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**16th Pacific Rim Conference on Ceramic and
Glass Technology/GOMD 2025**

ABSTRACT BOOK

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Introduction

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How to Use the Abstract Book

Refer to the Table of Contents to determine page numbers on which specific session abstracts begin. At the beginning of each session are headings that list session title, location and session chair. Starting times for presentations and paper numbers precede each paper title. The Author Index lists each author and the page number on which their abstract can be found.

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Monday, May 5, 2025

PACRIM Plenary Lectures

PACRIM Plenary Lectures

Room: Regency ABC

Session Chairs: Yiquan Wu, Alfred University; Bryan Huey, University of Connecticut

8:20 AM

(PACRIM-PLEN 01-001-2025) A Commentary on Complexions: Conception, Controversy and Adoption

M. Harmer*¹

1. Lehigh University, USA

What are interface complexions and how has this concept evolved? What has been the controversy behind this subject during its evolution? How can the concept of complexions be applied to design, tailor and engineer materials with controlled microstructures and greatly improved material properties and performance? How widely has it been successfully applied in other disciplines? What are the obstacles to getting a new concept adopted by a community and how can they be minimized? What are the future predictions, directions and needs in complexions research? If you are interested in these sorts of questions I welcome you to participate in this plenary lecture and share your thoughts.

9:10 AM

(PACRIM-PLEN 01-002-2025) Grain Boundary Atomic Structures and Their Dynamics in Ceramics

Y. Ikuhara*¹

1. University of Tokyo, Institute of Engineering Innovation, Japan

Grain boundary (GB) properties in ceramics are known to be strongly influenced by factors such as misorientation angle and the orientation of the GB plane, but the exact effects of these factors have yet to be fully understood. Additionally, dopant segregation at GBs plays a crucial role in modifying these properties. In this study, we systematically fabricated various types of bicrystals from ceramics like such as Al₂O₃, ZrO₂, SrTiO₃, with and without dopants, in order to investigate their GB atomic structures. Using aberration-corrected scanning transmission electron microscopy (STEM), the atomic structures and chemical compositions of these GBs were thoroughly characterized. Beyond structural analysis, the dynamics of GBs, such as fracture and migration, were also studied using in-situ TEM straining experiments combined with nano-indentation and MEMS techniques. The results showed that GB fractures tend to occur along specific crystal planes, and dislocations were observed to emit from the crack front. Furthermore, we recently demonstrated that high-energy electron beam irradiation can precisely control GB migration in ceramics. This migration occurs via the cooperative shuffling of atoms in the GB ledges along defined routes, offering new insights into how GB migration proceeds. These findings provide valuable contributions to understanding various GB phenomena in ceramics.

10:20 AM

(PACRIM-PLEN 01-003-2025) From Ultrafast Sintering to Controlling Microstructures with Electric Fields

J. Luo*¹

1. University of California San Diego, USA

This talk will first review a series of mechanistic studies of flash sintering. In 2015, we reported that flash sintering generally starts as a thermal runaway. In 2017, we further reported a mechanistic study to suggest ultrahigh heating rates as the key factor in enabling ultrafast sintering by demonstrating that similar densification rates

can be achieved for ZnO via (1) flash sintering and (2) rapid thermal annealing (infrared heating without an electric field) with similar heating rates of ~200 K/s. Similar conclusions were also obtained by independent studies. Subsequently, general ultrafast sintering methods such as ultrafast high-temperature sintering (UHS), enabled by the same underlying mechanism, were demonstrated in collaborative studies. Although we have demonstrated that ultrafast sintering can be achieved without an electric field, we recognize that electric fields can influence microstructural evolution. For example, we discovered an electrochemically induced grain boundary disorder-to-order transition to trigger abnormal grain growth in Bi₂O₃-doped ZnO. Furthermore, combined aberration-corrected electron microscopy and ab initio molecular dynamics simulations showed that applied electric fields can induce grain boundary oxidation transitions near the anode to create continuously graded microstructures in undoped ZnO in a controlled manner.

11:10 AM

(PACRIM-PLEN 01-004-2025) Complex Hybrid Metamaterials Designs based on Functional Ceramics and Beyond

H. Wang*¹

1. Purdue University, School of Materials Engineering, USA

Functional ceramics are widely used in various electronic, optical and magnetic devices, as well as structural components. Coupling their unique multifunctionalities, ceramics and their nanocomposites with unique nanoscale interfaces and defect designs have allowed a new class of ceramic-based hybrid metamaterial designs. In this talk, multiple ceramic-based hybrid metamaterial systems that couple 2 or more functional materials in a vertically aligned nanocomposite (VAN) thin film form, are introduced. Such hybrid metamaterial designs provide unlimited possibilities in developing new materials with multifunctionalities and/or unique functionalities for future plasmonics and optics, electronics and energy applications. The talk will cover some of the pioneering VAN demonstrations in oxide-oxide systems for low field magnetoresistance materials and multiferroics, recent oxide-metal nanocomposites with superior anisotropic optical and magnetic properties, and very recent nitride-metal and nitride-oxide based VANs coupling ferroelectric, ferromagnetic, plasmonic, hyperbolic optical response, and superconductivity in a single material platform. We also demonstrate that it is possible to transfer these epitaxially grown complex hybrid metamaterials onto various device relevant substrates for on-chip integration and flexible sensors.

PacRim S4 - Polymer-Derived Ceramics/ Composites/Nanocomposites as Functional Inorganic Materials

PACRIM Symposium 4 - Environmental, energy, health and functional applications I

Room: Plaza C

Session Chairs: Diletta Sciti, CNR-ISSMC; Thomas Konegger, TU Wien

1:15 PM

(PACRIM-S04-001-2025) Synthesis and characterization of polymer-based CaO/SiOC based nanocomposites for CO₂ capture (Invited)

S. Kaur¹; K. Rezwan¹; M. Wilhelm*¹

1. University of Bremen, Production Engineering, Germany

The global energy crisis underscores the need for sustainable solutions as the majority of energy consumption depends on carbon-based fossil fuels. Carbon capture technologies aim to mitigate CO₂ emissions, but conventional methods like monoethanolamine-based wet-scrubbing are energy-intensive and pose environmental

challenges such as solvent recycling and corrosion. Calcium oxide (CaO)-based solid sorbents offer advantages like high capture capacity and abundance but face challenges, including sintering and high decarbonization temperatures. Strategies to address these include nanosized metal oxides, porous supports, and alkali/alkaline metal salt doping. Porous supports like Al_2O_3 enhance active site exposure but suffer from poor heat conductivity and the formation of inactive phases (e.g., $\text{Ca}_3\text{Al}_2\text{O}_6$), which limit performance. Polymer-Derived Ceramics (PDCs) offer a promising alternative, enabling homogeneous dispersion of metal oxides within a micro-porous matrix. Preliminary research on CaO/SiCO-based ceramics for CO_2 capture demonstrated a nanosized CaO distribution in the SiC(O) matrix, achieving significant CO_2 adsorption at moderate temperatures. While pure CaO showed higher absorption, it lacked decarbonation at this temperature. In contrast, polymer-derived CaO/SiC(O) achieved efficient decarbonation, facilitating direct methane conversion and eliminating CO_2 transport.

1:45 PM

(PACRIM-S04-002-2025) Oxidation protection coatings for Mo-based refractory alloys (Invited)

T. Loskutova¹; R. Nizinkovskiy²; V. Taran¹; G. Hasemann²; M. Krueger²; M. Scheffler^{*1}

1. Otto-von-Guericke-Universität Magdeburg, Non-Metallic Inorganic Materials, Germany
2. Otto-von-Guericke-Universität Magdeburg, High-Temperature Materials group, Germany

Mo alloys possess a distinct high-temperature strength exceeding that of Ni-based super alloys making them candidates for stationary gas turbine applications. However, they degrade rapidly when exposed to air; thus, a comprehensive protection from oxygen attack is mandatory. This lead in the past to numerous approaches for the development of protective coatings. A great promise is the use of Si and B as components of such coatings, independent on the coating processing such as pack cementation (PC), polymer-to-ceramic processing (PDC) or methods involving vacuum processing; a fairly good protective effect has been shown in a great number of publications for a wide range of processing methods. In this paper the combination of PC and PDC processing for oxidation protection coatings on Mo alloys is demonstrated for the first time. Several Mo alloys were coated with the PDC approach, with PC processing and with a combination of both in an alternating sequence. It was found, that, beside Si, B is essential, were high B amounts influence the protective effect negatively; thus, the B amount needs to be minimized. Finally, selected samples of coated Mo alloys were long-term exposed to air at 800 °C and 1100 °C and the protective effect was demonstrated for the different coating systems. From these findings novel coating strategies may be developed, e.g. for real-part geometries with complex surfaces.

2:15 PM

(PACRIM-S04-003-2025) In situ design of nanoscale transition metal-based particles in porous Polymer-Derived Ceramic supports for hydrogen evolution reaction

M. J. Potestas^{*1}; M. Ben Miled¹; S. Valette¹; A. Habrioux²; S. Bernard³

1. Université de Limoges, France
2. Université de Poitiers, France
3. CNRS, IRCER, France

The polymer-derived ceramics (PDC) method represents a transformative approach to ceramic processing, leveraging soluble and crosslinkable precursors to enable enhanced shaping capabilities and the formation of ceramics at significantly lower temperatures compared to conventional techniques. Notably, these precursors can be tailored with metal complexes to produce, via in situ heat treatment, metal and transition metal carbides nanoparticles embedded within porous ceramic matrices. Among transition metal carbides, molybdenum carbide and nickel carbide have emerged as key

candidates for electrocatalytic applications, particularly in the hydrogen evolution reaction (HER). To further enhance their performance, these carbides are often doped or integrated into composite materials. This study presents the in situ synthesis of nanoscale molybdenum carbide and nickel carbide particles within a PDC matrix, achieved through the strategic combination of various metal precursors and preceramic polymers. The materials' evolution through the processing steps will be comprehensively characterized, and their HER performance will be evaluated and discussed.

2:35 PM

(PACRIM-S04-004-2025) Nanoscale high-entropy alloy-based pre-catalysts stabilized in polymer-derived micro/macroporous ceramics for sustainable energy

S. Vendra^{*1}; M. Ben Miled¹; A. Bouzid¹; O. Masson¹; A. Habrioux²; S. Bernard¹

1. Institut de Recherche sur les Ceramiques, Univ. Limoges, CNRS, IRCER, UMR 7315, France
2. Université de Poitiers, CNRS, IC2MP, UMR 7285, France

Technological advancements in energy storage systems (ESSs) such as fuel cells, metal-air batteries and electrolyzers to lower the carbon emissions and protect the environment. Among them, electrocatalysis for the water-splitting reactions such as hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) play a prominent role. However, this clean reaction only represents 4% of the actual method of H_2 production around the world. The recent development of anion exchange membrane materials has led to the emergence of the anion exchange membrane electrolyzers allowing the use of non-noble transition metals in the composition of pre-catalysts for HER and OER in alkaline media. However, their nanoscale synthesis is highly challenging to limit the overpotential, particularly at the anode (OER). In this work we exploited the Polymer-Derived Ceramics (PDC) route to design self-supported nanosized high entropy alloy (HEA) as pre-nanocatalysts confined in a porous amorphous SiOCN ceramic matrix for OER applications. The presence of HEA has been confirmed by X-ray diffraction (XRD) and the morphological features of the nanoparticles have been imaged through electron microscopy. These composites exhibit micro/macroporous matrices with surface area above 250 m^2/g . The electrochemical measurements for OER have been performed and will be discussed.

3:30 PM

(PACRIM-S04-006-2025) Single-source-precursor synthesis of SiC-based Nanocomposites as Electrocatalysts for Water Splitting (Invited)

Z. Yu^{*1}

1. Xiamen University, China

Among all of the strategies to yield hydrogen fuel, electrochemical water splitting is one of the most efficient ways due to its renewability and environmental-friendliness. For the first time, we reported on the in-situ formation of a nano-sized Nowotny phase (NP) $\text{Mo}_4.8\text{Si}_3\text{C}_0.6$ embedded in a porous SiC/C-based matrix via a polymer-derived ceramic (PDC) approach. Again, for the first time, the NP was discovered to possess electrocatalytic activity and excellent durability in terms of the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) for electrochemical water splitting. The outstanding electrocatalytic properties include: i) low overpotentials of 22 and 138 mV vs. reversible hydrogen electrode for driving cathodic current densities of 1 and 10 mA cm^{-2} in acidic media, respectively; ii) high stability ratio (over 90 %) during 35 h. In general, the above-mentioned performance exceeds that of almost all the reported Mo-based electrocatalysts. Our discovery broadens the potential applications of PDC in the energy field.

4:00 PM

(PACRIM-S04-007-2025) Electrochemical energy and conversion devices based on polymer derived ceramic carbon (Invited)

A. Tamayo*¹; E. Chinarro¹; A. Mazo¹; J. Rubio¹

1. Institute of Ceramics and Glass, CSIC, Spain

Carbon-based materials play an important role in the development of electrochemical energy storage and conversion devices. The combination of high specific surface area and the tunable morphology of the carbon phase contained in the sol-gel and polymer derived ceramics turns these materials excellent candidates for the electrodes in the electrochemical systems. By selective etching in dry atmospheres, the conductivity of the mesoporous carbon reaches the values comprised within the state of the art of the carbon electrodes in the fuel cells. On the other side, the high functionality of the surface obtained through wet etching is highly valuable for their application in electrolytic double layer capacitors. In this work it will be presented the most significant parameters affecting the conductivity and the electrochemical performance of carbide and oxycarbide derived carbons obtained from the sol gel method and preceramic polymers. To evaluate the performance of the materials in fuel cells, there have been produced MEAs with the different carbon materials decorated with an electrocatalyst and processed via warm pressing methods. Their use as capacitor electrodes were tested in pouch-cell assemblies and using aqueous electrolytes. There are correlated the textural, microstructural and surface active functionalities with their behavior in each device.

4:30 PM

(PACRIM-S04-009-2025) Amorphous SiOC Coatings: Polymer-Derived Ceramics for Nuclear Applications

M. Gaweda*¹; P. Jelen²; D. Kalita¹; F. J. Domínguez-Gutiérrez¹; M. T. Sitarz²; I. Jozwik¹

1. Narodowe Centrum Badan Jadrowych, NOMATEN, Poland

2. Akademia Gorniczo-Hutnicza im Stanislaw Staszica w Krakowie, Poland

Advanced nuclear technologies require materials with high performance under extreme conditions. Although currently available alloys exhibit adequate mechanical properties, their oxidation resistance and radiation tolerance remains insufficient. Enhancement may be achieved by introduction of additional grain boundaries and interfaces, as in ODS alloys, or by creating a barrier between the metal and its environment. This study proposes amorphous coatings based on silicon oxycarbide (SiOC), obtained as the polymer-derived ceramics (PDCs). The materials were proven to be effective protective coatings due to their high thermal and chemical resistance. Their unique structure, analogous to amorphous silica, allows structural reorganisation under irradiation, preventing deterioration. Self-synthesised ladder-like polysilsesquioxanes, with a controlled silicon-to-carbon ratio, were used as precursors, enabling precise control over the material's composition. The coatings, deposited on AISI 316L steel via dip-coating, underwent ceramization. The use of self-synthesised precursors also facilitates doping with ions to enhance or introduce new properties. In this work, iron ions were incorporated to inhibit diffusion of substrate's compounds through the protective layer. The coatings' suitability for nuclear applications was evaluated via neutron irradiation simulations using noble gases and structural analyses.

4:50 PM

(PACRIM-S04-010-2025) Polymer derived SiOC/Sn nanocomposites as anode materials for lithium storage applications

G. Blugan*¹; H. Ramlow¹; M. Wilamowska-Zawlocka²; S. Paz³; M. Koebel³

1. Swiss Federal Laboratories for Materials Science and Technology,

Laboratory for High Performance Ceramics, Switzerland

2. Politechnika Gdanska Wydział Chemiczny, Poland

3. Siloxene AG, Switzerland

Metal-based materials capable of lithium (Li) alloy formation are key to realization of new high-energy density anodes for Li-ion batteries, owing to their high storage capacity. Designing a matrix is essential for homogeneously nesting these metallic nanodomains, to effectively utilize their high capacity while tackling the volume expansion issues. Silicon oxycarbides (SiOC), obtained via a polymer derived approach, have recently gained interest as efficient host matrices. Sn nanoparticles, measuring less than 100 nm in size, are formed in-situ within an amorphous SiOC matrix using an economical single-source precursor. The polymeric precursor was indigenously developed from a novel, low cost vinyl functionalized polysiloxane and tin dioleate as the Sn source. Tin dioleate at different wt%, viz. 33–56 %, was uniformly crosslinked with the Q-T polysiloxane and was pyrolysed at 1000 °C in an argon atmosphere to obtain the SiOC/Sn nanocomposites. The electrochemical characterization of SiOC/Sn ceramic nanocomposite anodes exhibit outstanding specific capacities of 650 and 750 mAh g⁻¹ at 372 and 18.6 mA g⁻¹, respectively after 400 charge/discharge cycles.

5:10 PM

(PACRIM-S04-031-2025) Low-temperature sintered MA@PDC-SiBCN ceramics: Mechanical properties and high-temperature oxidation behavior

D. Jia*¹

1. Harbin Institute of Technology, School of Materials Science and Engineering, China

In this study, the densification of SiBCN ceramics with an MA@PDC-SiBCN structure at low temperatures (<1600 °C) without any sintering aids was achieved by depositing a partially cured polyborazylene coating layer on the surface of MA-SiBCN nanoparticles, followed by warm pressing of coated powder and pyrolysis/sintering of powder compact. Due to the significant viscoelastic deformation behavior, the partially cured precursor layer surrounding the MA-SiBCN particles in the coated powder could merge together to form a three-dimensional precursor network that encapsulates and connects MA-SiBCN particles in a dense powder compact. Serving as a template, the structure in the powder compact transforms to dense SiBCN ceramics with MA@PDC-SiBCN structure during subsequent pyrolysis and sintering and the resulting ceramics exhibit enhanced mechanical performance and oxidation resistance.

PacRim S6 - Dielectric Ceramics for Microwave and Submillimeter-Wave Applications

PACRIM Symposium 6 - Dielectric Measurements

Room: Balmoral

Session Chairs: Nate Orloff, NIST; Rick Ubic, Boise State University

1:15 PM

(PACRIM-S06-001-2025) A SI-traceable standard for complex permittivity (Invited)

B. Bosworth^{*1}; L. Enright¹; B. Jamroz¹; N. Jungwirth¹; N. Orloff¹

1. NIST, USA

All electronic circuits use dielectrics of one form or another, whether it is as a substrate or as a functional material for an integrated circuit. Today, there is no standard for complex permittivity traceable to international system of units (SI). Without a standard, designers, system integrators, and manufacturers have no way to evaluate the accuracy of measurement instrumentation, develop meaningful calibration procedures, or evaluate new materials that could offer cost savings or design improvements. Making an SI-traceable standard for complex permittivity is no easy feat; it requires a comprehensive set of SI-traceable measurements of independent variables with a detailed uncertainty analysis propagated to the measurand. This work represents the first attempt to develop a fit-for-purpose SI-traceable standard for complex permittivity. Our approach uses split cylinder resonators (SCRs) and a comprehensive measurement chain traceable to the meter and hertz. This talk will present the measurement chain and NIST's effort to release 150 micron thick fused silica as an SRM for permittivity. We introduce several modifications to SCR, enabling robotic automation of repeated pick and place measurements of the fused silica sheets at 7 frequencies from 20 GHz to 60 GHz. With this approach, NIST will scale to 200 SRMs per year for dissemination in the very near future.

1:45 PM

(PACRIM-S06-002-2025) Split-cylinder resonator measurements of the complex permittivity of substrates and thin films

L. Enright^{*1}; B. Jamroz¹; B. Bosworth¹; G. Brennecke²; N. Orloff¹

1. National Institute of Standards & Technology, Communications Technology Laboratory, USA
2. Colorado School of Mines, USA

Dielectric properties (i.e., relative permittivity and loss tangent) are key inputs for the design and modeling of electronic devices. The importance and the difficulty of reliably measuring these properties increase with increasing frequencies, e.g. millimeter-wave (30 GHz – 300 GHz). Here, we show the use of split-cylinder resonators and fused silica substrates to develop SI-traceable standards for complex permittivity at 28 GHz, and potentially up to 80 GHz. We describe the electromagnetic theory, uncertainty analysis, and limitations of split-cylinder resonator measurements. We then extend these split-cylinder resonator measurements, theory, and uncertainty analysis from the simple case of homogeneous substrates to the more complicated case of thin films on substrates including ceramics (e.g., AlN) and polymers (e.g., SU-8). Taken as a whole, this work allows us to deliver reliable material measurements of homogeneous substrates and heterogeneous material stacks with applications that have broad impacts across the electronics industry.

2:05 PM

(PACRIM-S06-003-2025) Understanding and predicting frequency-dependent dielectric permittivity and loss in ferroelectric ceramics (Invited)

S. Nakhmanson^{*1}

1. University of Connecticut, Materials Science and Engineering, USA

A paramount characteristic of ferroelectric ceramics, underpinning numerous applications in tunable microwave and optical devices, is their dielectric permittivity, which is a function of applied field frequency, temperature and other applied conditions. Due to remarkable structural complexity of these materials -- encompassing the presence of grains (and grain boundaries), polar domains and potentially other dipole vector patterns, composition variations, defects, etc. -- a unified understanding of their dielectric response remains elusive. Here, we present a phenomenological mesoscale-level approach for evaluating frequency- and temperature-dependent dielectric permittivity and loss in perovskite ferroelectrics, and discuss our attempts to employ it for establishing some structure-properties-performance relations for these materials. Specifically, we utilize $\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$, a relaxor system with compositional disorder, and a 'classical' example of an Ising 180-degree domain wall in BaTiO_3 as benchmark cases to unfold the complexities of dielectric response inherently present in ferroelectric perovskites, as well as make suggestions for possible improvements of their useful properties.

2:35 PM

(PACRIM-S06-004-2025) Temperature Dependent Dielectric Properties at GHz frequency (Invited)

M. Lanagan^{*1}; S. Perini²; A. Hossain²; S. Voyton²; M. Rahman²; M. E. Eltantawy²; C. Nieves³

1. Penn State University, Dept. of Engineering Science and Mechanics, USA
2. The Pennsylvania State University, Materials Research Institute, USA
3. Air Force Research Laboratory, USA

Key dielectric properties for electronic devices include permittivity, loss, and the temperature dependence of permittivity. Among these, the temperature dependence of permittivity is the least studied. Dielectric properties are crucial not only for electronic package design but also for understanding the fundamental polarization states of a wide array of materials, including ceramics, glass, polymers, and liquids. The presentation will focus on the fundamental aspects of how different polarization mechanisms affect temperature dependent dielectric properties in the microwave and millimeter frequency ranges. Glass and polymers are leading candidates for microelectronic packaging materials that support signal propagation in the GHz frequency range. For glass, ionic and space charge polarization mechanisms contribute to a positive temperature coefficient. Polymers tend to have a negative temperature coefficient as electronic polarization dominates. The temperature dependent dielectric properties of water are monitored through the freeze-thaw cycle at microwave frequency, where the dipolar polarization response can be significantly altered by surfaces. Examples will be provided for water entrained in pores.

PACRIM Symposium 6 - Glass for Microwave and Submillimeter-Wave Applications

Room: Balmoral

Session Chairs: Nate Orloff, NIST; Martin Letz, Schott AG

3:30 PM

(PACRIM-S06-005-2025) Glasses and glass ceramics: Dielectric properties and Applications in Microwave and Submillimeter-wave ranges (Invited)

M. Letz*¹

1. Schott AG, R&D, Germany

Glasses and glass ceramics are highly homogeneous, can be manufactured free of pores and have extremely smooth surfaces. Depending on the range of microwave frequency there are different needs for a dielectric material. At small GHz frequencies below 10GHz the wavelength is large, 30 mm and more, and there is a need to miniaturize antennas or filters. Miniaturization can be done by dielectric loading. Here materials with large dielectric constant are needed. We present antennas and filters which are made by a dielectric glass-ceramic with $\text{Ba}_4\text{Al}_2\text{Ti}_{10}\text{O}_{27}$ as a crystalline phase, a dielectric constant of $\epsilon' = 33.5$ and a dielectric loss of order $\tan\delta = 0.001$. At larger frequencies, above 30GHz, materials with low dielectric constant are needed. Here also a close packaging of active and passive components, antenna in package (AIP) concepts, become important, since any transport of microwave or even millimeter wave signals is extremely lossy. AIP concepts can benefit from the current trend in semiconductor industry to glass panel based packaging. Here cost efficient and highly precise laser manufacturing methods for glass panels are being developed. Using these emerging manufacturing methods highly accurate hollow waveguide structures can be realized. We show a band pass filter at 88GHz and a high bandwidth corrugated horn antenna at 130GHz.

4:00 PM

(PACRIM-S06-006-2025) Glass Composition and Post Forming Process Impacts on mm-Wave Dielectric Properties

L. Lamberson*¹; L. Cai²

1. Corning Incorporated, Glass Research, USA
2. Corning Incorporated, Characterization Science and Services, USA

The present drive for higher bandwidth has moved the mobile carrier frequency range to >5 GHz and possibly to >20 GHz in the near future. This has fueled the rapid development of 5 G and mm-wave technologies. The increased bandwidths available in the mm-wave frequency range allow for applications that require high-data-rate communications, which is not possible at lower frequencies due to Shannon's Capacity Theorem. However, the mm-wave frequency also presents a challenge to device performance due to the limitation on material properties. Many incumbent materials, such as silicon, ceramic, and polymer based substrates, suffer from high dielectric loss, rough surface, or poor durability to process chemistry. Silicate glass, on the other hand, has been shown to exhibit low dielectric loss, smooth surface, and high resistance to process chemistry. In addition, modern manufacturing technology has enabled silicate glass to be made with large size and thin form factor, which provides a clear advantage to lowering the cost. While many attributes of glass may be already familiar to the general scientific community, dielectric properties in the mm-wave frequency range have not been extensively reviewed. In this report, we show that mm-wave dielectric property can be changed by glass composition and post-forming processes. We also show examples of mm-wave devices that can be made with glass.

4:20 PM

(PACRIM-S06-007-2025) Dielectric response of glass materials in the GHz-THz band and demonstration of filter devices using glass-ceramic substrates (Invited)

K. Kanehara*¹; S. Urata³; K. Niwano¹; S. Yasuhara²; T. Tsurumi²; T. Hoshina²

1. AGC Kabushiki Kaisha, Material Integration Laboratories, Japan
2. Tokyo Kagaku Daigaku, Japan
3. AGC Kabushiki Kaisha, Innovative Technology Research Center, Japan

The faster data transmission in 5G telecommunications has deepened interest in the characterization and prediction of electrical properties at microwave and mm-wave frequencies. Glass and/or glass ceramics have been attracting particular attention as materials possessing a low dielectric constant and dielectric loss, together with high flatness and easy processing. However, the mechanism underlying the dielectric properties of glass in the frequency range above 10 GHz has hardly been studied so far. In this study, we attempted to measure the complex permittivity of simple silicate glasses in the GHz-THz region using our original measurement system. Further, we calculated the complex permittivity of some glasses by molecular dynamics (MD) simulations to theoretically understand the role of alkaline species. The calculated frequency dependence of the dielectric constant and loss is in reasonable agreement with the experimentally measured data. In addition, filter devices fabricated with glass ceramics substrates are demonstrated. The obtained substrates are suitable for filter devices because the temperature dependence of the dielectric constant is reduced by using separated rutile crystals in glass. The filter device operates at millimeter-waves, and devices with very small temperature dependence and low insertion loss have been obtained.

4:50 PM

(PACRIM-S06-008-2025) Low loss and permittivity borosilicate glass for packaging applications (Invited)

R. Rodriguez Cano*¹; M. Lanagan²

1. Aalborg Universitet, Electronic Systems, Denmark
2. Penn State University, Dept. of Engineering Science and Mechanics, USA

The increasing demand for higher data rates, is pushing the exploration of higher frequency bands beyond 5G. Achieving data rates of 100 Gbps and beyond requires the use of carrier frequencies above 100 GHz, prompting to examine the largely unexplored sub-THz spectrum. Supporting wireless applications at these higher frequencies requires the development and fabrication of new RF components and waveguides. While attenuation characteristics of different guiding structures are relatively similar at lower frequencies, significant differences arise as frequencies approach the sub-THz range. This divergence is primarily due to the increasing dominance of dielectric losses, which scale quadratically with frequency, compared to conductor losses that grow more slowly, at the square root of the frequency. As dielectric losses become the primary factor at higher frequencies, the selection of dielectric material becomes critical in the design process. Materials with a low-loss tangent are essential for minimizing these losses, and permittivity also plays a crucial role, as it influences both dielectric and conductive losses. To address these challenges, we propose a low-permittivity, low-loss borosilicate glass interposer for packaging applications. This material demonstrates excellent potential for reducing losses and improving performance in sub-THz frequency applications.

PacRim S7 - Direct Heat-to-Electricity Energy Conversion Mtls & Thermal Energy Harnessing Challenges

PACRIM Symposium 7 - Direct Heat-to-Electricity Energy Conv Materials & Thermal Energy Harnessing Challenges I

Room: Dover/Tennyson

Session Chairs: Michitaka Ohtaki, Kyushu Daigaku; Min Hong, University of Southern Queensland; Mary Anne White, Dalhousie University; Yuzuru Miyazaki, Tohoku Daigaku

1:15 PM

(PACRIM-S07-001-2025) Porous Ceramics Based Composite Phase Change Materials for Thermal Energy Storage (Invited)

M. White*¹; J. Noel¹

1. Dalhousie University, Chemistry, Canada

Phase change materials (PCMs) can be used to efficiently store thermal energy for later release. Two of the main issues preventing wider PCM use are the need for containment (the phase change is generally solid to liquid), and low intrinsic thermal conductivity of PCMs, especially for organic PCMs. We have addressed both issues through preparation of novel composite materials: porous ceramics impregnated with PCMs. We have shown that many different scaffold materials can be used as matrices for a wide variety of PCMs, to prepare a range of composite phase change materials. The PCM-matrix interaction is physical not chemical, so the porous ceramic matrix does not substantially influence the PCM melting points, but does control the fill, thermal conductivity and mechanical properties of the form-stable PCM. Different matrices can be used to optimize thermal conductivity, or form stability, or PCM loading, depending on the application.

1:45 PM

(PACRIM-S07-002-2025) Data-driven approach to find potential Fe-based half-Heusler thermoelectric materials for the near-room-temperature applications (Invited)

Y. Miyazaki*¹; X. Nan¹; Z. Huang¹; K. Hayashi¹

1. Tohoku Daigaku, Department of Applied Physics, Japan

Half-Heusler alloys (HHs) have attracted much interest as potential thermoelectric (TE) materials to be utilised at a mid-temperature range around 800 K. Despite their high TE power factor $P = S^2\sigma$ (S: Seebeck coefficient, σ : electrical conductivity), room temperature (RT) applications have not been much considered due to their relatively high lattice thermal conductivity $\kappa_L \sim 10$ -15 W/Km. In order to reduce κ_L while maintaining high P, we have performed a data-driven approach by combining DFT (density functional theory) calculations and chemical bonding analyses. We extracted 23 chemically stable Fe-based HHs, XFeZ (X: electropositive transition metals, Z: semi-metals), out of 230 candidates, and discovered that 3 of them would exhibit reasonable TE properties, without any carrier-doping and nano structural modifications. Based on the strategy, we designed and fabricated several HH alloys and evaluated TE properties at 300-400 K. In the conference, we will demonstrate recent efforts to maximise the dimension-less figure-of-merit, around RT.

2:15 PM

(PACRIM-S07-003-2025) Exploration of the Effect of Nanoscale Transport on Thermoelectric Energy Conversion (Invited)

Q. Zhu¹; J. Maassen*¹

1. Dalhousie University, Canada

Thermoelectric materials can convert thermal energy into electrical energy, and vice versa, thereby enabling applications in power generation and solid-state cooling. The performance of a thermoelectric

depends sensitively on the interplay between its electronic and thermal properties. According to traditional thermoelectric theory, the efficiency of a material does not depend on its size. However, when the length of a material is scaled down and becomes comparable to a carrier's mean-free-path, deviations from diffusive transport behavior emerge. For example, on the nanoscale, ballistic effects lead to a length-dependent conductivity and a breakdown of the classical Joule heating formula. In this talk, we theoretically explore how such non-diffusive phenomena can impact thermoelectric performance by varying the material length from the diffusive to the near-ballistic transport regime. A coupled electro-thermal transport framework, based on the McKelvey-Shockley flux method which captures ballistic and nonequilibrium effects, is adopted. Our findings illustrate how thermoelectric conversion on the nanoscale can deviate from, and potentially outperform, that of bulk materials.

2:45 PM

(PACRIM-S07-004-2025) Development of novel thermoelectric materials by database approach and of miniaturized thermoelectric devices toward IoT (Invited)

I. Ohkubo*¹

1. Busshitsu Zairyo Kenkyu Kiko Kokusai Nanoarchitectonics Kenkyu Kyoten, Japan

Developing novel thermoelectric materials and devices has attracted attention due to its contribution to the Internet of Things (IoT) and green innovation. This presentation will introduce two recent studies exploring novel thermoelectric materials and devices. (1) A database of electronic structure parameters of the charge-transfer energy (Δ) and the onsite Coulomb repulsion energy (U) for 566 transition-metal compounds (nitrides, oxides, fluorides, phosphides, sulfides, chlorides, arsenides, selenides, bromides, tellurides, and iodides) was constructed. High-performance thermoelectric transition-metal compounds were mainly located in two specific regions in the Δ - U diagram. Attractive thermoelectric materials will be developed by searching undeveloped transition-metal compounds in the two particular areas of the Δ - U diagram. (2) Miniaturized thin-film-based thermoelectric devices have been developed using microfabrication technology. Miniaturization and integration of thermoelectric devices with other electronic devices are required for IoT applications. Our thin-film-based thermoelectric devices contain a relatively large number of π junctions and show high output voltage and power density.

3:30 PM

(PACRIM-S07-005-2025) Advancing High-temperature Energy Conversion: Theory and Experiment (Invited)

A. Nojeh*¹

1. University of British Columbia, Electrical and Computer Engineering, Canada

Converters of heat to electricity power much of today's world. This will likely continue with both traditional and new sources of heat such as concentrated sunlight and stored thermal energy. Given the challenges of turbine generators, static heat engines appear as a promising alternative for harnessing high-temperature heat. Thermionic energy converters, in which electrons are directly transferred from a hot emitter to a cold collector, represent the ultimate static engine in conceptual simplicity. However, the performance of these devices has not met expectations. Improving this performance entails closely controlling charge and heat exchange channels between the two sides of the device. Historically, at high temperatures, the relevant transport phenomena have been treated semi-classically and without detailed links to the specific materials physics of the emitter and the collector. This is partly due to the assumption that, at such temperatures, the rich physics emanating from quantum effects become mostly irrelevant. However, discussing both theory and experiment, we will see that that may not always be the case, and that advancing thermionic energy conversion

*Denotes Presenter

may necessitate an integrated approach to treating materials and device physics which involves quantum phenomena and draws on theoretical and experimental techniques similar to those used in condensed matter physics research.

4:00 PM

(PACRIM-S07-006-2025) Various device architecture of thermoelectric devices (Invited)

W. Kim*¹

1. Yonsei University, School of Mechanical Engineering, Republic of Korea

In this talk, we present various device architecture of thermoelectric devices. First, I am going to talk about architecture of thermoelectric device for body heat harvesting application aiming to operate sensors and actuators for healthcare application. Continuous monitoring of vital signs and timely treatment are the future trends for wearable and implantable healthcare systems, which inevitably require ceaseless power supply. Discharged batteries could be detrimental to the health of people, such as those with type 1 diabetes, whose glucose levels should be monitored and controlled through timely insulin injections. Here, we demonstrate a feasible true continuous healthcare system for type 1 diabetes by combining a low-energy micropump, self-powered glucose sensor, and ceaseless power supply based on thermoelectrics. In addition, we are going to present our recent efforts to build a compact vital band which contains wearable sensors, unintermittent power supply, and flexible circuits located at a single location (i.e., the forearm). The vital band is specially designed for the continuous monitoring of the core body temperature (CBT) with novel CBT sensors and pulse rate sensor operated by intermittent power. These findings can help realize a true continuous healthcare system in the future. Secondly, we present a new device architecture for waste heat recovering for low S/W system.

4:30 PM

(PACRIM-S07-007-2025) Interface Optimization for Low-Contact Resistance and High-Thermal Reliability between Bismuth Telluride and Barrier Metals in TEG Devices

A. Katsura*¹; M. Tsurumoto¹; Y. Hirose¹; M. Daniele³; E. Iwase²; T. Sugahara¹

1. Kyoto Kogei Sen'i Daigaku, Japan
2. Waseda Daigaku, Japan
3. Politecnico di Torino, Italy

Thermoelectric generation (TEG) devices with bismuth telluride (Bi_2Te_3) are most advanced toward commercialization as an energy harvesting technology. However, contact resistance at the interface between Bi_2Te_3 and the barrier metal hinders the thermoelectric conversion efficiency and reliability of TEG devices. In this study, we fabricated 189 samples including barrier metals (Ti, Cr, Ni) / Bi_2Te_3 interfaces, and evaluated specific contact resistivity (ρ_c) and its temperature dependence using an advanced transfer length method (TLM). Our TLM measurements revealed that specific contact resistivity of Bi_2Te_3 increased independently of the barrier metal. Furthermore, results showed that the Ti/ Bi_2Te_3 interface had the lowest ρ_c at 298 K, whereas the Ni/ Bi_2Te_3 interface exhibited the lowest ρ_c at 378 K. In addition, we evaluated element diffusion and the degradation, distortion of interfaces under high-temperature environments. Therefore, the results demonstrated that using Ti as a barrier metal on the cool side and Ni on the hot side of Bi_2Te_3 can enhance the thermoelectric conversion efficiency and thermal interfacial reliability of TEG devices.

4:50 PM

(PACRIM-S07-008-2025) Defect engineering towards high-performance thermoelectric germanium telluride

Y. Jiang*¹; J. Li¹

1. Tsinghua University, School of Materials Science and Engineering, China

GeTe is a promising mid-temperature thermoelectric compound, but inevitably contains excessive Ge vacancies that hinder the performance maximization. In the present work, we demonstrate several successful paradigms of enhancing the dimensionless figure of merit (ZT) of GeTe by defect engineering. First, by driving the evolution from zero to high-dimensional defects through the optimized heat-treatment, abundant phonon scattering centers, including the dislocations and nanodomains, are generated in GeTe , leading to a significant reduction of lattice thermal conductivity. Meanwhile, these dislocations and planar defects resulting from the accumulation of cationic vacancies prove to weaken the carrier scattering, contributing to enhanced carrier mobility and hence a maximum ZT > 2.3 at 648 K. Second, by incorporating the boron inclusions into GeTe matrix, similar defect evolution can be evoked, which helps to strengthen the scattering of mid-frequency phonons. Due to the presence of heterogeneous interfaces, the adversely dependent σ and S are efficiently decoupled, giving rise to an enhanced power factor (PF) and hence a high ZT of 2.45 at 613 K.

5:10 PM

(PACRIM-S07-009-2025) Solid solution alloying strategy to enhance thermoelectric efficiency of metal chalcogenides; $(\text{Bi,Sb})_2\text{Te}_3$, $\text{Bi}_2(\text{Se,Te})_3$ and beyond

S. Kim*¹

1. University of Seoul, Department of Materials Science and Engineering, Republic of Korea

Solid solution alloying (SSA) of metal chalcogenide compounds (M_xX_y) can be formed either by alloying cation or anion site. SSA by cation (i.e. $(\text{M,N})_x\text{X}_y$) could provide a gradual change of electronic dispersions, which could optimize thermoelectric (TE) power factor by controlling band structure and band convergence. SSA by anion (i.e. $\text{M}_x(\text{Se,Te})_y$) enables to control the band gap, which optimize level of bipolar conduction for high power factors. In addition, lattice thermal conductivity can be reduced by SSA by additional phonon scattering, which could further increase the TE figure of merit. Therefore, SSA approach can enhance TE efficiency of chalcogenides effectively. Herein, I would like to first revisit the origin of high TE efficiency of $(\text{Bi,Sb})_2\text{Te}_3$ and $\text{Bi}_2(\text{Se,Te})_3$ solid solution alloys in these respects, which are the most conventional TE chalcogenides. Then, investigations to enhance TE efficiency of chalcogenides in a similar way are discussed, including simple SSA, including $(\text{Fe,Co})\text{Te}_2$, $\text{Co}(\text{Se,Te})_2$, and $\text{Cr}_2(\text{Se,Te})_3$, and rather complex SSA, including $\text{Cu}_2\text{ZnSnSe}_4$ - Cu_3SbSe_4 and Bi_2Te_3 - PbBi_2Te_3 . Analysis based on single parabolic band model, which estimates TE transport properties by varying carrier concentration, suggests additional condition in enhancing TE efficiency of solid solution chalcogenide family.

PRS9 - Fndmtls of interfaces/grain boundaries/surfaces - interatomic bonding to macroscopic prop

PACRIM Symposium 9 - Thermodynamic and kinetic stability of interfaces

Room: Oxford

Session Chair: Klaus van Benthem, University of California, Davis

1:15 PM

(PACRIM-S09-001-2025) Equilibrium, Phase Transitions, and Kinetics of Charged Interfaces in Ionic Ceramics (Invited)

R. Garcia^{*1}; K. Vikrant²; C. M. Bishop³

1. Purdue University, Materials Engineering, USA
2. Indian Institute of Technology, India
3. University of Canterbury, New Zealand

A thermodynamically consistent phase field framework is presented to understand the effects of ionic species and point defects on the stability of interfaces in polycrystalline ionic ceramics. The properties induced by the broad region of electrochemical influence in front of a grain boundary are quantified, and the effect of non-electrochemical driving forces, including stresses, ferroelectric polarization, misorientations, and structural disorder are considered. The spatial extent of these effects spans anywhere from a few angstroms to entire grains, greatly impacting equilibrium and switching properties. In addition, the effects of electrostatic charge on grain boundary motion during grain growth as a function of electrical, chemical, mechanical, or structural driving forces are quantified as a direct extension of John Cahn's solute drag theory for metallic systems. Example applications to GCO, YSZ, STO, BTO, and PZT are presented.

1:45 PM

(PACRIM-S09-002-2025) Grain boundary studies by magnetic-field-free atomic resolution electron microscopy (Invited)

N. Shibata^{*1}

1. The University of Tokyo, Japan

Atomic resolution scanning transmission electron microscopy (STEM) is a powerful technique for characterizing atomic-scale structures inside materials and devices. However, it has been very difficult to observe magnetic materials at very high spatial resolution because high magnetic fields (>2T) are always exerted on samples inside the magnetic objective lens. In recent years, we have developed a new magnetic objective lens system that realizes a magnetic field free environment at the sample position. Using this new objective lens system in combination with higher order aberration corrector, spatial resolution of 82 pm has been achieved under magnetic field free condition. The novel electron microscope with this new objective lens system (Magnetic-field-free Atomic Resolution STEM: MARS) is expected to be powerful for research and development of many magnetic materials and devices. In this talk, some recent applications using MARS for grain boundaries in magnetic materials and oxides will be presented.

2:15 PM

(PACRIM-S09-003-2025) Using Interface Layer Quantities to Compute Thermodynamic Quantities from Atomic Probe Microscopy

W. Carter^{*1}; C. M. Bishop²

1. Massachusetts Institute of Technology, Materials Science and Engineering, USA
2. University of Canterbury, Mechanical Engineering, New Zealand

Quantities such as the interfacial segregation coefficient have been measured with atomic probe microscopy. Interface quantities are always excess thermodynamic quantities and have been treated by Gibbs and by Cahn. These thermodynamic treatments commence

by specifying an arbitrary volume of material that encloses the interface and then proceed to derive unambiguous quantities that could be measured experimentally. Atomic probe experiments mirror this approach: data is obtained, a volume is chosen, and the counts and locations of atomic species are obtained. The interface's location within the chosen volume does not enter into the data reduction; but, is typically indicated graphically. In the thermodynamic treatments, the interface location is completely specified by the specific choice of the interface's linearly independent variables: Gibbs chose to eliminate the excess volume and excess concentration of the solute; this was generalized Cahn by symbolically delaying the choice the reduced set with his "layer quantities". In each case, the thermodynamic quantities are not those which are obtained from atomic probe data by straightforward counting. The layer quantities provide a recipe for how atomic probe data should be extracted as quantities that are appropriate for thermodynamic relationships—such as the adsorption isotherm. We explain this procedure.

2:35 PM

(PACRIM-S09-004-2025) Characterizing the atomic-level structure and stability of interfaces of Pt nanoparticles in contact with transition aluminas

A. L. Clauser¹; K. Oware Sarfo²; R. Giulian³; J. Ciston⁴; C. Ophus⁵; L. Árnadóttir²; M. K. Santala^{*1}

1. Oregon State University, Materials Science Program, USA
2. Oregon State University, Chemical, Biological, and Environmental Engineering, USA
3. Universidade Federal do Rio Grande do Sul, Institute of Physics, Brazil
4. Molecular Foundry, Lawrence Berkeley National Laboratory, The National Center for Electron Microscopy, USA
5. Stanford University, Materials Science and Engineering, USA

Metal nanoparticles (NPs) supported on metal-oxides play a critical role in catalytic processes. In this work, transmission electron microscopy (TEM) is used to guide and validate density functional theory (DFT) based models of Pt/ γ -Al₂O₃ and Pt/ θ -Al₂O₃ interfaces. Pt NPs were formed in dense γ - and θ -alumina through solid-state precipitation into sapphire partially amorphized by ion implantation of Pt. Thermal annealing re-crystallizes the amorphized alumina and precipitates Pt NPs, which are mainly bound by {111} Pt facets. Atomic-resolution STEM images of Pt/alumina interfaces are compared to DFT-based models of the interfaces with different alumina terminations (O, Al1, Al2). The O-terminated interface model provides the best match to experiments for both γ - and θ -alumina and is predicted to be the most stable for the processing conditions, based on thermodynamic calculations of the interfacial energy as a function of temperature and oxygen partial pressure. The Pt/ γ -Al₂O₃ model matches experiments well at the interface but does not capture the bulk structure as well. This is attributed to compromises in the γ -Al₂O₃ model made to limit the computational time required for the calculations, which were not needed for θ -Al₂O₃ model. This work furthers the understanding the limits of models of transition aluminas and Pt/alumina interfaces.

2:55 PM

(PACRIM-S09-005-2025) The interplay between surface chemistry and energetics on controlling the shapes of transition metal carbide ceramics

Y. Huang¹; A. Stubbers²; G. Thompson²; O. A. Graeve³; C. R. Weinberger^{*1}

1. Colorado State University, Department of Mechanical Engineering, USA
2. University of Alabama, Metallurgical & Materials Engineering, USA
3. University of California, San Diego, Mechanical and Aerospace Engineering, USA

There is no consensus on the shapes of synthesized transition metal carbides – varying from cubes to octahedra and can be influenced based on processing routes and chemistry. In this talk, we examine how carbide crystals can be controlled through their surface energies via carbon vacancies and transition metal doping. Specifically, we

*Denotes Presenter

use DFT modeling to examine how carbide stoichiometry changes the surface energies and subsequent shapes of cubic carbide crystals. Then, we demonstrate how doping with different transition metals can also change these equilibrium shapes. These results are then compared to experimental observations of transition metal carbide powders to provide a better understanding of what controls carbide particle shapes and how processing conditions can affect it.

3:30 PM

(PACRIM-S09-006-2025) Diffusion bonding of iron doped 45 degree (100) twist grain boundaries in SrTiO₃

W. Hahn^{*1}; K. Kawahara²; S. Sasano³; B. Feng³; Y. Ikuhara⁴; K. van Benthem⁵

1. University of California Davis, Materials Science and Engineering, USA
2. Tokyo Daigaku, Japan
3. The University of Tokyo, Japan
4. University of Tokyo, Institute of Engineering Innovation, Japan
5. University of California, Davis, Dept. of Chemical Engineering and Materials Science, USA

45 degree (100) twist grain boundaries in SrTiO₃ were fabricated by diffusion bonding of single crystals. Doping of the grain boundaries was accomplished either by the utilization of Fe-doped single crystals, or sputter deposition of ultra-thin iron layers on one of the (100) surfaces prior to diffusion bonding. TEM samples were subsequently prepared by focused ion beam sectioning and Ar ion milling. Atomic and electronic interface structures were determined by aberration-corrected scanning transmission electron microscopy. Initial energy dispersive X-ray spectroscopy (EDS) experiments using spatial difference techniques revealed interfacial dopant concentrations that varied between the different bicrystals. More detailed atomic resolution EDS experiments are underway to investigate equilibrium dopant segregation of Fe. Additional experiments are planned to verify whether interfacial segregation can be affected by electric field annealing.

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(PACRIM-S09-007-2025) Solute segregation process and kinetics in yttria stabilized zirconia grain boundary

J. Tam^{*1}; B. Feng¹; A. Nakamura²; S. Kondo¹; N. Shibata¹; Y. Ikuhara³

1. The University of Tokyo, Japan
2. Osaka Daigaku, Department of Mechanical Science and Bioengineering, Japan
3. University of Tokyo, Institute of Engineering Innovation, Japan

Yttria stabilized zirconia (YSZ) is a technologically important ceramic with diverse applications. However, the structure and chemistry at the atomic scale need to be well-controlled to optimize the macroscopic properties and behaviour. In YSZ, Y³⁺ tends to segregate to grain boundaries in a substitutional manner as in the bulk. Currently, little is known on the segregation process and the conditions that trigger segregation. A novel bicrystal fabrication process was developed to fabricate specimens without Y³⁺ segregation. As a model system, the grain boundary geometry selected for this study is $\Sigma 3$ {111}<110>. To induce grain boundary segregation, the specimen was annealed at various temperatures and their structure and chemistry were tracked by atomic resolution scanning transmission electron microscopy (STEM) imaging and energy dispersive X-ray spectroscopy (EDS). Furthermore, the driving force and kinetics of segregation were determined by applying classical interfacial phenomena equations. The results of this study can be used as a guideline to control the decoration of solutes at the grain boundary to enable desirable physical and functional properties.

PacRim S11 - Optical and Electronic Phase Change Materials - Science and Application

PACRIM Symposium 11 - Optical and Electronic Phase Change Materials: Science and Application I

Room: Georgia A

Session Chair: Matthias Wuttig, RWTH Aachen University

1:15 PM

(PACRIM-S11-001-2025) Tunable Free-space Optics via Phase Change Materials (Invited)

A. Majumdar^{*1}

1. University of Washington, USA

Shaping an optical wavefront with sub-wavelength spatial resolution is important for various applications with far-reaching scientific and technological impacts (e.g., in adaptive optics and imaging through turbid, disordered media) and commercial interest (e.g., LIDAR for autonomous transportation and pixelated holography). The primary enabling technology for such capability is a compact optical phase shifter, which can change the phase of the incident light by a full 360 degree with low energy and high frequency (~MHz). Existing tunable optical technologies cannot provide this functionality; mechanically tunable modulators can reach a speed of only a few kHz, while liquid-crystal based modulators operate at 100's of Hz. The pixel size of the spatial light modulator is also on the order of tens of wavelengths, which increases the energy consumption per pixel. In this talk, I will discuss our effort to tune meta-optics using chalcogenide based non-volatile phase-change materials. Using wide bandgap phase change materials, we reported a transmissive tunable metasurface, and also reported independent tuning of ~14 meta-atoms. Finally, we reported the first visible tunable transmissive metasurface using phase change materials.

1:45 PM

(PACRIM-S11-002-2025) Back-end integration of phase change materials in foundry-fabricated silicon photonics and its performance bounds (Invited)

J. Li^{*1}; H. Lin²; L. Li³; J. Hu⁴

1. Hangzhou Institute for Advanced Study, University of Chinese Academy of Sciences, China
2. Zhejiang University, China
3. Westlake University, China
4. Massachusetts Institute of Technology, USA

Chalcogenide phase change materials (PCMs) are a promising candidate for ultra-compact and zero-static-power-consumption photonic devices due to their high refractive index contrast during the reversible and nonvolatile phase transition. With the recent advancements of low-loss PCMs and their integrated photonic devices, the large-scale integration of PCM-based photonics becomes an essential technique for further study and practical applications. Here we report the realization of back-end integration of phase change materials (for instance, Sb₂Se₃ and Ge₂Sb₂Se₄Te₁) in foundry-fabricated silicon photonics. Notably, the use of low-throughput e-beam lithography is avoided in the entire fabrication process. Based on this PCM back-end integration platform, quasi-continuous nonvolatile switching and arbitrary-states configuration are achieved, thus enabling electrically reconfigurable post-fabrication trimming, multi-level phase shifting, and intensity modulation. We then analyze the performance bounds of back-end integrated PCM-based silicon photonic devices. The primary factors constraining the device performances and potential mitigation strategies are also discussed.

2:15 PM

(PACRIM-S11-003-2025) Photonic computing using phase-change materials (Invited)Z. Cheng*¹

1. Fudan University, China

Thanks to the great success of optical fiber communication in the field of ultra-high-speed data transmission, as well as the rapid development of silicon-based photonics and optoelectronics integration, photonic computing has been widely and deeply studied, which is one of the important directions for the development of integrated circuits in the Post-Moore era. At the same time, the rise of artificial intelligence is rapidly driving the development of new computing architectures, such as neuromorphic computing inspired by the human brain. To mimic the function of the brain from a hardware perspective, neuromorphic computing needs to focus on two levels: collocation of storage and computing and artificial neural networks. Here, we combine non-volatile phase-change materials (PCMs) and optical waveguides to implement photonic in-memory computing and associative learning networks to construct the above two neuromorphic paradigms. Moreover, in recent years, we have focused on the development of new phase-change materials in photonics applications.

2:45 PM

(PACRIM-S11-004-2025) Reconfigurable metasurfaces using optical phase change materials (Invited)C. Constantin Popescu¹; K. Dao¹; B. Mills³; H. Kim²; C. A. Rios Ocampo⁴; J. Hu¹; T. Gu*¹

1. Massachusetts Institute of Technology, USA
2. Korea Advanced Institute of Science and Technology, Republic of Korea
3. Massachusetts Institute of Technology, Materials Science and Engineering, USA
4. University of Maryland, USA

Metasurface flat optics herald a new era of dynamic control over light propagation, processing, and interaction with matter, offering improved performance and introducing novel capabilities. In this talk, I will discuss the prospects and hurdles of utilizing reconfigurable metasurfaces across multiple applications. Leveraging advanced phase change materials and designs, we develop ultra-compact meta-optics with high performance and new functionalities.

PACRIM Symposium 11 - Optical and Electronic Phase Change Materials: Science and Application II

Room: Georgia A

Session Chair: Tian Gu, Massachusetts Institute of Technology

3:30 PM

(PACRIM-S11-005-2025) Neuromorphic Photonic Computing Devices Based on Electrically Controlled Phase-Change MemoryW. Zhou*¹

1. Xi'an Jiaotong University, China

Neuromorphic computing hardware aims to mimic biological neural networks and has emerged as a viable path in overcoming limitations of the von Neumann architecture. By eliminating the latency and energy losses associated with transferring data between the memory and central processing unit, these systems promise to improve on both speed and energy. Here, we report photonic implementation using on-chip, nonvolatile waveguide memories to deliver energy efficient, high-speed, and high-density data processing within the photonic memory. We developed a non-volatile electronically reprogrammable PCM memory cell with a record-high 4-bit weight encoding levels using a non-resonant waveguide microheater. For system-level application, a compact photonic-electronic dot-product engine for in-memory computing was demonstrated with a high computational precision for image processing and classification.

*Denotes Presenter

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(PACRIM-S11-006-2025) AI-assisted Discovery of Phase Change Materials for Electronic DevicesC. Lee*¹; H. Sun¹; C. A. Rios Ocampo¹; I. Takeuchi¹

1. University of Maryland, Materials Science and Engineering, USA

Chalcogenide-based phase change materials (PCMs) have been exploited in advanced non-volatile electrical memories and neuromorphic computing devices, relying on rapid and reversible switching. Since each application requires a set of unique characteristics, developing high-throughput methods to expand the current PCM library driven by specific performance metrics is paramount. In neuromorphic computing, some key features for building high-performance devices, such as stochasticity, switching energy, switching speed, endurance, retention, etc. PCM-based devices have been considered promising integration owing to high resolution integration, high cyclability, and data retention. However, power consumption for switching and electrical drift is still high compared to other technologies, such as conductive filament memristors, magnetic tunneling junctions and ferroelectric tunneling junctions. Novel materials are in need as current PCMs ($\text{Ge}_2\text{Se}_2\text{Te}_3$, GeTe , or Sb_2Te_3) fall short. Here, we tackle this challenge by leveraging the reliable response of doped-PCMs following a wafer-scale combinatorial sputtering study on electronic device arrays. We combine autonomous experiments with active learning under a multi-objective scheme, aiming to find materials with lower switching energy, large resistance contrast, and no drift. We demonstrate a combinatorial study on this unique platform enabling on-chip switching.

(PACRIM-S11-007-2025) Harnessing Losses in Phase-Change Materials for Novel Nanophotonic DevicesC. Lian*¹; Y. Huang¹; H. Sun¹; N. Acharjee²; A. Dewland³; S. Wang¹; I. Takeuchi³; C. A. Rios Ocampo¹

1. University of Maryland, Materials Science and Engineering, USA
2. University of Maryland, Electrical & Computer Engineering, USA
3. University of Maryland, Institute for Research in Electronics and Applied Physics, USA

The integration of phase-change materials (PCMs) with photonic devices enables precise and dynamic tuning of light. The optical responses stem from the contrast in the real (n) and imaginary (k) parts of refractive indices upon PCM phase transformation. However, the simultaneous coupling of Δn and Δk in $\text{Ge}_2\text{Se}_2\text{Te}_3$ and $\text{Ge}_2\text{Sb}_2\text{Se}_4\text{Te}_3$, for example, limits the performance of these PCMs as we lose the ability to independently control phase and amplitude of light. This limitation highlights the unique advantage of Sb_2Se_3 , as it exhibits a large contrast in refractive index and no loss in either state in the telecom wavelength, making it ideal for phase only modulation. Many studies have focused on controlling the real part of the refractive index in PCMs, with significant efforts dedicated to minimizing losses in optical systems by exploring low-loss PCMs. However, most PCMs display large losses, which are often considered undesirable. Instead, we can harness this property to tune from low to high losses and strategically engineer optical phenomena, such as inducing parity-time (PT) symmetry breaking and unbreaking in waveguides, controlling Fano resonances, and more. These approaches enable low-loss and unprecedented modulations even when high-loss PCMs are integrated into novel nanophotonic devices.

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(PACRIM-S11-008-2025) Tellurium: A phase-change selector materialS. Elliott*¹

1. University of Oxford, United Kingdom

3D-cross-point PCRAM memory arrays need selector switches for each memory cell to select particular cells on applying voltages to word and bit lines and avoid sneak current paths involving other cells.

Amorphous chalcogenides are often used for this purpose. These employ Ovshinsky threshold switching (OTS); an applied voltage above a threshold value causes a big increase in electrical conductivity (ON state) but the material stays amorphous; the material returns to the low-conductivity OFF state when the applied voltage is reduced below a holding value. The OTS effect is thought to be electronic in nature. Recently, we have shown that elemental Te exhibits voltage-dependent switching, and can be used as a selector, but the mechanism is not OTS-like. Instead, Te exhibits a volatile phase-change (PC) behaviour, different from the conventional non-volatile PC behaviour for tellurides (e.g. Ge-Sb-Te) for memory applications, where voltage-induced switching between glassy and crystalline phases occurs. In Te selectors, the OFF state is the semiconducting crystal; the ON state is the transient metallic liquid formed when a Joule-heating voltage is applied. I will present experimental results on the operation of Te selectors and results from molecular-dynamics simulations of Te using a machine-learned potential, revealing the origin of the difference in threshold voltage between first and later voltage pulses, as well as chiral growth.

4:30 PM

(PACRIM-S11-009-2025) In Situ TEM and Nanocalorimetry Study of the Thermodynamics and Kinetics of Crystallization of Sb-rich Phase Change Materials

T. D. Koledin^{*1}; I. McGieson²; K. Bustillo³; J. Pettibone⁴; W. A. Osborn⁴; F. Yi⁴; D. A. LaVan⁴; M. K. Santala⁵

1. Oregon State University, Materials Science Program, USA
2. Oregon State University, Department of Physics, USA
3. E O Lawrence Berkeley National Laboratory, NCEM, USA
4. National Institute of Standards and Technology Material Measurement Laboratory, MML, USA
5. Oregon State University, School of Mechanical, Industrial and Manufacturing Engineering, USA

Phase change materials (PCM) are marginal glass formers that may be used in memristors and neuromorphic memory, because they may be rapidly switched between amorphous and crystalline phases. Due to the rapid crystallization and small grain size, until recently it had not been possible to image and directly measure the crystal growth much above the glass transition temperature, T_g . Ultrafast differential scanning calorimetry (DSC) and reflectivity have been used to extract growth rates from the measurement of the fraction crystallized, but this requires assumptions about the relative contribution of nucleation and growth. This work utilized nanocalorimeters designed and fabricated at the National Institute of Standards and Technology to be run in a transmission electron microscope (TEM). Simultaneous nanocalorimetry and TEM imaging was performed on thin films of $\text{Ag}_3\text{In}_4\text{Sb}_7\text{Te}_{17}$ and $\text{Ge}_7\text{Sb}_{93}$, at up to 9,000 K/s and 30,000 frame/s using high-speed electron detectors at the National Center for Electron Microscopy. The growth rates were directly measured, and the enthalpy of crystallization was quantified for a range of temperatures above T_g . These measurements contribute to the picture of crystallization kinetics of PCMs and suggest that assumptions made about nucleation in the analysis of ultrafast DSC experiments have led to the overestimation of fragility.

4:50 PM

(PACRIM-S11-010-2025) Tailoring the Switching in Phase Change Materials: The Role of Chemical Bonding

M. Wuttig^{*1}

1. RWTH Aachen University, Germany

Controlling a state of material between its crystalline and glassy phase has fostered many real-world applications. Nevertheless, design rules for crystallization and vitrification kinetics still lack predictive power. Here, we identify stoichiometry trends for these processes in phase change materials (PCMs) crucial to tailor devices based on these PCMs. We investigate alloys along the GeTe-GeSe, GeTe-SnTe, and GeTe-Sb₂Te₃ pseudo-binary lines employing

a pump-probe laser setup and calorimetry. A clear stoichiometry dependence of crystallization speed is discovered along a line connecting regions characterized by two fundamental bonding types, metallic and covalent bonding. Increasing covalency slows down crystallization by six orders of magnitude and promotes vitrification. The stoichiometry dependence is correlated with material properties, such as the optical properties of the crystalline phase and a bond indicator, the number of electrons shared between adjacent atoms. A quantum-chemical map explains these trends and provides a blueprint to design crystallization kinetics in optical and electronic memories employing PCMs.

5:10 PM

(PACRIM-S11-011-2025) Autonomous high-throughput exploration of phase change memory materials (Invited)

I. Takeuchi^{*1}

1. University of Maryland, USA

We are applying the combinatorial thin film high-throughput platform for rapid exploration of novel phase change memory materials for photonic and electronic device applications. Composition spreads are fabricated in a high vacuum co-sputtering system. In order to rapidly identify compositions with desirable properties, we have developed the closed-loop autonomous materials exploration and optimization (CAMEO) technique. This technique allows effective self-navigation of compositional phase space without the need to map the entire search space. Through this approach, we have previously identified $\text{Ge}_4\text{Sb}_6\text{Te}_7$ (GST467), a coherent nanocomposite, as the composition with the largest bandgap difference between amorphous and crystalline states within a large compositional space in the Ge-Sb-Te ternary. Subsequent device studies based on GST467 have revealed that owing to the epitaxial nanocomposite structure, the material has superior electrical and photonic switching properties compared to other compositions within the ternary. Details of the autonomous exploration technique as well as the properties of GST467 will be discussed. This work has been carried out in collaboration with Heshan Yu, Gilad Kusne, Changming Wu, Mo Li, Asir Khan, Eric Pop, Chih-Yu Lee, and Carlos O'Campo, and has been funded by an SRC nCORE program, ONR MURI N00014-17-1-2661, and NSF DMR-2329087.

PacRim S12 - Eng Ceramics and Ceramic Matrix Composites - Processing/Design/Applications

PACRIM Symposium 12 - Advanced design, processing, and manufacturing of CMC I

Room: Plaza B

Session Chairs: Hua-Tay Lin, Guangdong University of Technology; Yanwen Zhang, Queen's University

1:15 PM

(PACRIM-S12-001-2025) From Materials Response at Extremes to Materials Design and Discovery (Invited)

Y. Zhang^{*1}; A. Datye²; A. R. Khanolkar³; W. J. Weber⁴; H. Lin⁵

1. Queen's University, Mechanical and Materials Engineering, Canada
2. Yale University, Material Science and Engineering, USA
3. Idaho National Laboratory, USA
4. University of Tennessee, Materials Science & Engineering, USA
5. Guangdong University of Technology, School of Electronic and Mechanical Engineering, China

Under radiation, materials with similar crystalline structures exhibit different responses to defect formation and damage accumulation, highlighting the interplay among various chemical bonds. The physical properties and irradiation response of the high-entropy transition metal (TM) diboride $\text{Hf}_{0.2}\text{Nb}_{0.2}\text{Ta}_{0.2}\text{Ti}_{0.2}\text{Zr}_{0.2}\text{B}_2$ and some of

its subsets have been investigated. Surprisingly, these TM diborides exhibit electronic heat/energy conduction as the predominant mechanism, rather than the ceramic-like behavior typically expected. The high-entropy diboride shows the greatest recovery in hardness and modulus at high fluences, demonstrating superior resistance to radiation-induced damage compared to its quaternary counterparts. An exception to this trend is observed in $(\text{Hf}_{1/3}\text{Ta}_{1/3}\text{Ti}_{1/3})\text{B}_2$ and differences in defect cluster formation in the VIB TM diboride $(\text{Hf}_{1/3}\text{Ti}_{1/3}\text{Zr}_{1/3})\text{B}_2$ warrant further investigation at the atomic and electronic levels. The findings highlight opportunities to design high-entropy ceramics by tailoring chemical disorder and bonding characteristics. Gaining insights into the role of element substitution and associated chemical disorder will enable the design of complex materials with specific functionality and improved performance, thus opening numerous exciting research directions and offering opportunities for materials discovery.

1:45 PM

(PACRIM-S12-002-2025) Preparation, Densification, and Strengthening-Toughening Studies of High-Entropy Nitride Ceramics (Invited)

Y. Lu¹; W. Song¹; C. Wang¹; M. Li¹; J. Li¹; Y. Li¹; B. Ma^{*1}

1. North Minzu University, China

In this study, SiC and Ni were used as sintering aids to investigate the effects of different sintering methods (solid-state and liquid-phase) on the densification behavior of high-entropy nitride ceramics. The densification mechanisms were summarized, and the strengthening and toughening mechanisms of additives in high-entropy bulk ceramics were explored. Meanwhile through first-principles calculations, the crystal structure and mechanical properties of $(\text{Hf}_{0.2}\text{Zr}_{0.2}\text{Ti}_{0.2}\text{Nb}_{0.2}\text{Ta}_{0.2})\text{N}$ high-entropy ceramics were modeled. Using submicron $(\text{Hf}_{0.2}\text{Zr}_{0.2}\text{Ti}_{0.2}\text{Nb}_{0.2}\text{Ta}_{0.2})\text{N}$ high-entropy powder as the raw material, $(\text{Hf}_{0.2}\text{Zr}_{0.2}\text{Ti}_{0.2}\text{Nb}_{0.2}\text{Ta}_{0.2})\text{N}$ high-entropy bulk ceramics were sintered via spark plasma sintering (SPS) at 2100°C. The final relative density of the ceramics was measured to be 93.08%. SiC and Ni as a sintering additive, when the SiC content reached 10.0 wt.%, the relative density of the ceramics achieved 98.32%. When the addition of SiC and Ni was optimized at 10 wt.% and 3 wt.%, respectively, the relative density of the bulk ceramics reached an impressive 99.81%. This near-theoretical densification resulted in exceptional mechanical performance. The Vickers hardness, fracture toughness, and flexural strength of the bulk ceramics achieved values of 24.87 ± 0.57 GPa, 6.44 ± 0.81 MPa m^{1/2}, and 445 ± 21 MPa, respectively.

2:15 PM

(PACRIM-S12-003-2025) Application of Electrophoretic Phenomenon for h-BN, Al₃SiC₄ and Ti₃SiC₂ Interphase Formation of SiC_f/SiC Composites (Invited)

K. Yoshida^{*2}; A. Gubarevich²; M. Kotani¹

1. Japan Aerospace Exploration Agency (JAXA), Japan

2. Institute of Science Tokyo, Japan

Silicon carbide fiber-reinforced silicon carbide matrix (SiC_f/SiC) composites have been expected to be used in aerospace, future nuclear and fusion fields as next-generation heat resistant structural materials with high reliability. The formation of the optimum interphase between fiber and matrix has been recognized one of the critical issues to achieve high performance SiC_f/SiC composites. At present, carbon or hexagonal-boron nitride (h-BN) has been coated on SiC fibers as the interphase for SiC_f/SiC composites, and they have been coated by chemical vapor deposition (CVD) or chemical vapor infiltration (CVI) method. The present authors proposed the novel interphase formation process for SiC_f/SiC composites based on electrophoretic deposition (EPD). In this symposium, interphase formation process of layered compounds, h-BN, Al₃SiC₄ and Ti₃SiC₂, which show better oxidation resistance than carbon, by EPD method, and properties of unidirectional SiC_f/SiC composites with h-BN, Al₃SiC₄ and Ti₃SiC₂ interphases formed by EPD method were reviewed.

2:45 PM

(PACRIM-S12-004-2025) Fabrication and property analysis of C_f/ZrB₂-SiC composites prepared via slurry infiltration and precursor impregnation and pyrolysis (Invited)

Y. Zou^{*1}; S. Lee¹

1. Korea Institute of Materials Science, Republic of Korea

Ultra-high temperature ceramic matrix composites (UHTCMCs) have recently attracted significant attention due to their excellent strength and stability at elevated temperatures, as well as their ability to overcome the intrinsic brittleness and low damage tolerance of pure UHTCs such as ZrB₂ and ZrC. For continuous carbon fiber reinforced UHTCMCs, the UHTC matrix is typically introduced using methods such as chemical vapor infiltration (CVI), precursor impregnation and pyrolysis (PIP), reactive melting infiltration (RMI), and slurry infiltration (SI). However, each of these techniques has limitations: CVI is expensive and time-consuming, RMI often results in poor mechanical properties, SI is restricted by limited infiltration depth, and PIP requires an extended processing cycle due to the low ceramic yield of the precursor. Consequently, the development of a hybrid technology is essential for the fabrication of UHTCMCs. In our study, C_f/ZrB₂-SiC composites were prepared using a combination of highly concentrated aqueous ZrB₂ slurry infiltration and SiC precursor impregnation and pyrolysis. The fabrication process and microstructure of the composites were analyzed, and their mechanical properties at elevated temperatures were also investigated. Additionally, the fracture behaviors of the composites and the underlying mechanisms were discussed.

PACRIM Symposium 12 - Advanced design, processing, and manufacturing of CMC II

Room: Plaza B

Session Chairs: Hua-Tay Lin, Guangdong University of Technology; Yanwen Zhang, Queen's University

3:30 PM

(PACRIM-S12-005-2025) Fracture Strength Recovery in Polycrystalline Zirconia by Crack Healing under Electric Field (Invited)

K. Morita^{*1}

1. National Institute for Materials Science (NIMS), Japan

Strong electric field/current can lower the sintering temperature and time of ceramic powders. The accelerated phenomena called as flash event is known to effectively work not only on the sintering of powders, but also on high temperature processing of bulk ceramics, such as deformation and joining. We confirmed that the flash event is also effective to accelerate crack healing. In this work, therefore, the effect of the flash healing on the mechanical strength was examined before and after FH treatment using 8Y-CSZ polycrystals as a reference material. The flash event under DC successfully healed the micro-crack with an initial length of 20 mm at a specimen temperature of 1223 °C for 10 min. As compared to the healing without the electric field/current (0 V), the crack healing was apparently accelerated by more than 180 times even at the same temperature of 1223 °C. The accelerated crack healing can be ascribed to accelerated grain boundary diffusivity of cations that caused additionally through the flash event. Although the room temperature bending strength decreases to about 180 MPa by forming the microcrack of 20 mm, it can be recovered to >400 MPa, which is almost the same to that of the as-sintered specimen, through the flash healing treatment at 1223 °C for 10 min.

4:00 PM

(PACRIM-S12-006-2025) Recent Progress in Environmental Barrier Coatings for 2700 °F (1482 °C) SiC/SiC Ceramic Matrix Composites (Invited)

K. Lee*¹; R. I. Webster¹; B. Puleo¹; B. J. Harder¹; M. J. Presby¹; J. Stuckner¹; J. Setlock²; L. C. Hoffman¹

1. NASA Glenn Research Center, USA
2. University of Toledo, USA

Environmental barrier coatings (EBCs) have enabled the implementation of SiC/SiC ceramic matrix composites (CMCs) in gas turbines by protecting CMCs from corrosive species. The upper use temperature of current CMCs is ~1316 °C (2400 °F). The next generation CMCs are targeting for 1482 °C (2700 °F) temperature capability. The Si bond coat employed in current state-of-the-art EBCs is not a viable bond coat for next generation CMCs due to its low melting point (1414 °C). The viability of next generation CMCs, therefore, is contingent upon the successful development of a higher temperature bond coat to replace the Si bond coat. Oxide-based bond coats are a logical option to replace the Si bond coat for 1482 °C temperature capability. NASA has recently developed a high-temperature EBC using an oxide-based bond coat via slurry process and demonstrated its performance on CMC coupons and sub-components via various rig tests simulating engine environments. Many challenges remain, including steam oxidation life, recession resistance under high velocity steam and CMAS (calcium-magnesium-aluminum-silicate) resistance. This paper will discuss the recent progress in the high-temperature EBC technology at NASA.

4:30 PM

(PACRIM-S12-007-2025) Chemical vapor deposition of rare-earth aluminum garnet-alumina nanocomposite coatings (Invited)

A. Ito*¹

1. Yokohama National University, Graduate School of Environment and Information Sciences, Japan

Directionally solidified eutectics (DSE) is a bulk composite in a ceramic eutectic system and have been studied as a high-temperature structural ceramic since the early reports on $Y_3Al_5O_{12}-Al_2O_3$ (YAG-alumina) and $GdAlO_3-Al_2O_3$ bulk composites indicated their excellent high-temperature strength and durability. Oxide-oxide ceramic matrix composites remain of interest as high-temperature components used in the aerospace and defense industries. Although the DSE composites show outstanding mechanical strength and heat resistance, their application as a ceramic coating is limited because a melt-solidification process was believed to be the only way to form ordered structures in eutectic systems. Chemical vapor deposition (CVD) is a practical coating technique in industrial manufacturing process; however, the conventional thermal CVD process is unfeasible to form thick protective coating and as a rapid production method. We have developed the laser-assisted CVD method to produce thick ceramic coatings rapidly. We propose a chemically vapor deposited eutectic system (CDE) of rare-earth aluminum garnet (REAG)-alumina composite coatings with ordered structures. In YAG-alumina eutectic system, YAG phase with rod and lamella structures grew unidirectionally in the alumina phase, which was homoepitaxially grown on a sapphire substrate.

5:00 PM

(PACRIM-S12-008-2025) Rapid pressureless densification of boron carbide with electromagnetic induction assistance

A. Gubarevich*¹; G. Homma¹; K. Yoshida¹

1. Tokyo Kagaku Daigaku, Japan

Dense boron carbide was fabricated from commercial powders using a standard electromagnetic induction heating equipment with a high-frequency solenoid coil and a graphite crucible. The induction coil served two primary roles: (1) heating the sample indirectly via the graphite crucible (susceptor) and (2) directly applying a

high-frequency electromagnetic field to the boron carbide sample. The shielding properties of the susceptor, influenced by its material and thickness, controlled the degree of electromagnetic field effect on the sample. The relationship between crucible thickness and densification was investigated, showing that using a graphite crucible thinner than the graphite characteristic skin depth promotes rapid densification. As a result, by applying current to the induction coil for less than 5 minutes, boron carbide achieved a relative density of 95% without the need for sintering additives or external mechanical pressure. Despite rapid heating and cooling rates, the densified samples were crack-free and demonstrated excellent mechanical properties, including a Vickers hardness of 30 GPa, a Young's modulus of 415 GPa, and a fracture toughness of $4.82 \text{ MPa}\cdot\text{m}^{1/2}$. Our results suggest that high-frequency electromagnetic fields affect atomic diffusion and promote rapid, pressureless densification of boron carbide at elevated temperatures.

PacRim S19 - Nanostructured Bioceramics and Ceramics for Biomedical Applications

PACRIM Symposium 19 - Nanostructured Bioceramics and Ceramics for Biomedical Applications I

Room: Stanley

Session Chairs: Leena Hupa, Åbo Akademi University;
Pelagia-Irene Gouma, The Ohio State University

1:15 PM

(PACRIM-S19-001-2025) Bioconjugated Nanocarriers for Precision Drug Delivery (Invited)

S. Mathur*¹

1. University of Cologne, Institute of Inorganic Chemistry, Germany

Chemical processing of functional ceramics has played a key role in converging disciplines, which is especially true for biomedical applications. For example, the development of biocompatible drug-carriers that can hold back the payloads and release the drugs or antibiotics at the specific diseased area is a materials processing challenge. The selective transport and retention of drugs in sufficiently high concentrations at the target site is inhibited by various physiological barriers, which reduces or even blocks the therapeutic efficiency of molecular drugs. Therefore, advanced drug-delivery systems designed to overcome biological barriers are needed to meet the specific traits of physiological and disease-related barriers. In this context, chemically functionalized nanoparticles act as efficient drug-carriers to transport higher amounts of therapeutic payloads to diseased sites that also reduces the undesired off-site effects. Moreover, hollow nanocarriers can incorporate more than one drug enabling theranostic and theraregenerative approaches. Finally, ceramic nanoparticles can be modified with surface-bound target ligands to exploit the overexpression of receptors and promote cell specific attachment of the carriers for a localized high concentration of drug around disease sites. This talk will discuss the potential benefits of inorganic nanoparticles towards precision drug delivery.

1:45 PM

(PACRIM-S19-002-2025) Biomass based skin-interfaced triboelectric sensors (Invited)

W. Wu*¹

1. Purdue University, USA

The capability of sensor systems to efficiently scavenge their operational power from stray, weak environmental energies through sustainable pathways could enable viable schemes for selfpowered health diagnostics and therapeutics. Triboelectric nanogenerators (TENG) can effectively transform otherwise wasted environmental mechanical energy into electrical power. However, obstacles hindering the development of efficient triboelectric devices based on

biocompatible materials continue to prevail. I will discuss our recent progress in the design and engineering of biomaterials for biocompatible, wearable triboelectric devices. Such wearable devices are conformable to human skins and can sustainably perform non-invasive functions by harvesting the operation power from the human body. The gained fundamental understanding and demonstrated capabilities enable the rational design and holistic engineering of novel materials for more capable biocompatible triboelectric devices that can continuously monitor vital physiological signals for creating unprecedented diagnostic tools for diagnosis, interpretation, and prediction of human status in ubiquitous resource-constrained conditions.

2:15 PM

(PACRIM-S19-003-2025) Bioactive Calcium Silicate and Aluminate Cements for Dentistry (Invited)

C. Primus*¹

1. Augusta University, Adjunct Assoc. Prof. Endodontics, USA

In the 1990s, the ordinary, hydraulic, calcium silicate, and calcium aluminate cements were discovered to be bioactive-forming hydroxyapatite when used in contact with subgingival oral tissue *in vivo*. These well-known cements have been revolutionary in improving the success of treatments for tooth-saving dental procedures – e.g., root canal therapy, surgical endodontics, perforation treatment, vital pulp therapy procedures, and other endodontic diseases of the enamel or pulp tissues. The benefits of these cements to pediatric dentistry will also be discussed. These cements are successful for their concomitant properties of dimensional stability, high pH, and calcium ion release. Low microleakage and adequate bond strength also contribute to these cements meeting the desired requirements for sealing materials used below the gum line (subgingival) to avoid further tooth destruction or extraction. State-of-the-art and the current requirements in ISO and ADA standards will be summarized for the calcium silicate/aluminate cements used in dentistry. Many formulas are available, with various liquids for mixing with the cement. An overview will be given for properties, including cement phase proportions, setting times, film thickness and flow, radiopacity, biocompatibility, and antimicrobial properties. Selected healing histology results will be shown to correlate with the ceramics' properties.

2:45 PM

(PACRIM-S19-004-2025) Developing Advanced Bioceramic Scaffolds for Bone Regeneration through Computer-aided Design, Computational Simulations and Additive Manufacturing (Invited)

M. Wang*¹

1. The University of Hong Kong, Department of Mechanical Engineering, Hong Kong

The traditional approach and also manufacturing technologies have limitations which hinder the development of advanced tissue engineering (TE) scaffolds with desired porous structures and biological properties. Computer-aided design (CAD) is a powerful tool for designing complex structures including advanced porous TE scaffolds, and additive manufacturing (i.e., 3D printing) technologies enable us to fabricate complicated (pore size-graded, functional gradient, etc.) and customized (i.e., patient-specific) TE scaffolds. Also, computational simulations (mechanical, fluidic, etc.) can assist us greatly in developing advanced TE scaffolds. By integrating CAD, computational simulations and 3D printing, advanced TE scaffolds can be developed effectively and efficiently, minimizing the cost, time and efforts. For bone regeneration, bioactive ceramics are commonly used to construct bone tissue engineering (BTE) scaffolds. Owing to its osteoconductivity and osteoinductivity and controllable biodegradation rate, the biphasic calcium phosphate (BCP) bioceramic is among best materials for BTE scaffolds. In this invited talk, our research on integrating CAD, computational simulations and 3D printing in developing BCP scaffolds is presented. These BCP scaffolds showed excellent *in vivo* performance in regenerating bone in an animal model.

PACRIM Symposium 19 - Nanostructured Bioceramics and Ceramics for Biomedical Applications II

Room: Stanley

Session Chairs: C. Primus, Avalon Biomed Inc.;

Min Wang, The University of Hong Kong

3:30 PM

(PACRIM-S19-005-2025) Electrospun Photocatalytic Nanogrids (Invited)

P. Gouma*¹

1. The Ohio State University, MSE, USA

Photocatalytic nanomats of metal oxides which float on water and using sunlight (both visible and UV spectrum) were employed to induce the photochemical decomposition of petroleum hydrocarbons or for water splitting and hydrogen production. Metal oxide semiconductors, such as titania (TiO₂) or tungsten trioxide (WO₃), when illuminated with light having a higher energy than their respective band gaps can decompose organic compounds. Electrospun nanomats, called nanogrids, are the only engineered nanomaterial that is self-supported and interconnected and while it has all the advantages of nanomaterials it has none of the disadvantages (e.g. dispersion and need for a filtration system to collect dispersed nanoparticles). They can be used in oil spills to break down harmful pollutants or they may convert any pool and pond into a power plant for production of hydrogen and oxygen. This unique and high promising sustainable and renewable energy technology has received a lot of attention by the media (press releases by Fast Company, mentions by NPR, CNCB, etc.) as oxide-based photoassisted oxidation is a most promising route to effective and eco-friendly oil decomposition. A scalable electrospinning process was invented and demonstrated by our research group to create photocatalytic blankets which are reusable. Uses in the biomedical field, such as treating tumors in cancer therapy are also discussed.

4:00 PM

(PACRIM-S19-006-2025) Bioactive Glasses React in Nanoscale (Invited)

L. Hupa*¹

1. Åbo Akademi University, Johan Gadolin Process Chemistry Centre, Finland

Most commercial bioactive glass-based medical devices are micron-sized particles used as bone void fillers, cancer treatment or wound-healing dressings. Intense efforts are paid to develop monolithic porous implants for moderately load-bearing bone applications. In bone healing applications, the development of the apatite surface layer, which provides bonding to the bone apatite, is not just a critical characteristic of bioactivity, but a key to successful bone healing. The nanosized needles and platelets with shortest distances varying from 5 to 40 nm and longest dimensions up to 100 nm in bone apatite question the compatibility of micron-sized materials for bone applications. This presentation discussed why granules and monoliths are accepted to treat bone trauma and lesions, although bone apatite is known to comprise nanosized hydroxyapatite crystals. One essential factor supporting the chemical bonding of the formed apatite crystals with bone apatite is the relatively thick, solution-impregnated silica-rich layer acting as nucleating sites for apatite precipitation and providing dimensional flexibility for the apatite crystals in the interface between the bone and implanted glass. The impact of various factors, such as the solution composition, flow rate, and contact time, will be discussed as critical factors for forming the nanosized hydroxyapatite crystals.

PacRim S21 - Cultural Heritage of the Pacific Rim

PACRIM Symposium 21 - Cultural Heritage of the Pacific Rim I

Room: English Bay

Session Chair: Fumie Iizuka, University of Wisconsin System

1:15 PM

(PACRIM-S21-002-2025) Green strategy for temporary reinforcement and conservation of ancient ivory relics: Calcium-based mineralized hydrogels

C. Shi¹; L. He^{*1}; A. Pan¹

1. Xi'an Jiaotong University, China

Ancient ivory serves as an important witness of time and historical events, offering highly significant insights into the fields of mineralogy, materials science, and geochemistry. However, ancient ivory various environmental factors as a result of its long-term burial, resulting in a loose porous structure and a loss of mechanical strength. The temporary reinforcement and preservation of ancient ivory artifacts is a well-known challenge. Designing a biomimetic mineralized material for non-destructive bonding, inspired by ivory, will be a valuable research endeavor. A methodology was presented in this article for the synthesis of calcium-based mineralized hydrogels (Ca-gel), which possess controllable adhesive strength, beneficial compatibility, environmentally friendly and noninvasive protection, as well as efficient and rapid adhesion for ancient ivory cultural relics. Controllable gel time and gel state can be achieved by manipulating the various components of Ca-gel. Furthermore, Ca-gel exhibited high hygrothermal and UV resistance. The obtained Ca-gel adhesive possessed universality adhesive properties for sandstone, ceramic, and temporary adhesive properties for cultural relics. It is expected that the Ca-gel will emerge as a prominent tool in the field of temporary reinforcement of authenticity, integrity, and continuity for cultural relics.

1:35 PM

(PACRIM-S21-003-2025) Analytical investigation of the glass artifacts and glaze of the blue and white of the mid-14th century Temasek shipwreck near Singapore

C. S. Lau^{*3}; J. Van Kan¹; A. Chi²; M. Ren¹; T. Osipowicz¹; Y. Taniguchi³; Y. Abe⁴; Z. Minrui¹

1. National University of Singapore, Physic, Singapore
2. Nanyang Technological University, Singapore
3. Tsukuba Daigaku, Japan
4. Tokyo Denki Daigaku, Japan

The mid-14th century Temasek shipwreck, discovered near Singapore, serves as a remarkable submerged time capsule, offering a unique window into Southeast Asia's ancient trade and exchange networks that connected the Indian Ocean and the South China Sea. The shipwreck has preserved a diverse array of artifacts which provide tangible evidence of the materials exchanged along these historic trade routes. This study employs non-destructive elemental analytical techniques, including portable XRF and SEM-EDS, to examine glass artifacts and the glazes of blue-and-white Chinese porcelain recovered from this shipwreck. The aims include understanding the manufacturing techniques, provenance, and origins of the ship's artifacts, alongside an assessment of their degradation. This study sheds further light on the extensive trade connections between Southeast Asia and other regions, showcasing the technological and cultural exchanges that emerged from these interactions. These findings provide valuable insight to the historical craftsmanship, material technologies, trade networks, and involved in the production and exchange of these goods while also establishing new baselines for the conservation and preservation strategies of these invaluable cultural treasures.

1:55 PM

(PACRIM-S21-004-2025) An experimental study on decoration manufacturing technique of ceramic bronze-casting molds from the Houma foundry, China

C. Wang^{*1}; Q. Wang¹

1. Shandong University, Institute of Cultural Heritage, China

The ceramic piece-mold casting technique was predominant in the Chinese Bronze Age, and the production of decorations was an important part of the mold-making process. The invention of the pattern-block method in the Houma foundry during the Eastern Zhou period (770-221BCE) was a revolutionary change to the decoration manufacturing technique, enabled the mass production of bronzes. While how extremely fine decoration patterns were made in clay mold with a very sandy texture? In this study, experimental approach was carried out based on the analytical results of the mold fragments from Houma foundry to investigate the decoration manufacturing technique used in this site. The results enable reconstructing the use of pattern-blocks, explain the layered structure and speculate the tools used for producing the pattern on the surface of the bronze-casting molds, and help understand the manufacturing techniques of ceramic bronze-casting molds.

2:15 PM

(PACRIM-S21-005-2025) Understanding manufacturing processes of glazed architectural bricks from Middle Eastern Antiquity coupling archaeometric and experimental approaches

D. Caurant^{*1}; E. Beauvoit²; A. Bouquillon²; O. Majérus¹; Y. Coquinot²; G. Wallez³; J. Cuny³; A. Thomas³

1. Chimie Paristech CNRS, IRCP, France
2. Centre de Recherche et de Restauration des Musées de France (C2RMF), France
3. Musée du Louvre, Département des Antiquités Orientales, France

Multi-colored glazed bricks were used between the 14th and 4th centuries BC to decorate palaces in the Middle East. In this study, we focused on two productions of colored glazed bricks, from Khorsabad (Iraq, 8th century BC) and Susa (Iran, 6th century BC), carrying out a comparative study of the yellow-orange and black glazes to understand the origin of their coloration and their manufacturing process. To achieve this, a double approach was adopted: firstly, millimetric samples of glazes from archaeological bricks were studied (microstructure, composition of the glassy phase, composition and structure of the crystalline phases) using several techniques (SEM-EDX, XRD, μ -Raman, μ -XANES). Secondly, to complete the data obtained from the archaeological samples and to specify their fabrication method, colored glazes were synthesized in the laboratory. The results obtained revealed similar manufacturing processes for the yellow-orange glazes (prior preparation of a pigment based on lead antimonate then mixed with a glass frit before air firing on the bricks at $T < 1000^\circ\text{C}$). For black glazes, major differences emerged between Susa and Khorsabad productions, with the use of ionic-type coloration (Mn^{3+} , Fe^{2+}) or iron-rich crystalline coloring particles for Susa, and the production of Cu_2S nanoparticles for Khorsabad.

2:35 PM

(PACRIM-S21-007-2025) Study the materials and techniques of the lacquer-painted pottery in China

S. Wei^{*1}; S. Shi¹

1. University of Science and Technology Beijing, China

In this study, the materials and technique of the paint on the pottery excavated from a late Neolithic site (6000-5300 BP) in China were comprehensively studied. The analytical techniques conducted include optical microscope (OM), scanning electron microscopy/energy dispersive X-ray spectrometry (SEM-EDS), Raman spectroscopy, Fourier transform infrared spectroscopy (FTIR), Ultra Performance Liquid Chromatography-quadrupole-time of flight-mass spectrometry (UPLC-Q-TOF-MS) and thermally assisted

hydrolysis-methylation pyrolysis-gas chromatography/mass spectrometry (THM-Py-GC/MS). The results revealed the painted pottery is lacquer-painted pottery, which is the earliest evidence of using laccol as binding media to paint pottery. Moreover, a two-layer structure of the paint technique was found. Cinnabar and a kind of yellow dye were detected in the first layer, while iron red was determined in the ground layer. Laccol, instead of urushiol as a binding medium, was identified in both two layers. Laccol is the maker compound from the tree of Toxicodendron (*Rhus*) succedanea, which mainly grows in Vietnam. Its presence in the painted pottery represents that the use of Toxicodendron (*Rhus*) succedanea resource can be as early as the late Neolithic period in China.

2:55 PM

(PACRIM-S21-009-2025) In search of the manufacturing process of tin oxide opacified glazes on terracotta sculptures from the Italian Renaissance

D. Caurant^{*1}; L. Boutenègre¹; L. Cutard¹; A. Bouquillon²; G. Wallez¹

1. Chimie Paristech CNRS, IRCP, France
2. Centre de Recherche et de Restauration des Musées de France (C2RMF), France

Glazes deposited on ceramic objects can be opacified by high refractive index particles dispersed in their bulk. SnO₂ particles were first used for glaze opacification around the 8th century in the Middle East, this technique then spread in Europe. The present work focused on the famous Della Robbia family of Italian artists that produced sculptures covered with opaque glazes during the Renaissance. Their white and blue glazes were opacified by SnO₂ particles, but the process used to produce them remains not well understood. According to contemporary written sources these glazes could have been made by using as intermediate phase a lead-tin calcine (mixture of oxides and lead stannate) obtained by simultaneous calcination of lead and tin metals. Using XRD and SEM-EDX, the present study aimed to precise the opacification process used by the Italian artists by comparing samples of museum with samples synthesized in laboratory at different temperatures. Calcine syntheses showed that between 650 and 900°C Pb₂SnO₄ was the main phase. With a silicate glass frit this phase totally transformed into PbSnO₃ above 800°C that then totally decomposed above 900°C into micrometric SnO₂ particles and PbO that entered the structure of the glassy phase. Comparison with museum glazes demonstrated that the Italian artists used a firing temperature above 900°C.

3:30 PM

(PACRIM-S21-011-2025) Non-invasive analysis of the production technology of Yayoi- and Kofun-period iron and bronze weapons from Japan using neutron imaging and diffraction

J. Ryan^{*1}; F. Grazzi²; F. Cantini²; A. Lo Giudice³; A. Re³; T. Shinohara⁴; S. Harjo⁴; G. Wu⁴

1. Okayama Daigaku, Japan
2. Consiglio Nazionale delle Ricerche Istituto di Fisica Applicata "N. Carrara" CNR-IFAC, Italy
3. University of Torino, Department of Physics, Italy
4. J-Parc Center Busshitsu Seimei Kagaku Kenkyu Shisetsu, Japan

The tombs of Japan's Late Yayoi and Kofun periods (1st to 7th century AD) were characterized by numerous bronze mirrors and metal weapons. While these burial goods are believed to have acted as prestige goods, there is still much that is unknown about the nature of their production and circulation. We present the results of our analysis of four Yayoi period bronze arrowheads and four Kofun period iron swords. We analyzed their morphological, microstructural, and compositional details by exploiting a combination of neutron imaging and diffraction techniques, complemented with XRF, XRD, and XCT. We exploited different neutron beam attenuation degrees related to metal and mineralization phases to achieve useful morphological results concerning conservation state and former shape. Imaging results can provide useful hints about thermal

gradients, mechanical work, artificial and natural patination, and mineralization. We used Rietveld multiphase diffraction analysis to determine relative concentration of metal and mineralization phases and we determined microstructural features by analyzing the diffraction peak profile and Bragg edge shape, correlated to specific parameters such as domain size, residual strain, and texture. These results reveal new details about metal production during the period of early state formation in Japan.

PacRim S22 - 7th International PacRim Richard M. Fulrath Memorial Symposium on Advanced Ceramics

PACRIM Symposium 22 - 7th International PacRim Richard M. Fulrath Memorial Symposium on Advanced Ceramics I

Room: Grouse

Session Chairs: Bryan Huey, University of Connecticut; Hirokazu Sasaki, Shoei Chemical Inc

1:15 PM

(PACRIM-S22-001-2025) Fascinated by amorphous materials for next generation battery application (Invited)

F. Mizuno^{*1}

1. Toyota Motor Corporation, Advanced Battery Development Division, Japan

Amorphous is a promising research subject to discover a new class of the energy storage materials. Today, I will introduce three key examples. First, we have developed lithium-ion conductive solid electrolytes obtained through crystallization of sulfide-based glassy materials. High temperature crystalline phase was well stabilized in the glass-ceramics, leading to superionic properties of the solid electrolyte. This methodology is indeed a good approach to design the materials and also to manufacture such functional materials. Using a solid electrolyte, all-solid-state lithium-ion batteries have been assembled. We have really recognized that the solid electrolyte plays an important role to maintain the solid-solid interface, determining the cell performances. Second, we have demonstrated a variety of materials which have been studied for Mg battery cathode. In multi-valent chemistry, we may need to change the methodology to design a host-guest relationship. Through high-throughput screening and highly advanced analysis, not only characteristic polymorphs but also unique molecule structures have been discovered so far. Amorphous compounds actually showed great features of electrochemical performances. Last, encouraged by solid-state chemistries, new approaches to imagine a sustainable future society have been studied. It would expand great potentials of metal-gas battery system, Li recycling and so on.

1:45 PM

(PACRIM-S22-002-2025) Development of Na-ion conducting glass electrolytes for all-solid-state batteries (Invited)

A. Hayashi^{*1}; K. Motohashi¹; A. Sakuda¹

1. Osaka Koritsu Daigaku, Japan

All-solid-state rechargeable batteries have attracted attention because of their long cycle life, high safety even at high temperature, and high power and energy densities. The key material for realizing solid-state batteries is a superior solid electrolyte with high ion conductivity and good formability. Sulfide electrolytes with sodium-ion conductivity have been developed during the last decade. In crystalline sulfide electrolytes, the sodium ion conductivity of Na_{2.88}Sb_{0.88}W_{0.12}S₄ is over 10⁻¹ S cm⁻¹ at 25°C, which is equal to or greater than the lithium ion conductivity in the LGPS-type sulfide electrolyte. On the other hand, glass electrolytes have relatively lower conductivities than the crystalline electrolyte, but they have better formability and compatibility

with electrode active materials. For example, Na_2BS_3 glass exhibited better Na plating/stripping performance because of forming an electronically insulating thin passivated interphase. Chloride sodium-ion conductor NaTaCl_6 with amorphous components was mechanochemically synthesized, and its oxychloride electrolyte showed a high conductivity of over $10^{-3} \text{ S cm}^{-1}$.

2:15 PM

(PACRIM-S22-003-2025) Mechanism of Suppressing Insulation Resistance Degradation in Sn-Doped Ni Internal Electrode Multi-Layer Ceramic Capacitors (Invited)

S. Suzuki^{*1}; T. Nakamura¹

1. Murata Seisakusho Kabushiki Kaisha Yasu Jigyosho, Japan

Multi-layer ceramic capacitors (MLCCs) have become integral components in modern electronic devices such as smartphones and personal computers due to their cost-effective miniaturization and high capacitance. This progress has been achieved through the thinning of BaTiO_3 -based dielectric ceramics. However, these MLCCs are prone to degradation in insulation resistance when exposed to high temperatures and voltages. On the other hand, it was found that the Sn-doped Ni inner electrode at the anode position effectively suppressed this degradation, but the same result was not obtained when the Sn-doped Ni inner electrode was placed at the cathode position. A series of studies were conducted to elucidate the mechanism of this phenomenon. X-ray photoelectron spectroscopy measurements indicated that increasing Sn content within Ni electrodes leads to a reduction in their work function. At the same time, transmission electron microscopy revealed that Sn is concentrated on the surface of these Ni internal electrodes. These findings suggest that the enrichment of Sn on the electrode surface reduces its work function, thereby enhancing the interfacial barrier between the ceramics and the anode interface. This high interfacial barrier means that ceramics adjacent to regions with degraded insulation resistance at the anode may exhibit p-type conduction characteristics.

2:45 PM

(PACRIM-S22-004-2025) Reliability of Multilayer Ceramic Capacitors (MLCC) in M2M Environments (Invited)

K. Morita^{*1}

1. Taiyo Yuden Kabushiki Kaisha, Japan

Multilayer Ceramic Capacitors (MLCCs) are among the most widely used electronic components, essential to a vast array of electronic circuits from smartphones and electric vehicles to satellites, underpinning today's electronics society. Recently, there has been an increasing demand for MLCCs with high reliability that can withstand high temperatures and voltages, particularly for AI servers and autonomous driving systems in electric vehicles. While substantial research has been conducted to enhance the reliability of MLCCs, advancing our understanding of fundamental degradation mechanisms, the material design to ensure MLCC reliability in the increasingly prevalent M2M environments has not been sufficiently discussed. This paper addresses this gap by discussing and reporting on the reliability of MLCCs in practical usage environments and the grain boundary design of dielectric materials necessary to ensure their reliability.

3:30 PM

(PACRIM-S22-005-2025) Application of Pulsed Electric Fields in Ceramics Processing (Invited)

T. Nakayama^{*1}

1. Nagaoka University of Technology, Japan

Features of pulsed power supplies include the ability to apply an electric field at the timing when an electric field is required and to induce electrochemical reactions for a short period of time. Furthermore, in nanosecond pulse power supplies, the electric field can be reduced to zero before dielectric breakdown occurs. Therefore, nanosecond pulse power supplies can be used to apply

voltages as high as 10 times or more than the breakdown voltage. We have used such nanosecond pulsed power supplies to expand into the fields of environmental remediation and energy conversion. Current water treatment is carried out by first precipitating large contamination, followed by microbial or chemical treatment. However, if the contamination is too severe, it cannot be precipitated sufficiently. In this study, the electrocoagulation method is used to quickly precipitate contaminants by electrically forming flocculant particles in the water. In this study, however, a pulsed electric field is used to achieve water treatment with about half the power consumption of conventional methods. In terms of energy conversion, more electricity can be generated in pyroelectric power generation by priming the input of an external electric field. At this time, a DC electric field is generally used to realize the Olsen cycle, but by replacing this with a nanosecond pulsed electric field, the input power can be reduced.

4:00 PM

(PACRIM-S22-006-2025) Response of ferroelectric nanodomains to external direct-current and alternative-current electric fields (Invited)

Y. Sato^{*1}

1. Kumamoto Daigaku, Research and Education Institute for Semiconductors and Informatics, Japan

Since piezoelectricity of materials is closely related with response of ferroelectric domains to external electric fields, control of domain structure is an important issue to develop a new piezoelectric material. For example, piezoelectrics are often subjected to prior electrical treatment known as poling, by which polarization direction of domains is aligned to a preferred direction to enhance the piezoelectricity. Although poling has long been carried out using direct-current electric fields, recent studies have clarified that poling by alternative-current electric fields can be more effective. In the present study, in order to understand the role of domain response to piezoelectricity of materials, in-situ electrical biasing transmission electron microscopy observation was carried out. Our study has clarified that ferroelectric nanodomains reorient by applying direct-current electric fields in a piezoelectric single crystal, $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-PbTiO}_3$. The domain response was reversible on application and removal of the fields. Recently, it was also visualized that ferroelectric nanodomains are reoriented by applying alternative-current electric fields. Application of alternative-current electric fields for shorter duration led to reduction of domain wall density, whereas that for longer duration caused growth of microdomain bands perpendicular to the electric fields.

4:30 PM

(PACRIM-S22-007-2025) Mechanical properties of single crystal BaTiO_3 at the microscopic scale measured by bending test of microcantilever beam specimens (Invited)

J. Tatami^{*1}; H. Yamaguchi¹; M. Iijima¹; T. Takahashi²

1. Yokohama National University, Japan

2. Kanagawa Institute of Industrial Science and Technology, Japan

Bending tests were carried out on microcantilever beam specimens fabricated on the surface of single crystal BaTiO_3 by focused ion beam technique, was carried out. After a bending stress of about 150 MPa was applied to a single-crystal BaTiO_3 microcantilever specimen with a strain deformation of about 0.15%, only the strain increased by about 1% without a significant increase in stress. Thereafter, the stress increased nonlinearly with strain, accompanied by discrete strain increases, and the specimen eventually failed brittle. The low-stress side of the nonlinear deformation was attributed to domain switching, while the high-stress side was attributed to stress-induced phase transition. The flexural strength and fracture strain were approximately 6.2 GPa and 10.7 %, respectively, indicating extremely high strength and fracture strain compared to the bulk material. Such properties as high strength and high fracture strain with a nonlinear stress-strain curve are expected to be used as a highly reliable structural material in microdevices and other applications.

5:00 PM

(PACRIM-S22-008-2025) Nanovolumetric Surface Milling and Tomographic Property Mapping of Functional MaterialsK. Lizu¹; K. Del Cid-Ledezma¹; A. Chen²; B. Huey^{*1}

1. University of Connecticut, MSE, USA
2. Los Alamos National Lab, USA

To investigate the local materials properties and device functionalities for perpetually shrinking microelectronics and other advanced semiconductor systems, various Atomic Force Microscopy methods have long been leveraged. It is challenging to use such a surface sensitive tool to investigate real-world devices, however, which increasingly rely upon 3-Dimensional and mesoscale designs and microstructures. Accordingly, we are advancing novel nanovolumetric property mapping methods based on simultaneous AFM imaging and in situ tip-induced polishing. This gradually reveals initially buried features, akin to serial sectioning but with down to Angstrom scale depth resolution. Examples are reported for polycrystalline ceramics, single crystals, and epitaxial thin films. The tomographic results literally uncover the 3D effects of composition, crystallographic orientation, polarization, and strain for local piezoelectricity and conductivity. An additional capability, leveraging 3-D resolved nanomilling rates, is found when studying <5 nm superlattice layers to even be sensitive to the shear strength of distinct interfaces.

5:20 PM

(PACRIM-S22-009-2025) Echoes of the past and new beginnings: Musings of a global scholar at a half centuryJ. McCloy^{*1}

1. Washington State University, School of Mechanical and Materials Engineering, USA

In this talk, I will reflect on themes in my work and life that have crystallized since I received the Fulrath-Okasaki award in 2018. I will focus on the opportunities I received as part of the award to visit Japan to build bridges with Japanese colleagues and I will discuss the long-term results of those interactions. While in 2018 my sole focus was on nuclear materials and glasses, the last five years have added a new area of research - oxide and chalcogenide crystal growth and the study of doping and opto-electronic properties - particularly work in Ga₂O₃ and CdTe. I will discuss some of this work as well, which provides new avenues for collaboration with the Pacific Rim ceramic societies. I will use this lecture to describe the evolution of a career trajectory as influenced by colleagues, friends, students, travel, global events, opportunities, and scientific curiosity.

PacRim S23 - Advanced Processing and Manufacturing Technologies for Ceramics**PACRIM Symposium 23 - Ultra-fast high-temperature sintering**

Room: Georgia B

Session Chair: Raul Bermejo, Montanuniversitaet Leoben

1:15 PM

(PACRIM-S23-001-2025) Ultrafast Sintering: A Review of Prior Mechanistic Studies and New Perspective (Invited)J. Luo^{*1}

1. University of California San Diego, USA

In a series of mechanistic studies of flash sintering, we reported that flash sintering generally starts as a thermal runaway, and we furthered suggest ultrahigh heating rates enable ultrafast sintering by demonstrating that similar densification rates can be achieved via (1) flash sintering and (2) rapid thermal annealing (intense infrared heating without an electric field) with similar heating rates of ~200 K/s.

Similar conclusions were also suggested by other researchers in simultaneous and independent studies. See an earlier review and perspective article. Subsequently, general ultrafast sintering methods, enabled by the same underlying mechanism, were demonstrated in collaborative studies led by Professor Liangbing Hu, e.g., ultrafast high-temperature sintering. Two ultrafast reactive sintering schemes have also been developed to synthesize and fully densify high-entropy metal diborides (representing one of the most-difficult-to-sinter ceramics) in ~ 2 minutes with or without electric currents in the specimens. Our on-going study on a new scheme of ultrafast sintering will also be presented and discussed (unpublished results).

1:55 PM

(PACRIM-S23-002-2025) Fabrication of single tetragonal phase 3YSZ using UHS sintering (Invited)B. Feng^{*1}; R. Murakami¹; N. Shibata¹; Y. Ikuhara¹

1. The University of Tokyo, Japan

3 mol% yttria-stabilized zirconia (3YSZ) with a tetragonal phase is widely used as a structural ceramic due to its exceptionally high toughness. However, conventional high-temperature sintering for extended durations often results in uneven Y³⁺ distribution. This non-uniformity leads to the formation of Y-rich regions that transform into the cubic phase, resulting in a mixed tetragonal-cubic microstructure. To enhance the toughness of zirconia, it is critical to develop 3YSZ polycrystals with uniform Y distribution and a single tetragonal phase. Here, we employed ultrafast high-temperature sintering (UHS) to produce fully dense 3YSZ with a single tetragonal phase by drastically reducing the sintering time. 3YSZ powder (Tosoh, TZ-3Y) was pressed into pellets and sintered in an argon atmosphere at approximately 1500°C for just 30 seconds using the UHS method. Our results demonstrate the successful fabrication of fully dense 3YSZ using the UHS method. XRD analysis confirmed that UHS-sintered samples consist of a single tetragonal phase, in contrast to conventional sintering, which results in a tetragonal-cubic dual-phase structure. Furthermore, STEM-EDS analysis revealed a uniform Y distribution in the UHS samples. These findings highlight that UHS effectively prevents phase separation, enabling the production of high-density 3YSZ with enhanced properties under non-equilibrium conditions.

2:25 PM

(PACRIM-S23-003-2025) Rapid sintering of telluride compounds for thermoelectric conversion applications (Invited)M. Mikami^{*1}; H. Miyazaki²; Y. Nishino²

1. National Institute of Advanced Industrial Science and Technology, Japan
2. Nagoya Kogyo Daigaku, Japan

Thermoelectric power generation (TEG) directly converts waste heat into electric power to improve energy utilization efficiency. To enhance the conversion efficiency of TEGs for practical applications, improving the performance of thermoelectric materials, which is evaluated using the thermoelectric figure of merit $Z (=S^2\sigma/\kappa)$, where S is Seebeck coefficient, σ is electrical conductivity, and κ is thermal conductivity), is indispensable. Microstructure modification is one of the effective ways to improve the Z value because the magnitude of σ and κ are highly dependent on microstructure. Therefore, optimization of sintering process plays an important role in obtaining high performance thermoelectric materials. Recently, we have been studying the rapid densification of thermoelectric materials by flash sintering (FS) based on the electric current activated/assisted sintering (ECAS) technique. For instance, Sb₂Te₃ was fully densified with a current feed duration of 1 s under mechanical pressure, and it was confirmed that energy consumption for sintering was considerably reduced compared to the conventional ECAS. In the case of nano-structured Sb₂Te₃ powder, we found that the reduced κ value by the suppression of grain growth during FS can enhance Z value. These results suggest that the energy-efficient FS is highly useful as a sintering technology for thermoelectric materials.

PACRIM Symposium 23 - Cold sintering and energy-efficient densification techniques

Room: Georgia B

Session Chair: Bin Feng, The University of Tokyo

3:30 PM

(PACRIM-S23-004-2025) Understanding the mechanical behavior of cold sintered ceramics (Invited)

R. Bermejo^{*1}; A. Jabr¹; D. Salamon¹

1. Montanuniversitat Leoben, Materials Science, Austria

The cold sintering process can densify various ceramic systems at exceptionally low temperatures (< 350°C), offering advantages in materials integration, grain boundaries design and microstructure control. Densification at such low temperatures is enabled by a chemically active transient liquid phase and an externally applied pressure. However, the effect of these peculiar processing conditions on the mechanical reliability, particularly grain boundary cohesion, remains poorly understood. This work investigates and compares the mechanical performance of cold (140°C) and conventionally sintered (1000°C) ZnO. To account for grain size effects, different samples were sintered using conventional and rapid sintering techniques. Biaxial bending tests and fractography were conducted to identify strength-limiting flaws. It is found that the strength of cold sintered samples can be compromised by improper processing conditions associated with temperature and/or pressure gradients, resulting in delamination effects. The prevention of such defects is demonstrated by selection of CSP parameters, resulting in structurally reliable cold sintered ZnO ceramics with strengths above 100 MPa. Fracture toughness and hardness measurements explain the lower fracture resistance of cold sintered materials, associated with their nano-crystalline microstructure, which should be taken into account for load bearing applications.

4:00 PM

(PACRIM-S23-005-2025) Structural and Mechanical Characteristics of Whitlockite Fabricated via Mineralization-Assisted Cold Sintering Process

S. Nawa^{*1}; Y. Seo¹; Y. Kondo¹; S. Chou¹; J. Stadulis²; A. Zarkov²; T. Goto¹; T. Sekino¹

1. Osaka University, SANKEN, Japan

2. Vilnius University, Lithuania

Whitlockite (WH; $\text{Ca}_{18}\text{Mg}_2(\text{HPO}_4)_2(\text{PO}_4)_{12}$), a type of calcium phosphate found in human hard tissues, exhibits excellent biocompatibility and osteoconductivity in vivo. However, due to the presence of hydrogen phosphate groups in its crystal structure, WH thermally decomposes at approximately 700 °C, making it challenging to fabricate dense WH in a single-phase. Additionally, this limitation has remained the mechanical and physical properties of WH unrevealed, thereby restricting its applications as biomaterials. To solve these issues, we focused on the cold sintering process (CSP), a technique for densifying inorganic materials at low temperatures below 300 °C. In CSP, raw particles mixed with a small amount of solution are subjected to pressure and heating, inducing particle arrangement and material diffusion driven by concentration gradients at the particle interfaces under hydrothermal-like conditions. In this study, we applied the low-temperature mineralization sintering process (LMSP), which combines the densification mechanism of CSP with a mineralization reaction, to fabricate highly densified bulk WH. Simulated body fluid (SBF) solution was used for the densification, which realized relative density of approximately 89% for the bulk WH prepared at 180 °C. Structural analysis and mechanical properties of the obtained bulk WH will be discussed in detail.

4:20 PM

(PACRIM-S23-006-2025) Transparent Hydroxyapatite Densified by Cold Sintering Process Combined with Biomineralization

Y. Seo^{*1}; T. Goto²; S. Chou¹; T. Sekino¹

1. Osaka University, SANKEN, Japan

2. Osaka University, Institute for Advanced Co-Creation Studies, Japan

Hydroxyapatite (HAp) stands out as a promising transparent ceramic material. To prepare the transparent HAp, various sintering methods such as spark plasma sintering and hot isostatic pressing, which require temperatures over 1000 °C, have been utilized so far. Recently, a cold sintering process (CSP) has been reported as the low-temperature densification method of inorganic materials. CSP employs a transient liquid phase to facilitate mass transport, enabling densification at temperatures below 300 °C. This study explores the fabrication of transparent HAp using a combination of CSP and biomineralization. The integration of these two processes is expected to facilitate the densification of HAp nanoparticles through the precipitation of HAp nanocrystalline phase via biomineralization. This approach resulted in transparent HAp achieving over 98% theoretical density and exhibiting over 80% transmittance in visible light. The densification behavior, microstructures, and optical and mechanical properties of the transparent HAp will be discussed in detail.

4:40 PM

(PACRIM-S23-007-2025) Designing low temperature sintered ultra-uniform nanocrystalline ceramics (Invited)

Y. Dong^{*1}

1. Tsinghua University, School of Materials Science and Engineering, China

Nanocrystalline ceramics with <100 nm grain sizes and superior properties are of great interest. Much has been discussed about ultrafine grain sizes, but little is known about ultra-uniformity, defined as grain size distribution narrower than predicted by the classical theory of Hillert. Here we provide a generalized growth theory unifying the textbook knowledge of Ostwald ripening and normal grain growth. For curvature driven grain growth, we find a steady-state size distribution that is analytically solvable for growth exponent $n > 1$ and it narrows with increasing n . Experimental validation of this prediction is found in porous alumina ceramics at various intermedium and final stage sintering, which sheds light on the hidden role of porosity to self-homogenize the microstructure.

PacRim S24 - Solid-State Optical Materials and Luminescence Properties

PACRIM Symposium 24 - Advanced processing of optical materials and devices

Room: Prince of Wales

Session Chair: Ivar Reimanis, Colorado School of Mines

1:15 PM

(PACRIM-S24-001-2025) Advanced Alumina Ceramics with Pseudo-Isotropic Optical Properties for IR Windows (Invited)

A. Ikesue^{*1}

1. World Lab. Co., Japan

We have succeeded in synthesizing polycrystalline alumina ceramics with a hexagonal structure that have extremely high transmittance and optical quality in the near-infrared to mid-infrared range. Although the fabricated alumina ceramics belongs to hexagonal crystal system, the amount of leakage light due to birefringence measured under cross nicols in the wavelength bands above the near-infrared is only less than 0.2 %, and the extinction ratio is above 30 dB, which is comparable to the characteristics of

birefringence-free materials such as C-axis single crystal sapphire and cubic Y_2O_3 ceramics. When observed with near-infrared (0.9 - 1.7 μm) and mid-infrared (3 - 5 μm) cameras through the fabricated alumina windows ($t = 2 - 6 \text{ mm}$), bright and clear images were obtained as in the case of a sapphire single crystal windows.

1:45 PM

(PACRIM-S24-002-2025) Fabrication of highly transparent Y_2O_3 ceramics via air pre-sintering by deionization treatment of suspension (Invited)

X. LI*¹

1. Northeastern University, China

The colloidal processing methods offer advantages over dry pressing routes by producing green bodies with improved microstructure uniformity, higher packing density, and by providing versatile geometrical options. Unfortunately, powders of Y_2O_3 are highly reactive in an aqueous medium, posing additional difficulties in preparing stable suspensions of high solid content for colloidal processing. An easy albeit quite effective deionization suspension treatment was adopted to alleviate the detrimental effects related to the hydrolysis of Y_2O_3 in an aqueous medium. Fabrication of highly transparent Y_2O_3 ceramics with a fine grain size via air pre-sintering and post-hot isostatic pressing (HIP) treatment without using any sintering additive was achieved using the treated suspensions. The hydrolysis issue of Y_2O_3 powder in an aqueous medium was effectively alleviated by using deionization treatment, and a well-dispersed suspension with a low concentration of dissolved Y^{3+} species was obtained. The green bodies showed an improved homogeneity with a relative density of 52.1%. The Y_2O_3 ceramic with high transparency was obtained by pre-sintering consolidated green compacts at a low temperature of 1400 °C for 16 h in air followed by a post-HIP treatment at 1550 °C for 2 h under 200 MPa pressure. The sample had a fine average grain size of 690 nm.

2:15 PM

(PACRIM-S24-003-2025) Strengthening of transparent AlON ceramics utilizing intermediate oxide layer (Invited)

X. Mao*¹

1. Shanghai Institute of Ceramics Chinese Academy of Sciences, China

Aluminum oxynitride, normally known as AlON or γ -AlON, is one of the strongest transparent ceramics and has received much attention since its emergence. The intermediate oxide γ' -AlON which has expanded lattice parameter was proposed to create strengthened AlON ceramics in first time simply by calcining the polished transparent AlON at 900-1000 °C in air. The microstructure topography of the calcined AlON surfaces were characterized by SEM, TEM and confocal laser scanning microscope (CLSM). The strength of AlON test bars increase by 62% after calcined at 1000 °C, with a loss of transmittance by 3-5 per cent. The obtained oxide layers have a gradient structure with an amorphous layer of alumina outside and crystallized γ' -AlON in between. The intermediate oxide γ' -AlON has larger lattice parameter with Al-O-N group determined by XPS and EPR. This work provides a novel idea for the strengthening of nitride ceramics, especially for transparent ceramics.

2:45 PM

(PACRIM-S24-022-2025) Transparent Ceramics: Challenges, Successes and Opportunities

M. Rubat du Merac*¹; S. Begand²

1. Consultant Technical Ceramics, Canada
2. Fraunhofer Institute for Ceramic Technologies and Systems IKTS, Germany

Transparent ceramics have steadily gained increasing attention, particularly when possessing additional functional properties like luminescence, lasing, electronic conductivity, photovoltaic effect and/or exceptional thermo-mechanical behavior. However, they face stiff competition from polymers, glasses, glass ceramics and single crystals,

typically requiring industrial-scale manufacturing for economic viability. They are also difficult to make without introducing defects and are extremely sensitive to raw materials and processing parameters, further complicating fabrication. Defects affect performance, increase waste and cost and can become limiting. However, the ability to easily see defects presents an opportunity to understand their origin and improve processing and properties. This presentation will focus on fabrication issues for bulk transparent ceramics using specific examples, showcase successes, and discuss future opportunities.

PACRIM Symposium 24 - Optical spectroscopy of crystalline and amorphous materials

Room: Prince of Wales

Structure Chair: Dariusz Hreniak, Institute of Low Temperature Structure Research

3:30 PM

(PACRIM-S24-004-2025) Residual Stresses in Transparent Ceramics and Glass: Control and Measurement with Raman Spectroscopy (Invited)

I. Reimanis*¹; A. J. Bellafatto¹

1. Colorado School of Mines, USA

Local residual stresses in transparent ceramics and glasses may arise from different sources. They may be intentionally formed within a microstructure during processing with the objective to increase strength and/or toughness; they may also result from extraneous damage processes during contact such as in scratching. It is of interest to identify the location and magnitude of those elastic stresses, but this may be challenging, especially when they are sub-surface. The present talk is divided into two parts. In the first, a methodology is described to design alumina particle-toughened magnesium aluminate spinel, demonstrating the potential to make a tough, transparent ceramic. In the second, Raman spectroscopy is employed to measure three-dimensional stress fields under indents in quartz, amorphous silica and sapphire. It is shown that Raman spectroscopy is a versatile and practical tool when changes in signal intensity and peak shape with depth of measurement are taken into account.

4:00 PM

(PACRIM-S24-005-2025) Laser Drilling and Cutting Machines for Glasses and Ceramics (Invited)

S. Jiang*¹

1. AdValue Photonics Inc, USA

We have developed laser drilling and cutting machines for glasses and ceramics by using different types of pulsed lasers. Green and 1 micron wavelength nanosecond pulsed lasers and picosecond pulsed lasers are used for glass drilling and cutting process. The processing speed and surface quality will be described in detail in this presentation. Long pulse and picosecond 1 micron wavelength lasers have been used for drilling and cutting ceramics. Many specific application examples will be presented.

4:30 PM

(PACRIM-S24-006-2025) Network Structure of Bi_2O_3 - Al_2O_3 - $NaPO_3$ Glasses Investigated via Solid-State Nuclear Magnetic Resonance Spectroscopy

R. Zhang*¹

1. University of Jinan, Material Science and Engineering, China

A comprehensive and detailed structural investigation has been carried out on a series of phosphate laser glasses with the composition xBi_2O_3 - yAl_2O_3 -(100-x-y)NaPO₃ (where $x = 0, 10$ and $y = 0, 5, 10, 15, 20$) by employing solid-state nuclear magnetic resonance (NMR) techniques and X-ray photoelectron spectroscopy (XPS). The 31P MAS NMR spectroscopy reveals that the incorporation of

Bi_2O_3 and Al_2O_3 induces the depolymerization of the phosphorus chain, following the transformation sequence of $\text{Q}^2 \rightarrow \text{Q}^1 \rightarrow \text{Q}^0$. The various phosphorus species (Q^n , $n=0, 1, 2$) are identified by ^{31}P single pulse, $^{31}\text{P}\{^{27}\text{Al}\}$ rotational echo adiabatic passage double resonance (REAPDOR), $^{31}\text{P}\{^{27}\text{Al}\}$ J-coupling-based heteronuclear multiple-quantum coherence (HMQC) and 1D refocused INADEQUATE experiments. The results of $^{23}\text{Na}\{^{31}\text{P}\}$, $^{31}\text{P}\{^{23}\text{Na}\}$, $^{27}\text{Al}\{^{31}\text{P}\}$ rotational echo double resonance (REDOR) and XPS consistently confirm that Na^+ , Al^{3+} , and Bi^{3+} ions are all bound by phosphorus tetrahedron $[\text{PO}_4]^{3-}$. No bond is formed between these glass modifiers. Based on the complementary evidence from above experiments, comprehensive local structure models are developed for these Bi_2O_3 - Al_2O_3 - NaPO_3 glasses.

4:50 PM

(PACRIM-S24-007-2025) Unveiling the Crystallization Mechanism of Rare Earth Doped Oxyfluoride Glass ceramics through Solid-State Nuclear Magnetic Resonance Spectroscopy (Invited)

J. Ren*¹

1. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai 201800, China, China

Rare earth doped oxyfluoride glass ceramics exhibit promising potential for use in 3D displays, solar cells, and white light illumination, primarily due to their exceptional up-conversion luminescence efficiency. The luminescent performance of these materials is intricately tied to the distribution of luminescent rare earth ions between the glass and fluorine crystalline phases. This presentation aims to elucidate the atomic-scale structural transformations of oxyfluoride glasses during the heat-induced crystallization process, utilizing advanced solid-state nuclear magnetic resonance (NMR) spectroscopy. By leveraging the structural insights provided by solid-state NMR, we will delve into the crystallization mechanism of fluoride within the glass matrix and investigate the multifaceted roles of rare earth ions during the crystallization process, as well as their distribution within the fluoride crystal and glass phase.

PacRim S25- Syn/Prcsng/Micro-structural Control of Mtls using Elec Currents/Magn fields/Press

PACRIM Symposium 25 - Processing & Micro-structural Control using Electric Currents, Magnetic fields and/or Pressures

Room: Seymour

Session Chairs: Alexander Dupuy, University of California, Irvine; Javier Garay, University of California, San Diego

1:15 PM

(PACRIM-S25-001-2025) Multiscale control strategies for sintering of advanced ceramics (Invited)

D. Giuntini*¹

1. Eindhoven University of Technology, Mechanical Engineering, Netherlands

Sintering is one of the longest-practiced material processing technologies, yet ceramics are complex material systems that retain major processing challenges. Emerging processing technologies, such as additive manufacturing and ultrarapid field-assisted sintering, are themselves enabling the production of previously unthinkable shapes and compositions, but at the same time introducing new process control challenges (shrinkage anisotropies, density and grain size non-uniformities, etc). To avoid time and energy-consuming trial-and-error experimental campaigns, sintering modeling is a valuable asset. The continuum theory of sintering can capture the fundamentals of ceramics densification processes with only a

limited set of fitting parameters, and it is able to provide valuable insights on how a part shrinks and deforms during processing, unlocking the targeted design of green parts. It can also be coupled with multiphysics simulations to virtually reconstruct the whole set of phenomena occurring during manufacturing, and with micro-scale methods to monitor phase changes and grain size evolution. This talk will provide an overview of modeling-empowered multi-scale control of ceramics processing, experimentally validated with a broad set of oxide and non-oxide ceramics.

1:45 PM

(PACRIM-S25-002-2025) Enhanced Sintering Behavior of Yttria during Spark-Plasma-Sintering (SPS) (Invited)

K. Morita*¹

1. National Institute for Materials Science (NIMS), Japan

The effect of pulsed electric current during spark-plasma-sintering (SPS) has been reported to enhance sintering behavior of various materials such as metals, ceramics and those composites. Although the SPS method has widely been employed in the sintering of various materials, the pulsed current effects on the sintering behavior remain unclear. Especially for insulator materials such as ceramics, the current effects of the SPS processing are under discussion. In this work, therefore, the current effects in the SPS technique were examined in yttria (Y_2O_3) ceramics by comparing the sintering behavior using conductive and non-conductive die set-ups. The sintering behavior of Y_2O_3 was apparently accelerated under the conductive set-up than under non-conductive die set-up. This suggests that during the SPS processing, applied pulsed electric current would contribute to the sintering of Y_2O_3 ceramics. Acknowledgment: This work was financially supported by Innovative Science and Technology Initiative for Security Grant Number JPJ004596, ATLA, Japan.

2:15 PM

(PACRIM-S25-003-2025) Controlling dislocation motion using an electric field

Y. Zou*¹

1. University of Toronto, Canada

Dislocation motion, an important mechanism underlying crystal plasticity, is critical for the hardening, processing and application of a wide range of structural and functional materials. For decades, the movement of dislocations has been widely observed in crystalline solids under mechanical loading. However, the goal of manipulating dislocation motion via a non-mechanical field alone remains elusive. Here we present real-time observations of dislocation motion controlled solely by using an external electric field in single-crystalline zinc sulfide—the dislocations can move back and forth depending on the direction of the electric field. We reveal the non-stoichiometric nature of dislocation cores and determine their charge characteristics. Both negatively and positively charged dislocations are directly resolved, and their glide barriers decrease under an electric field, explaining the experimental observations. This study provides direct evidence of dislocation dynamics controlled by a non-mechanical stimulus and opens up the possibility of modulating dislocation-related properties.

2:35 PM

(PACRIM-S25-004-2025) Electric Fields Effects on Microstructural Evolution: The Role of Electrochemical Coupling and Electrochemically Induced Grain Boundary Transitions (Invited)

J. Luo*¹

1. University of California San Diego, USA

In a series of mechanistic studies of flash sintering, we reported that flash sintering generally starts as a thermal runaway, and further suggested ultrahigh heating rates on the order of 100 K/s can enable ultrafast sintering with and without electric fields (in flash sintering vs. rapid thermal annealing). Although we have demonstrated that

ultrafast sintering can be achieved without an electric field, we recognize that electric fields can influence microstructural evolution. Specifically, we discovered an electrochemically induced grain boundary disorder-to-order transition to trigger abnormal grain growth in Bi₂O₃-doped ZnO. We further studied the electric field-induced microstructural evolution in polycrystalline Bi₂O₃-doped ZnO in presence of a secondary liquid phase. Moreover, we showed that applied electric fields can induce grain boundary oxidation transitions near the anode to create continuously graded microstructures in undoped ZnO. Unpublished results in electric field effects on microstructural evolution in SrTiO₃ and BaTiO₃ based systems will also be discussed.

3:20 PM

(PACRIM-S25-005-2025) Leveraging Electric Fields in Large Format Field Assisted Sintering for Materials in Harsh Environments (Invited)

J. Rufner^{*1}; A. Preston¹; X. Zhang¹; A. Gorman¹

1. Idaho National Lab, Materials Science and Manufacturing, USA

An important part of enabling clean energy deployment requires creating material solutions specific to each of their operating environments, which are quite harsh. INL has been at the forefront of researching and developing such materials capable of withstanding harsh environments and extreme conditions, including high temperatures, radiation, mechanical stress, and corrosive environments. Advanced manufacturing, specifically with advanced sintering technologies such as electric field assisted sintering (EFAS), is a powerful pathway that is poised to open access to many materials for harsh environments that were previously out of reach. INL is driving the scientific research, development, and deployment (RD&D) of field assisted sintering at both small and large length scales. Methodology, benefits, and recent project results using EFAS to enable technologies such as fusion and fission energy, near net shape part processing, embedded sensors for material health surveillance, materials for aerospace utilization, corrosion resistant alloy fabrication, molten salt and concentrated solar power/thermal systems, and critical material manufacturing will be presented.

3:50 PM

(PACRIM-S25-006-2025) Multiple Densification Mechanisms in Na₂Mo₂O₇ Dielectric Composites under the Cold Sintering Process (Invited)

C. Randall^{*1}

1. Penn State University, Materials Science and Engineering, USA

A powerful aspect of cold sintering is the ability to densify different materials and powders to enable new types of composites. This is enabled because of the low temperatures pressure solution creep, however beyond this mechanism there is little known on other processes that could contribute especially to composite densification. In this presentation, we will outline a densification study to determine the activation energies and mechanisms on a microwave material, Na₂Mo₂O₇ (NMO) and filler materials of micro diamond (MD) and hexagonal Boron Nitride (h-BN). Rearrangement is a major part of the densification with the h-BN -NMO composites, and this is followed by the pressure solution creep. In contrast the NMO-MD composites has a limited rearrangement in the early stages, then there is a major densification through pressure solution creep, and finally the last stage is controlled by a diffusional creep process.

4:20 PM

(PACRIM-S25-007-2025) Modeling Flash Sintering of Ionic Ceramics: From Individual Defects to Engineering Level (Invited)

R. Garcia^{*1}

1. Purdue University, Materials Engineering, USA

A wide variety of processing routes exist to consolidate an initial granular powder that will be later used as a starting point for the fabrication of carefully thought out layers and multifunctional architectures. Sintering of ceramics, in particular, is a processing methodology that is a result of the underlying contributions from individual point (vacancies and interstitials) line defects (dislocations), and surfaces and interfaces, as they interact in a local microstructural, mechanical, chemical, and electrical field induced through local or external stimuli. In this presentation, by starting from fundamental thermodynamic concepts, a generalized phase field theory is presented to describe the chemical and electric field-induced mechanisms that control the flash sintering of ceramics. Well known aging phenomena observed in metals, such as the Cottrell effect and the Portevin-Le Chatelier effect, are revisited in the context of the underlying ionic character of ceramics. The impact of these mechanisms at the particle level are assessed, and its coupling to the macroscopic sintering curves are discussed and quantified. Applications to Y₂O₃, 3YSZ, TiO₂, and Al₂O₃ will be presented.

4:50 PM

(PACRIM-S25-008-2025) Microstructure control of polycrystalline aluminum oxide densified body with high transparency

Y. Kodera^{*1}; K. Ikeda¹; D. Shikata¹; J. E. Garay²

1. Ryukoku Daigaku - Seta Campus, Materials Chemistry, Japan

2. University of California, San Diego, Dept. of Mechanical and Aerospace Engrg., USA

Current Activated Pressure Assisted Densification (CAPAD) method (also known as Spark Plasma Sintering) comes with the capability of applying direct current and pressure simultaneously. High heating rate is the one of the advantages of CAPAD and it can develop non-conventional microstructure and properties on conventional materials. This method allows a wide variety of tooling options such as graphite or non-graphite mold/plunger. One other advantage of this method is high pressure capability. Most common pressure is < 150 MPa which is the limit of graphite tooling. However, it has been demonstrated that selecting C/C composite as plunger can result > 400 MPa. Moreover, non-graphite materials with superior mechanical strength allow to reach 1GPa range. This is well combined with other characteristics of CAPAD. For instance, the combination of high heating rate and high pressure can result in obtaining the fully dense bulk specimen with far-from equilibrium structure such as nano grain sizes. In this presentation, we densified alpha aluminum oxide which exhibits unique characteristics as transparent materials. Because of its non-cubic crystal symmetry and birefringence, in-line transmission is sensitive to the grain sizes of bulk sample. We will demonstrate microstructure controllability (grain size) on polycrystalline a-aluminum oxide densified body with high transparency.

PacRim S27 - International Symposium of Fundamental and Frontier Sciences of Ceramics

PACRIM Symposium 27 - International Symposium of Fundamental and Frontier Sciences of Ceramics I

Room: Cypress

Session Chairs: Gregory Rohrer, Carnegie Mellon University;
William Fahrenholtz, Missouri University of Science & Technology

1:15 PM

(PACRIM-S27-001-2025) Leveraging Machine-learning and High Throughput Powder Processing for Efficient Design of Ceramics – Challenges and Opportunities (Invited)

R. Bordia^{*1}; F. Peng¹; K. G. Webber²; H. Xiao³; X. Geng¹; U. Eckstein²

1. Clemson University, Materials Science and Engineering, USA
2. Friedrich-Alexander-Universität Erlangen-Nürnberg, Materials Science and Engineering, Germany
3. Clemson University, Electrical and Computer Engineering, USA

Machine learning approaches are being extensively used in a variety of research fields in material science. Notable success has been demonstrated in using machine learning for the design of chemical composition of both polymeric and inorganic materials. However, success has been limited in using machine learning to design and predict optimal microstructures, especially for ceramics. We will review the status of machine learning for the design of ceramic microstructures and highlight an important limitation for ceramic microstructures – lack of high throughput experiments and the lack of large datasets. We will then focus on some of the key developments in high throughput experiments in the areas of powder processing, green state processing, laser sintering of alumina, and a machine learning approach to predict the microstructure and microstructure-property relationships for ceramics. For each one of these steps, the state-of-the-art techniques will be discussed together with specific examples. The advantages and the limitations of these approaches will be summarized. Finally, a perspective on the challenges and opportunities will be presented.

1:45 PM

(PACRIM-S27-002-2025) A Combined Computational and Experimental Approach For Discovery of Novel Hard Ceramics (Invited)

W. Fahrenholtz^{*1}; S. Filipovic²; N. Obradovic²; G. Hilmis¹; S. Curtarolo³

1. Missouri University of Science & Technology, Dept. of Materials Science and Engineering, USA
2. Institute of Technical Sciences of SASA, Materials, Serbia
3. Duke University, Materials Science, Electrical Engineering and Physics, USA

This presentation focuses on the discovery of new superhard compounds using computational methods followed by synthesis and property measurement. Machine learning was used to identify a composition of (Hf,Mo,Ti,V,W)B₂ as a potential superhard material. This composition was predicted to be thermodynamically stable using high-throughput thermodynamic computational methods based on a combined entropy-enthalpy descriptor. Then, (Hf,Mo,Ti,V,W)B₂ was synthesized as a single phase compound with a hexagonal AlB₂ type structure. Subsequent densification by direct current sintering produced a fully dense ceramic with a grain size of 3.8 μm and homogeneous distribution of metals. The Vickers hardness exhibited the indentation size effect, increasing from 27 GPa at a load of 9.8 N to as high as 66 GPa at a load of 0.49 N. This is the highest hardness reported to date for high entropy boride ceramics. This methodology provides a framework for faster route for discovery of new materials based on selection of a desired property, hardness in this case, and a combination of computational tools.

2:15 PM

(PACRIM-S27-003-2025) Solute Adsorption, Diffusion, and Disconnection Motion for Microstructure Control of Monolithic and Particle Reinforced Alumina (Invited)

W. D. Kaplan^{*1}

1. Technion - Israel Institute of Technology, Dept. of Materials Science and Engineering, Israel

During densification, grain boundary (GB) motion often occurs, resulting in grain growth driven by the reduction of GB area. GB motion can result in occluded porosity, requiring bulk diffusion for densification. Grain growth is often attributed to diffusional processes similar to those occurring during densification. However, recent evidence suggests that the mechanism of GB motion is via the motion of GB disconnections, which do not require long-range diffusional transport. Alumina is a paradigm for microstructural evolution studies. Mg is known to promote densification and limit grain growth by solute-drag. Ca in alumina at concentrations below the solubility limit increases GB mobility (solute-acceleration). The mechanism for solute-drag and solute-acceleration is believed to be adsorbing dopants (and their charge compensating defects) interacting with disconnections at GBs. Dopant adsorption to the surfaces of pores can change their relative mobility, where Mg is known to increase surface diffusion (preventing pore detachment). Cr apparently reduces surface diffusivity, increasing the probability for pore detachment and retarding densification. These concepts can be extended to controlling the position of reinforcing particles of a second phase, which will be discussed in terms of ceramic matrix nanocomposites.

2:45 PM

(PACRIM-S27-004-2025) The local driving force for grain growth in textured alumina (Invited)

A. Krause^{*1}

1. Carnegie Mellon University, Materials Science and Engineering, USA

Modeling grain growth is critical to improving processing control of microstructures and, thus, properties of ceramics. Recent grain growth studies using non-destructive 3D x-ray diffraction microscopy have revealed that current simulations cannot reproduce real behavior. Furthermore, curvature and number of neighbors do not correlate with grain growth behavior as predicted. This study investigates whether grain boundary stiffness, which is a function of the energy's dependence on plane inclination, is a better descriptor for grain growth behavior in alumina. Alumina is a model system because grain boundary energy exhibits a strong dependence on plane inclination. 3D laboratory-based diffraction contrast tomography (LabDCT) will be used to evaluate relationships between local microstructural features and grain boundary velocity and area changes. Additionally, a comparison of grain growth behavior in textured and untextured Ca-doped alumina will be used to evaluate the effect of connectivity of different grain boundary types. The results are compared to a Monte Carlo Potts simulation that incorporates anisotropic grain boundary energy and mobility as a function of plane inclination. The simulations that match experimental observations suggest that grain boundary stiffness may be a governing factor for grain growth. The implications of these results on predicting grain growth in ceramics will be discussed.

3:30 PM

(PACRIM-S27-005-2025) Processing and Microstructural Evolution of Entropy Stabilized Materials: New Insights (Invited)

H. M. Chan^{*1}; J. Zhang¹; J. Rickman¹

1. Lehigh University P C Rossin College of Engineering and Applied Science, Materials Science & Engineering, USA

For a special class of ceramic compounds, the increased configurational entropy due to disorder on the cation sites can more than compensate for the enthalpy of formation. These ceramics are thermodynamically stable only above a critical temperature (T_c), and

hence can be described as entropy stabilized. One such material occurs in the Co-Ti-O system; at temperatures below ~ 1140 °C, a 1:2 molar mixture of CoTiO_3 and TiO_2 will exist as a two phase mixture, whereas at higher temperatures, reaction between the binary oxides will take place to form CoTi_2O_5 . This latter transformation was studied by fabricating a series of dense, 1:2 duplex mixtures of CoTiO_3 and TiO_2 , where the starting grain size was varied by modifying the sintering conditions. The samples were then up-quenched to temperatures above T_c and isothermally annealed for varying times. The transformation kinetics and microstructural evolution were studied by XRD, SEM and EBSD. The talk will focus on several unusual and interesting characteristics of the transformation, including the pseudo-single crystal nature of the transformed dititanate and resemblance of aspects of the transformation to discontinuous dissolution (DD). A model will be discussed that accounts for the complex nature of the transformation process.

4:00 PM

(PACRIM-S27-006-2025) Accelerated DEED discovery of high-entropy ceramics with multi-component interatomic Hamiltonians (Invited)

S. Curtarolo^{*1}; H. Eckert¹; S. Divilov¹

1. Duke University, Materials Science, Electrical Engineering and Physics, USA

The need for improved functionalities in extreme environments is fuelling interest in high-entropy ceramics. In 2024, the disordered enthalpy-entropy descriptor (DEED) was introduced to capture the balance between entropy gains and enthalpy costs, allowing the correct classification of functional synthesizability of multi-component ceramics, regardless of chemistry and structure. In this presentation, we extend the formalism by parameterizing 5- and 6-metal high-entropy transition-metal carbide/carbonitride/boride model Hamiltonians. The chaotic harmony of metal mixing is addressed by studying Bayesian synthesizability across the periodic table. One- and two-metal correlations in the 5- and 6-metal synthesizability give surprising hints on mixing directions. Somehow, both dinosaurs and HE carbides/carbonitrides have something in common.

4:30 PM

(PACRIM-S27-007-2025) Room-temperature dislocations in ceramics: from understanding to active engineering (Invited)

X. Fang^{*1}; A. Frisch¹; C. Okafor¹; O. Preuß²; K. Durst²; J. Rödel²

1. Karlsruhe Institute of Technology, Institute for Applied Materials, Germany
2. Technical University of Darmstadt, Department of Materials and Earth Sciences, Germany

Ceramics are often considered brittle and exhibit little or no plasticity at room temperature. However, research of recent years suggests that dislocations (line defects) may have been much under-appreciated in ceramics. Demonstrated promising proofs-of-concept for dislocation-tuned functional properties suggest that dislocations may hold great technological potential in advanced ceramics. As the prerequisite to harvest dislocation-tuned properties, engineering dislocations into ceramics without brittle fracture has thus become a pressing bottleneck. To tackle this challenge, we have separately examined the dislocation behavior including dislocation nucleation, multiplication, and motion, enabling us to tune dislocations into ceramic oxides such as SrTiO_3 at room temperature. We can now achieve a dislocation density of up to $\sim 10^{15}/\text{m}^2$ with a plastic zone size of up to centimeters using a mechanical deformation toolbox developed in our group. We also extend the material toolbox by discovering and reporting more oxide perovskites that can be plastically deformed at room temperature across the length scale. These combined deformation and material toolboxes offer a new platform for studying the dislocation-tuned functional properties (e.g., electrical conductivity as well as catalysis) and the mechanical properties (plasticity, toughness, and damage tolerance) over a wide range of length scales.

5:00 PM

(PACRIM-S27-008-2025) Understanding the fracture behaviour of tough ceramic inspired by nacre (Invited)

V. Vilchez¹; S. Zhou¹; S. Rawson²; P. J. Withers²; F. Bouville^{*1}

1. Imperial College London, Department of Materials, United Kingdom
2. The Henry Royce Institute, United Kingdom

Millions of years of evolution have gifted natural materials with sophisticated structures that enable them to resist fracture despite being primarily composed of brittle ceramics. Nacre stands out as having one of the simplest microstructures, resembling a brick-and-mortar wall, yet exhibiting many toughening mechanisms leading to a pseudo-ductile behaviour in tension. Today's nacre-like composites exhibit higher values of fracture toughness and improved crack-resistance curves compared to bulk ceramics. However, understanding the link between the microstructure and crack resistance is necessary to improve these materials further. We studied fracture in nacre-like ceramics composed of alumina bricks and ceramic mortar and in tightly packed colloidal crystal made from silica rods and polymer interface. The first system allowed us to establish links between grain boundaries properties and toughening through highly deflected and branched cracks, supported by in-situ synchrotron tomography fracture testing. The second system, with its highly ordered microstructure, reveals a close link between the regularity of a microstructure and the development of process zone toughening, a toughening mechanism up to now limited to zirconia and natural materials. These two analyses reveal important lessons on the effect of the microstructure and mortar properties to guide the improvement of these materials.

PacRim S29 - Progress in High-Entropy Materials

PACRIM Symposium 29 - AI/ML- AI/ML- Model development and applications I

Room: Plaza A

Session Chairs: Raymundo Arroyave, Texas A&M University;
Liang Qi, University of Michigan

1:15 PM

(PACRIM-S29-001-2025) Multi-scale Studies of High-Entropy Materials with Machine Learning (Invited)

S. Ong^{*1}; J. Qi¹; I. Beyerlein²; L. Fey²

1. University of California San Diego, USA
2. University of California System, Santa Barbara, USA

A fundamental challenge in computational materials science is bridging length and time scales from quantum to atomistic to continuum. In this talk, I will present a roadmap to attacking this challenge in the context of complex concentrated materials, aka high entropy materials, in an automated fashion through machine learning (ML). In the past decade, ML interatomic potentials (MLPs) have emerged as a robust approach to bridge the quantum and atomistic scales by learning the potential energy surface from high-throughput ab initio calculations. In turn, simulations from MLPs can be used to learn statistical parameters for continuum scale models. I will illustrate this process using several prototypical examples from multi-principal element alloys and solid ceramic electrolytes for lithium-ion batteries. Finally, I will outline the major gaps that remain to the realization of high-throughput multi-scale simulations of materials.

1:55 PM

(PACRIM-S29-002-2025) Accelerated Discovery and Optimization of High Entropy Alloys through Bayesian Optimization (Invited)

R. Arroyave*¹

1. Texas A&M University, Materials Science and Engineering, USA

Traditional approaches to alloy design, such as ICME and high-throughput methods, are neither efficient nor optimal for navigating the vast design spaces of High Entropy Alloys (HEAs). ICME is computationally expensive and sequential, while high-throughput frameworks often lack iterative feedback, limiting their ability to optimize alloy properties. In this talk, I will present how Bayesian approaches, specifically Bayesian Optimization (BO), offer a solution by dramatically accelerating materials discovery. BO efficiently balances exploration and exploitation, using prior knowledge to guide decisions and iteratively refine predictions with each new data point, significantly outpacing conventional methods in identifying optimal materials. Our integrated framework combines BO with advanced simulations and experimental workflows, allowing us to optimize multiple alloy properties—such as strength, hardness, and strain rate sensitivity—while exploring only a small fraction of the total design space. This comprehensive computational-experimental approach has been applied to both FCC and BCC HEA systems, demonstrating remarkable improvements in discovery speed and effectiveness. Examples from these systems will be shared to illustrate the transformative potential of this approach in accelerating alloy development.

2:25 PM

(PACRIM-S29-003-2025) Compositional Design of Refractory High-Entropy Alloys Using Machine Learning Models (Invited)

H. Xu*¹

1. The University of Tennessee Knoxville Tickle College of Engineering, Materials Science and Engineering, USA

Refractory high-entropy alloys (RHEAs) have gained significant attention as potential next-generation materials for high-temperature applications due to their outstanding mechanical properties. This study focuses on exploring phase stability and employing machine learning (ML) models to predict critical mechanical properties, such as yield strength at elevated temperatures. By examining nine refractory elements (Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, and W), the research spans 466 multicomponent systems, ranging from ternary to novenary alloys, and evaluates 43,425 compositions with incremental concentration steps of 10%. ML-predicted mechanical properties are projected into a latent space to guide the selection of optimal compositions. Using this approach, we identified several new equiatomic RHEAs with yield strengths between 551 and 639 MPa at 1800 K, demonstrating the efficiency of this methodology. Furthermore, systematic design rules derived from these models provide a streamlined framework for accelerating the discovery and optimization of RHEAs for demanding high-temperature environments.

2:55 PM

(PACRIM-S29-004-2025) Physics-informed Machine Learning Design of Refractory Complex Concentrated Alloys for Advanced Manufacturing (Invited)

Y. Hu²; A. Sundar¹; D. Jobses¹; J. Gordon¹; A. Misra¹; L. Qi*¹

1. University of Michigan, USA

2. Drexel University, USA

Body-centered cubic (bcc) refractory complex concentrated alloys (RCCAs) are of great interest due to their remarkable strength at high temperatures. Optimizing the chemical compositions of these alloys to achieve a combination of high strength, room-temperature ductility, and high-temperature corrosion resistance remains challenging. We first developed regression models to accurately and efficiently predict the unstable stacking fault energy (γ_{usf}) and surface

energy (γ_{surf}) for RCCAs. Using the regression models, we performed a systematic screening of γ_{usf} , γ_{surf} and their ratio in the high-order multicomponent systems to search for alloy candidates that may have enhanced strength-ductile synergies. Then we develop hierarchical screening models to identify promising alloys from a 13-element composition space (Ti-Zr-Hf-V-Nb-Ta-Mo-W-Re-Ru-Al-Cr-Si). The results combined with high-throughput thermodynamics calculations are used to discover promising bcc alloys with high ductility, thermodynamic stability at high temperatures, and thermodynamic capability to passive oxide films. Finally, laser powder bed fusion (L-PBF) processing is applied to two representative RCCAs with promising results in both yield strengths and failure tensile strains.

3:45 PM

(PACRIM-S29-005-2025) Compositional Space Graphs as a Novel Tool for Efficient Exploration of High-Dimensional Design Spaces (Invited)

A. M. Krajewski*¹; Z. Liu¹

1. The Pennsylvania State University, Materials Science and Engineering, USA

All chemical compositions exist in non-Euclidean simplex spaces where component fractions sum to 100%, rendering many standard design tools and machine learning (ML) models inefficient or even qualitatively inaccurate. We present a new mathematical algorithm implemented within an open-source tool (nimplex.phaseslab.org) that represents compositional spaces of arbitrary dimensionality as graphs consisting of discretized compositions and all possible neighbor-to-neighbor transitions, orders of magnitude faster than before (e.g., seconds vs years for 6-component system at 1% resolution). The use of such graph representations is also agnostic to the number of components, making screening and optimization of 9-component high entropy alloys (HEAs) no more complex than ternary, since the same efficient algorithms for graph traversal, gradient descent, and custom approaches can be deployed. Furthermore, compositional graphs can be procedurally combined together to represent design problems like “optimize this alloy considering at most 6 out of 14 components at a time” and run without any adjustments. To demonstrate the power of this novel approach, we deploy it in the discovery of refractory HEAs (RHEAs) in conjunction with high-throughput CALPHAD and ML models trained on our ULTERA Database (ultera.org) spanning over 10,000 experimental HEA data-points from over 700 publications.

4:15 PM

(PACRIM-S29-006-2025) Physics Inspired Graph Neural Network Model for Inverse Design and Synthesizability Prediction of TiZrNb Based High Entropy Alloys

A. Malik*¹; H. Malik²; H. Ryu³

1. Korea Advanced Institute of Science and Technology, Department of Materials Science and Engineering, Republic of Korea

2. University of Toronto, Department of Computer and Mathematical Sciences, Canada

3. Korea Advanced Institute of Science and Technology, Department of Nuclear and Quantum Engineering, Republic of Korea

High entropy alloys (HEAs) are among the most versatile alloy systems because of their ability to tailor properties for a wide range of applications. The extensive compositional variation mandates the use of advanced screening systems to design alloys with optimum properties. This is where advanced machine learning models can greatly help find the right alloys for specific applications. However, most machine learning models use only compositional descriptors to represent alloys in the model, whereas the structural features, which are among the unique aspects of HEAs, are mostly ignored. In this study, we developed a physics-inspired graph neural network (GNN) model to represent HEAs, with graph nodes representing elemental compositions and graph edges computed using physical hardening interaction models. The high entropy graph developed is trained on hardness and Young's modulus data reported in the literature to

design alloys with an optimum combination of high hardness and low modulus for biomedical implant applications. Additionally, a positive and unlabeled (PU) learning scheme is used to determine the synthesizability of the predicted compositions from the model. The approach outlined in our study offers a guideline to incorporate not only the compositional information but also the structural information that gives a unique character to HEAs.

4:35 PM

(PACRIM-S29-007-2025) Nanocrystalline High-Entropy Alloys (Invited)

Y. Zou*¹

1. University of Toronto, Canada

High-entropy alloy (HEA) design is an emerging methodology that stabilizes nanocrystalline materials, which themselves are highly sought after due to their high strength and hardness resulting from grain boundary hardening. In the past decade, studies have examined the synthesis and performance of such materials made primarily from vapour- and solid-state processing methods, which offer little flexibility in scalability. By contrast, electrodeposition is a relatively low-cost, highly scalable fabrication route for nanocrystalline materials that can be applied to almost any substrate shape or material, which also has industrial-scale infrastructure already in place. Here, we report the first comprehensive study on the synthesis and characterization of electrodeposited HEAs made from aqueous electrolytes, building on the groundwork of past work on electrodeposited medium-entropy alloys. Our study continues to build a framework for electrodeposition of HEAs, paving the way for developing new high-strength, thermally stable, and scalable nanostructured materials.

Tuesday, May 6, 2025

PACRIM Plenary Lectures

PACRIM Plenary Lectures

Room: Regency ABC

Session Chairs: Yiquan Wu, Alfred University;
Bryan Huey, University of Connecticut

8:10 AM

(PACRIM-PLEN 01-005-2025) Imaging Polarization and Ion Distribution in Functional Materials

S. Hong*¹

1. Korea Advanced Institute of Science and Technology, Materials Science Division, Republic of Korea

Ion is the building block of most of the ceramic materials. In ceramic materials, positive ions and negative ions are neighboring each other with mostly ionic bonding at atomic scale. Sometimes, polymer and semiconductor materials contain ions that can diffuse in and out of them. In the meantime, polarization charges of ferroelectric materials are screened by equal amount of surface charges with opposite polarity in ambient conditions. As such, imaging the location, charge as well as the velocity of each ion and polarization will greatly enhance our understanding of electrochemical properties of ferroelectric materials. Here I present our research on various imaging methods of polarization using proxies like piezoelectric strain, screening charges, and friction coefficient, which can be used to image ferroelectric polarization. Furthermore, I will show how these contrast mechanisms can be applied to energy harvesting and chemical mechanical polishing. In addition, I present our research

on various imaging methods of ions and charged defects using proxies like electrochemical strain, and electric charges, which can be used to image ion distribution. Finally, I will show how imaging ion and electron conduction path can help understand the nanoscale behavior of battery materials.

9:00 AM

(PACRIM-PLEN 01-006-2025) Local structure tailoring of rare-earth doped fluoride materials for optical applications

L. Su*¹

1. Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

The traditional strategy for development of novel laser crystals mainly adopts the combination of lattice crystals and active ions, therefore the availability of spectroscopic parameters is seriously limited and can not meet the requirements of the rapidly developing laser applications. Alkaline earth fluoride crystals MF₂ (M=Ca, Sr, Ba) combine the characteristics of wide transmittance range, high thermal conductivity and low phonon energy, which is favorable for application as optical components. Additionally, rare earth (RE) dopants tend to form atomic scale clusters of various structure, thus could serve as platform for tailoring local coordination of rare earth laser active ions. We proposed the strategy of designing the luminescent behaviors of rare earth doped MF₂ crystals by tailoring the local coordinate structure via co-doping regulating ions. The spectroscopic parameters of RE ions could be modulated within a large range, meanwhile the energy transfers between RE dopants could be well controlled.

PacRim S4 - Polymer-Derived Ceramics/Composites/Nanocomposites as Functional Inorganic Materials

PACRIM Symposium 4 - Environmental, energy, health and functional applications II

Room: Plaza C

Session Chair: Michaela Wilhelm, University of Bremen

10:10 AM

(PACRIM-S04-011-2025) Polymer Derived Ceramic Graded Environmental Barrier Coatings for Ceramic Matrix Composites

R. Bordia*¹; S. Maiti¹; Z. Zhang¹; F. Peng¹; J. Delvaux²; M. Hafner²

1. Clemson University, Materials Science and Engineering, USA
2. GE Vernova, USA

We report on the design, processing and performance of graded composition polymer derived environmental barrier coatings (EBC) for ceramic matrix composites. The compositional gradient was designed using simulations to minimize thermal stresses. Additionally, the coating composition was optimized to substantially slow down the oxygen transport and oxide volatilization of EBC under high-velocity steam and oxidizing conditions at elevated temperatures (up to 1300 °C). Taking advantage of the demonstrated excellent compositional tailorability of polymer derived ceramics (PDCs), we developed a graded coating that smoothly transitions from the bond interface at the bottom to a hermetic Y₂O₃ top layer. This smooth compositional transition was shown to result in coatings with excellent thermal and environmental performance, including enhanced oxidation resistance under high velocity steam conditions, and high thermal shock resistance

10:30 AM

(PACRIM-S04-012-2025) Polymer-derived Ni nanoparticle-dispersed amorphous silicon nitrides for catalytic application to RWGS reaction

N. Asakuma³; M. Iijima¹; T. Tamura¹; S. Honda¹; A. Bouzid²; S. Bernard²; Y. Iwamoto*¹

1. Nagoya Institute of Technology, Japan
2. CNRS, IRCER, France
3. Graduate School of Engineering, Nagoya Institute of Technology, Life Science and Applied Chemistry, Japan

Hydrogen (H₂) has been widely used in chemical processes such as the hydrogenation reactions of organic compounds and CO₂. Most of these reactions can be facilitated by the transition metal catalyst, and especially, precious metals exhibit excellent catalytic performance. Recently, increasing attention has been directed to developing precious-metal-free catalysts to allow their widespread deployment and applications. In this study, Ni supported on polymer-derived amorphous silicon nitride (Ni/a-Si₃N₄) was designed and synthesized for catalytic application to CO₂ hydrogenation reactions. Our material design was based on the electronic metal-support interaction (EMSI) for modifying the electronic structure of Ni, adjusting catalytic performance for the reverse water gas shift (RWGS) reaction to afford CO. The Ni/a-Si₃N₄ sample exhibited a high CO selectivity of over 90 % even below 400 °C while the reference sample of Ni/a-SiO₂ sample showed a low CO selectivity of below 50 % at the same low-temperature regions. Spectroscopic analysis and DFT calculations were performed to elucidate the dominant mechanisms for the unique high CO selectivity of the Ni/a-Si₃N₄ sample. The results will be shown and discussed aiming at developing novel precious metal-free catalysts for CO₂ hydrogenation reactions.

10:50 AM

(PACRIM-S04-013-2025) Synthesis of nitride and carbide antiperovskite composite materials as electrocatalyst for the water splitting reaction

M. Cheype*¹; Y. Iwamoto¹; M. Ben Miled²; S. Bernard²

1. Nagoya Institute of Technology, Japan
2. CNRS, IRCER, France

Electrochemical water splitting is one of the most attractive methods to produce dihydrogen (H₂). Indeed, electrocatalysts play a crucial role in water electrolysis to lower the kinetic energy barriers of the oxygen evolution reaction (OER) and of the hydrogen evolution reaction (HER). Electrocatalysts based on non-noble transition metals (TM) like Fe, Ni and Mo are inexpensive, abundant and environmentally friendly. Consequently, different materials have been considered to rank water electrolysis among the most efficient, environmentally friendly and decarbonized routes to dihydrogen. Among them antiperovskite material (X₃BA), exhibiting a similar crystal structure than perovskite with inverted cation-anion arrangement, seems to present an interesting catalytic property due to the specific electronic configuration obtained from 3d transition metals in position X and A. Therefore, we present a synthesis approach by the Polymer-Derived Ceramics (PDCs) route, which offers the opportunity to elaborate composite materials formed by antiperovskite nitrides or carbides particles embedded in an amorphous SiN or SiC matrix. The chemistry behind the synthesis and pyrolysis behavior of these materials as well as their microstructure will be presented and discussed. The characterization of the materials will be done at each step of their elaboration process.

PacRim S6 - Dielectric Ceramics for Microwave and Submillimeter-Wave Applications

PACRIM Symposium 6 - Low-Temperature & Additive Fabrication I

Room: Balmoral

Session Chairs: Jorg Topfer, Ernst-Abbe-Hochschule Jena;

10:10 AM

(PACRIM-S06-009-2025) Energy Efficient Fabrication of Microwave Materials and Devices (Invited)

I. M. Reaney*¹

1. The University of Sheffield, School of Chemical, Materials and Biological Engineering, United Kingdom

Cold sintering is a low energy process that facilitates the densification of ceramics using a transient solvent at low temperature and moderate pressure. The use of cold sintering to fabricate novel MW ceramics and composites for use as substrates is discussed along with examples of prototype devices, such as antennas on COG multilayers. The use of multimaterial 3D printing to construct MW devices using low loss polymers and ceramics is also presented.

10:40 AM

(PACRIM-S06-010-2025) Cold sintering of microwave dielectric ceramics and devices (Invited)

J. Guo*¹; X. Li¹

1. Xi'an Jiaotong University, China

With the rapid development of internet, wireless communication technology has gradually developed from 4G to 5G and its successor 6G, which puts higher requirements for microwave dielectric ceramics. Limited by the variety of materials known to be suitable and the deficiency of low temperature sintering technology, exploring new microwave dielectric materials with improved sintering methods has become one of the focused areas. Recently, cold sintering process (CSP) was proposed to fabricate ceramics at extremely low temperatures (≤ 300 °C). During cold sintering process, a mediated liquid phase such as water, acid, or aqueous alkali is employed to facilitate the densification by a dissolution-precipitation process. Based on CSP, we have further established a protocol for low temperature sintering processes by combining CSP with other sintering technologies, such as microwave and spark plasma sintering. In this talk, I will discuss the recent development of microwave dielectric ceramics and devices fabricated by cold sintering assisted routes with several examples, such as molybdate, tungstate and TiO₂. The frameworks of fundamental mechanisms are outlined together with the experimental data. It is expected that cold sintering process is promising for the fabrication of microwave dielectric materials and offers inspirations on sintering combinations to develop low-temperature sintering processes with high efficiencies.

11:10 AM

(PACRIM-S06-011-2025) Cold Sintering of Boron Nitride Ceramics

H. Nishiyama*¹; J. Mena-Garcia¹; H. Shimizu³; C. Randall²

1. The Pennsylvania State University, USA
2. Penn State University, Materials Science and Engineering, USA
3. Taiyo Yuden Kabushiki Kaisha R and D Center, Japan

Hexagonal boron nitride (hBN) exhibits electrical insulation properties and possesses high in-plane thermal conductivity, making it a promising candidate for various high-temperature applications as both a structural and functional material. Nevertheless, due to its flaky morphology and inherent chemical inertness, sintering hBN into dense bulk ceramics necessitates temperatures exceeding 1600°C.

Recently, there has been an increasing interest in the cold sintering process, which is a low-temperature and energy-efficient technique that involves applying uniaxial pressure to a powder mixed with a solvent under moderate heat. In this study, we present a method for fabricating dense bulk hBN ceramics via the cold sintering process, where shear forces and particle rearrangement facilitate high-density compaction through the utilization of transient phases.

11:30 AM

(PACRIM-S06-012-2025) New Inorganic Binders for Room Temperature Fabrication of Upside-down SrTiO₃-based Ceramic Composites (Invited)

M. Spreitzer*¹; N. Kuzmic¹; S. Skapin¹; M. Nelo²; H. Jantunen²

1. Jozef Stefan Institute, Advanced Materials Department, Slovenia
2. University of Oulu, Finland

In this study, inorganic binders are prepared and successfully applied as alternatives to Li₂MoO₄ for room-temperature fabrication of binder-SrTiO₃ composites. The inorganic compounds Na₂MoO₄, Na₂WO₄, Na₂SiO₃, and MgSO₄, were used as binding phases (15 vol%) in the room-temperature fabricated composite systems, resulting in pellets with relative density ($\rho = 83\text{--}88\%$) and dielectric properties applicable in radio and microwave (MW) frequency ranges. The relative permittivity values of the as-prepared binder-SrTiO₃ composites varied from 68–124 at 1 MHz and between 67–129 in the MW frequency range. The dielectric losses exhibited a range of 0.0029–0.0142 at 1 MHz, with corresponding $Q \times f$ values ranging from 689–1335 GHz. The microstructure, binder-SrTiO₃ interactions, and thermal behavior of the binders and composites were studied using SEM, XRD, and TG analysis. This study provides valuable insights into the use of inorganic binders to fabricate binder-SrTiO₃ composite systems, which could have significant implications in various fields, including electronics and telecommunications, owing to their enhanced properties.

PacRim S7 - Direct Heat-to-Electricity Energy Conversion Mtls & Thermal Energy Harnessing Challenges

PACRIM Symposium 7 - Direct Heat-to-Electricity Energy Conv Mtls & Thermal Energy Harnessing Challenges II

Room: Dover/Tennyson

Session Chairs: Alireza Nojeh, University of British Columbia; Woochul Kim, Yonsei University

10:10 AM

(PACRIM-S07-010-2025) Reinforcing Phonon Scatterings to Enhance zT (Invited)

M. Hong*¹

1. University of Southern Queensland, Australia

Lattice thermal conductivity (k_l) is independently governed by phonon transport. In thermoelectrics, a net increase in zT can be achieved by reducing k_l . First, we introduced the concept of tuning phonon dispersion to enhance phonon-phonon scatterings in GeTe alloys. By modifying the phonon dispersion, we were able to improve the scattering of phonons, leading to a reduction in k_l . Additionally, in polycrystalline thermoelectric materials, to enhance the mid-frequency phonon scattering, we introduced high-density dislocations in the Bi₂Te₃ material and stacking faults in AgSbTe₂. Furthermore, we developed high-density planar vacancies and superlattice precipitates in GeTe alloys, leading to a significant reduction in k_l . To gain a deeper understanding of the underlying connection between structural/lattice imperfections and low k_l , we employed electron microscopy characterizations and first principle calculations.

10:40 AM

(PACRIM-S07-011-2025) Multiscale modeling of thermoelectric properties in complex materials

M. Morshed¹; A. Gautam²; K. Nepal²; C. Ugwumadu²; B. Feygelson³; D. Drabold²; S. Nakhmanson*¹

1. University of Connecticut, Materials Science and Engineering, USA
2. Ohio University, Dept. of Physics and Astronomy, USA
3. U.S. Naval Research Laboratory, Electronics Science and Technology Division, USA

Thermoelectric performance of a complex nanostructured material or composite is strongly dependent on the morphology and transport properties of interfacial areas that connect individual crystal grains or composite constituent phases. However, relatively few experimental and theoretical investigations have been focused on probing the interfacial transport properties of relevant materials. We developed a multiscale approach combining predictive atomistic-level simulations of spatially resolved thermal and electronic conductivity with finite element method based mesoscale-level modeling to evaluate the effective transport properties of structurally complex materials including their figure of merit ZT(T). In this presentation, we highlight the capabilities of this approach, discuss the results obtained for a few popular nanocrystalline thermoelectric systems – such as Si, SiGe, BiTe and SnSe – and outline some ideas for developing better performing thermoelectrics that these results suggest.

11:00 AM

(PACRIM-S07-012-2025) Decoupling the Electrical Conductivity and the Thermopower by Consolidating SrTiO₃ and Metallic Phases

M. Ohtaki*¹; L. Aoki¹; K. Suekuni¹

1. Kyushu Daigaku, Interdisciplinary Graduate School of Engineering Sciences, Japan

Strontium titanate SrTiO₃ (STO) has been known to show a promising thermoelectric performance as an oxide upon n-type doping under reducing conditions. However, the electron doping strong enough to attain a sufficiently high electrical conductivity deteriorates the thermopower of the materials, always making it difficult to achieve high ZT values. We synthesized Sr_{1-x}(Ti_{0.8}Nb_{0.2})_{1-y}Ni_yO₃ ($x, y = 0, 0.05, 0.10$) by solid state reaction. After sintering in air at 1420 °C, the samples were reduced under 20% H₂/N₂ or 100% H₂ at 1350 °C. Whereas the electrical conductivity σ of the samples showed metallic behavior and significantly varied from 200 to 1900 S/cm at room temperature, the Seebeck coefficient S at the same temperature was within a narrow range of –50 to –80 μ V/K. The molar fractions of Ni⁰, $f(\text{Ni}^0)$, obtained from the XPS spectra widely varies from 0.5 to 55% depending on the reducing conditions such as the H₂ concentrations in the reaction atmosphere, while $f(\text{Ti}^{3+})$ stays within 16 – 18% for all the samples. This analysis clearly explains the discrepant behavior of σ and S, the former being tuned by the amount of the metallic Ni particles forming conduction paths, while the latter being governed by the carrier concentrations in the STO matrix. A highest ZT of 0.37 at 800 °C was achieved by the sample with the largest amount of Ni⁰.

PRS9 - Fndmtls of interfaces/grain boundaries/ surfaces - interatomic bonding to macroscopic prop

PACRIM Symposium 9 - Novel Characterizations Techniques

Room: Oxford

Session Chair: Naoya Shibata, The University of Tokyo

10:10 AM

(PACRIM-S09-008-2025) Accurate determination of atomic structures and segregation at grain boundaries in Al_2O_3 (Invited)

K. Matsunaga*¹

1. Nagoya University, Materials Physics, Japan

Al_2O_3 is a representative ceramic material used for structural and functional applications. It is well known that macroscopic Al_2O_3 properties are strongly dependent on physical properties of its grain boundaries. Therefore, it is essential to obtain in-depth understanding of electronic and atomic structures of the grain boundaries for materials development. However, the crystal structure of Al_2O_3 is in low symmetry and thus contain many atoms in the unit cell, so that a great number of atoms should be inevitably handled in the grain boundary modeling. This often makes it difficult to systematically treat Al_2O_3 grain boundaries at the DFT level. In the present study, artificial neural network interatomic potentials trained by DFT data were developed for $\alpha\text{-Al}_2\text{O}_3$, and were applied for the grain boundaries. Grain boundary structures obtained theoretically were compared with experimental STEM images to verify accuracy of the present potentials. Dopant segregation behavior at a specific grain boundary was also investigated, and it turned out that complicated dopant locations observed experimentally can be clearly understood.

10:40 AM

(PACRIM-S09-009-2025) What happens when grain boundary energies approach zero in nanoceramics? (Invited)

R. Castro*¹; I. Loureiro Muller Costa²; D. Fonseca¹

1. Lehigh University, Material Science & Engineering, USA
2. UC Davis, Materials Science and Engineering, USA

In this talk, we explore the implications of achieving a (quasi) zero-energy grain boundary on the stability and mechanical properties of nanocrystalline oxides. While it is understood that grain boundary energies cannot be truly zero, a theoretical framework based on the Gibbs adsorption isotherm suggests that these excess energies can be substantially reduced through grain boundary excesses—often referred to as segregation, though without forming a distinct second phase. Our study demonstrates that yttria-stabilized zirconia (YSZ) can achieve a near-zero grain boundary energy by doping with gadolinium (Gd). This reduction in energy confers remarkable stability against grain growth, a property however strongly influenced by temperature due to the changing solubility limits of the dopant. Additionally, this reduction extends the initiation grain size associated with the inverse Hall-Petch relationship, effectively enhancing the material's mechanical behavior at the nanoscale. These findings provide a robust foundation for grain boundary engineering in nanocrystalline ceramics, offering new pathways to optimize performance through precise control of grain boundary energetics and associated phenomena.

11:10 AM

(PACRIM-S09-010-2025) The Influence of Solutes and Fields on Anisotropic Grain Growth of Alumina (Invited)

I. Naamne¹; R. Marder¹; W. D. Kaplan*¹

1. Technion - Israel Institute of Technology, Dept. of Materials Science and Engineering, Israel

Grain growth occurs alongside densification during the sintering of polycrystalline ceramics. The size and shape of grains can significantly influence a material's properties, while grain boundary motion can lead to the occlusion of second-phase particles and pores, altering residual stress fields and strengthening mechanisms. Understanding the factors driving morphological changes is therefore critical. Although dopants are often used to limit grain growth via solute-drag, recent studies have shown that certain dopants can accelerate grain growth. In alumina, dopants can also alter the relative anisotropic grain boundary mobility, causing notable changes in morphology and properties. This presentation examines anisotropic grain boundary mobility by measuring the interface motion of oriented single crystals of sapphire into undoped and Ca-doped polycrystalline alumina. The findings show that while Ca increases the mean mobility, it dramatically enhances the mobility of boundaries parallel to the rhombohedral plane, resulting in elongated grains. These results are compared with the effects of electric fields on grain growth in dense alumina, highlighting the role of oxygen vacancies in this process. Finally, the role of disconnections as the mechanism for grain boundary motion will be discussed.

11:40 AM

(PACRIM-S09-011-2025) Electric field-induced defect redistribution along a near 23 degree (100) tilt grain boundary in SrTiO_3

W. Hahn*¹; A. R. Lupini³; K. van Benthem²

1. University of California Davis, Materials Science and Engineering, USA
2. University of California, Davis, Dept. of Chemical Engineering and Materials Science, USA
3. Oak Ridge National Laboratory, USA

An electrostatic field strength of 11.6 V/mm was applied during thermal annealing along the grain boundary plane of a near 23 degree (100) tilt grain boundary in SrTiO_3 . Electron microscopy characterization revealed an increased number of pores located at the boundary plane near the positive electrode. Towards the negative electrode a lower physical density at the interface and a wider boundary core structure were observed compared to areas near the positive electrode. Atomic resolution scanning transmission electron microscopy identified different structural units for the boundary core in the proximity of the two electrodes, and a higher density of interfacial steps close to the negative electrode. Electron energy-loss spectroscopy confirms modifications of the local interfacial bonding, stronger reduction of Ti cations, and distorted Ti-O octahedra near the negative electrode. Experimental observations demonstrate field-induced redistribution of oxygen vacancies along the interface plane accommodated by disconnection movement. iDPC experiments are underway to investigate changes in space charge distribution at the boundary region due to oxygen vacancy redistribution. A second trial of experiments are in progress with an identical boundary annealed at a field strength of 5.85V/mm to investigate field strength influence on vacancy redistribution and changes to the boundary.

PacRim S11 - Optical and Electronic Phase Change Materials - Science and Application

PACRIM Symposium 11 - Optical and Electronic Phase Change Materials: Science and Application III

Room: Georgia A

Session Chair: Zengguang Chen, Fudan University

10:10 AM

(PACRIM-S11-012-2025) Crystallization kinetics of phase change materials for non-volatile photonic and electronic applications (Invited)

P. Lucas^{*1}; M. Muller²; F. Hoff²; J. Pries²; M. Wuttig³

1. Univ of Arizona, USA
2. Rheinisch-Westfälische Technische Hochschule Aachen, Germany
3. RWTH Aachen University, Germany

The kinetics of crystallization is a key parameter for applications of phase change materials (PCMs) in photonic and electronic devices. While ultrafast switching is desired for electronic data storage applications, lower speeds are acceptable for many photonic devices, if other requirements such as low optical losses are met. This evolution in requirements has broadened the compositional range of chalcogenide PCMs from tellurides to selenides and sulfides. This compositional change brings about significant changes in bonding as well as crystallization mechanism. Here we decouple nucleation and growth in a series of PCMs and show that the crystallization speed is largely controlled by the nucleation time while the growth rate remains mostly constant with change in stoichiometry. Importantly, fast nucleating samples are found to crystallize with very low stochasticity, which is also an important feature for application requiring fractional crystallization such as neuromorphic computing. It is also found that changes in morphology from bulk to film permits to switch the crystallization kinetic from growth driven to nucleation driven.

10:40 AM

(PACRIM-S11-013-2025) Multiphysics Modeling of Large-Volume Switching in Phase-Change Materials Using Nanosecond Laser Pulses

W. Takeda^{*1}; P. Lucas¹

1. The University of Arizona, Department of Materials Science and Engineering, USA

Ultrafast switching and large property contrast between crystalline and amorphous phases in chalcogenide phase-change materials (C-PCMs) enable both electrical resistive switching in electric devices and the manipulation of light in photonic devices. In photonic applications, C-PCMs are typically deposited on optical components with thicknesses less than 100 nm. However, novel non-volatile photonic devices could benefit from switching thicker films to achieve novel functionality such as reconfigurable waveguides. In this work, using a multiphysics model, we investigate the phase-switching dynamics of micrometer-thick C-PCM films induced by nanosecond laser pulses. Key features that facilitate the switching of such thick C-PCM films are proposed, including material selection, architectural design, and laser setup optimization.

11:00 AM

(PACRIM-S11-014-2025) Multiscale simulations of chalcogenide phase-change materials for non-volatile optical devices (Invited)

W. Zhang^{*1}

1. Xi'an Jiaotong University, China

Chalcogenide phase-change materials (PCMs) are widely applied in electronic and photonic applications, such as non-volatile memory and neuro-inspired computing. Ab initio simulations have been extensively applied to advance the understanding of PCMs for the past

twenty years, enabling rational design of novel materials. In this talk, I will discuss how to combine the advantages of ab initio simulations with the coarse-grained device simulations via the finite-difference time-domain (FDTD) method to promote the design and optimization of phase-change optical devices. For instance, by carrying out ab initio calculations, the essential input parameters, such as refractive index (n) and extinction coefficient (k), are provided for FDTD simulations of devices. In this way, the performance of waveguide memory devices, color display and metasurface devices can be simulated and predicted. I will discuss the use of various PCMs for these optical applications, and provide suggestions on how to improve the device performances further with atomic level knowledge.

11:30 AM

(PACRIM-S11-015-2025) Machine-learning-driven advances in modelling phase-change memory materials (Invited)

V. L. Deringer^{*1}

1. University of Oxford, Department of Chemistry, United Kingdom

Phase-change materials (PCMs) from the Ge-Sb-Te system are widely used in data storage and computing applications, and their intriguing properties have long been studied at the atomic scale using computer simulations. Building on the long-standing success of density-functional theory methods, recent advances in atomistic machine learning (ML) are now bringing “device-scale” molecular-dynamics simulations of PCMs within reach. In this presentation, I will review recent work on the development of ML-based interatomic potential models that can describe the atomistic mechanisms of structural transitions in Ge-Sb-Te PCMs. Following a brief discussion of the methodology and its validation, I will focus on the increasingly realistic simulations of PCMs that are now possible with the help of machine-learned potentials, and showcase recent applications. I will discuss future methodological developments, challenges, and possible long-term perspectives.

PacRim S12 - Eng Ceramics and Ceramic Matrix Composites - Processing/Design/Applications

PACRIM Symposium 12 - Innovative processing and synthesis methods

Room: Plaza B

Session Chair: Jingxian Zhang, Shanghai Institute of Ceramics Chinese Academy of Sciences

10:10 AM

(PACRIM-S12-009-2025) Research and Industrialization of Si_3N_4 substrate from tape casting and gas pressure sintering (Invited)

J. Zhang^{*1}

1. Shanghai Institute of Ceramics Chinese Academy of Sciences, China

Si_3N_4 ceramics is a prospective substrate candidate for power electronic devices due to its excellent mechanical properties and high theoretical thermal conductivity. However, the development of high thermal conductivity and high strength Si_3N_4 is still a challenge especially considering the reliability and the dielectric breakdown strength. The microstructure and crack control is still a challenge. In this presentation, the research and industrialization of high thermal conductivity silicon nitride ceramic substrates is discussed. High thermal conductivity Si_3N_4 ceramic was prepared through tape casting and gas pressure sintering. The influence of carbon addition on the sintering behavior, phase, microstructure, mechanical properties, and thermal conductivity of Si_3N_4 was studied. The grain boundary and the second phase character is studied. Si_3N_4 ceramics with relative density and thermal conductivity as 99% and 98 W/m×K

respectively can be obtained. The mechanism for the microstructure development and the resulting thermal and mechanical properties were discussed. Finally, the influence of defects on dielectric breakdown strength and the performance consistency control of high thermal conductivity silicon nitride ceramic substrates is presented.

10:40 AM

(PACRIM-S12-010-2025) Application and challenge of high throughput mechanical property testing technology for ceramic coatings (Invited)

D. Wan*¹

1. China Building Materials Academy State Key Laboratory of Green Building Materials, China

Ceramic materials are widely used in engineering applications, particularly as thermal barrier coatings, due to their high modulus, strength, high-temperature resistance, and corrosion resistance. However, the evaluation of ceramic coating mechanical properties has long faced challenges due to a lack of technology, standards, and equipment, primarily because coatings are difficult to peel from substrate. Current standard techniques are inadequate for directly measuring these properties, especially at high temperatures. This paper introduces the relative method as an indirect testing technology that effectively solve this problem. The core of this method is establishing the analytical relationship among the properties of the coating, the matrix, and the composite. Based on the relative method technology, the elastic modulus, thermal expansion coefficient and residual stress of ceramic coatings are evaluated, effective testing technologies for mechanical properties of ceramic coatings at room temperature and high temperature are developed, and relevant new testing technologies are transformed into international standards (ISO). Additionally, the difficulties of rapid characterization technology and equipment development of high-throughput mechanical properties of ceramic coatings are also introduced, and the potential application of relative method technology is prospected.

11:10 AM

(PACRIM-S12-011-2025) Recycled Wind Turbine Blades in Clay Bricks: A Sustainable Solution or a Structural Risk?

M. B. Østergaard*¹; T. Ulrich²; H. Johra³; U. Hribar⁴; M. R. Fischer¹; J. König⁴; Y. Yue⁵

1. Aalborg University, Chemistry and Bioscience, Denmark
2. Aarhus Universitet, Department of Geoscience, Denmark
3. SINTEF Community, Architectural Engineering, Norway
4. Jozef Stefan Institute, Advanced Materials, Slovenia
5. Aalborg University, Denmark

Wind energy has become a key element in the green transition. While the use of turbines is beneficial to the green energy generation, the disposal of wind turbine blades at end-of-use is a serious burden to the environment as they are a strong composite materials consisting of glass fibers and an organic epoxy matrix. Currently, the blades are difficult or impossible to recycle. Thus, new actions must be taken to reduce this problem. We investigate the possibility to recycle shredded wind turbine blade material as a component of clay bricks in industry. The turbine blades possess two potential advantages as raw materials. First, the glass fibers could act as a fluxing agent to promote sintering, thereby enhancing the mechanical properties of bricks. Second, burning of the epoxy resin could provide additional energy to the firing process of bricks, thereby reducing the energy input during the brick production. In this presentation, we will introduce the potential obstacles in producing composite bricks with wind turbine blade material on both lab and industrial scale. We present an optimization route of the clay-blade-water suspension by varying ratios of the three components. The effect of the suspension viscosity on firing process and the impact of firing temperature on properties of the bricks is discussed.

11:30 AM

(PACRIM-S12-012-2025) Research on the preparation methods and influencing mechanisms of prestressed ceramics

S. Fu*¹; D. Wan¹

1. China Building Materials Academy State Key Laboratory of Green Building Materials, China

Surface compressive stress can significantly enhance the flexural strength and impact resistance of brittle materials, such as prestressed concrete and tempered glass. However, the ability to achieve predetermined compressive stress on ceramic surfaces is the core issue in the study of prestressed ceramics. This report presents the latest developments in the formation of surface compressive stress in ceramics, specifically through the surface coating method. Prestress enhancement can substantially improve the strength and durability of both traditional and advanced ceramics. For advanced oxide ceramics, prestress enhancement can increase flexural strength by 40% to 50%, while traditional ceramics can achieve approximately double the strength. Additionally, the mixed coating method has enabled the simultaneous enhancement of strength and thermal conductivity in alumina ceramic substrates, demonstrating the immense potential of prestressed ceramics.

PacRim S19 - Nanostructured Bioceramics and Ceramics for Biomedical Applications

PACRIM Symposium 19 - Nanostructured Bioceramics and Ceramics for Biomedical Applications III

Room: Stanley

Session Chairs: Monica Ferraris, Politecnico di Torino;

Junghyun Cho, Binghamton University

10:10 AM

(PACRIM-S19-008-2025) Lanthanide-Doped Nanomaterials for Biomedical Applications – Impact of Surface Chemistry (Invited)

E. Hemmer*¹

1. University of Ottawa, Chemistry and Biomolecular Sciences, Canada

The remarkable optical and magnetic properties of the lanthanides (Ln) make Ln-based nanoparticles (Ln-NPs) ideal for biomedical applications, including diagnostic and therapeutic approaches. This is due to the unique electronic properties of the Ln³⁺ ions allowing for upconversion and near-infrared (NIR) emission under NIR excitation as well as high magnetic moments. Sodium lanthanide fluorides (NaLnF₄) are our favorite materials, and we developed a fast and reliable microwave-assisted synthetic approach allowing crystalline phase and size control in the sub 20 nm realm. Rendering the nanoparticles water-dispersible is key for their potential application in biomedicine, e.g., for imaging, thermal sensing or drug delivery. While a large variety of surface modifications towards water-dispersible Ln-NPs has been reported in the literature, their chemical, optical, and dispersion stability as well as cytotoxicity and interaction in vivo has not yet been fully understood. In this presentation, pros and cons of established and recently developed approaches will be discussed, including silica-coated Ln-NPs for operation in the NIR spectral region and Gum Arabic as straight-forward, biocompatible approach, while we also revisit open toxicity questions by assessing nano-bio-interactions as a function of surface chemistry.

10:40 AM

(PACRIM-S19-009-2025) Effects of Calcium Precursors on Bioactive Glass Nanoparticles: Properties and Applications in Bone Tissue RepairU. Pantulap¹; P. Jampeerung¹; N. Sawangboon¹; E. Meechoowas^{*1}

1. Department of Science Service, Thailand

Mesoporous bioactive glass nanoparticles (MBGNs) are widely studied for bone tissue engineering due to their nanoscale size, mesoporous structure, and large surface area. However, the traditional Stöber method struggles to incorporate CaO content above 15% when using calcium nitrate as a precursor, which limits the nanoparticles' bioactivity and potential for bone regeneration. This study explores a modified Stöber process by using calcium hydroxide as an alternative precursor to calcium nitrate. The resulting MBGNs were analyzed for their morphology, composition, and bioactivity. The results revealed that the MBGNs were amorphous, with spherical or oval shapes and particle sizes between 200–300 nm. Importantly, using calcium hydroxide nearly doubled the CaO content compared to calcium nitrate. In vitro studies in simulated body fluid (SBF) confirmed bioactivity through the formation of hydroxyapatite-carbonate layers on the MBGN surfaces. MBGNs synthesized with calcium hydroxide exhibited enhanced bioactivity, attributed to the higher CaO content. In conclusion, the choice of calcium precursor is critical in optimizing the physicochemical properties and bioactivity of MBGNs. Using calcium hydroxide significantly improves CaO incorporation, positioning these nanoparticles as promising materials for bone tissue repair applications.

11:00 AM

(PACRIM-S19-010-2025) Mixing Energized Fields with Freeze Casting for Future Biomaterials (Invited)S. E. Naleway^{*1}

1. University of Utah, Department of Mechanical Engineering, USA

Freeze casting is a bioinspired technique for the fabrication of tailored, porous ceramic materials with structuring down to the nanoscale. Mimetic of the growth of mammalian bone and other biomaterials where biopolymers template the deposit of biominerals to create complex composites, freeze casting employs a template of growing ice crystals to create a complex porous microstructure in any ceramic. We propose that this bioinspired technique can be controlled through either intrinsic (those that modify from within by altering the constituents) or extrinsic (those that apply external forces or templates) means. Through these classifications, examples of extrinsic (through energized external fields) freeze cast, bioinspired structures will be discussed with a focus mimicking the structure of natural bone. In vitro results and applications as bone filler materials will be discussed.

11:30 AM

(PACRIM-S19-015-2025) Can nanostructured material, hydroxyapatite/collagen bone-like nanocomposite, make available selective cell recruitment? (Invited)M. Kikuchi^{*1}; T. Hasegawa²; N. Amizuka²

1. National Institute for Materials Science (NIMS), Bioceramics Group, Japan
2. Hokkaido Daigaku, Japan

Appropriate cell recruitment is important for regenerative medicine including bone void repair by implantation of artificial bone void fillers. Even hydroxyapatite/collagen bone-like nanocomposite (HAp/Col) porous body is good for comparatively small bone void filler; however, in case of huge bone defects, osteoclastic resorption sometimes occurred at too early stages and insufficient bone formation was observed at the center of defects. In this presentation, our recent results that improvement of bone formation prior to osteoclastic resorption without using any drugs. Lamellar disk of the HAp/Col was prepared by uniaxial-press dehydration of the HAp/Col

fibers in a specially designed mold. The flat surface of the disk was mainly composed of long axis of collagen molecules and m-surface of HAp and the perpendicular surface was randomly distributed but comparatively dominated by edge of collagen molecules and c-surface of HAp. The disk was implanted into SD-rats tibia and histochemically observed at 5 to 28 days post-operation. The results showed that the flat surface recruited osteoblasts to form new bone followed by bone remodeling and the perpendicular surface recruited osteoclasts to resorb the HAp/Col directly. Thus, the nanostructured composite, HAp/Col, can control cell recruitments by orientation of HAp and collagen.

PacRim S21 - Cultural Heritage of the Pacific Rim**PACRIM Symposium 21 - Cultural Heritage of the Pacific Rim II**

Room: English Bay

Session Chair: Fumie Iizuka, University of Wisconsin System

10:10 AM

(PACRIM-S21-012-2025) Study on the Influence of Calcination Temperature of Iron Vitriol on the Coloration of Ancient Chinese Traditional Iron Red Overglaze ColorA. Wu^{*1}; D. Yi¹

1. Donghua University, China

Iron red, a traditional Jingdezhen overglaze color, is primarily colored with iron oxide (Fe_2O_3). In traditional processes, the main ingredient for the iron red overglaze color, raw iron red, is produced by calcining iron vitriol. Analysis of ancient iron red porcelain samples indicates that the coloration is unstable, ranging from bright red to dark red, and occasionally to black. Addressing this, the present study, from a ceramic technology standpoint, conducts a series of calcination experiments on industrial iron vitriol at varying temperatures. Utilizing methodologies such as differential scanning calorimetry-thermogravimetry (DSC-TG), Raman spectroscopy, X-ray diffraction (XRD), scanning electron microscopy with X-ray energy dispersive spectrometry (SEM-EDS), and optical microscopy (OM), this research scientifically explores the impact of iron vitriol's calcination temperature on the coloration of traditional Jingdezhen iron red overglaze color.

10:30 AM

(PACRIM-S21-013-2025) New insights behind the polychrome of Philippine ivories – Archangel Saint Michael leading the wayA. S. Ortiz Miranda^{*1}; J. Lauffenburger¹; A. Proser²; D. Chan²

1. The Walters Art Museum, Conservation, USA
2. The Walters Art Museum, Curatorial, USA

The 17th-century ivory sculpture of the Archangel Saint Michael at the Walters Art Museum stands as a masterpiece of Philippine devotional art distinguished by its size and exceptional craftsmanship. This abstract reports on the characterization of the polychromy and gilding components that embellish the ivory surface of this complex sculpture. XRF and FORS were used to identify the pigments of the palette. THM-Py-GCMS was used to determine the components of the resinous brown material used as a mordant for gilded decoration—this constitutes a new approach to studying the Philippine ivories. Laccol, tung oil, and pine resin were the major components identified in the resinous material used in the gilded design. Verdigris, vermilion, organic-origin red, and lead white were identified in the polychrome palette. The identification of laccol, a natural lacquer from *Rhus succedanea*, marks a groundbreaking development, shedding light on the cross-cultural exchanges that shaped artists' production during and after the Spanish colonial period. It is known that the ivory carving was done by Chinese craftsmen working in

Manila in the 17th c., but less is known about polychrome decoration. Laccol, known and used in Asia, ties the polychrome decoration to Asia and the Philippines for the first time rather than the Spanish Americas, as some scholars have previously speculated.

10:50 AM

(PACRIM-S21-014-2025) Basic copper chloride pigments and silk deterioration in Korean Buddhist painting

C. Bisulca*¹

1. Detroit Institute of Arts, USA

Synthetic basic copper chloride pigments are commonly found in Buddhist paintings and are sometimes linked to severe deterioration of the silk support. As part of ongoing research at the DIA, the composition of this pigment was analyzed in ten Choson Dynasty Korean Buddhist paintings. Basic copper chlorides occur as three polymorphs—atacamite, paratacamite, and botallackite—which can be distinguished noninvasively using Vis-NIR fiber optics reflectance spectroscopy in the 1700–2500 nm range. The analysis revealed that the pigment consists of varying proportions of atacamite and botallackite, with differences observed across the paintings. These variations in composition suggest differences in manufacturing processes, which may contribute to the variability in silk deterioration noted from painting to painting.

11:10 AM

(PACRIM-S21-015-2025) Pigments or degradation products? The arsenate pigments in ancient Chinese grotto murals

L. Shen*¹

1. Hangzhou City University, China

Arsenic-containing ancient pigments were relatively limited, primarily consisting of orpiment, realgar, or some lead arsenates such as mimetite, all showing a yellowish appearance. However, in recent non-destructive investigation of the Yungang Grottoes and the Kizil Caves, arsenic(V) was detected in many color shades of the grotto murals, including purple-red, pink, white, brown, and blue-green. Yet no yellow residues were observed under the microscope on-site, indicating the absence of an underlayer of orpiment or realgar. Through micro-sampling, Raman spectroscopy, infrared spectroscopy, SEM-EDS, and EPMA-WDS analysis, it was found that both Arsenic(V) oxide and anhydrous arsenates are present. The purple-red color is mostly lead arsenate, the light red is probably calcium arsenate, some browns are copper arsenate, and the blue-green is lavendulan. According to the microscopic morphology and color, arsenic(V) oxide, blue-green lavendulan, and brown copper arsenate are likely degradation products, while the others are probably ancient arsenic-containing pigments that have been reported for the first time.

11:30 AM

(PACRIM-S21-016-2025) A study on Japanese folk art of the 18th - 19th centuries: crêpe print, doro-e painting, and glass painting

Y. Ichimiya*¹

1. Tokyo Geijutsu Daigaku, Japan

This study examines Japanese folk art of the 18-19th centuries, when art forms emerged that were accessible to the general public. Little scientific research on folk art has led to misunderstandings, particularly regarding the colorants used. For example, the idea that folk paintings used cheaper colorants represent only part of the work and are misconceptions. This study focused on three distinctive art forms: crêpe print, doro-e, and glass painting. Crêpe prints, a unique variation of ukiyo-e, involves shrinking an existing print to create textured designs. A survey of 1,286 privately owned prints revealed a short production period and evolving techniques to meet changing demands. Doro-e, a form of painting that introduced Western techniques to the public. This study revealed the use of smalt, indigo

and brass, suggesting that doro-e were more innovative than previously thought. Glass painting, introduced by European and Chinese techniques, uses the transparency of glass to enhance the brightness of the artwork. XRF analysis of the pigments further revealed their unique characteristics. These three art forms highlight the artisans' openness to experimentation, blending Western influences with traditional Japanese aesthetics. This study enriches our understanding of these art forms and supports efforts to preserve these fragile works.

PacRim S22 - 7th International PacRim Richard M. Fulrath Memorial Symposium on Advanced Ceramics

PACRIM Symposium 22 - 7th International PacRim Richard M. Fulrath Memorial Symposium on Advanced Ceramics II

Room: Grouse

Session Chair: Tomoyuki Nakamura, Murata Mfg. Co. LTD

10:10 AM

(PACRIM-S22-010-2025) Scientific Surprises in Electroceramic Materials when Undergoing New Non-Equilibrium Processes (Invited)

C. Randall*¹

1. Penn State University, Materials Science and Engineering, USA

In general, we consider non-equilibrium thermodynamic processes as those that describe a material undergoing change and not being in a stable state. In this presentation, we will describe two cases under this general framework. The first example introduces a new model to understand transient densification under isothermal conditions. Here, we consider the time evolution with a double relaxation process. This provides a comprehensive methodology with different temperature and pressure dependences that permits the energetics to be determined and accurately predicts the strain and strain rates as the material undergoes densification. The second case revisits the electrical poling of ferroelectric materials into piezoelectric materials. Poling is a process that orients the domain structures. Traditionally, this has been performed by applying a DC field at room temperature or an elevated temperature. More recently, in single crystals, an AC poling strategy has become a method whereby higher properties have been observed. In this study, we have considered pulse poling as a new method to control the nucleation and domain growth processes.

10:40 AM

(PACRIM-S22-011-2025) Failure Modes in Oxide Solid State Electrolytes: Direct Observations of the Stress Accompanying Dendrite Growth (Invited)

C. D. Fincher¹; Y. Chiang¹; B. Sheldon²; M. D. Thouless³; W. Carter*¹

1. Massachusetts Institute of Technology, Materials Science and Engineering, USA

2. Brown University, Mechanical Engineering, USA

3. University of Michigan, Mechanical Engineering, USA

Although solid-state batteries with metal anodes promise to enable safer, higher energy density batteries, metal protrusions (dendrites) short-circuit the cell when charging faster than a critical current density. Dendrite growth is accompanied by stress and we have previously shown that applied stresses affect a dendrite's growth. We used operando birefringence microscopy to directly observe dendrite-induced stresses. The stress intensity is determined by fitting the experimentally measured stress distribution to that expected around an internally loaded crack. These operando

experiments, combined with cryogenic scanning transmission electron microscopy (STEM) characterization of the dendrite tip, allow separate study of electrochemical and mechanical phenomena underlying dendrite growth in ceramic electrolytes. All experiments were conducted on the most electrochemically stable Li-ion conducting solid electrolyte (tantalum-doped lithium lanthanum zirconium oxide).

11:10 AM

(PACRIM-S22-012-2025) Charge separation mechanisms in transition metal oxide photocatalysts (Invited)

G. Rohrer*¹

1. Carnegie Mellon University, USA

Many transition metal oxides, such as BiVO₄ and SrTiO₃, catalyze photochemical reactions. The photochemical reaction that splits water is one of the most widely studied. The best photocatalytic materials have mechanisms to spatially separate photogenerated charge carriers. This prevents charge carrier recombination and the back reaction of intermediate reaction products. This presentation will compare findings from non-polar oxides (SrTiO₃, BiVO₄, CaTiO₃, WO₃) and polar oxides (BaTiO₃, AgNbO₃, La₂Ti₂O₇, Sr₂Nb₂O₇) and discuss charge separation driven by different surface charges, ferroelectric domains, and inhomogeneous distributions of charged point defects.

11:40 AM

(PACRIM-S22-013-2025) From Studying Metal Oxide Polymorphism to Developing “The RISE Breath Test” (Invited)

P. Gouma*¹

1. The Ohio State University, MSE, USA

The Richard M. Fulrath Award of The American Ceramic Society was awarded to this author in “recognition of technical contributions relating to novel ceramics for bio-sensing and olfaction”. Metal oxides are ceramics that change their electrical resistance in the presence of a gaseous analyte. They are polymorphic materials, crystallizing in different phases based on temperature, pressure, or crystal size. A crystallo-chemical map was constructed, empirically at first and now proven experimentally, which predicts the affinity of certain crystallographic configurations (rutile vs perovskite vs layered vs acentric structures, to name a few) to specific gases. This crystallo-chemical approach led to selective chemical sensors and opened the pathway for detecting trace amounts of signaling volatile biomarkers of disease in exhaled breath. Our work pioneered breathalyzer devices for the detection of Nitric Oxide, Ammonia, or Acetone, and these devices led to the COVID-19 breath test which detects the host response to infection by SARS-CoV-2. The need for simple, rapid tests that are fundamentally different from the clinical tests currently being used has become common knowledge following the pandemic. Currently, we develop a breath test for Respiratory Panel infections from pathogens, such as viruses and bacteria, to mitigate the spread of infectious diseases via portable, easy to use breathalyzers.

PacRim S23 - Advanced Processing and Manufacturing Technologies for Ceramics

PACRIM Symposium 23 - Flash sintering

Room: Georgia B

Session Chairs: Wilhelm Meulenber, Forschungszentrum

Julich Institut für Energie- und Klimaforschung; Hiroshi Masuda,

The University of Tokyo

10:10 AM

(PACRIM-S23-008-2025) Toward High-Speed Forming and Joining of Structural Ceramics Assisted by Flash Events (Invited)

H. Yoshida*¹; K. A. Shariffuddin¹; Y. Yang¹; H. Masuda²; K. Morita³;

T. Yamamoto⁴

1. Tokyo Daigaku Daigakuin Kogakukei Kenkyuka Kogakubu, Materials Science and Engineering, Japan
2. The University of Tokyo, Department of Materials Engineering, Japan
3. National Institute for Materials Science (NIMS), Japan
4. Nagoya Daigaku, Materials Design Innovation Engineering, Japan

Since the pioneering works by H. Conrad's group, it has been pointed out that the application of an external strong electric field may enhance the plastic deformability of structural ceramics, such as TZP ceramics, analogous to the electroplasticity of metals and alloys. We have recently demonstrated that high-speed (strain rates $>10^{-3} \text{ s}^{-1}$) tensile or bending deformation of fine-grained TZP ceramics is possible even at ambient temperatures below 1000°C under the occurrence of flash events under a strong electric field. This high-speed forming is attributed to enhanced cationic diffusion under an electric field as well as flash sintering. Furthermore, high-speed diffusion (superplastic) joining is also possible under a flash event. In the present presentation, our recent results on the effects of flash events on the mechanical response of structural ceramics will be summarized, and strategies for high-speed forming and joining of structural ceramics will be discussed.

10:50 AM

(PACRIM-S23-010-2025) Effect of Electric Field/Current on Grain Growth of Zirconia (8Y-CSZ)

K. Morita*¹

1. National Institute for Materials Science (NIMS), Japan

Flash event, which takes place under strong electric fields, have been attracted many attentions because it can accelerate the sintering of ceramic powders. The flash event has firstly been reported by Raj and his colleagues in sintering, but it is known to be effective also to other high temperature processing, such as deformation, joining and crack healing. Although the flash event has widely been examined, the effect of electric field/current on the sintering is still unclear. This is because the flash sintering generally completes within a few seconds. The steep behavior is an advantage for industrial applications, but it makes it difficult to understand the rate-controlling mechanisms. In order to clarify the field/current effect on the high temperature processing of ceramics, therefore, the present study was carried out to examine the electric field/current effects on grain growth behavior of polycrystalline zirconia ceramics (8YSZ) under the DC and AC current conditions. In the presentation, the more detailed field/current dependent high temperature processing will be reported. This work was financially supported by JST CREST (JPMJCR1996) and by KAKENHI (20H02444), Japan.

PacRim S24 - Solid-State Optical Materials and Luminescence Properties

PACRIM Symposium 24 - Novel optical materials design and their properties I

Room: Prince of Wales

Session Chair: Dariusz Hreniak, Institute of Low Temperature and Structure Research

10:10 AM

(PACRIM-S24-008-2025) Structure Evolution of the Clusters in Er Doped Fluorite Crystals and Their High Power Mid-infrared Laser (Invited)

Z. Zhang^{*1}; Z. Zhang¹; F. Ma²; D. Jiang¹; L. Su¹

1. Shanghai Institute of Ceramics Chinese Academy of Sciences, Synthetic Single Crystal Research Center, China
2. Jinan University, Department of Optoelectronic Engineering, China

Er-laser around $3\mu\text{m}$ has significant applications in laser surgery, gas detection and IR countermeasure. Er doped gain materials are of significant interest to achieve a compact and high-efficiency $\sim 3\mu\text{m}$ laser. However, due to the strong dependence of high concentration doping and severe thermal effect of Er doped gain materials, achieving high-power continuous-wave (CW) laser remains a big challenge in laser field. Taking advantage of the unique “clustering effect” of trivalent rare earth ions in fluorite crystals, efficient $\sim 3\mu\text{m}$ laser could be realized at a rather lower doping level. Accordingly, we grew series of Er doped fluorite crystals and investigated the effect of doping concentration on the clusters’ structure. Through combining the spectral analysis and the first principles calculations, we reveal the evolution behavior of Er^{3+} cluster structure with doping concentration as well as the changes in luminescent behavior. It is found that in $\text{Er}:\text{CaF}_2$ system the clustered Er ions come to dominant place at about 1at.% doping level and apparently promote the inter-ionic energy transfer process. We achieved a LD direct-pumped CW $\sim 2.8\mu\text{m}$ laser with a slope efficiency of 40% in $\text{Er}:\text{SrF}_2$ crystal, the efficiency surpasses the Stokes limit of 35%. Besides, a high-efficiency and high-stability 20W level CW $\sim 3\mu\text{m}$ laser was first achieved by LD double-end-pumped a $\text{Er}:\text{CaF}_2$ crystal slab.

10:40 AM

(PACRIM-S24-009-2025) An innovative method for synthesizing luminescent and magnetic garnets from glass melts (Invited)

M. Nalin^{*1}

1. Universidade Estadual Paulista Julio de Mesquita Filho, Inorganic Chemistry, Brazil

Garnet single crystals have received increasing attention in recent years due to their versatile compositions and growing range of applications, particularly those based on luminescence and magnetic properties. Garnets containing rare earth elements are especially important from commercial and technological perspectives. In this work, we present an innovative methodology for synthesizing $\text{TR}_3\text{Ga}_5\text{O}_{12}$, $\text{TR}_3\text{Al}_5\text{O}_{12}$, and $\text{TR}_3\text{Fe}_5\text{O}_{12}$ (where TR = rare earths) single crystals using a glass matrix as the reaction medium. A heavy metal oxide composition based on lead-germanate glass containing the appropriate oxide is melted, and the cooling rate is controlled to obtain cubic single crystals via phase separation. Systematic characterization has been conducted to confirm the garnet compositions, including X-ray diffraction, Raman and UV-Vis spectroscopies, photoluminescent spectroscopy, transmission electron microscopy, and energy-dispersive spectroscopy. Additionally, magnetic properties were assessed using SQUID analysis. Acknowledgements: The authors thank the São Paulo Research Foundation FAPESP (grants n° 2013/07793-6), CNPq, and SISFOTON-MCTI for financial support.

11:10 AM

(PACRIM-S24-010-2025) Photonic-Plasmonic Coupling Color Materials Using SiO_2 -Metal Nitride Patchy Particles

S. Noguchi^{*1}; M. Lama³; Y. Fujii²; A. Miura²; K. Tadanaga²

1. Hokkaido University, Graduate School of Chemical Sciences and Engineering, Japan
2. Hokkaido University, Faculty of Engineering, Japan
3. Hokkaido University, Institute for Chemical Reaction Design and Discovery, Japan

Color materials with photonic and plasmonic properties were developed using SiO_2 -metal nitride (MN) patchy particles. Nanoparticles (10–30 nm) of MN (M=Ti, Zr, Hf) exhibiting localized surface plasmon resonances (LSPRs) were attached to the surface of mono-dispersed SiO_2 particles modified with polyvinylpyrrolidone. The monodispersity of SiO_2 particles was preserved after the deposition of MN nanoparticles. The prepared SiO_2 -MN patchy particles exhibited a plasmon resonance absorption band at 820 nm in the TiN system, 670 nm in the ZrN system, and 620 nm in the HfN system. The particle-stacked films from the SiO_2 -MN patchy particles were fabricated using the drop-casting method. The particle-stacked films of the SiO_2 -MN patchy particles exhibited the Bragg diffraction-based maximum reflection depending on the particle size of the SiO_2 core. In addition, the plasmonic absorption of the metal nitride nanoparticles attached to SiO_2 was reflected in the reflectance spectrum of the particle-stacked film. Materials exhibiting a gamut of colors were achieved to a certain extent by controlling the core particle size (photonic effect) and the type and amount of metal nitride attached to the SiO_2 surface (plasmonic effect). The materials are expected to serve as a colorant that exhibits different hues without relying on noble or harmful heavy metals.

11:30 AM

(PACRIM-S24-011-2025) Development of transparent and fluorescent α -SiAlON ceramic by co-doping of Ce^{3+} and Lu^{3+}

J. Tatami^{*1}; K. Amianka¹; M. Iijima¹; A. Ito¹; S. Matsumoto¹; T. Takahashi²; T. Ohji¹

1. Yokohama National University, Japan
2. Kanagawa Institute of Industrial Science and Technology, Japan

The effects of Ce/Lu co-doping and its ratio, as well as the particle size of the raw powder, on the transparency and fluorescence of α -SiAlON ceramics were investigated. Although the addition of only Ce did not result in transparent α -SiAlON ceramics, we succeeded in fabricating $\text{Ce}^{3+}:\text{Lu}-\alpha$ -SiAlON ceramics with both transparency and Ce^{3+} -derived fluorescence by co-doping with Lu, which has the smallest ionic radius. It was also found that the transparency improves with decreasing Ce concentration and the fluorescence wavelength becomes shorter. In addition, it was found that the use of finer rare-earth oxide raw powder improved transparency due to the reduction of oxynitride glass caused by homogenization of the α -SiAlON formation reaction. The transparent $\text{Ce}^{3+}:\text{Lu}-\alpha$ -SiAlON ceramics developed by controlling these powder processes were also found to exhibit scintillation in response to α -rays and X-rays.

PacRim S27 - International Symposium of Fundamental and Frontier Sciences of Ceramics

PACRIM Symposium 27 - International Symposium of Fundamental and Frontier Sciences of Ceramics II

Room: Cypress

Session Chairs: Michael Stuer, Swiss Federal Laboratories for Materials Science and Technology, Empa; Florian Bouville, ETH Zürich

10:10 AM

(PACRIM-S27-009-2025) Dielectric behavior of high entropy ferroelectric ceramics (Invited)

H. Yan^{*1}

1. Queen Mary University of London, School of Engineering and Materials Science, United Kingdom

High entropy materials represent interesting properties, with unexpected properties that go beyond the rule of mixtures of their constituent components. Recently three groups of high entropy ceramics, including perovskite ABO_3 , Aurivillius phase and perovskite layer structured (PLS) ferroelectrics, were successfully prepared and characterized. ABO_3 ferroelectric $(Pb_{0.25}Ba_{0.25}Sr_{0.25}Ca_{0.25})TiO_3$, including 4 elements at A-site, contains minor secondary phase and perovskite structured ferroelectric phase which includes nano domains. When the elements at A-site were increased from 4 to 6 in the structure, single phase ferroelectric $(Pb_{1/6}Ba_{1/6}Sr_{1/6}Ca_{1/6}Na_{1/6}Bi_{1/6})TiO_3$ was prepared, due to high entropy effect. Single phase Aurivillius structured $ABi_4Ti_4O_{15}$ ceramics with 3, 4, 5 and 6 elements at A-site were separately prepared. Their dielectric breakdown strength (BDS) increased with entropy increase due to maximized local stress field. Relaxor ferroelectric behaviour was observed in PLS $(Ca_{0.5}Sr_{0.5}Ba_{0.5}Pb_{0.5})Nb_2O_7$ high entropy ceramic which is single-phase structure with space group $Cmcm$. Its value of the relative permittivity $\epsilon' = 130$ at 1 kHz and room temperature is much larger than that for conventional PLS ceramics $Sr_2Nb_2O_7$ ($\epsilon' = 42$) and $Ca_2Nb_2O_7$ ($\epsilon' = 38$). This can be attributed to the presence of polar nano regions and the lattice distortion effect in high entropy materials.

10:40 AM

(PACRIM-S27-010-2025) Montmorillonite Nanosheets for Polymer-Derived MMT-SiOC Nanocomposites (Invited)

K. Lu^{*1}; A. Rau²

1. University of Alabama at Birmingham, USA
2. Virginia Polytechnic Institute and State University, USA

In this study, twice-functionalized MMT nanosheets were randomly dispersed in the SiOC matrix with α -SiO₂ forming at the MMT-SiOC interface. Pyrolysis to 1400°C induced the formation of SiC nanowhiskers that were observed up to 20 μ m in length and 200 nm in diameter. After selective etching of SiO₂ domains with HF, pore sizes and specific surface areas of MMT-SiOC were analyzed with nitrogen adsorption. While water vapor-assisted pyrolysis selectively removes free C in pure SiOC, surprisingly, MMT and water vapor in combination led to encapsulation, shielding, and retention of C as graphene oxide in MMT-SiOC-H₂O ceramics. Crystalline α -SiO₂ phases in MMT-SiOC were converted to amorphous SiO₂ phases during water vapor-assisted pyrolysis, leading to 25-50% reductions in specific surface areas of HF-etched MMT-SiOC without changes to the intrinsic pore structure of water vapor-pyrolyzed SiOC. Further pyrolysis to 1400°C led to the dissolution of the aforementioned pore structure due to more extensive carbothermal reduction and refinement of β -SiC nanowhiskers. The methodology and results presented improve the understanding and viability of 2D nanomaterial-reinforced ceramic composites and MMT as a precursor for nanostructured SiC.

11:10 AM

(PACRIM-S27-011-2025) New Metastable Oxides via Crystallisation of Glasses and Undercooled Melts (Invited)

M. Pitcher^{*1}

1. Centre National de la Recherche Scientifique, France

The full and congruent crystallisation of a glass precursor is an established route to new transparent ceramics with different optical applications. This approach is enabled for a wide range of compositions by containerless processing of melts using aerodynamic levitation, and features glass synthesis (by melt-quenching) followed by a separate heat treatment to partially- or fully-crystallise the material into a (glass-) ceramic. The crystallisation step often produces metastable compounds or polymorphs with functions that complement those of known materials. Recently, the aerodynamic levitation approach has led to the emergence of direct crystallisation of the undercooled melt as an alternative single-step pathway to new (glass-) ceramics: here, instead of freezing into glass, the deeply-undercooled melt (a non-equilibrium state) crystallises directly, producing a range of interesting materials featuring metastable compounds and crystal structures, with microstructures ranging from classic ceramic-type micro-crystallinity through to millimetric crystalline domains with bulk samples resembling large single crystals. I will describe some recent examples of novel (glass-) ceramic materials that can be synthesised by these two approaches, from typical glass-forming systems (e.g. ternary aluminosilicates) through to refractory non-glassformers (e.g. rare-earth niobates).

11:40 AM

(PACRIM-S27-012-2025) Scale-bridging processing of advanced ceramics

D. Giuntini^{*1}

1. Eindhoven University of Technology, Mechanical Engineering, Netherlands

With their ever-increasing applications in key engineering sectors, ceramics occupy a prominent spot in materials engineering. Their processing, nevertheless, remains challenging. Additional to overcoming the difficulties in shaping and sintering, the controlled formation and evolution of nano- and micro-structures during processing is crucial to tune their performance. There is a strong need for scale-bridging ceramics processing strategies, to simultaneously control the material evolution at the nano-, micro- and macro-scale. The recent advancements in colloidal assembly, additive manufacturing and sintering technologies are key enablers. We show here how scale-bridging in ceramics processing entails material design, tailored particle- and powder-based manufacturing, advanced characterization tools, and the support of analytical and numerical modeling. Performance-targeted material design guided by optimization algorithms is applied to microcomposites with enhanced mechanical properties and nanocomposites with tunable magnetic response. The continuum theory of sintering is broadened to capture not only macroscopic shrinkage and deformations during processing, but also microstructural changes in layered and hierarchically porous ceramics. By tuning the rheological and mass transfer phenomena driving each processing step, the development of hierarchical ceramics with tailorable mechanical and functional properties is demonstrated.

PacRim S29 - Progress in High-Entropy Materials

PACRIM Symposium 29 - AI/ML- Model development and applications II

Room: Plaza A

Session Chair: Adam Krajewski, The Pennsylvania State University

10:10 AM

(PACRIM-S29-008-2025) High Entropy Materials for Clean Energy: Unique Electrochemical Application, Specialized Database and Universal Predictor (Invited)

B. Ouyang^{*1}

1. Florida State University, Chemistry and Biochemistry, USA

High-entropy materials (HEMs) initially emerged as promising candidates for structural applications, exemplified by the extensively studied high-entropy alloys. Recently, the application of HEMs expanded into broader fields, including energy storage and conversion. We will demonstrate the potential of these materials as high-performance, low-cost materials for battery electrode/electrolytes and electrocatalysis. To facilitate rapid discovery of synthesizable and high-performance compositions and structures, we developed a specialized database containing over 200,000 DFT-computed high-entropy alloys and metal oxides. Furthermore, we will illustrate how integrating physical models with advanced deep learning algorithms enables the development of a universal stability predictor to assess the synthetic accessibility of these materials. Finally, we will present case studies that delve into unique phenomena, including enhanced diffusivity and compositional dependent corrosion resistance in HEMs.

10:40 AM

(PACRIM-S29-009-2025) Integrated Data Driven Methodology Development for the Design of Multicomponent Alloy Chemistries Given Property Trade-offs (Invited)

S. Broderick^{*1}

1. University at Buffalo, USA

This presentation will discuss the role of materials informatics in the design of multi-component systems. The primary focus will be on the design of high entropy alloys and the challenges in trade-offs between strength, ductility and various environmental effects. To address the limitations in traditional regression approaches which can generate large amounts of data rapidly but do not account for the complexities in unknown property data, an approach for introducing a new design index is discussed. This approach is designed to capture the interplay between chemistry, microstructure and phase stability, which allows us to identify chemical design rules for improving mechanical properties with minimal trade-offs. These results are integrated with Bayesian Neural Networks and DFT calculations to design target alloys. The approach permits one to understand how different and/or the same alloying element has a multifunctional role in defining engineering properties. The implications of this work for design of ceramic systems for given applications will also be discussed.

11:10 AM

(PACRIM-S29-010-2025) Accelerated discovery of high entropy ultra-high temperature ceramics by machine learning and high throughput experiments (Invited)

K. Wang^{*1}

1. Alfred University, USA

Machine learning (ML) methods have been successfully applied to predict phase formation and properties of novel materials, such as high entropy materials. However, the application of ML approach in

high entropy ceramics (HECs) used in extreme environments, such as nuclear reactors and hypersonic vehicles etc., remains limited due to the serious data scarcity as well as data quality issues. Herein, the machine learning (ML) model is trained on data collected via high-throughput experiments (HTEs). Because the experiment was conducted under the same conditions, HTEs enable generating high-quality dataset for ML training. The experimental validation is performed to examine the performance of the ML model. In addition, the ML is also applied to inversely understand the underlying physical mechanisms. For instance, we demonstrate that a mismatch of the bonds between boron and transition metals (δ B-TM) dominates the formation of HEBs. We propose an empirical rule that HEBs favor forming a single phase when δ B-TM < 3.66; otherwise, multiphase. The rule has a high accuracy of 93.33% for new HEBs predictions. Additionally, we are the first attempt to apply high-throughput experiments (HTEs) assisted data-driven strategy in the prediction of oxidation recession of HEBs-SiC ceramic composites.

11:40 AM

(PACRIM-S29-011-2025) Active Learning Driven Materials Discovery for Low Thermal Conductivity Rare-Earth Pyrochlore-Oxide

A. Chowdhury^{*1}; A. R. Romero²; G. Figueredo³

1. University of Nottingham, M3, United Kingdom
2. Fundacion Tecnalia Research & Innovation, Spain
3. University of Nottingham, Health Science, United Kingdom

Machine learning holds promise in expediting the materials discovery process. By combining the fast prediction of material properties, provided by a trained machine learning model, with an efficient search algorithm like Bayesian optimisation, this study aims to develop a high-throughput method to generate new compositions with low thermal conductivity. The compositions used in this study are rare-earth oxides with a pyrochlore/flourite structure due to their promise as low thermal conductivity ceramics and their capacity to form high-entropy (HEC) and multi-component (MCC) compositions. This provides an expansive search space to show the potential of Bayesian optimisation in materials discovery.

PacRim S32 - Advanced Characterization, Testing, and Analysis of Materials

PACRIM Symposium 32 - Advanced Characterization, Testing, and Analysis of Materials I

Room: Seymour

Session Chairs: Amanda Krause, Carnegie Mellon University;

Scott Misture, Alfred University

10:10 AM

(PACRIM-S32-001-2025) Direct Nanovolumetric Investigation of Domain Walls and Grain Boundaries in Functional Oxides (Invited)

A. Akoma¹; K. Del Cid-Ledezma¹; K. Lizu¹; J. Schultheiss²; D. Meier²;

B. Huey^{*1}

1. University of Connecticut, MSE, USA
2. Norges teknisk-naturvitenskapelige universitet, Norway

It is experimentally difficult to truly correlate the local properties of functional materials with the microstructure given the three-dimensional nature of key features and defects such as grain boundaries, stacking faults, layer interfaces, and domain walls. We have therefore advanced Tomographic AFM, which combines high resolution surface imaging with serial sectioning, especially to investigate phase, grain, and domain boundary effects for manganate and pzt thin films. This includes mapping domain morphologies in 3D as a function of grain orientation, and proximity to grain boundaries, with voxel resolution as fine as 10^*10^*2 nm³. 3-dimensional

localized curvature along domain walls is also uniquely resolved and statistically analyzed. Such research extends the limits of resolution for more traditional tomographic methods such as microCT and FIB-SEM sectioning. Such insights are important for the advanced modelling, enhanced processing, novel engineered devices, and optimized applications of functional oxides.

10:40 AM

(PACRIM-S32-003-2025) Advancing Electron Microscopy for uncovering Oxide and Sulfide Catalysts at the Atomic-Scale

M. Ek²; L. Hansen³; F. Chen⁴; D. van Dyck⁵; C. Kisielowski⁶; P. Specht⁶; C. Damsgaard¹; J. Jinschek^{*1}; S. Helveg¹

1. Danmarks Tekniske Universitet, Denmark
2. Lunds Universitet, Centre for Analysis and Synthesis & NanoLund, Sweden
3. Topsoe A/S, Denmark
4. City University of Hong Kong, Hong Kong
5. Universiteit Antwerpen, Belgium
6. Electron Scattering Solutions, USA

The current quest for sustainability calls for a new view on catalysts. While electron microscopy (EM) operating at the highest spatial, temporal, and energetic resolution offer unprecedented opportunities to resolve atomic-scale structural and chemical information of catalyst surfaces, such investigations are challenged by sample alterations induced by the electron illumination. To address this issue, we have advanced bright-field EM in combination with exit-wave reconstruction to detect catalysts at the level of single atoms using a minimal amount of scattered electrons. Image acquisitions using low-dose-rate illumination is furthermore critical to suppress object excitations and advance chemical meaningful insight. We showcase these advancements for two catalyst systems. First we have studied single-layer MoS₂ nanocatalysts and demonstrate how a new analytical model for the exit wave is able to extract the three-dimensional atomic structure, stoichiometry as well as vibrational blur to give a consistent structural and dynamical characterization at the level of single atoms. Next we have studied VO_x/TiO₂ nanocatalysts. We show that the present concepts can be applied for in situ and operando conditions and favorably combined using low-dose-rate scanning EM in combination with electron energy loss spectroscopy to resolve reaction-induced redox dynamics at the catalyst surface.

PacRim S4 - Polymer-Derived Ceramics/Composites/Nanocomposites as Functional Inorganic Materials

PACRIM Symposium 4 - Design-oriented manufacturing and processing of composites

Room: Plaza C

Session Chair: Yuichiro Hirota, Nagoya Institute of Technology

1:15 PM

(PACRIM-S04-015-2025) Synthesis and water-vapor corrosion resistance of (5RE_{0.2})₂Si_xO_{2x+3}/SiOC nanocomposites at 1200-1500°C (RE= Yb, Ho, Er, Lu, Tb, Tm, Gd) (Invited)

Q. Wen^{*1}; X. Huang¹

1. Central South University, Powder Metallurgy Research Institute, China

Dense monolithic (5RE_{0.2})₂Si_xO_{2x+3}/SiOC nanocomposites (RE= Yb, Ho, Er, Lu, Tb, Tm, Gd, x=1 or 2) containing a high-entropy rare-earth (RE) silicate phase were prepared using a PDC method combined with spark plasma sintering. The nanocomposites were characterized by a microstructure with a homogeneous dispersion of (5RE_{0.2})₂Si_xO_{2x+3} nanoparticles within an amorphous SiOC matrix. The atomic ratios of rare-earth (RE) metal elements within the in situ generated (5RE_{0.2})₂Si_xO_{2x+3} nanoparticles can be controlled precisely by tailoring the composition of the preceramic

precursors. Interestingly, the (5RE_{0.2})₂SiO₅ is stable up to 1500 °C, which is different from that of the silicates with only one rare-earth elements (generally, RE₂Si₂O₇ formed at such a high temperatures). That means the (5RE_{0.2})₂SiO₅ was stabilized owing to the high-entropy effect. High-temperature water-vapor corrosion resistance of the (5RE_{0.2})₂Si_xO_{2x+3}/SiOC nanocomposites was investigated at 1200-1500°C for 100 h. The results show that, compared with SiOC, the (5RE_{0.2})₂Si_xO_{2x+3}/SiOC exhibit significantly enhanced water-vapor corrosion resistance, and the nanocomposites with different RE elements exhibit different water-vapor corrosion behaviors.

1:45 PM

(PACRIM-S04-016-2025) Preparation of high temperature resistant ceramic coatings based on preceramic polymer-derived ultrahigh-temperature ceramic nanocomposites (UHTC-NCs)

A. D. Camacho Ramirez^{*1}; S. Kredel¹; J. Bernauer¹; E. Ionescu²; R. Riedel¹

1. Technische Universität Darmstadt Fachbereich Material- und Geowissenschaften, Germany
2. Fraunhofer-Einrichtung für Wertstoffkreisläufe und Ressourcenstrategie IWKS, Germany

In this work, preceramic polymers were synthesized by modifying the commercially available organopolysilazane Durazane 1800 with Hf and Ta amido complexes and borane dimethyl sulfide complex. The incorporation of transition metals into the polymer structure, their influence on ceramization and processability were investigated. The preceramics were coated onto substrates such as eutectic Mo-20Si-52.8Ti and silicon wafers via spin coating, forming crack-free, amorphous SiHfTa(B)CN-based ceramic coatings with excellent adhesion. A new multilayer coating process was developed to produce thicker, filler-free, crack-free coatings exceeding 10 μm in thickness. The composition of the ceramic coatings was investigated via X-ray photoelectron spectroscopy (XPS), and their high-temperature behavior was examined through oxidation tests in the range of 1000-1200°C. A thermal cycling procedure to temperatures above 1250°C with rapid heating and cooling rates in the range of (100-120K s⁻¹) was applied to the ceramic coating, which showed no damage even after ten thermal cycles, indicating their outstanding thermal shock resistance and their potential for use as environmental barrier coatings at high temperatures. The authors acknowledge the funding of Deutsche Forschungsgemeinschaft (DFG) in the frame of the MatCom-ComMat project (GRK 2561).

2:05 PM

(PACRIM-S04-017-2025) Straightforward design of 3D polymer-derived SiC architectures via a granule-derived FDM technology

D. Sazarin¹; M. Cheype¹; V. Pateloup¹; S. Bernard^{*1}

1. CNRS, IRCER, France

There is a trend toward more performant or competitive materials with the objective to improve the efficiency of actual systems and to repel technological boundaries. Silicon Carbide (SiC) attracts strong interests due to its properties targeted for future materials and technologies especially in aerospace. Inherent difficulties to the traditional techniques for manufacturing such dense materials with a complex geometry can be overcome by the development of new manufacturing approaches and the deployment of synthetic paths where chemistry of materials and ceramic science are combined rationally. The Polymer-Derived Ceramics (PDC) route offers great opportunities in material sciences when combined with 3D printing. Here, the aim of this talk is to introduce a straightforward design approach consisting in tailoring the extrusion ability of polycarbosilanes to fit with a granule-based fused deposition modeling process and form after a two-step heat-treatment process at a relatively low temperature 3D stoichiometric SiC and derived composites parts.

PACRIM Symposium 4 - Organic-inorganic hybrid materials: from synthesis to application

Room: Plaza C

Session Chairs: Christel Gervais, UPMC; Timothy Pruyn, Air Force Research Laboratory

2:25 PM

(PACRIM-S04-019-2025) Hybrid Cu(II)acrylate/Silazane thin coatings with hydrophobic and antibacterial properties

M. Zahedtalaban^{*1}; S. Schafföner¹; G. Motz¹

1. Universität Bayreuth Fakultät für Ingenieurwissenschaften, Ceramic Materials Engineering, Germany

Healthcare acquired infections (HAIs) are caused by the transmission of pathogens in hospitals, threatening both patients and staff. Surfaces play a major role in the indirect spread of pathogens, and hygiene practices have proven insufficient to alleviate this matter. Therefore, development of antibacterial coatings grants the best approach to reduce the prevalence of HAIs. This study presents a novel hybrid coating combining the biocidal activity of Cu(II)acrylate with the hydrophobic character of the oligosilazane Durazane 1800. SEM and EDS analysis of the as-crosslinked coating on steel substrate revealed the formation of a 4 µm thick and well-adhered layer with uniformly distributed Si and Cu atoms. Cross-cut and scratch tests revealed a good coating adhesion (GT2) and a 20 N scratch tolerance, ascribed to the covalent Fe-O-Si bonds formed between the coating and steel substrate. The exposure of methyl and vinyl groups from Durazane 1800 on coating's surface led to its hydrophobicity, denoted by a static water contact angle of 99°, while its biocidal activity against *E. coli* and *S. aureus* was accredited to the presence of Cu²⁺ ions from the metal acrylate. Moreover, the coating demonstrated an improved chemical resistance against common disinfectants such as isopropanol and H₂O₂, showing minimal signs of degradation and thickness loss after 24 h immersion at room temperature.

3:30 PM

(PACRIM-S04-020-2025) Development of ionic liquid-siloxane hybrid membranes and their application to vapor and liquid separation (Invited)

Y. Hirota^{*1}

1. Nagoya Institute of Technology, Department of Life Science and Applied Chemistry, Japan

Ionic liquids (ILs) have superior physical and chemical properties, so have been widely studied in membrane separation processes. We have developed IL-siloxane hybrid membranes using silylated ILs as precursor chemicals. The membrane showed selective permeation of CH₃OH against H₂ at the temperature range from 373 to 473 K. Although separation performance was decreased with increasing the permeation temperature, separation factor of more than 10 was still obtained at 473 K. We have also applied the developed membrane to the separation of organic mixtures via pervaporation method. The membrane showed selective permeation of toluene against n-hexane in the toluene concentration range from 10 to 50 wt% at 293 K. The toluene selectivity was increased with the toluene concentration. The toluene/n-hexane permeance ratio of 19 was obtained with the toluene permeance of 2.6×10⁻⁶ mol m⁻²s⁻¹Pa⁻¹ in a 50 wt% toluene solution. The results of vapor permeation and pervaporation tests suggest that permselectivity of the membranes is strongly controlled by the affinity of the permeate molecules toward the IL group.

4:00 PM

(PACRIM-S04-021-2025) Aligned Carbon/Ceramic Hybrid Fibers with improved Oxidation Resistance

G. Motz^{*1}; J. Denk¹; X. Liao²; S. Agarwal³; S. Schafföner¹

1. University of Bayreuth, Ceramic Materials Engineering, Germany
2. Tianjin University, China
3. Universität Bayreuth Fakultät für Biologie Chemie Geowissenschaften, Macromolecular Chemistry II, Germany

Carbon and ceramic fibers were initially developed for extreme conditions in aerospace and military applications. These fiber types with specific advantages and disadvantages especially regarding oxidation stability and costs are now used on a large scale for civil applications. Recently we developed hybrid polymers composed of silazanes and polyacrylonitrile, leading to fibers which can fill the gap between carbon and ceramic fibers regarding properties and costs. Especially the oxidation resistance is remarkably due to the formation of a well distributed ceramic nano-phase within the carbon matrix, which forms a protective silica layer under oxidative conditions. Since PAN cannot be melt-spun wet-spinning and electrospinning were chosen for polymer fiber processing followed by stretching, curing in air and pyrolysis in nitrogen atmosphere. By using wet spinning fibers with a diameter of 20 µm, high tensile strengths of 2.0 GPa and a Young's modulus of 175 GPa were produced. Considering the simple process setup in the lab, these are excellent mechanical properties, comparable to commercial ceramic fibers. Electrospinning of the hybrid polymer led to a novel multifibrillar C/SiCON fiber type with a diameter of 15 to 20 µm consisting of thousands of individual fibers in the nanometer range. The tensile strength of about 700 MPa can be extremely improved if sticking of the nanofibers can be avoided.

4:20 PM

(PACRIM-S04-022-2025) Design at Nanoscale of Thermostable Hybrid Sol-Gel Bondlayer to Functionalize Aeronautical CFRP by Thermal Spray

S. Senani - de Monredon^{*1}; L. Rozes²; G. Penvern¹; A. Joulia¹; S. Bonebeau³

1. Safran SA, France
2. Sorbonne Université, LCMCP, France
3. SAFIR, France

Composite Fibers Reinforced Parts are widely used in aeronautic since more than 40 years to decrease the aircrafts environmental footprint. Indeed CO₂ and NOx emissions have been considerably decreased by lightweighting correlated to significant fuel consumption reduction. To go further and reach the new ambitious target of 20% reduction for the next aircraft engine, functionalization of CFRP is mandatory to extend them to more aggressive use cases. To reach this goal, thermal spray coatings are widely studied, even if it remains very complex to implement. Metallization of CFRP by coldspray is favored by numerous teams, with interesting results but not sufficient to fit performance required for aeronautic qualification. Our approach aims to design a thermostable sol-gel hybrid bondcoat. We will discuss how we succeed to control the nanostructuration and the nature of the substrate/bondlayer/topcoat interfaces to influence the thermomechanical bondcoat's properties and thus the building and the thickness increase of the thermal sprayed topcoat layer linked to the adhesion of the stack. Understanding the relation between nanostructuration of the hybrid sol-gel layer and their thermomechanical properties is essential to optimize the whole system. Finally, this will widely open the variety of materials reachable to functionalize CFRP part and allow new use cases.

4:40 PM

(PACRIM-S04-023-2025) Novel BCN and HfBCN nanocomposites for energy conversion applicationK. Lu^{*1}; W. Li¹; J. Ding²

1. University of Alabama at Birmingham, USA
2. Technische Universität Darmstadt, Germany

Multicomponent MBCN ceramics, where M represents a transition metal, are garnering increased interest due to their multifunctionality and ultrahigh-temperature stability. Currently, research on MBCN primarily focuses on its preparation and application in the form of thin films. In this study, we prepared monolithic BCN and HfBCN nanocomposites using a single-source precursor approach for the first time and explored their potential application as thermoelectric materials for energy conversion. Cubic $\text{HfB}_x\text{C}_y\text{N}_{1-x-y}$ nanocrystallites ranging from 10 to 200 nm were formed in-situ within amorphous HfBCN materials after sintering at 1600 °C. Furthermore, the presence of turbostratic $\text{BC}_x\text{N}_{1-x}$ phase within the matrix, significantly surpassing the percolation threshold, contributes to both BCN and HfBCN nanocomposites, exhibiting exceptionally high electrical conductivity exceeding $100 \text{ S}\cdot\text{cm}^{-1}$. A power factor of approximately $40 \mu\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-2}$ was achieved in HfBCN-based nanocomposites, setting a record high among polymer-derived ceramics.

PacRim S6 - Dielectric Ceramics for Microwave and Submillimeter-Wave Applications

PACRIM Symposium 6 - Low-Temperature & Additive Fabrication II

Room: Balmoral

Session Chairs: Matjaz Spreitzer, Jozef Stefan Institute; Ian Reaney, University of Sheffield

1:15 PM

(PACRIM-S06-013-2025) Low temperature sintering of the BaO-CuO-SiO₂ ternary microwave dielectric ceramics with low permittivity values (Invited)

D. Zhou^{*1}; W. Wang¹; Y. Lou¹

1. Xi'an Jiaotong University, School of Electronic Science and Engineering, China

In low permittivity microwave dielectric ceramic systems, silicate-based ceramics have low dielectric constant. Silicate ceramics are usually crystalline materials with silica-oxygen tetrahedral coordination, generally forming $[\text{SiO}_4]^{4-}$. The ionic and covalent bonding ratios of Si-O bonds in $[\text{SiO}_4]^{4-}$ are 45 % and 55 % respectively, and the Si-O bonds are shorter in length and stronger, closer to rigid bonds. Therefore, silicate ceramics are suitable for millimeter-wave dielectric materials. In the BaO-CuO-SiO₂ ternary system, there are a couple of single compounds microwave dielectric ceramics reported, such as $\text{BaCuSi}_4\text{O}_{10}$, $\text{BaCuSi}_2\text{O}_6$, $\text{BaCu}_2\text{Si}_2\text{O}_7$ etc. In this presentation, we will introduce our recent progress in low temperature co-fired ceramics technology (LTCC) of the BaO-CuO-SiO₂ ternary ceramics using low-melting-point oxides and low-softening-point glasses as sintering aids to meet the requirements of LTCC technology.

1:45 PM

(PACRIM-S06-014-2025) Development of LTCC Materials and Processes for Microwave and Mili-meter Wave Devices (Invited)

Y. Sugimoto^{*1}

1. Murata Seisakusho Kabushiki Kaisha, Inorganic materials development Dept., Japan

Low-Temperature Co-fired Ceramics (LTCC) have become a key technology for further miniaturization of RF circuits. Capacitors and inductors can be buried in the ceramics because LTCC can be co-fired with Cu or Ag electrode, which have low electric resistivity. LTCC, which have various dielectric constant and high Q-value, are applied to functional circuit boards and chip monolithic devices. Recently constrained sintering technology, co-firing technologies of various materials and high Q-value LTCC materials have been developed. Constrained sintering technology improve size accuracy and flatness of substrates, and co-firing technologies contribute to further integration of microwave devices by co-firing various materials, for example high or low dielectric constant materials, printed resistors and so on. And high Q-Value LTCC materials can reduce electric loss of devices. In the recent trend of using higher frequencies for wireless communication, e.g. 5G system, controlling electric loss is the biggest challenge. The higher the used frequency is, the higher the electrical loss of wireless devices is. In order to suppress stray capacitance between electric circuits, substrate materials of lower dielectric constant have been developed. Therefore, these technologies will integrate more passive circuit elements and contribute to further miniaturization of microwave devices and higher frequencies.

2:15 PM

(PACRIM-S06-015-2025) Integration of functional materials in LTCC layers of SiCer composite substrate modules (Invited)

M. Heidenreich¹; T. Schulz¹; B. Capraro²; J. Topfer^{*1}

1. Ernst-Abbe-Hochschule Jena, Germany
2. Fraunhofer IKTS, Germany

We have studied the integration of functional materials into the LTCC layers of the SiCer composite substrate. The SiCer process includes the combination of Si wafers and LTCC multilayer systems by cofiring at 900°C, wafer processing, and assembly of the complete module. SiCer composite substrates allow fabrication of MEMS, sensor- and communication modules. The LTCC tape BCT was used for shrinkage matching with Si. Examples for the integration of functional materials into the BCT multilayer system include ferrites for integrated transformers, dielectrics for integrated capacitors, and NTC spinels for thermistor applications. LTCC multilayer modules with integrated magnetic microwave components for satellite communication systems in the K_a-band (26-40 GHz) were also studied. Sc-substituted ferrites $\text{BaMe}_x\text{Fe}_{12-x}\text{O}_{19}$ were used for self-biasing microwave components, e.g., in circulators. Static magnetic measurements show that both the saturation magnetization and coercivity decrease with x, indicating a reduction of the anisotropy field. The ferromagnetic resonance frequency for x = 0.5 is at 30 GHz. Ferrites were integrated into LTCC multilayer modules as drop-in bulk components into LTCC cavities, or anisotropic ferrite films obtained by screen-printing or tape casting, drying in a magnetic field and cofiring. Such oriented self-biasing ferrite layers were used in microwave components.

2:45 PM

(PACRIM-S06-016-2025) Alkali Modified Borosilicate Glass-SiO₂ Composites for Electronic Packaging and High Frequency Applications

M. E. Eltantawy^{*1}; A. Shearer¹; U. Sanjeevani²; Y. Liao²; J. C. Mauro¹; S. Wang²; M. Lanagan¹

1. The Pennsylvania State University, Materials Research Institute, USA
2. National Taipei University of Technology, Taiwan

This research primarily focuses on developing high-density borosilicate glass for advanced electronic packaging applications through viscous sintering and sol-gel processing. The project aims to explore the structure-properties-processing relationships of alkali borosilicate glass-SiO₂ composites, focusing on optimizing the dielectric properties. The composite design features a borosilicate glass matrix with embedded SiO₂ particles, and the system is expected to remain fully amorphous to enhance its functional properties. By emphasizing the role of the glass structure, the research investigates how the dielectric constant and loss in the GHz frequency range are influenced by the material's composition and processing conditions. Effective medium theories will be applied to predict and tailor the dielectric properties of glass composites. Viscous sintering and sol-gel techniques will be optimized to achieve a fully amorphous, high-density glass with minimal porosity. Advanced characterization techniques will be employed to assess the structure and properties of the sintered composites. The expected outcome is a high-density borosilicate glass-SiO₂ composite with a low dielectric constant, low dielectric loss, high thermal stability, and improved mechanical integrity, suitable for next-generation communication devices and high-frequency electronic circuits.

3:20 PM

(PACRIM-S06-017-2025) Contribution of additive manufacturing to the production of ceramic dielectric resonators with adapted permittivity (Invited)

C. Le Paven^{*1}; T. Lavie¹; M. Julian¹; L. Le Gendre¹; R. Benzerga¹; A. Sharaiha¹; F. Cheviré²

1. University of Rennes 1, Institute of Electronics and Telecommunications of Rennes (IETR), France
2. Institut des Sciences Chimiques de Rennes, Equipe Verres et Céramiques, France

The advancement of telecommunications necessitates dielectric materials with optimized permittivity, high quality factor, and near-zero temperature coefficient for integration into dielectric resonator antennas (DRAs). Additive manufacturing (AM) offers opportunities to tune permittivity via complex geometries and this study investigates ceramic resonators with controlled permittivity, achieved by introducing air inclusions without altering the material composition. Using gyroids—mathematically defined triply periodic minimal surfaces—we fabricated ceramic/air composite resonators from alumina and zirconia as test materials, integrated into DRAs. Digital light processing (DLP) was employed to produce cylindrical gyroid resonators, which were debinded and sintered to achieve high relative density. Dielectric measurements (1–16 GHz) by means of a resonant cavity revealed that effective permittivity of resonators actually decreases with air inclusion volume, from 32.7 to 1.3 using zirconia and then alumina; results are in accordance with current models. Increased air inclusion also reduces dielectric loss. Prototyped DRAs demonstrate comparable performance, achieving a weight reduction of 50% for zirconia gyroid resonators relative to solid alumina parts. Future work includes exploring the temperature coefficient of resonance frequency and gradient gyroid resonators.

3:50 PM

(PACRIM-S06-018-2025) Structured dielectric composite deflector fabricated by 3D printing (Invited)

J. Heintz^{*1}; C. Elissalde²; N. Penin⁴; T. Fournier³; V. Hoang⁵; E. Vandelle⁵; B. Loiseaux⁵; P. Pouliguen⁶

1. ENSMAC-Bordeaux INP, ICMCB, France
2. ICMCB-CNRS, France
3. CANOE, France
4. ICMCB-University of Bordeaux, France
5. Thales Research and Technology France, France
6. DGA, France

3D printing of dielectric composites is an interesting alternative for the design and manufacture of compact, low-cost antennas for applications in the microwave band, such as on-board Internet access distribution. In this work, we exploited FDM (Fused Deposition Modelling) technique since it is considered as one of the most mature additive manufacturing methods. First, the advantages and limitations of FDM in the field of dielectric composites for antenna applications will be highlighted. Then, the selection of a low loss dielectric oxide powder (TiO₂) and polymer matrix (Cyclic Olefin Copolymer) will be explained. The powder preparation and the optimisation of the ceramic charge in the filaments will be described. Printable composite filaments containing up to 36 vol% dielectric particles and exhibiting high dielectric permittivity ($\epsilon_r = 7.7$) and low losses ($\tan \delta = 1.10^{-3}$) over a wide frequency range (10 - 40 GHz) were successfully produced. To demonstrate the benefits of this material, a sub-wavelength deflector was designed in COC-TiO₂ composite and compared to its counterpart in ABS (acrylonitrile butadiene styrene). The simulation results demonstrate the numerous advantages of high permittivity material, particularly in terms of reduced thickness and weight of the component, increasing efficiency and reducing side-lobe levels. Finally, the successfully printed COC-TiO₂ demonstrator will be presented.

4:20 PM

(PACRIM-S06-019-2025) The effects of Zn substitution on the Phase, Microstructure, Dielectric and Electrical properties of Y_{2.95}Dy_{0.05}MgAl₃SiO₁₂ Garnet Structured ceramics

A. Manan^{*1}; O. Ullah¹; M. Lanagan²; A. Hossain²

1. University of Science & Technology Bannu, Department of Physics, Pakistan
2. Penn State University, Dept. of Engineering Science and Mechanics, USA

Y_{2.95}Dy_{0.05}Mg_{1-x}Zn_xAl₃SiO₁₂ (x=0.0, 0.05, 0.10, 0.15) ceramics were processed via solid state sintering method. Phase, microstructure, dielectric and electrical properties were determined for the ceramics. XRD data analysis revealed a single phase ceramic for each composition. The ϵ_r measured at 1 MHz for all compositions sintered at 1575 °C for 4h increases from 12.16 to 13.15 with an increase in x content from 0 to 0.15 due to the fact that Zn²⁺ has high ionic dielectric polarizability (2.04 Å³) than Mg²⁺ (1.32 Å³). The dielectric loss initially increased slightly from 0.007 to 0.015 as the x value increased from 0 to 0.05 and then decreased to 0.012 for x 0.10 measured at 1 MHz. Dense microstructure is obtained for all Zn doped samples, however, the average grain size is the lowest (3.2 μm) for x=0.10 that also led to a lower electrical conductivity and higher electrical impedance for x=0.10 in comparison to other x values. The material could find application in millimeterwave devices.

PacRim S8 - STE(A)M Outreach/Education/Engagement/Retention (Joint with GOMD)

PACRIM Symposium 8 & GOMD Symposium 4 - STEAM Outreach, Education, Engagement and Retention

Room: Dover/Tennison

Session Chairs: Charmayne Lonergan, Missouri University of Science & Technology; Casey Schwarz, Ursinus College

1:15 PM

(PACRIM-S08-001-2025) Making Glass with High, Middle and Elementary Schoolers (Invited)

S. Feller*¹; M. Affatigato¹; C. B. Bragatto¹

1. Coe College, Physics Department, USA

We use three ways to make glass with school children: 1. We bring glass making directly to high school science labs. Only a Bunsen burner with a spark or matches, 20 cc porcelain or alumina crucibles, furnace gloves, tongs, a spatula, boric acid, and a weighing balance are needed. The reaction $2\text{H}_3\text{BO}_3 \rightarrow \text{B}_2\text{O}_3 + 3\text{H}_2\text{O}$ readily goes to near completion in about 15 minutes. About 6-8 grams of boric acid are weighed and heated until the water vapor ceases to emerge and the sample is molten glass. The weight loss (about 46%) may be measured and compared to the periodic table prediction. Deviations of about 10% from the predicted loss are typical. A small 1000 °C electric furnace may be substituted for the Bunsen burner. With a little water it is easy to run the reaction backwards and create boric acid from boron oxide glass. 2. We have hosted the Coe College Playground of Science over 20 times. This multi demonstration event with over 50 interactive demos includes glass making in a public display area at the entrance to the Coe Physics Department. We draw over a thousand visitors from four counties most of whom see glass made. 3. We invite high school classes for tours and demos in the Coe College glass labs. The students get to do proscribed experiments using equipment such as furnaces, dscs, glove boxes, electron microscopes, AFMs, and Raman spectrometers in our ongoing Coe Nanoworkshops. We acknowledge NSF through grant DMR-2203142.

1:45 PM

(PACRIM-S08-002-2025) Science for Society: Expanding access to materials science education in both formal and informal learning settings

L. McDonald*¹

1. The American Ceramic Society, USA

In a rapidly evolving world driven by technological progress and innovation, it is more critical than ever that people have at least a basic understanding of materials science. Engineered materials play a foundational role in a wide range of industries, from electronics and aerospace to healthcare and energy. Paradoxically, although such materials are key enablers of our modern world, materials science education tends to be less visible than other engineering disciplines due to a lack of materials science curriculum in K-12 schooling and a dearth of university programs on ceramic and glass materials specifically. These constraints limit access to this vital career path. This presentation highlights the importance of materials science education and also showcases tangible initiatives and resources available through The American Ceramic Society (ACerS) and the Ceramic and Glass Industry Foundation (CGIF) to educate people about materials science, with an emphasis on ceramics and glass, at every stage of their career.

2:05 PM

(PACRIM-S08-003-2025) Asynchronous Education for an Intro to Materials Science Course: When and How to Do It Well

M. D. Losego*¹

1. Georgia Institute of Technology, School of Materials Science and Engineering, USA

This talk will discuss the development of an entirely asynchronous version of "Introduction to Materials Science" designed for non-majors. This asynchronous course has now been delivered at least five times to often over 250 students per semester, with student feedback that is comparable to the in-person synchronous course, including high levels of student engagement. Well-established pedagogical methods of chunking content to 10 min or less are at the foundation of the course but, mixed with good helpings of diversity in content type (e.g., lectures, demos, activities, and quizzes), intentional reminders that students are still part of a class, well-defined and communicated course scheduling, and at-home experiments that are both engaging and meaningful. Interestingly, the asynchronous version is also more easily delivered equitably by being easily able to accommodate student emergencies as they arise. Such a course is also powerful in providing support for other instructors, in-coming graduate students from non-MSE majors, and potentially for high school recruitment through college-level coursework.

2:25 PM

(PACRIM-S08-004-2025) Empowering the Next Generation of STE(A)M Innovators Through Real-World Simulations, Mentorship, and Outreach in Glass and Ceramics

C. Schwarz*¹; R. Sharma²; J. Donnelly³; M. Lam³; K. Richardson²

1. Ursinus College, Physics & Astronomy, USA
2. University of Central Florida, CREOL, USA
3. University of Central Florida, Chemistry, USA

Our team presents a multi-faceted approach to inspire and retain the next generation of STE(A)M professionals, with a focus on engaging students in the dynamic field of glass science and ceramics research. In this work, we integrate real-world simulations using advanced characterization tools, providing students with hands-on experiences that connect theoretical knowledge to practical applications while serving underrepresented and/or low-income communities. We also build a pathway for small colleges to gain access to state-of-the-art equipment and expand engagement. We introduce our methods for high school lab integration, outreach, peer-to-peer mentorship, unique research experiences, and industry connections. By connecting students to these activities, we hope to enhance their understanding of critical concepts and spark their interest in pursuing careers in STE(A)M fields. Recent qualitative and quantitative results on these efforts will be presented.

3:30 PM

(PACRIM-S08-005-2025) Design and Implementation of STEAM Outreach Initiatives in Educational Settings: Insights, Challenges, and Key Takeaways (Invited)

A. Yadav*¹; S. Gupta²; R. Sharma²; K. Sonowal³

1. Sri Aurobindo College, University of Delhi, Department of Physics, India
2. Sri Aurobindo College, University of Delhi, Department of Electronics, India
3. Sri Aurobindo College, University of Delhi, Department of Environmental Science, India

This presentation highlights ongoing efforts to foster awareness and increase interest in Science, Technology, Engineering, Arts and Mathematics (STEAM) among diverse audiences, with a particular emphasis on fostering interests in glass and ceramics-related topics. These efforts include community outreach initiatives, interactive workshops, and mentorship programs, all aimed at demystifying complex concepts and making STEAM fields more accessible and engaging. Special attention is given to integrating artistic creativity

into STEAM disciplines to create interdisciplinary learning experiences. Through a review of existing programs, case studies, and participant feedback, we identify key strategies that have contributed to the effectiveness of these initiatives. The study also highlights the challenges faced, including limited funding, disparities in access, and the need for sustained engagement across diverse student populations. Key lessons learned emphasize the importance of tailored programming to meet the specific needs of different student groups, as well as the role of collaboration between educational institutions, industry, and local communities. The presentation concludes with recommendations for improving future STEAM outreach efforts to better address equity, enhance student engagement, and ensure long-term impact in promoting STEAM education.

4:00 PM

(PACRIM-S08-006-2025) Training opportunities as a tool to guide student outcomes (Invited)

R. Sharma*¹; K. Richardson²

1. University of Central Florida, College of Optics and Photonics, USA
2. University of Central Florida, CREOL, USA

As academic researcher leaders working in the inter-disciplinary area of optical materials, our research teams are comprised of students and staff members of varying academic levels and technical backgrounds. 'Training' has multiple meanings that can include hands-on experimental experiences, as well as an exposure to experiences in literature review, technical writing and speaking. Training opportunities for undergraduate students serve as an important 'test drive' by which students assess the possibility of future careers in technical areas that could lead to further graduate studies or employment. For graduate students, post docs and scientists, 'training' of new students can involve day to day supervision, mentorship, management (time management, definition of expectations, managing budgets and deliverables), as well as problem solving. This talk discusses academic group strategies and industry group needs and how these efforts can be mutually linked for both teams' benefit.

4:30 PM

(PACRIM-S08-007-2025) Needs, potential solutions and challenges for making US STEM doctoral training that is aligned with student career paths

H. Jain*¹; V. Dierolf²; A. Jagota³; Z. Pan³

1. Lehigh University, International Materials Institute for New Functionality in Glass, USA
2. Lehigh University, Physics, USA
3. Lehigh University, USA

Driven by the fact that a great majority of STEM PhD graduates will be employed in non-academic jobs, primarily in industry, there is a growing recognition that the present format of doctoral training does not prepare them sufficiently for a career outside academia. In response to this need to fill the gap, recently a new student-centered model of STEM doctorate, Pasteur Partners PhD (P3), based on use-inspired research was developed. Industry-university partnership is a requirement of this model, which calls for a concerted participation of industry experts in the training of student through identification of industry-relevant research problem, mentoring by co-advising about how to approach its practical solution, and other non-technical skills that are equally important for success in industry. We will examine an assessment of this model, which shows overwhelming student interest. However, faculty participation, intellectual property agreements, and expectations of faculty tenure/promotion and funding agencies remain as major challenges. We will share the results of student demand and their experience with its non-traditional features, support of university administration, feedback from industry co-advisers and the challenges felt by interested faculty advisers in implementing the industry-university doctoral training (P3) program.

4:50 PM

(PACRIM-S08-008-2025) Building Bridges: The Evolution and Impact of the PRE-CCAP Consortium

R. Grodsky*¹; A. Moser²

1. National Nuclear Security Administration Kansas City National Security Campus, Inorganic Materials, USA
2. National Nuclear Security Administration Kansas City National Security Campus, Center of Excellence Lead, USA

The Minority Serving Institute Partnership Program (MSIPP) was designed for DOE/NNSA to develop a sustainable pathway from Minority Serving Institutions (MSIs) to industry partners in the Nuclear Security Enterprise (NSE). Over the years, the Kansas City National Security Campus has participated in several MSIPP consortia, but one stands out for its longevity, high-quality research, strong partnerships, and impressive track record of students hired. Launched in 2018, the Partnership for Research and Education Consortium in Ceramics and Polymers (PRE-CCAP) is now in its seventh year of funding. Originally focused on attracting bright students to applied materials science research and potential job opportunities, it has since expanded to include middle school and high school outreach, research symposia, and opportunities beyond the NSE. This presentation will highlight how the consortium was developed, its growth, future plans, and the challenges and rewards of the consortium model.

5:10 PM

(PACRIM-S08-009-2025) Challenges of organizing a multi-departmental STEAM night in a rural community: Alfred University's Night of Science and Arts

R. Welch*¹

1. Alfred University, Materials Science and Engineering, USA

Rural K-12 schools can be greatly limited in their accessibility to STEM education. It is critical for young children to see and identify with other minorities and genders that math and science is an option for them. In addition, continued exposure to the sciences increases awareness for career paths in STEM and ultimately benefits the growth of all scientific fields including engineering and materials science. To address these shortcomings present in rural areas, the Night of Science and Arts was created at Alfred University two years prior. This event, which involves over 15 different departments and over 75 student and faculty volunteers, has consistently brought in over 400 kids and families each year. The lessons learned from continuing and organizing such an event will be discussed as well as the key steps needed to start such an event.

PRS9 - Fndmtls of interfaces/grain boundaries/ surfaces - interatomic bonding to macroscopic prop

PACRIM Symposium 9 - Microstructure evolution through sintering and grain growth

Room: Oxford

Session Chair: Katsuyuki Matsunaga, Nagoya University

1:15 PM

(PACRIM-S09-012-2025) Direct Observation of Atomic-Scale Surface Evolution in Oxide Catalysts during OER (Invited)

S. Chung*¹

1. Korea Advanced Institute of Science and Technology, Republic of Korea

Hydrogen-evolution/oxygen-evolution reactions (HER/OER) are key electrochemical processes at the cathode and anode sides, respectively, in electrolyzers for hydrogen production via water splitting. It is generally accepted that the activation barrier of the OER associated with transfer of multiple electrons and protons is larger

than that of the HER, resulting in a comparatively higher anodic overpotential to split water. Therefore, the OER is a predominant pathway that can notably affect the overall efficiency of electrolysis. Furthermore, the stability of catalysts at the anode side is another significant issue in addition to the high catalytic activity. In this presentation, we focus on recent breakthroughs in OER electrocatalysts on the basis of atomic-scale surface structure and composition variations along with the electronic structure changes. To this end, we highlight the critical roles of atomic-level defects, including lattice distortion, encompassing oxygen octahedral displacements, in oxides, many of which are largely utilized for OER catalysis in alkaline electrolytes under strong anodic potentials. The issues of surface instability and subsequent element dissolution at the nanoscale in both acid and alkaline electrolytes are also covered and thereupon exploiting such instability in alternative methods toward surface modification for better catalytic properties is suggested.

1:45 PM

(PACRIM-S09-013-2025) In-situ Manipulation of the Ferroelectric Domain and Domain Walls (Invited)

H. Tian*¹

1. Zhejiang University, China

Domain and domain-wall nanoelectronics are considered new paradigms for logic technologies and memory, where domain structures serve as the key element. The controllable configurations of ferroelectric domains and domain walls offer the opportunity to develop useful nanoelectronic applications, such as microelectronic devices and high-density memories. Despite the increasing experimental and theoretical insights into various domain structures and domain walls, manipulating the polar structures and comprehensively understanding their underlying mechanism still need to be improved. Here, we report a strategy for controlling domain configurations at atomic level and real-time scale. Using an in-situ biasing technique, we constructed and controlled in-plane charged domain walls and polar structures and investigated the dynamic switching mechanism and topological transformations. We demonstrate how in-line holography offers extraction of charge distribution and detects dynamic charge redistribution. Voltage control of charged domain walls also gives rise to multiple non-volatile resistance states, thus demonstrating the key functional property of a few unit-cell thick memristors. These results promote a better understanding of ferroelectric switching behavior and provide a new strategy for creating unit-cell-scale devices.

2:15 PM

(PACRIM-S09-014-2025) The Effects of Domain Walls on Plastic Deformation Behavior of Bulk Barium Titanate Single Crystals

T. Shibamoto*¹; K. Kasai²; Y. Li¹; F. Zhuo³; T. Shimada²; A. Nakamura¹

1. Osaka Daigaku, Department of Mechanical Science and Bioengineering, Japan
2. Kyoto Daigaku, Department of Mechanical Engineering and Science, Japan
3. Technische Universität Darmstadt, Department of Materials and Earth Sciences, Germany

Ferroelectrics are essential in modern society because they can convert electrical, mechanical, and thermal energy. Ferroelectrics have spontaneous electric polarization, which can be tuned by electric fields. Regions polarized in specific directions are called domains, and domain walls are the boundaries of two domains. Though the thickness of domain walls is only several atomic layers, it is well known that domain walls affect the electrical properties of ferroelectrics. On the other hand, significant attention has been paid to the relationship between domain walls and mechanical properties, especially plastic deformation behavior. However, at room temperature, the effect of domain walls on plastic deformation behavior is still unclear. In this study, uniaxial compression tests were conducted on bulk barium titanate single crystals to

investigate how domain structures and domain walls influence the room-temperature plastic deformation. As a result, obvious effects of domain walls on plastic compression deformation were found. Though the fracture strain of barium titanate crystals with domain walls was only a few %, single-domain barium titanate crystals showed much higher strain to fracture, indicating the presence of room-temperature plasticity.

2:35 PM

(PACRIM-S09-015-2025) In situ visualization of crystallization interface in vertical Bridgman growth of fluoride crystals

Z. Zhang*¹; L. Su¹

1. Shanghai Institute of Ceramics Chinese Academy of Sciences, China

Functional crystals synthesized by modern industrial crystal growth techniques are widely used in semiconductor industry, optoelectronics, information technologies, etc. Despite that crystal growth processes have been dramatically improved nowadays during the past decades from a technical perspective, detailed kinetics of crystallization interfaces during practical crystal growth still remain mysterious, which becomes a critical bottleneck for the developments of crystal growth techniques. Herein, we report the experimental investigation of in situ detections of solid-liquid (S-L) crystallization interfaces of large-size fluoride crystals based on a vertical Bridgman (VB) apparatus with capability of real-time visualization. Evolutions of S-L interface of $\Phi 140$ mm CaF_2 crystals, especially the multifarious shifts of interface positions along vertical direction, was unveiled for the first time. Quantitative descriptions of deviations between the crystallization and crucible pulling rates were obtained by extracting the coordinates of S-L interface in images of crystallization regions, meanwhile evolutions of the heat transfers at various growth stages were calculated by numerical simulations to analyze their influences on such deviations. The phenomenon observed by this apparatus could provide innovative vision for the development of VB techniques as well as numerical simulations.

PACRIM Symposium 9 - Fundamentals of Space Charge

Room: Oxford

Session Chair: Sung-Yoon Chung, Korea Advanced Institute of Science and Technology

2:55 PM

(PACRIM-S09-016-2025) The role of grain boundary interfaces on the increased fracture toughness in transition metal carbides (Invited)

A. Stubbers⁴; S. Hossain²; E. Schwind¹; O. A. Graeve³; C. R. Weinberger²; G. Thompson*¹

1. University of Alabama, Metallurgical & Materials Engineering, USA
2. Colorado State University, Department of Mechanical Engineering, USA
3. University of California, San Diego, Mechanical and Aerospace Engineering, USA
4. Alabama Materials Institute, USA

Historically, generation of micro- to meso-scale models to predict mechanical performance have been hampered by the difficulty to measure and understanding the influence of grain boundary interfaces on fracture phenomenon. In this presentation, we address the use of combined focus ion milling with in situ SEM mechanical testing of directionally oriented microcantilevers to measure fracture toughness in a series of transition metal carbides. Initially, the single-plane fracture toughness has been measured and compared to values of cleavage energy and fracture toughness from computational models. Building from these results, the systematic incorporation of an increasing number of grain boundaries, as well as secondary phase precipitate interfaces, in the micro-cantilever beam were measured and their influence on the fracture toughness

recorded. This collective data is then compared to the accuracy of cleavage energy and fracture toughness meso-scale models. Finally, serial sectioning of crack bifurcation through the microstructure along with post-mortem TEM imaging of plasticity mechanisms are developed within context of the meso-scale model.

3:40 PM

(PACRIM-S09-017-2025) Microstructure and chemical analysis of layer samples with Si-based polymer-derived ceramic nanocomposites (PDC-NCs) coatings

I. S. Nurak*¹

1. Karlsruhe Institut für Technologie, IAM-WK, Germany

Generally, a fundamental understanding of the microstructural and chemical evolution at the interface of different layer samples depending on heat treatment conditions: temperature, atmosphere, and sample roughness is important to tailor the material intrinsic properties and improve the interconnection between the layers at elevated temperatures. Therefore, different electron microscopy techniques will be applied to study the interfaces between (i) Si-based polymer-derived ceramic (PDC) nanocomposites (NCs) (ii) Cr and Al bond coat layer (iii) Mo-Si-Ti as substrate. In this present work, three different layer systems will be investigated. All three systems have Mo-Si-Ti as a substrate and are coated with the same Si-based PDC-NCs: $\text{Si}(\text{Hf}_{0.7}\text{Ta}_{0.3})(\text{B,C})\text{NO}$. The first layer system consists of Mo-Si-Ti directly coated with Si-based PDC-NCs, and the other two-layer systems have a bond coat in between, Cr or Al. The samples are heat treated at 1200°C and 1400°C in air and argon atmosphere. Chemical intermixing and phase formation were observed using SEM and conventional TEM techniques. The authors gratefully acknowledge the funding of Deutsche Forschungsgemeinschaft (DFG) in the frame of the MatCom-ComMat project (GRK 2561).

4:00 PM

(PACRIM-S09-018-2025) Microstructure analysis of Polycrystalline Monoclinic Zirconia

K. Yoo*¹; J. Tam²; B. Feng¹; S. Kondo¹; K. Matsui¹; N. Shibata¹; Y. Ikuhara¹

1. The University of Tokyo, Japan
2. University of Alberta, Canada

Zirconia has gained significant interest across various fields, including dental, structural, and catalytic materials. It has three representative phases: monoclinic, tetragonal, and cubic phase. Among these, the monoclinic zirconia is the most stable phase in low temperatures (up to about 1170 °C), which has been widely used in catalysis. However, little is known about the microstructure of polycrystal monoclinic zirconia. In this study, we investigated the microstructure of monoclinic zirconia, focusing on its grain boundary and twin boundary atomic structures. To get a dense monoclinic zirconia sintered body, we first performed the cold isotropic pressing (CIP) at 300 MPa for 10 min and then sintered the green body at 1200 °C for 2h. We successfully fabricated high-density monoclinic zirconia polycrystal with a relative density of 92%. The microstructure was analyzed by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The atomic structure of grain boundary and twin boundaries were analyzed by atomic-resolution scanning TEM (STEM). Details will be discussed in the presentation.

4:20 PM

(PACRIM-S09-019-2025) Strengthening and Toughening of Thin Film Materials Based on Micro/Nano-Structured Design (Invited)

K. Zhang*¹

1. Jilin University, China

For non-intrinsic hard thin film materials, researchers have used interface engineering to introduce numerous interfaces that hinder dislocation motion, significantly enhancing hardness. However,

high hardness often leads to high brittleness, posing a safety risk for material performance. We developed a 3D co-registered micro/nano structure, overcoming spatial limitations. Using a layer deposition technique that activates “solid-state dewetting,” we obtained a TaC@Ta nanocore-shell thin film. This structure suppresses interface crack formation in three dimensions, overcoming the limitation of toughening metals in phase separation processes, and resolves the trade-off between hardness and toughness. We also proposed an atomic-scale tailoring strategy using “high negative mixing enthalpy + high lattice distortion” to induce local disorder clusters. This approach transformed transition metal high-entropy alloys into sub-nanometer-scale hierarchical structures, achieving 100% hardness and 69.2% compressive strength improvements, with greatly enhanced plastic deformation. Additionally, a “bamboo-like” copper thin film, reinforced with an amorphous boron framework, achieved an indentation hardness of 10.8 GPa, with excellent strength and ductility. These strategies provide new insights for designing strong, tough thin films.

PacRim S11 - Optical and Electronic Phase Change Materials - Science and Application

PACRIM Symposium 11 - Optical and Electronic Phase Change Materials: Science and Application IV

Room: Georgia A

Session Chair: Wei Zhang, Xi'an Jiaotong University

1:15 PM

(PACRIM-S11-016-2025) Re-evaluation of calorimetry-based PCM fragility and crystal growth rate using measurements from synchronous in situ TEM and nanocalorimetry

I. McGieson²; T. Koledin¹; K. Bustillo⁴; J. Ciston⁴; L. Ravi Narayan³; W. A. Osborn³; J. Pettibone³; F. Yi¹; D. A. LaVan³; M. K. Santala*¹

1. Oregon State University, Materials Science Program, USA
2. Oregon State University, Department of Physics, USA
3. National Institute of Standards and Technology, Materials Measurement Science Division, Materials Measurement Laboratory, USA
4. Molecular Foundry, Lawrence Berkeley National Laboratory, The National Center for Electron Microscopy, USA

The thermodynamics and kinetics of crystallization are key to understanding glass-forming materials, including poor glass formers such as phase change materials (PCMs). In PCMs, it is challenging to measure the crystal growth rate, u , directly with microscopic methods between the glass transition, T_g , and the temperature where the maximum growth rate occurs, because the limited time between nucleation and the impingement of grains and the small grain size demand both high spatial and temporal resolution. This has led to the use of indirect methods to study PCM crystallization, such as differential scanning calorimetry (DSC). Here, nanocalorimeters designed to be run in transmission electron microscopes (TEM) were used to measure the enthalpy of crystallization of $\text{Ag}_3\text{In}_4\text{Sb}_7\text{Te}_{17}$ (AIST) and GeTe and to make direct microscopic measurement of u . The nanocalorimeters provide the high heating rates necessary to observe PCM crystallization above T_g and have better characterized temperature profiles than other in-situ TEM platforms. A classical model for crystal growth is fit to these data and is compared to predictions of u based solely on DCS data. Growth rates extracted from DSC alone appear to overestimate u by as much as two orders of magnitude for both AIST and GeTe in a key temperature regime from 500 to 600 K.

1:35 PM

(PACRIM-S11-017-2025) Mapping Local Dielectric Behavior of Phase Change Material Sb_2S_3 by Scanning Probe TechniquesJ. W. Kaman^{*1}; E. J. Musterman³; H. Jain²; V. Dierolf⁴; N. Domingo-Marimon⁵; K. P. Kelley⁵

1. Iowa State University, Materials Science and Engineering, USA
2. Lehigh University, International Materials Institute for New Functionality in Glass, USA
3. Brookhaven National Laboratory, USA
4. Lehigh University, Physics, USA
5. Oak Ridge National Laboratory, USA

Piezoresponse Force Microscopy is a scanning probe technique often used to study electromechanical phenomena on the nanoscale, but suffers from ‘artifacts’ that lead to false positives for piezoelectric coupling. These have been attributed to a number of phenomena, from chemical strain to surface charge-induced electrostriction to electrostatic forces. Crystalline Sb_2S_3 , an optical and electrical phase change material, is an example of a material where PFM artifacts have led to such a false positive, where glassy Sb_2S_3 shows no such response. Here, we show a great similarity between frequency-domain impedance spectroscopy measurements and time-domain PFM experiments. While the mechanism for electromechanical coupling remains ambiguous, it is nonetheless shown that its dynamics correspond to the same low-frequency dielectric behavior as on the macroscale. Using the distinctly different electrical characteristics of glassy and crystalline Sb_2S_3 , we show that it can be used to probe local dielectric characteristics with high sensitivity and spatial resolution. We identify characteristics of this system that enable this comparison between PFM and dielectric spectroscopy as well as its limitations.

1:55 PM

(PACRIM-S11-018-2025) Prospect and Challenges of Solution-Derived Ge-Sb-Se-Te Phase-Change Chalcogenide Films (Invited)M. Kang^{*2}; R. Sharma⁵; D. Wiedeman⁵; Q. Altomose¹; P. Lynch²; G. Sop Tagne³; Y. Zhang³; M. Shalaginov³; C. Constantin Popescu³; B. Triplett⁴; C. R. Baleine⁴; C. Schwarz¹; A. M. Agarwal³; T. Gu³; J. Hu³; K. Richardson⁵

1. Ursinus College, USA
2. Alfred University, USA
3. Massachusetts Institute of Technology, USA
4. Lockheed Martin Corporation, USA
5. University of Central Florida, USA

We present our ongoing and future efforts to optimize available choice of processing-material combinations to enable solution-derived Ge-Sb-Se-Te chalcogenide layers to be deployable as versatile high performance optical phase change materials (PCMs). The need for the integration of such new PCMs onto a variety of photonic platforms has necessitated the development of fabrication processes compatible with diverse material compositions as well as substrates of varying material types, shapes, and sizes. Our study explores the application of chemical solution deposition as a fabrication method and delves into the resulting modifications in the structural and optical properties of Ge-Sb-Se-Te PCMs. Our finding provides an insight on the solution-based process’ key parameters and challenges as well as our strategies to mitigate the issues and prepare starting glass layers that can structurally transform into desirable target crystalline phases, assessed by a range of cross-correlating characterization methods. Both fundamental and practical natures of the novel deposition approach studied here may shed light on the lingering questions on the microscopic origin behind the thermodynamics and kinetics of chalcogenide optical PCMs. Our study would set a stage for their versatile incorporation into a variety of photonic devices, thus being of broad interest to both materials and optics communities.

PacRim S12 - Eng Ceramics and Ceramic Matrix Composites - Processing/Design/Applications**PACRIM Symposium 12 - Novel sintering and microstructure control I**

Room: Plaza B

Session Chairs: Federico Smeacetto, Politecnico di Torino; Kexin Chen, University of Science and Technology Beijing

1:15 PM

(PACRIM-S12-013-2025) Ductile Ceramics from Dream to Reality (Invited)K. Chen^{*1}

1. University of Science and Technology Beijing, China

Ceramics exhibit intriguing properties, including high hardness, high strength, and notable tolerance to high temperatures, making them attractive for a range of applications across diverse fields such as aerospace and automotive engineering. However, the inherent brittleness of ceramics at ambient temperatures, primarily due to restricted atomic motions from rigid ionic or covalent bonded structures, is a persistent challenge. In recent years, our group have realized the compressive and tensile ductility in covalently bonded ceramics at room temperature. Specifically, an α/β dual-phase structure with coherent interfaces has been constructed in covalently bonded silicon nitride ceramic, which facilitates a stress-induced β -to- α phase transformation and eventually generates plastic deformability at room temperature (Science, 2022, 378, 371-376). Very recently, we further proposed a “borrowing-dislocations” strategy that uses a tailored metal-ceramic interfacial structure with well-ordered bonds between Mo metal and ionic bonded La_2O_3 ceramic. Such an approach enables the generation of remarkable tensile ductility in La_2O_3 by mobilizing numerous dislocations in ceramic borrowed from metal through the interface, thereby overcoming the challenge associated with direct dislocation nucleation within ceramics (Science, 2024, 385, 422-427). Our works have paved an innovative way for the development of ductile ceramics at room temperature.

1:45 PM

(PACRIM-S12-014-2025) Large internal stress induced nonlinear current-voltage behavior in nanodiamond strengthened ZnO ceramics (Invited)Y. Fan^{*1}

1. Donghua University, China

The modulation of the electrostatic potential barrier at grain boundaries determines the performance of many ceramic-based electronics such as varistors. However, conventional protocols relying on complex doping and sintering processes inevitably increase the inhomogeneity of microstructure, which may jeopardize the performance stability and mechanical reliability in service. Instead of doping, herein we demonstrate an effective strategy to modulate the potential barrier in ZnO-based low-voltage varistors by exploiting internal stress-induced piezoelectric polarization. The local residual stress as large as ~ 1 GPa can be created in the ZnO matrix by incorporating ultra-stiff nanodiamond particles using a cold sintering process. As a result, the composite with only 2wt% of nanodiamond exhibits a prominent nonlinear current-voltage response at a low switch voltage of 15.7V/mm. More strikingly, the large internal stress can significantly enhance the strength of the composite by more than 230% compared with the monolith. These findings add internal stress as a new dimension to design mechanically robust ceramic electronics with high performance.

2:15 PM

(PACRIM-S12-015-2025) In-situ liquid phase sintering of MgAl₂O₄ spinel ceramics by inhomogeneous addition of sintering additives (Invited)

H. Kim^{*1}; Y. Park¹; J. Ko¹; H. Ma¹; J. Lee¹

1. Korea Institute of Materials Science, Republic of Korea

In this study, we aimed to clarify the principles behind improving the sinterability of MgAl₂O₄ containing identical amounts of added Ca by focusing on the non-uniform distribution of Ca. To achieve this, we prepared samples with intentionally non-uniform Ca distributions through solution impregnation and drying, as well as samples with uniformly distributed Ca achieved by either freeze granulation or the addition of CaCO₃ nanopowder. By monitoring the differences that arise during intermediate stages of the forming and sintering processes, we sought to identify the underlying mechanisms. Based on these insights, we propose a novel in-situ liquid phase sintering process employing minimal amounts of additives.

2:45 PM

(PACRIM-S12-016-2025) Double-tough ceramics

D. Giuntini^{*1}

1. Eindhoven University of Technology, Mechanical Engineering, Netherlands

The traditional labeling of ceramics as brittle materials has been challenged by the last decades of efforts in toughening them with a variety of strategies. Multiscale designs, tailored additions of material constituents and controlled phase transformations have shown promising results. Both the processing and mechanical characterization of toughened ceramics, however, require innovative approaches. We show here how multiple toughening strategies can be combined into bulk all-ceramic materials. Specifically, we present an optimization-driven approach to creating a double-tough ceramic material with a brick-and-mortar microstructure, where the mortar is itself transformation-toughened, engineered with the goal of simultaneously achieving high strength and fracture toughness levels. As the design of such a material, driven by multiscale toughening mechanisms, requires a laborious trial-and-error approach, we propose a Bayesian optimization framework as an integral part of our methodology to streamline and accelerate the design process. As a result, we develop a bio-inspired all-ceramic composite that exhibits an exceptional balance between bending strength and fracture toughness.

PACRIM Symposium 12 - Novel sintering and microstructure control II

Room: Plaza B

Session Chairs: Kexin Chen, University of Science and Technology Beijing; Federico Smeacetto, Politecnico di Torino

3:30 PM

(PACRIM-S12-017-2025) β -MoO₃ powder/whisker for medical radioactive isotope production (Invited)

H. Suematsu^{*1}; Y. Yang¹; M. Ngo²; T. Kitagawa³; Y. Fujita³; Y. Takahashi⁴; T. Nakayama¹; T. Suzuki⁵; T. Do¹; K. Niihara⁶

1. Nagaoka University of Technology, Extreme Energy-Density Research Institute, Japan
2. National Institute of Advanced Industrial Science and Technology (AIST), Multi-material Research Institute, Japan
3. Japan Atomic Energy Agency, Japan
4. Nagaoka University of Technology, Department of Materials Science and Engineering/Bioengineering, Japan
5. Nagaoka University of Technology, Department of Nuclear Technology, Japan
6. Nagaoka Sutoku Daigaku, Japan

Among many nuclear medicines, Tc-99m has been widely used radioactive isotope. Because of its short half-life (6 h), the parent nuclide of Mo-99 with a half-life of 66 h is delivered to each medical

facility and Tc-99m is obtained by the decay. Most of Mo-99 is produced as a fission product in a nuclear reactor using highly enriched uranium fuel, which is currently difficult to be utilized because of the nuclear security reasons. Instead, nuclear reaction methods by irradiating neutrons on various Mo-98 compounds including MoO₃ have been attempted. Among them, β -MoO₃ draws interests of researchers because the high kinetic energy given by the nuclear reaction to Mo-99 assists the diffusion from the β -MoO₃ target. These Mo-99 "hot atoms" can be easily extracted into water. In this study, β -MoO₃ particles and whiskers were synthesized by a thermal evaporation of α -MoO₃ powder and were irradiated by neutrons in Kyoto University Research Reactor. The extraction rate of Mo-99 from the irradiated β -MoO₃ particles and whiskers to water was measured. The measured extraction rate reached 66% at 60 °C for 5.5 h. From the measured activation energies, possible extraction process is discussed.

4:00 PM

(PACRIM-S12-018-2025) Integration of engineering ceramics for energy conversion and hydrogen technologies (Invited)

F. Smeacetto^{*1}

1. Politecnico di Torino, Applied Science and Technology, Italy

Hydrogen-related technologies are crucial for achieving deep decarbonisation of the energy system. Advanced glass and engineering ceramics play a key role in enhancing the efficiency and durability of electrochemical energy conversion systems, including reversible solid oxide cells, electrolyzers, and proton-conducting membranes. This presentation will cover current solutions and challenges in the design, processing, and microstructure-property-performance relationships of various glass and ceramic-based systems and their integration processes specifically developed for hydrogen-related technologies. A critical aspect of integrating ceramic matrix composites is the development of reliable joining techniques. One promising method involves the in-situ production of the Yb₂Si₂O₇ phase using a reactive viscous sintering approach to join SiC/SiC and C/SiC composites. This presentation will highlight the significant potential of advanced glass and engineering ceramics for disruptive innovations in energy conversion. It will also address unresolved questions regarding their durability, reliability, challenges, and future research perspectives.

PACRIM Symposium 12 - Novel sintering and microstructure control III

Room: Plaza B

Session Chairs: Federico Smeacetto, Politecnico di Torino; Kexin Chen, University of Science and Technology Beijing

4:30 PM

(PACRIM-S12-019-2025) Physics-based Machine Learning-Aided Design of Freeze-cast Si₃N₄-Si₂N₂O Scaffolds and its Enhancement on Properties of BAS-based Glass Ceramic

X. Liao^{*1}; Z. Yang¹; D. Jia¹; Y. Zhou¹

1. Harbin Institute of Technology, China

The bi-continuous structure, as an effective form of composite material design, features a uniform interlocking microstructure that integrates the advantages of two continuous phases. Optimizing the structure and properties of the scaffolds is essential for the development of high-performance bi-continuous composites. In this work, using freeze-casting Si₃N₄-Si₂N₂O scaffolds as a model system, a hybrid model for the quantitative design of the microstructure and mechanical properties is developed from four physics-based process-microstructure models with sintering, solidification, phase transformation and grain growth kinetic theories, and the subsequent data-driven structure-property model utilizing a machine learning method, artificial neural network (ANN). Through this hybrid model, the rapid, on-demand quantitative design of

$\text{Si}_3\text{N}_4\text{-Si}_2\text{N}_2\text{O}$ scaffolds is achieved. Based on the optimized scaffold, a bi-continuous $\text{Si}_3\text{N}_4\text{-Si}_2\text{N}_2\text{O/BAS}$ composite is successfully fabricated via pressureless melt infiltration. The resulting bi-continuous composite exhibits excellent thermal shock resistance, retaining 70.5% of its residual strength retention rate even under a thermal shock temperature difference of $\Delta T=1000$ °C.

4:50 PM

(PACRIM-S12-020-2025) Engineering Flexible Ceramics: A Multilayered Approach

H. Yazdani Sarvestani^{*1}; J. Patel¹; E. Azad¹; B. Ashrafi¹

1. National Research Council Canada, Canada

Traditional ceramics, renowned for their hardness and durability, are often brittle, limiting their use in applications requiring flexibility and impact resistance. This study explores the mechanical behavior of soft, multilayered ceramic structures, investigating the influence of hexagonal tile size, adhesive interlayer thickness, and layer configuration on flexural compliance, penetration resistance, and energy absorption. Utilizing precision laser cutting and adhesive bonding, we fabricated multilayered ceramic beams with varying structural parameters. Experimental results demonstrate that smaller tile sizes and thinner adhesives enhance flexibility, while larger tiles and thicker adhesives improve penetration resistance and energy absorption. Compared to conventional ceramics, these soft, multilayered structures exhibit significantly higher weight-specific compliance while maintaining competitive impact resistance and energy absorption. This novel approach paves the way for lightweight, durable, and flexible ceramics with applications in diverse fields such as personal protective equipment, aerospace, and robotics.

5:10 PM

(PACRIM-S12-021-2025) Influence of the glass phase on the elastic properties and thermal conductivity of fireclay and high-alumina refractories

W. Pabst^{*1}; E. Gregorova²

1. University of Chemistry and Technology, Prague, Department of Glass and Ceramics, Czechia

2. UCT Prague, Department of Glass and Ceramics, Czechia

The elastic properties and thermal conductivity are of fundamental importance for the mechanical behavior and heat transfer performance of engineering ceramics and refractories. However, the prediction of these properties by modeling requires not only the knowledge of the porosity but also complete information on the solid phase composition, including reliable estimates of the content and composition of the glass phase. In the present work and concerns siliceous fireclay model materials prepared in our laboratory, as well as commercially available fireclay and high-alumina refractories, this information is obtained by a multimethod approach (project GA25-16482S, Czech Science Foundation). Based on this information, digital proxies are generated, for which the effective properties (Young's modulus and thermal conductivity), are calculated under periodic boundary conditions. The numerical calculations for this work are performed via the commercial software package GeoDict and compared to the analytical predictions. Experimental measurements of elastic properties are performed via the impulse excitation technique, while the thermal conductivity is measured via transient plane source techniques. The correlation between relative Young's modulus and relative thermal conductivity is compared to the predictions via different cross-property relations.

PacRim S13 - Functional Defects in Ceramic Materials

PACRIM Symposium 13 - Defects for energy, thermal, mechanical, and electronic applications I

Room: Grouse

Session Chair: Eric Gabriel, Boise State University

3:30 PM

(PACRIM-S13-001-2025) Electrochemical Modification of Anion Defects in Energy Functional Materials (Invited)

T. Nakamura^{*1}; T. Katsumata²; Y. Kimura²; K. Amezawa²

1. Nagoya University, Institute of Materials and Systems for Sustainability, Japan

2. Tohoku University, Japan

Cation doping has been adopted as a rational strategy for material development because of its effectiveness, broad applicability and high feasibility. However, the effectiveness of cation doping is approaching the limit, due to extensive studies such as data-driven exploration, high-throughput combinatorial synthesis and autonomous exploration combined with artificial intelligence. As a new strategy for further material development, anion-mixing, in other words, the control of anion defect structures is a promising approach. So far, anion-mixing has been carried out by topochemical synthesis, high-pressure synthesis, mechanical milling as well as conventional solid-state reaction. For further advancement of anion-mixing strategy, we developed an electrochemical reactor for the modification of anion defect structures as designed. In the presentation, the concept of an electrochemical reactor and its demonstration on energy materials will be shown.

4:00 PM

(PACRIM-S13-002-2025) Mechanochemical coupling in strained SrFeO_x thin films (Invited)

Y. Du^{*1}

1. Pacific Northwest National Laboratory, USA

Defect-ordered oxides represent a versatile class of materials with a wide array of structural, compositional, and functional properties. However, their performance under operating or extreme conditions is often compromised by significant structural and chemical changes, which can lead to degradation and device failure. To address these challenges, we have explored the use of heteroepitaxy to achieve tunable functional properties in complex oxides, focusing on the interplay between defect chemistry and mechanochemical coupling. I will discuss our recent work on Brownmillerite-phase $\text{SrFeO}_{2.5}$ (BM-SFO) thin films, a perovskite-derived material exhibiting oxygen vacancy ordering. By leveraging advanced characterization techniques, including in situ and environmental TEM, ToF-SIMS, synchrotron-based spectroscopy, and ab initio simulations—we uncover the pathways of defect and chemical evolution in isotopically and atomically defined systems. These insights allow us to directly link the observed dynamic lattice oscillations of SrFeO_x to their catalytic behaviors. Our results demonstrate that interfacial tensile strain can greatly decrease the temperature needed for water splitting, offering a framework for understanding mechanochemical coupling and developing strategies for rational materials design.

4:30 PM

(PACRIM-S13-003-2025) Radiation-induced disorder and defects in epitaxial oxide thin films and heterostructures (Invited)

T. Kaspar*¹

1. Pacific Northwest National Laboratory, Physical and Computational Sciences Directorate, USA

Neutron and ion irradiation generate a nonequilibrium concentration of point defects that greatly increase rates of mass transport in an effect known as radiation-enhanced diffusion (RED). Irradiation of oxides introduces additional complications including the different responses of the anion and cation sublattices to irradiation and the generation, recombination, and/or transport of charged point defects. These processes lead to electronic and structural changes that are poorly understood. Fe, Cr, and their oxides are ubiquitous both in the natural environment and as the corrosion products of steels that are widely utilized in structural components of the built environment. We have studied epitaxial thin films and heterostructures of Fe₂O₃, Fe₃O₄, and Cr₂O₃ as model systems to understand fundamental disordering and defect generation processes and elucidate the role of interfaces. Incorporation of isotopic tracers (¹⁸O, ⁵⁷Fe) in distinct layers of the epitaxial films facilitates quantification of RED rates on the nanometer scale using atom probe tomography (APT). Scanning transmission electron microscopy (STEM) and positron annihilation spectroscopy (PAS) have provided key insights into defect formation, particularly near interfaces. This work has led to a deeper understanding of radiation-induced processes that govern coupled irradiation and corrosion of structural reactor materials.

5:00 PM

(PACRIM-S13-004-2025) The role of chemical, polar and octahedral tilt disorder in high voltage/energy density ceramic ceramics (Invited)

I. M. Reaney*¹

1. The University of Sheffield, School of Chemical, Materials and Biological Engineering, United Kingdom

High voltage/energy capacitors are used within power electronic modules for near engine management systems in electric vehicles. The high, temperature and voltage prohibit the use of classic X7R barium titanate based ceramics and currently low permittivity (~40) materials are used based on calcium zirconate. However, greater volumetric efficiency is required which necessitates the development of higher permittivity (>1000) ceramics. This contribution explores the role of chemical, polar and octahedral tilt disorder in the development of high voltage/energy density ceramics in ferroic oxides.

PacRim S19 - Nanostructured Bioceramics and Ceramics for Biomedical Applications

PACRIM Symposium 19 - Nanostructured Bioceramics and Ceramics for Biomedical Applications IV

Room: Stanley

Session Chairs: Eva Hemmer, University of Ottawa; Steven Naleway, University of Utah

1:15 PM

(PACRIM-S19-011-2025) Colorimetric Dye-Grafted Hydrogels As Platform for Chemical Sensors (Invited)

H. Chung*¹

1. University of Alberta College of Natural and Applied Sciences, Chemical and Materials Engineering, Canada

Hydrogels contain water that often incorporates various solutes; unless hydrogels are encapsulated by a barrier, the solutes in the hydrogels reach an equilibrium with the environment. The most attractive feature of hydrogels is that the aqueous environment

becomes a substantial part of the material itself, while the hydrogels maintain their mechanical consistency with a physical boundary. For these reasons, hydrogel is an ideal sensor platform in aqueous media. Colorimetric assays deliver information intuitively; keeping chromophores free from leaching has been a challenge in aqueous media. Direct ink writing is a versatile freeform manufacturing method for hydrogels; a generalizable formula to enable 3D printability can be impactful. In this study, dual network hydrogels of polyacrylamide and alginate with acrylated chromophores are printed by incorporating Laponite[®] as a universal rheological modifier. Here, a co-polymerization of the acrylated chromophores with polyacrylamide enables colorimetric response to various chemical analytes. Our 3D printed colorimetric pH sensing hydrogels combine sensitivity, intuitive data interpretation, mechanical strength, and structural integrity to operate in various aqueous environments while having arbitrary shapes to address various needs in environmental, underwater, and healthcare applications with a robust and versatile platform.

1:45 PM

(PACRIM-S19-012-2025) Silver nanocluster-embedded ceramic coatings: Scalable Antimicrobial Coatings via Co-Sputtering (Invited)

C. Balagna¹; A. Luceri¹; S. Perero¹; M. Ferraris*¹

1. Politecnico di Torino, Department of Applied Science and Technology, Italy

Emerging infectious diseases, like the recent COVID-19 pandemic, highlight the urgent need for innovative antimicrobial solutions. We developed and patented antipathogen composite coatings using a versatile co-sputtering technique. These coatings, composed of silver nanoclusters embedded in a glass or ceramic matrix, enable controlled ionic release without environmental or dermal dispersion. The coatings demonstrate broad-spectrum efficacy, preventing bacterial adhesion, fungal proliferation, and inactivating airborne viruses such as respiratory syncytial virus, influenza virus type A, human coronavirus (OC43), and SARS-CoV-2. Co-sputtering offers an industrially scalable, green deposition method that uses only gases and bulk materials, avoiding the production of hazardous liquid byproducts. This breakthrough in ceramic-based coatings offers sustainable, high-performance antimicrobial protection, advancing the field of functional materials for public health applications. Results from the EU project "NANOBLLOC" will be reviewed and further advancements will be discussed.

2:15 PM

(PACRIM-S19-013-2025) Design and DLP 3D Printing of Biphasic Calcium Phosphate Scaffolds for Bone Regeneration

J. Chen¹; M. Wang*¹

1. The University of Hong Kong, Department of Mechanical Engineering, Hong Kong

Porous bioactive ceramic scaffolds are often used for bone regeneration and biphasic calcium phosphate (BCP) consisting of hydroxyapatite (HAp) and β -tricalcium phosphate (β -TCP) at different ratios, which has shown excellent bioactivity and controllable biodegradation rate, is a prime candidate for such scaffolds. Through computer-aided design (CAD), complex porous architectures as bone tissue engineering (BTE) scaffolds can be designed and these scaffolds can be fabricated accurately via digital light processing (DLP) 3D printing. In this study, bone-mimicking random-distributed Voronoi scaffolds were firstly designed via CAD by seeding points stochastically. Mechanical behaviors of CAD-designed scaffold models were then simulated using simulation softwares. Concurrently, highly printable DLP printing inks were formulated from BCP (70:30 for HAp:TCP), dispersant, photocurable polymer, photoinitiator and light absorber. The solid loading in inks was up to 70 wt.%, and scaffolds with 60%-80% porosities could be 3D printed via DLP, which then underwent debinding and sintering to obtain final BCP scaffolds.

Characterization and compression testing were performed for these scaffolds. Mechanical evaluation results were in agreement with simulation results for scaffolds, indicating the potential and importance of computational simulation in scaffold development.

2:35 PM

(PACRIM-S19-014-2025) Nanostructured Metal Oxide Coatings for Antibacterial and Self-Cleaning Surfaces (Invited)

J. Cho*¹

1. Binghamton University, Mechanical Engineering / Materials Science and Engineering, USA

Surface and air contamination by harmful pathogens poses significant risks to public health, necessitating frequent disinfection to mitigate the spread of bacteria and viruses. Ceramic coatings composed of metal oxides offer a unique solution by making the coated surface toxic to such microorganisms, thereby creating a self-cleaning surface. Achieving this functionality requires surfaces engineered with high-crystalline nanostructures to inactivate pathogens effectively. In this study, we employed a low-temperature hydrothermal processing to fabricate various nanostructures of TiO₂, ZnO, and their hybrid structures. These nanostructures demonstrate antimicrobial properties not only through photocatalytic reactions under UV or visible light, but also through contact-based inactivation even in the absence of light illumination. Our findings indicate that specific nanostructure features play a critical role in triggering effective antibacterial performance. Several examples of metal oxides are explored in this work to establish key nanostructure features for developing advanced antimicrobial and self-cleaning surfaces.

PacRim S20 - Advanced Functional Materials for Clean Energy Solutions

PACRIM Symposium 20 - Adv synthesis, characterization and modeling of catalytic and energy storage materials

Room: Georgia A

Session Chairs: Sanjay Mathur, University of Cologne;

Gunnar Westin, Uppsala University; Nicola Pinna, Humboldt University

3:30 PM

(PACRIM-S20-001-2025) Disordered versus ordered niobates as electrode materials for rechargeable batteries (Invited)

Y. Liu¹; P. Russo¹; N. Pinna*¹

1. Humboldt-Universität zu Berlin, Department of Chemistry, Germany

A well-ordered structure with high crystallinity is crucial in various applications, particularly in electrode materials for batteries. The dimensionality and connectivity of the interstitial sites, determined by the crystal structure, inherently influence alkali ions diffusion kinetics. Niobium-based oxides structures are built by the assembly of ReO₃-type blocks of specific sizes with metal sites having well defined positions within the crystalline structure. Structural disorder generally disrupts the regular pathways for ion and electron transport, leading to a lower overall conductivity. Here, we report a new anomalous disordered niobium tungsten oxide structure that significantly enhances the Li-ion storage performance compared to the ordered phase. The disordered tetragonal phase consists of corner-shared NbO₆ octahedra blocks of varied sizes, including [5x4], [4x4], and [4x3], with a disordered arrangement of the tungsten tetrahedra at the corners of the blocks, together with strong distortion of the WO₄ tetrahedra. This structural arrangement is found to be extremely robust during lithiation/delithiation, with a homeostatic local structure evolution during cycling, as determined by operando X-ray diffraction and X-ray absorption spectroscopy. This study highlights the benefits of introducing disorder into niobium tungsten oxide shear structures.

4:00 PM

(PACRIM-S20-002-2025) Plasma-Enhanced Thin Films on Current Collectors for Safer Anode-Free Batteries

D. Patrun*¹; B. Witulski¹; Z. Aytuna¹; T. Fischer¹; Y. Yamada³; T. Sekino²; S. Mathur¹

1. University of Cologne, Institute of Inorganic and Materials Chemistry, Germany

2. Osaka University, SANKEN (The Institute of Scientific and Industrial Research), Japan

3. Osaka University, SANKEN, Japan

Anode-free alkali metal batteries are a safer and lighter alternative, because they eliminate the traditional host anode for the alkali-ions, resulting in enhanced energy density and reduced battery weight. However, challenges like dendritic growth and electrolyte decomposition persist, influencing the battery life. Here, we present plasma enhanced chemical vapor deposition (PECVD) as scalable technique to directly deposit an artificial solid electrolyte interface (SEI) on different current collectors. Our work includes metal oxide coated (SnO₂) copper for Li metal batteries as well as the transition to next generation Na metal batteries with the cheap and more abundant alternative, carbon coated aluminium as current collector. The obtained coatings exhibited remarkable electrochemical properties. X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy is employed to examine the surface composition and impact of plasma treatment, while long-term cycling and electrochemical impedance spectroscopy (EIS) confirm battery durability. Scanning electron microscopy (SEM) and contact angle measurements elucidate coating homogeneity, with reduced nucleation overpotential during first cycle providing further evidence for homogeneity during de-/plating. Our anode-free metal battery design reduces thermal runaway and suppresses dendritic growth, two common causes of fires and explosions in batteries.

4:20 PM

(PACRIM-S20-003-2025) Using synthetic design to control the electrochemical performance of electrode materials for sodium- and lithium-ion batteries (Invited)

A. Zambotti*¹; Q. Nguyen¹; B. Dunn¹

1. University of California Los Angeles, Materials Science and Engineering, USA

With the growing demand for high-energy and high-power density lithium and sodium-ion batteries, there is a need to identify and create intercalation host materials that exhibit solid-solution behaviour during lithiation and sodiation reactions. Several factors influence the overall performance of these intercalation hosts, including ionic and electronic transport, as well as morphological and crystallographic properties. However, the interplay among these factors is still not fully understood. This presentation reviews our approach to designing a new generation of fast-charging electrodes, highlighting some of our recent findings on 0D, 1D, and 2D nanostructured oxides synthesized by hydrothermal methods. Our results with these different nanostructures show that selectively exposing specific crystal facets to the electrolyte solution can either enhance or hinder the intercalation of lithium or sodium. Special focus will be placed on nanostructured TiO₂ polymorphs where we have used bronze-phase TiO₂ as a model system in which to achieve designed intercalation in nanoparticle, nanorod and nanosheet morphologies.

4:50 PM

(PACRIM-S20-004-2025) Oxygen reaction activities in Li-ion battery cathodes materials studied through resonant inelastic soft x-ray spectroscopy (RIXS) (Invited)

Z. Zhuo^{*1}; W. Yang¹; J. Guo¹

1. E O Lawrence Berkeley National Laboratory, Advanced Light Source, USA

Recent advancements in RIXS have elucidated distinct oxygen redox activities in three representative Li-ion parent compounds, Li_2MO_3 (M = Mn, Ru, Ir). These findings reveal fundamentally different behaviors: irreversible oxygen oxidation in the Mn system, distinct reversible Ru and O redox activities in the Ru system, and exclusive divalent cationic redox in the Ir system. Here, through quantification of transition metal redox and characterizations of the lattice oxygen states, we finally provide a direct comparison among the three representative Li_2MO_3 compounds. Firstly, Li-rich configuration does not naturally trigger reversible oxygen redox, as there is no oxygen redox observed in Mn and Ir systems. It indicates that extra critical TM factors are required to maintain the reversible oxygen redox. Secondly, compared with Ru and Ir systems with both Ru/O redox involved and only Ir redox involved, separately, it indicates that oxygen redox is not necessarily enabled until the Li extraction amount which cationic redox could compensate is exhausted. Thirdly, comparison between irreversible oxygen oxidation process in Li_2MnO_3 and the high reversible oxygen redox activities in Ru systems, suggests the critical role for stabilization effect of TMs-O hybridization in oxygen activities.

5:20 PM

(PACRIM-S20-005-2025) Energy Challenges from a materials perspective (Invited)

F. Rosei^{*1}

1. Università degli Studi di Trieste, Department of Chemical and Pharmaceutical Sciences, Italy

The quest for sustainable development dictates an urgent transition from fossil fuels to renewables. This presentation focuses on next generation solar technologies from a materials perspective. We study structure property/relationships in advanced materials, emphasizing multifunctional systems that exhibit several functionalities. Such systems are then used as building blocks to fabricate emerging technologies. In particular, chemically synthesized nanomaterials are promising for future generation low cost and low energy intensive device manufacturing. We focus on 3rd generation photovoltaics, solar hydrogen production, solar windows and other optoelectronic devices, highlighting the role of critical raw materials.

PacRim S21 - Cultural Heritage of the Pacific Rim

PACRIM Symposium 21 - Cultural Heritage of the Pacific Rim III

Room: English Bay

Session Chair: Christina Bisulca, Detroit Institute of Arts

1:15 PM

(PACRIM-S21-017-2025) Ancient Glazes in China

W. Li^{*1}

1. Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

Ancient Chinese glaze is implicative and mysterious. Traditional ancient Chinese high-fired glaze falls into the category of calcium glaze or calcium-alkali glaze, originating from the plant ash glaze of the Shang Dynasty. The physico-chemical basis of Chinese high-fired glazes can be supposed within the confines of the phase

equilibrium relationships of $\text{CaO-Al}_2\text{O}_3\text{-SiO}_2$ system and the meta-stable liquid-liquid immiscibility region above 950 degrees Celsius in the system. The color and texture of glaze is determined by its chemical composition and microstructure. Glaze texture can be described by its transparency and gloss, which is firmly related to the amount, size and distribution of the scatterers (bubble, crystal, liquid-liquid immiscible structure) exiting in the glaze as well as at the glaze surface. Factors affecting glaze color include chemical factor (coloring agent such as iron ion) and physical factor (structural coloring), which factor is predominate depends on specific cases. In general, the investigation upon the correlation among composition, microstructure, color and texture of ancient Chinese glaze is of great importance and will help us scientifically understand the essence of ancient Chinese ceramics.

1:35 PM

(PACRIM-S21-018-2025) The first pottery from the last Ice Age in Hokkaido, Northern Japan

F. Iizuka^{*1}; D. Natsuki²; M. Izuho³

1. University of Wisconsin-Madison, Anthropology, USA
2. University of Tokyo, Graduate School of Humanities and Sociology, Japan
3. Tokyo Metropolitan University, Faculty of Social Sciences and Humanities, Japan

The Japanese Archipelago is a regions with pottery appearing by the last Ice Age. On Honshu, the central island of Japan, the earliest pottery appeared by ~15,500 cal BP during the Oldest Dryas (~19,000-14,700 cal BP). Numerous sites appear in Honshu by the Bølling-Allerød (~14,700-12,900 cal BP). In contrast, on Hokkaido in the north, there are only two pottery-bearing sites that clearly associate with the last Ice Age. They appear between the Oldest Dryas to the Bølling-Allerød. This limited evidence may be attributed to the freeze-thaw processes reducing the visibility of pottery as well as distinct adaptation of foragers in the the colder climatic condition. In this study, we examine ceramics from the Tachikarushunai M-I site in Hokkaido, with inferred occupational dates, ~15,000-13,800 cal BP, with one of the two sites with clear evidence of pottery. We conducted (1) visual and digital microscope analyses characterizing technological properties, (2) ceramic petrographic and chemical compositional study with polarizing microscope and a laser-based high-resolution spectrometer comparing results with geological context some raw materials from the site area, (3) measured grain distribution and porosity sizes and characterized pore forms. With analytical results, we provide inferences on post-depositional alteration and hunter-gatherer behaviors, providing insights on the origins of pottery in Hokkaido.

1:55 PM

(PACRIM-S21-019-2025) A scientific study of ceramic bronze-casting molds from Bronze Age foundries in the Central Plain of China

Q. Wang^{*1}

1. Shandong University, Institute of Cultural Heritage, China

Different from other civilizations, Chinese bronzes with lavish decoration were cast in ceramic piece-molds. How very fine designs were made on such sandy and porous molding material? In this study, complementary analyses including petrography, chemical and phytolith analysis, as well as measurement of firing temperature, were carried out on Bronze Age ceramic bronze-casting molds from the Central Plain of China to explore the feature of the molding material. A large number of mold fragments from five foundries, including Houma, the largest foundry site found to date in China were analyzed. The results show that the molds were made of loess, containing high silt, high porosity and low clay, with mainly husks of foxtail and broomcorn millet and charcoal particles as tempers. Main differences in the body fabrics between these molds from different sites lie in: the presence/absence of calcite, the particle size

distribution, and firing temperatures, suggesting a diachronic and spatial change in mold material processing. This study will help understand bronze production in different regions of the Central Plain during the Chinese Bronze Age.

2:15 PM

(PACRIM-S21-020-2025) The origin and early development of Chinese high-fired glaze-From Proto-porcelain to Celadon

X. Zhou^{*3}; J. Cui¹; T. Rehren²

1. Peking University, China
2. The Cyprus Institute, Cyprus
3. Hangzhou City University, China

The emergence of high-fired glaze is an integral part of the origin of porcelain. To investigate how the high-fired glaze originated and improved, we carried out several replicative experiments. Based on the results, we compared the replicative specimens and archaeological samples, to study the development of high-fired glaze products. Our study of archaeological samples showed that fuel ash glaze, wood ash glaze (slurry glazing), and the glaze made by wood ash in combination with clay, match the three stages of the early development of Chinese high-fired glaze. The first stage occurred during the Xia and Shang dynasties when the earliest period of proto-porcelain occurred, indicating the emergence of high-fired glazes and the attempts at production. The second stage also occurred during this period. For now, the information indicates that the glaze slurry glazing method first appeared at the kiln site group in Quanzhou, Fujian Province, represented by kiln sites in Quanzhou. However, this technique was not widely used until the end of the Shang dynasty and during the Western Zhou period, when the fuel ash-glazed products disappeared. The third stage occurred in the East Han Dynasty, the craftsmen began to use binary recipes for glazes in mature celadon, marking a significant revolution of high-fired glaze.

2:35 PM

(XACRIM-S21-021-2025) Study of Faience in the Bronze Age Xinjiang, China: Origins, Transmission, and Localization

N. Liu^{*1}

1. Chinese Academy of Social Sciences Institute of Archaeology, China

This study examines the origins, transmission, and localization of faience in Bronze Age Xinjiang, China. Through the detailed analysis of microstructure and chemical composition of faience beads excavated from various archaeological sites in Xinjiang, the research identifies diverse transmission routes and sources of faience during the Bronze Age. The soda-rich faience unearthed at the Xiaohe Cemetery, located south of the Tianshan Mountains, shows a connection to the Harappan civilization of the Indus Valley, suggesting that it might have spread to the Tarim Basin via Central Asia. Meanwhile, faience beads found in the northern Tianshan Mountain reveal influences from the North Caucasus, accompanied by evidence of technological adaptation and localization. This study of faience beads uncovers distinct cultural exchange routes and mechanisms between the northern and southern regions of the Tianshan Mountains during the Bronze Age, offering new perspectives on the transmission of technology across the Eurasian continent during this period.

2:55 PM

(PACRIM-S21-022-2025) Reassessing the Circulation of Enamelled Objects between France and China: Technological, Cultural, and Diplomatic Interactions

X. Jiang^{*1}

1. Peking University School of Archaeology and Museology, China

Enamelled porcelain from the Qing imperial court, celebrated as the pinnacle of artistic achievement and a sophisticated expertise within the “firing arts”, symbolises the unprecedented intercultural exchanges between China and Europe during the early modern period. Over the past decade, Franco-Chinese research teams have undertaken several large-scale international collaboration projects and conclude, in effect: (1) that some early Qing enamelled porcelain pieces in European museums are either fakes or ancient copies; (2) that the technical know-how and trade in raw materials essential for enamel production originated in France, predominantly in Limoges; and (3) that the localisation of enamel techniques was achieved during the Yongzheng period. However, a critical reassessment of the provided scientific data and historical archives challenges these prevailing assertions. First, the presence of “pure cobalt” should not be considered a definitive criterion for authenticity. Second, there is no reliable evidence linking the technological roots of painted enamel on porcelain specifically to France; rather, they are more plausibly traced to the German region. Third, the enamel pigments continued to rely on imported materials throughout the Qing dynasty, with inadequate evidence to substantiate the claim of complete localisation.

3:30 PM

(PACRIM-S21-025-2025) Simulation Experimental Study on the Transition from Proto-Porcelain to Celadon

J. Cui^{*1}

1. Peking University, China

To investigate how the high-fired glaze originated, the factors influencing the appearance of proto-porcelain glazes, and the reasons for the difference in glaze evenness between proto-porcelain and mature celadon, we carried out replicative experiments to make high-fired glazes by fuel glazes, high-calcium wood ash only and high-calcium wood ash with different proportions of clay as raw materials for glaze preparation. Based on the results, we compared the replicative specimens and archaeological samples, to study the development and spread of high-fired glaze products. Experiments of high-fired glaze showed that the formation of glaze follows the phase diagram under the laws of thermodynamics and that the final composition can only be located in the eutectic trough, regardless of the recipe. Thus, the composition of the high-fired calcium glaze formed by the fuel glaze, the glaze applied with a pure ash glaze slurry, and the glaze applied with wood ash in combination with clay are similar for all three. However, they will differ in their glaze morphology, based on which the glazing recipe and process of the finished product can still be told.

PacRim S23 - Advanced Processing and Manufacturing Technologies for Ceramics

PACRIM Symposium 23 - Novel forming technologies

Room: Georgia B

Session Chairs: Hidehiro Yoshida, The University of Tokyo; Yasuhiro Kodera, University of California, San Diego

1:15 PM

(PACRIM-S23-011-2025) Fabrication of Proton Conducting Membranes by Tape Casting and Additive Manufacturing (Invited)

W. A. Meulenber^{*1}; J. L. Wolter¹; W. Deibert¹; O. Guillon¹; S. Gross-Barsnick²; I. Jevtovikj³; C. Mai³; M. Hassan³; S. Schunk³; A. Pelka⁴; D. Nikolay⁴

1. Forschungszentrum Julich GmbH, Institute of Energy Materials and Devices (IMD-2), Germany
2. Forschungszentrum Julich GmbH, Central Institute of Engineering (ZEA-1), Germany
3. hte GmbH, Germany
4. WZR ceramic solutions GmbH, Germany

The lecture addresses a high-temperature cracking processes with a membrane reactor to produce chemical building blocks. The core of the cell assembly is a ceramic membrane made from mixed proton and electron conducting $\text{La}_{6-x}\text{W}_{0.8}\text{Mo}_{0.2}\text{O}_{12-\delta}$. The powder is in-house produced and the particle size, specific surface area and chemical composition is determined before the ceramic layers are formed. The first manufacturing approach is sequential tape-casting to fabricate an asymmetric structure of a dense membrane layer and a porous support. Furthermore 3D-printing techniques are implemented to achieve defined support structures. Firstly, a combination of tape casting and material extrusion is introduced, where the support structure is printed directly on a tape-cast membrane layer. This technique allows a good membrane quality but suffers during the co-firing of the final layers. Secondly, a pure 3D-printing approach is introduced, which utilizes 3D-screen printing. With this technique both, membrane and support layer, are formed subsequently in one machine allowing good membrane quality and precise support structures. After co-firing all membrane components undergo a quality testing procedure. The next step is the joining of the ceramic membrane into a metal frame to form a membrane module, which can easily be built in a test reactor and quickly exchanged for multiple tests.

1:55 PM

(PACRIM-S23-012-2025) Exploration of Novel Lead-free Halides Towards Optoelectronic Applications (Invited)

T. Zhou¹; Y. Wang¹; H. Chen^{*1}

1. Donghua University, China

Metal halides have garnered significant attention due to their convenient synthesis, low cost and superior performance. Among them, lead-free halides demonstrate immense commercial potential due to their low toxicity. We will introduce our work on the construction and synthesis of some unknown lead-free halides (Zn, Cu and Sb). For metal halides, they could be viewed as being composed by two parts of the inorganic/organic cations and metal-halide ligands. The metal-halide ligands usually contribute to the optoelectronic properties, while the other part plays the role of the electron donors and structure stabilizer. By integrating organic cations with Zn-halide tetrahedra, six novel compounds were synthesized. We have successfully used them for X-ray imaging and anti-counterfeiting. For the Cu halides, with the same design idea, we have found four Cu halides assembled from aromatic molecules. They have been used

for the green lighting. To construct novel Sb halides, we chose rigid bulk triphenylphosphine as organic cations to obtain a series of novel Sb halides with a maximal PLQY of 99.3%. The luminescent fibers were successfully assembled using the 3D printing and electrospinning methods for advanced anti-counterfeiting and information encryption. Our work provides a promising way for the design of new metal halides, paving the way for sustainable advancements in multiple optoelectronic fields.

PACRIM Symposium 23 - Spark plasma sintering

Room: Georgia B

Session Chair: Haijie Chen, Donghua University

3:30 PM

(PACRIM-S23-015-2025) Obtaining non-conventional properties from conventional materials with far from equilibrium state via tailored powder-densification process (Invited)

Y. Kodera^{*1}

1. Ryukoku Daigaku - Seta Campus, Materials Chemistry, Japan

Non-conventional functional properties can be obtained from conventional materials when the material exhibits far from equilibrium (FFE) state, such as nano-grain size, over-doping, metastable/transitional phase and so on. Obtaining FFE bulk materials through powder consolidation approaches requires the specifically designed powder synthesis method for the particular consolidation method (tailored powder-densification process). Because an appropriate heat is required to obtain bulk form and maintain FFE state of powder. FFE materials can be obtained only within the specific processing condition (processing window). FFE will be converted to be an equilibrium state resulting conventional properties, when FFE materials are overheated. In this presentation, we will discuss a few examples of processing of material with FFE state. We demonstrate that tailored powder-densification process can widen processing window to obtain unique magnetic and optical properties from conventional compositions such as iron oxide and aluminum oxide based material.

4:00 PM

(PACRIM-S23-016-2025) High-Temperature Sintered Ceramic Electrolytes for Solid-State Batteries (Invited)

E. J. Cheng^{*1}

1. Tohoku Daigaku, Japan

Solid-state batteries have attracted considerable attention for next-generation energy storage because of their potential high energy densities and improved safety. Solid electrolytes (SEs) are central to the development of solid-state batteries. Garnet ceramic oxide $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) and sodium superionic conductor $\text{Na}_3\text{Zr}_2\text{Si}_2\text{PO}_{12}$ (NZSP) are among the few that show good chemical stability against Li and Na metal anodes, respectively. Furthermore, their high oxidation stability allows the integration of high-voltage cathodes. In this study, we briefly discuss recent advancements in LLZO and NZSP SEs, highlighting the key challenges that hinder their practical implementation in solid-state batteries. Specifically, we systematically investigate the effects of the sintering techniques, including spark plasma sintering (SPS) and hot pressing (HP), as well as the influence of sintering additives (e.g. NaF) on the microstructure and ionic conductivity of LLZO and NZSP. Additionally, the electrochemical performance of these high-temperature sintering SEs is evaluated using symmetric cells. These results aim to inform strategies for optimizing the performance of SEs in solid-state batteries.

4:30 PM

(PACRIM-S23-017-2025) Revolutionizing Advanced Ceramics Manufacturing: Spark Plasma Sintering as a Low-Cost, Energy-Efficient SolutionC. Melnyk¹; E. Eyermaⁿ*¹

1. California Nanotechnologies, USA

California Nanotechnologies is driving innovation in advanced powder processing and sintering technologies to meet the growing demands for sustainable, high-performance materials in cutting-edge industries. Among these technologies, Spark Plasma Sintering (SPS) has emerged as a transformative low-cost, energy-efficient solution for advanced ceramics. By enabling rapid densification at lower temperatures and significantly shorter sintering times, SPS reduces energy consumption while maintaining or enhancing mechanical and functional properties. With precise control over nano- and micro-structure development, SPS facilitates the production of ceramics with tailored properties, including superior strength, thermal stability, and controlled porosity. This capability has unlocked new opportunities for ceramics in clean energy, nuclear, and aerospace applications. California Nanotechnologies leads the charge in scaling SPS for reliable and cost-effective manufacturing, offering solutions that prioritize sustainability and innovation. This presentation will explore the unique advantages of SPS as a next-generation sintering and bonding process, emphasizing its role in consolidating advanced ceramics that meet the stringent performance requirements of modern, sustainability-focused industries.

PacRim S24 - Solid-State Optical Materials and Luminescence Properties**PACRIM Symposium 24 - Novel optical materials design and their properties II**

Room: Prince of Wales

Session Chairs: Junichi Tatami, Yokohama National University; Shibin Jiang, AdValue Photonics Inc

1:15 PM

(PACRIM-S24-012-2025) Transparent tellurite ceramics obtained by full crystallization of glass (Invited)S. Chenu^{*1}; H. Benchorfi²; J. Cornette¹; M. Dutreilh-Colas³; V. Couderc⁴; J. Duclere¹; C. Genevois⁵; M. Allix⁶; G. Delaizir¹

1. Institut de Recherche sur les Ceramiques, France
2. Université Laval, Chemistry, Canada
3. IRCER, France
4. XLIM, France
5. Conditions Extremes et Matériaux Haute Temperature et Irradiation, France
6. CNRS (CEMHTI), France

Transparent ceramics are polycrystalline materials that allow for incoming photons to pass through without significant absorption and internal scattering occurring, which reduces the optical transparency of the material. However, the elaboration process of ceramics usually requires challenging powder sintering conditions as it remains difficult to completely eliminate the residual pores during their densification which attenuate transparency. The full crystallization of a bulk glass into a transparent ceramic is a promising alternative to circumvent the disadvantages and technical challenges related to the ceramics obtained by conventional powder sintering processing. Here, we report the elaboration of TeO₂-based ceramics by full crystallization of the parent glasses. The transmittance in both visible and IR ranges is measured and discussed in light of the composition, microstructure (crystals size, porosity, and grain boundaries thickness). By doping with rare earth ions such as Nd³⁺,

these transparent ceramics can present broadband near infrared luminescence. Bulk laser emission has been demonstrated attesting the potential of such polycrystalline transparent ceramics as optically active materials.

1:45 PM

(PACRIM-S24-013-2025) Crystal Structure and luminescence properties of yellow persistent Ca₃Ta_{1.5}Ga_{3.5}O₁₂ and red persistent Ca₃Ta_{1.5}Ga_{3.5}O₁₂:Pr³⁺ phosphorT. Onoe^{*1}; Y. Tonogai¹; M. Okamoto¹; K. Murai¹; T. Moriga¹

1. Tokushima Daigaku, Japan

Persistent luminescence(persL) phosphors are widely used in evacuation guiding signs, anti-counterfeiting markers, in vivo imaging, and so on. However, red persL phosphors still lack the persistent duration time, compared with commercially used blue emitting CaAl₂O₄:Eu²⁺, Nd³⁺ and green emitting SrAl₂O₄:Eu²⁺, Dy³⁺, so that applications of persL phosphors emitting these three primary lights have been limited. The Ca₃Ta_{1.5}Ga_{3.5}O₁₂ has a garnet structure with the general composition A₃B₂C₃O₁₂ and the B site is occupied by Ta⁵⁺ and Ga³⁺. We considered that such a disordered crystal structure could form trap centers, which is necessary for persL. Hence, new persL phosphors, Ca_{3-x}Ta_{1.5}Ga_{3.5}O₁₂:xPr³⁺ (x = 0, 0.003, 0.006, 0.009, 0.015, 0.03, and 0.06) were synthesized by solid state reaction method. The Ca₃Ta_{1.5}Ga_{3.5}O₁₂ host showed yellow persL with a peak emission at 557 nm, lasting for more than 4000 seconds under a 254 nm UV excitation. On the other hand, The Ca₃Ta_{1.5}Ga_{3.5}O₁₂:Pr³⁺ showed red persL peaked at 606 nm with a similarly persL duration time for more than 4000 seconds. Thermoluminescence measurements revealed the presence of trap centers, and shallow trap depths observed in both the host and the Ca₃Ta_{1.5}Ga_{3.5}O₁₂:Pr³⁺ were found to be similar. Therefore, we concluded the host plays an important role in the red persL properties of Pr³⁺.

PACRIM Symposium 24 - Optical Materials

Room: Prince of Wales

Session Chair: Sébastien Chenu, Institut des Sciences Chimiques de Rennes

2:05 PM

(PACRIM-S24-014-2025) Rare earth-doped borogermanate glasses from electronic waste for advanced magneto-optical applicationsD. F. Franco^{*1}; A. Berno¹; F. Caixeta¹; S. J. Ribeiro¹

1. São Paulo State University- UNESP, Institute of Chemistry, Brazil

Magneto-optical (MO) glasses are of growing interest for their potential in developing MO sensors. Borogermanate glasses enable the solubilization of high concentrations of rare earth (RE) ions. This work presents the synthesis and characterization of borogermanate (BGeB) glasses incorporating e-waste from fluorescent lamps containing rare earth (RE) ions with high magnetic moments. Glasses with x = 0, 10, 20, 30, and 50 %wst were prepared using the melt-quenching method at 1400 °C. Characterization techniques included Differential Scanning Calorimetry (DSC), X-ray Diffraction (XRD), Photoluminescence (PL), UV-Vis-NIR absorption spectroscopy, and MO characterization. XRD patterns confirmed the amorphous nature of all samples, and DSC curves identified glass transition temperatures (T_g) of around 516 °C. The transmission spectra of BGeBx%wst glasses revealed a broad optical transmission window (0.55–1.6 μm), with notable Tb³⁺ and Eu³⁺ transitions observed in emission spectra. The maximum Verdet constant achieved was -40.8 rad T⁻¹ m⁻¹ for the BGeB50%wst glass. This study emphasizes the importance of recycling e-waste containing RE ions and demonstrates the potential of oxide glasses doped with Tb³⁺ and Eu³⁺ for advanced magneto-optical applications.

2:25 PM

(PACRIM-S24-015-2025) Glasses and Optical Fibers Containing Tb³⁺ for Magneto-Optical Applications

T. A. Lodi^{*1}; E. O. Ghezzi¹; L. V. Albino¹; D. F. Franco¹; M. Nalin¹

1. Universidade Estadual Paulista Julio de Mesquita Filho, Analytical, Physical and Inorganic Chemistry, Brazil

The Faraday effect is a magneto-optical (MO) phenomenon in which the polarization direction of linearly polarized light rotates as it passes through a transparent material, under the influence of a magnetic field applied along the light's propagation direction. Typically, MO devices are based on crystalline materials and have a wide range of applications, including magneto-optical sensors, optical isolators, and magneto-optical fibers. However, the growth of single crystals is time-consuming, expensive, and results in materials with limited sizes and shapes. Compared to crystals, glass is a non-crystalline material that offers advantages such as durability, good optical and mechanical properties, along with the possibility of being produced in the form of optical fibers. Terbium is the most popular rare earth element in magneto-optical glasses due to its large magnetic moment and small absorption coefficient in the visible and IR regions. In this work, we report the potential of Tb³⁺-containing gallium-borogermanate (BGG) and gallium-boroaluminate (BAG) glass compositions for the construction of magnetic field and electric current sensor devices. BGG and BAG magneto-optical glasses doped with terbium were prepared by a conventional melt-quenching method, and their physical properties, magneto-optical effect, and luminescent properties were studied.

2:45 PM

(PACRIM-S24-016-2025) Development of novel NIR emission phosphor and their application

S. Kim^{*1}; T. Kang¹; B. Bae²

1. Korea Institute of Ceramic Engineering and Technology (KICET), Republic of Korea
2. Yeongwol Industrial Promotion Agency, Republic of Korea

Near-infrared (NIR) emissions are highly important in anti-counterfeiting, secret signals, medical, pharmaceutical, and agricultural industries. As counterfeiting technology for security materials develops, the importance of anti-counterfeiting and authentication technology increases, and new materials need to be developed. Recently, certification materials for waste plastic recycling and application products using eco-friendly Global Recycling Standard (GRS)-based materials are attracting attention. These anti-counterfeiting and certification materials can be applied as NIR materials with high efficiency, high thermal stability, and NIR-excitation to NIR-emission beyond existing UV-excitation. In this study, we used Yb³⁺ as the luminescence ion to develop new NIR emission phosphor with high thermal stability for use in the anti-counterfeiting and certification materials. Yb³⁺-doped NIR phosphors showed a broad NIR emission which was attributed to the ²F_{5/2} → ²F_{7/2} transition of Yb³⁺ ions in NIR region excitation. The NIR phosphor showed excellent thermal stability and recovered close to 100% of the initial emission intensity at room temperature after cooling. It was confirmed that significant NIR emission was detected by adding near-infrared phosphors to produce a master batch for application to fiber products. These results suggest applicability to advanced anti-counterfeiting and certification applications.

3:30 PM

(PACRIM-S24-017-2025) Tunable NIR luminescence in Bi-doped phosphosilicate fibers for optical amplifier applications

A. Cheriyaathu Valappil^{*1}; T. Meyneng¹; J. Lefebvre¹; P. Labranche¹; S. LaRochelle¹; Y. Messaddeq¹

1. Université Laval, Optic-Photonics Pavillion, Canada

Bismuth-doped optical fibers (BDFs) are gaining significant attention in the field of optical telecommunications due to their broad near-infrared (NIR) emission ranging from 1000 up to 1600 nm, where the optical losses in silica fibers are minimized, making them highly advantageous for optical amplifier applications. Among them, Bismuth-doped phosphosilicate fibers (BDPFs) are an upcoming and widely researched topic due to its potential to use as an optical fiber amplifier in the wavelength range of 1260-1430 nm. While the technological maturity of BDFs have improved, with commercial products already available, additional work is still required to fully unveil their potential. Our current work mainly focuses on the fabrication of BDPF via MCVD in conjunction with solution doping technique. Compared to other BDFs, phosphosilicate fibers are attractive, as phosphorus (P) doping can be achieved using both gas-phase and solution doping methods. In this work, we are exploring the tunability of NIR luminescence properties such as the luminescence intensity, emission width and peak position under different excitation wavelengths such as 464, 808, 980 and 1320 nm. Under each excitation wavelength, a broad emission in the wavelength range of 1000 – 1600 nm was observed. Moreover, we also present the changes in the luminescence properties in accordance with the Bismuth doping concentration.

PacRim S27 - International Symposium of Fundamental and Frontier Sciences of Ceramics

PACRIM Symposium 27 - International Symposium of Fundamental and Frontier Sciences of Ceramics III

Room: Cypress

Session Chairs: Amanda Krause, Carnegie Mellon University; Rajendra Bordia, Clemson University

1:15 PM

(PACRIM-S27-013-2025) Current status and challenges in understanding room-temperature impact consolidation (RTIC) phenomena in the AD process (Invited)

J. Akedo^{*1}

1. National Institute of Advanced Industrial Science and Technology Tsukuba, Sangyo Gijutsu Sogo Kenkyujo Tsukuba, Tsukuba, Ibaraki Prefecture, JP, academic/tech, Device Technology Research Institute, Japan

The AD method is a very interesting new ceramic process that realizes dense and highly adhesive ceramic coating at room temperature. For the past 25 years, it has been applied and researched in the fields of electronic ceramics such as piezoelectric devices, storage battery devices, and solar cells, functional ceramics, and engineering ceramics such as wear resistance and rust prevention. Since around 2012, yttria material coatings have been commercialized as low-dust plasma corrosion-resistant parts and are mass-produced as essential engineering parts for advanced semiconductor manufacturing equipment. However, there are still some unclear points about the film formation mechanism of the AD method and it is not fully understood. In this presentation, we will introduce the current status of understanding of the room temperature impact consolidation phenomenon, which is important for the wide practical deployment of the AD method, and discuss the root issues that will be addressed in the future.

1:45 PM

(PACRIM-S27-014-2025) Using mechanochemistry to obtain sulfur-based glass-ceramics and ceramics for solid state electrolytes applications (Invited)L. Verger^{*1}; S. Chenu¹; J. Zhang¹; J. Trébosco²; O. Lafon²; V. Nazabal¹; D. Le Coq¹; L. Calvez¹

1. University of Rennes, ISCR, France
2. Université de Lille, France

Sulfur-based materials are attracting growing interest as solid-state electrolytes due to their high ionic conductivity compared to their oxide counterparts, and their soft mechanical properties. They are classically synthesized by the melt quenching method in silica tubes. However, this process poses problems of safety, scalability and cost, and limits the compositions available, due to the reactivity of alkali with silica. An alternative to high-temperature syntheses and solvent-based processes is the use of mechanical milling techniques. In this talk, we will focus on sodium ion-conducting materials and show how mechanochemistry can be used to (i) extend the glass formation domain of sodium-rich glasses or (ii) obtain mechanically activated precursors for ceramics. The conductivity properties and structure of these new Na-rich materials are discussed. Crystallization tests are then carried out to obtain glass-ceramics and ceramics in these systems. This synthesis route offers significant advantages over the state-of-the-art: the synthesis temperature is typically lowered by about 50 %, it is a solvent-free route and a large quantity of material can be synthesized.

2:15 PM

(PACRIM-S27-015-2025) Microcantilever Bending Tests Leading to Reliability Innovation in Ceramics (Invited)J. Tatami^{*1}

1. Yokohama National University, Japan

Microcantilever bending tests provide knowledge of mechanical properties in regions unaffected by coarse defects such as cracks. This corresponds to the potentially superior mechanical properties of ceramics that can be expected to be realized in materials where the size of defects has been reduced to the limit by the advancement of the powder ceramics process. For example, the bending strength of silicon nitride ceramics measured on microcantilever specimens of a few microns in width and height is 5 to 10 GPa, which is extremely higher than that of conventional silicon nitride ceramics. Understanding degradation is also extremely important for material design to extend the lifetime of ceramics used in extreme environments. In our previous study, the strength and fracture toughness of silicon nitride ceramic surfaces after brief contact with molten aluminum were reduced when Y_2O_3 was used as a sintering aid, whereas no degradation was found with the addition of Lu_2O_3 . These differences correspond to structural changes at the nanoscale, such as the composition and structure of grain boundaries. Furthermore, plastic deformation of ceramics under tensile stress also occurs at this scale, even at room temperature, which should lead to new understandings of the mechanical properties of ceramics and innovations in materials design.

2:45 PM

(PACRIM-S27-016-2025) Lead-free ferroelectric ceramics for capacitive energy-storage applications (Invited)J. Li^{*1}

1. Tsinghua University, School of Materials Science and Engineering, China

Dielectric capacitors are fundamental energy storage components in advanced electronics and electrical power systems, for which relaxor ferroelectrics and antiferroelectrics have received significant attention as promising materials. This talk will highlight our recent advances in lead-free antiferroelectric ceramics and relaxor-ferroelectric thin films for capacitive energy storage. The presentation begins with

$AgNbO_3$, a representative lead-free antiferroelectric compound. I will present our findings on the electric-field-induced antiferroelectric to ferroelectric phase transition and the enhanced energy storage properties achieved through Ta and Sm doping. Phase-pure $AgNbO_3$ films were fabricated by a facile sol-gel method, but double PE loops characteristic of antiferroelectricity were not observed due to high current leakage, suggesting limited suitability of $AgNbO_3$ films for energy storage applications. However, significant progress was made with sol-gel-processed $Bi(Mg,Ti)O_3$ -based relaxor ferroelectric thin films, demonstrating high energy-storage performance. By implementing a partitioning polar-slush strategy, we realized simultaneous enhancement in reversible polarization and breakdown strength, resulting in a record-high energy density of 202 joules per cubic centimeter. Detailed structural design and experimental results will be elaborated during the talk.

3:30 PM

(PACRIM-S27-017-2025) New perspectives on grain boundary migration during grain growth (Invited)G. Rohrer^{*1}

1. Carnegie Mellon University, USA

Recent studies of polycrystalline Ni, $SrTiO_3$, and Fe have shown no correlation between curvature and migration velocity, contradicting the observed migration behavior of individual grain boundaries in bicrystals. In this presentation I will discuss the influence of grain boundary energy anisotropy on the driving force and, more specifically, the anisotropy associated with the grain boundary plane inclination. Application of this driving leads to the prediction that the area expansion of a given grain boundary is correlated to the difference in the energies of the grain boundaries that meet at a triple line. Experimental evidence, derived from the time evolution of three-dimensional polycrystalline microstructures measured by diffraction microscopy, is consistent with this prediction. Furthermore, the data show that grain boundaries migrate in such a way as to replace higher energy grain boundaries with relatively lower energy boundaries.

4:00 PM

(PACRIM-S27-018-2025) Sintering Ceramics in Seconds: Ion Conductors for Solid State Batteries, Hydrogen Electrolyzers and Thermal Barrier Coatings (Invited)L. Hu^{*1}

1. Yale University, Electrical and Computer Engineering, USA

We recently reported an ultrafast high temperature sintering (UHS) for solid state electrolytes (Science, 2020, May Cover). I will discuss our progress in applying UHS in various applications, including solid state batteries, solid oxide electrolyzer, and high temperature thermal barrier coating. (1) High-performance solid-state electrolyte. The long sintering time of conventional syntheses can lead to Li loss in garnet SSEs caused by the evaporation of Li and the formation of secondary phases that lead to lower ionic conductivity. Our UHS technique enables us to tune the sintering time in units of seconds, which provides excellent control in terms of the Li content and grain growth. (2) Solid oxide electrolyzer. UHS can address these challenges by reducing the number of sintering steps shortening sintering times from days to minutes, and enabling more continuous sintering. (3) High temperature thermal barrier coating. The UHS method allows sintering of various thermal barrier coatings (including bond coats), either as self-standing or on candidate substrates, within tens of seconds. By evaluating thermal expansion coefficient and steam recession rate, the materials databases were developed to provide guidance to coating composition selection.

4:30 PM

(PACRIM-S27-019-2025) Production of high-temperature ceramics by flash sintering (Invited)

V. M. Sglavo*¹

1. University of Trento, Italy

Numerous research activities are trying to identify processes with limited environmental impact and energy consumption to produce ceramics. Among these, the recently proposed technique identified as flash sintering appears promising although its application at an industrial level still requires extensive work. An area where the above-mentioned issue is even more problematic is that of refractory or high-temperature ceramics, which can be typically consolidated only at very high temperature under the action of significant pressures or through the addition of dopants, always working in inert atmosphere. In this work, the application of flash sintering on tungsten carbide, zirconium diboride and their composites is presented. Such materials behave like metals from an electrical point of view and therefore do not show the well known thermal runaway phenomenon when subjected to the simultaneous effect of temperature and electric field as observed in most ceramics. In addition, their chemical nature makes them prone to oxidize at high temperature in non-protecting environment. The conditions are discussed here to achieve high density and no oxidation by using flash sintering with the aim to identify possible evolution of the process to real applications and actual issues which need further investigations.

5:00 PM

(PACRIM-S27-020-2025) How Do Nanoscale Effects Alter Ceramic Phase Diagrams? (Invited)

R. Castro*¹; K. Joshi¹

1. Lehigh University, Material Science & Engineering, USA

At the nanoscale, the behavior of oxide ceramics deviates significantly from bulk predictions due to the pronounced influence of surface and grain boundary energies. These nanoscale thermodynamic effects can shift phase stability, alter polymorphic transitions, and redefine the equilibrium boundaries within phase diagrams. This talk explores recent advancements in quantifying surface and grain boundary energies using calorimetric method and their integration into thermodynamic models of oxide ceramics. We discuss how these nanoscale-specific phenomena reshape traditional phase diagrams, highlighting examples where metastable polymorphs are stabilized or entirely new phases emerge in systems such as yttria-zirconia, titania, magnesia-zirconia, and even the technologically relevant LiMn₂O₄. Such findings hold profound implications for material design, enabling the targeted synthesis of ceramics with tailored properties for applications in energy, electronics, and catalysis.

PacRim S29 - Progress in High-Entropy Materials

PACRIM Symposium 29 - Mechanical Properties

Room: Plaza A

Session Chairs: Mingwei Zhang, University of California Davis;

1:15 PM

(PACRIM-S29-012-2025) From High-Entropy Ceramics (HECs) to Compositionally Complex Ceramics (CCCs): A New Perspective (Invited)

J. Luo*¹

1. University of California San Diego, USA

This talk will review a series of our studies to push the boundary of the emergent field of high-entropy ceramics (HECs). Since 2016, we first reported a series of single-phase equimolar five-

HECs, e.g., MB₂, MB, M₃B₄, MB₄ and MB₆ borides, perovskite and YSZ-like fluorite oxides, and MSi₂ and M₅Si₃, as well as single-phase high-entropy intermetallic compounds. In 2020, we further proposed to extend HECs to “compositionally complex ceramics (CCCs)” to include non-equimolar compositions and short- and long-range ordering, which reduce configurational entropies, but offer additional dimensions to tailor and improve properties. We also reported the first dual-phase HECs/CCCs. We discovered long- and short- range orders, order-disorder transitions, and ultrahigh-entropy phases in a variety of 10- to 21-component CCCs in defect fluorite, pyrochlore, weberite, and other fluorite-derived crystal structures. Our recent research also investigates compositionally complex perovskite oxides (CCPOs) as new classes of materials for solar thermochemical hydrogen generation and as solid lithium-ion conductors.

1:55 PM

(PACRIM-S29-013-2025) Status of FCC and BCC high-entropy alloys (Invited)

E. P. George*¹

1. The University of Tennessee Knoxville Tickle College of Engineering, Department of Materials Science and Engineering, USA

The field of HEAs is now two decades old and this milestone is an opportune time to review progress made to date. Because of the vastness of the field, and the impossibility of covering everything in a single talk, I will restrict myself to mechanical behavior and phase transformations. Additionally, the focus of my talk will be on metallic alloys. Among these, I will concentrate on model alloys belonging to the FCC and BCC crystal structures since they are the most extensively investigated. Mainly, properties of relevance to structural applications, such as tensile properties (strength, ductility, toughness) for cryogenic applications, and creep properties and phase stability for high-temperature applications, will be discussed. Wherever possible, the observed macroscopic behavior will be related to the underlying (governing) physical mechanisms. While some HEAs will be shown to be best in class, others are severely lacking when compared to state-of-the-art commercial alloys. I will conclude with some thoughts on opportunities for future research in HEAs for structural applications.

2:35 PM

(PACRIM-S29-014-2025) Current Progress and Future Perspectives on High-Temperature Creep-Resistant Refractory High Entropy Alloys (Invited)

M. Zhang*¹

1. University of California Davis, Materials Science and Engineering, USA

There is a pressing need to develop new alloy systems capable of operating at temperatures beyond the limits of current Ni-based superalloys for space exploration, energy sustainability, and defense applications. Refractory High Entropy Alloys (RHEAs) show great promise due to their high melting points and elevated-temperature strength. However, significant challenges are still present in achieving a balance between room-temperature tensile ductility and high-temperature creep resistance, as well as oxidation resistance. We show that many (Mo, W, Cr, Zr)-rich RHEAs with high compressive strength exhibit little to no tensile ductility due to grain boundary embrittlement caused by oxide formation and phase decomposition. On the other hand, ductile NbTaTiHf-based RHEAs show insufficient creep resistance due to a lack of high-temperature strength for screw dislocation glide-controlled materials. The development of dispersion-strengthened, edge dislocation glide-controlled, and ductile RHEAs is seemingly the most promising route to achieve phase stability, creep strength, and recrystallization resistance. Furthermore, the majority of RHEAs face significant limitations in oxidation resistance, necessitating the development of effective and reliable coatings.

3:30 PM

(PACRIM-S29-041-2025) Exploring Non-Equimolar High-Entropy Diborides: From Atomic Structure to Mechanical and Thermodynamic Performance WITHDRAWNI. Zhukova^{*1}; D. Zagorac²; M. Tatarková¹; B. Matovic²; P. Tatarko¹

1. Slovak Academy of Sciences, Slovakia
2. Belgrade University, Serbia

This work presents the design, modeling, and experimental investigation of high-entropy diboride ceramics based on (TiZrHfNbTa)B₂ with varying non-equimolar compositions. The study aims to understand the impact of different atomic ratios on the structural, energetic, and mechanical properties of high-entropy boride systems. Density Functional Theory (DFT) calculations were performed using VASP with structural disorder modeled via the Special Quasirandom Structures (SQS) approach. Key parameters, such as formation energy and vacancy formation energy were evaluated to identify the most stable compositions. Experimentally, three selected non-equimolar compositions were synthesized using boro/carbothermal reduction followed by Spark Plasma Sintering (SPS) at 1800–2000 °C. Microstructural analysis was conducted using TEM and SEM, and mechanical properties—including hardness, Young's modulus, and wear resistance—were assessed via nanoindentation and tribological testing. The combined theoretical and experimental results offer insight into the structure–property relationships of high-entropy diborides and support their potential application in extreme environments.

PacRim S32 - Advanced Characterization, Testing, and Analysis of Materials**PACRIM Symposium 32 - Advanced Characterization, Testing, and Analysis of Materials II**

Room: Seymour

Session Chair: Scott Misture, Alfred University

1:15 PM

(PACRIM-S32-005-2025) Advanced Characterization of Disorder: Insights into High Entropy and Amorphous Phases (Invited)C. M. Rost^{*2}; G. R. Bejger²; J. Barber²; B. Jiang³; K. Lam⁴; Y. Son⁶; G. Niculescu¹; K. Holsgrove⁵; A. Kumar⁵; S. Troler-McKinstry⁶; J. Ihfeldt⁴; K. L. Page³

1. James Madison University, Physics and Astronomy, USA
2. Virginia Polytechnic Institute and State University, Materials Science & Engineering, USA
3. The University of Tennessee Knoxville Tickle College of Engineering, USA
4. University of Virginia, USA
5. Queens University Belfast, United Kingdom
6. The Pennsylvania State University, USA

Material properties are fundamentally influenced by composition and local structure, with atomic-level disorder emerging as a critical driver of novel functionalities and applications. By probing these local structures, we aim to manipulate materials to unlock opportunities for evolving technologies. High entropy oxides (HEOs) and amorphous materials are particularly compelling due to their intrinsic disorder, which facilitates tunable and metastable properties. HEOs, characterized by a near-equimolar distribution of multiple elements without a primary host, exhibit unique compositional and structural disorder. This disorder, coupled with localized structural distortions, profoundly impacts electronic, magnetic, and thermal behaviors, enabling broad functionality tunability. The local structure of amorphous phases may influence metastable phase nucleation, resulting in improved functionality. This presentation highlights our efforts in characterizing disordered materials using advanced techniques to probe local length scales. Leveraging X-ray absorption fine structure (XAFS) spectroscopy and neutron

total scattering combined with computational modeling, we reveal the role of local disorder in phase evolution and functionality. These methodologies not only provide insights into the impact of atomic-level complexity but also help accelerate the discovery of next-generation materials.

1:45 PM

(PACRIM-S32-006-2025) Radiation damage characterization of ion-irradiated high entropy ceramicsK. Wang^{*1}; D. Chen²

1. Alfred University, USA
2. Idaho National Laboratory, USA

Ultrahigh temperature ceramics, such as carbide, boride, and MAX phase, exhibited exceptional high-temperature thermomechanical properties. Also, the emerging high entropy materials have indicated superior radiation tolerance. Therefore, high entropy ceramics (HECs) are supposed to be excellent candidate materials for advanced nuclear reactors. However, the radiation response of HECs is still not well investigated. Herein, we fabricate bulk HECs by mechanical alloying and the subsequent spark plasma sintering (SPS). The HECs are irradiated by heavy ions under various irradiation conditions. The microstructural evolution, including radiation-induced dislocation loops, cavities, segregation, phase stability etc., is interrogated using analytical scanning/transmission electron microscopy (S/TEM). The radiation response of HECs is compared with binary ceramics. The results of this work will provide insights into the radiation behavior of HECs under extreme irradiation environments.

2:05 PM

(PACRIM-S32-007-2025) Glass goes DIGITAL – Digitalization of glass data through full automated screeningA. Diegeler^{*1}

1. Fraunhofer ISC, Center of Device Development, Germany

Glass development works traditionally iteratively by melting series of samples, investigating their properties, and then melting more samples with modified composition. The whole process might be pretty long and can take several months, up to one year in special cases. Fraunhofer ISC has developed a rapid-screening systems during the last years [1], which is currently being optimised in collaboration with the BAM in Berlin. The robotic glass melting systems currently running in Berlin allows the melting of 20 samples during 24 hours and is backed up with high throughput RFA, LIBS and DSC devices for chemical composition, glass transition and crystallization characterization. As an additional option, the system can be extended with a robotic in-line characterisation module for fundamental glass properties like viscosity, thermal expansion and crystallisation behaviour. Recent advances include the preparation of larger samples with masses of up to 200 g, an optimised cooling process and a better batch as well as glass melt homogenisation system. Further advancements of the system towards the development of glass-ceramics as well as enamel systems are discussed.

2:25 PM

(PACRIM-S32-008-2025) Material Characterization of Mixed Glass-Former Sodium Germanophosphate GlassesB. M. AlHasni^{*1}

1. University of Technology and Applied Sciences, Oman

Successful models originally developed to describe how the structure of mixed glass formers with a wide range of glass compositions. The structure factor comparison reveals a reasonable agreement between the model and experimental results, supporting the proposed structural arrangement. The model's outcomes closely aligned the experimental data, taking into account the uncertainties reported in the measurements. The intermediate structural ordering in glasses has been investigated by calculating both the total structure factors

*Denotes Presenter

and the partial pair correlation functions. Although the glass-modifying ions, Na⁺, are partially shared between the two glass-forming species, the modification of the phosphate component is favored. The effect of Na₂O addition on network connectivity of the glass matrix has been explored. Sodium act as a modifier and tend to interact more with the phosphate component of the network than with the germanate component. The Structural properties of the mixed glass former depend on the nature and concentration of the alkali modifiers and the concentrations of each glass former. The current model highlights the local environment of Ge-Ge and Ge-P to go insight to the connectivity between glass formers polyhedra.

2:45 PM

(PACRIM-S32-009-2025) A structural characterization study of iron-bearing aluminosilicate mineral wool fibres upon heating under oxidizing conditions

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1. Aarhus Universitet, Interdisciplinary Nanoscience Center, Denmark
2. Rockwool International A/S, Denmark
3. Aarhus Universitet, Department of Chemistry, Denmark

Stone Wool Fibers (SWFs) are mineral wool fibers used for building insulation. An important property of SWFs is fire resilience, i.e., the ability to withstand high temperatures (~1000°C). This fire resilience is inextricably linked to atomic scale features. The melting technologies create different redox conditions, altering chemistry and the structure of SWFs. Our goal is to elucidate the structural network of SWFs on multiple length scales by combining electron microscopy, X-ray absorption spectroscopy of the Fe K-edge, and X-ray scattering methods to provide new insights into the link between production process, atomic structure, and fire properties. It is hypothesized that Fe ions modulate SWFs in various ways depending on their valence state and coordination environment (Fe²⁺ acts as a network modifier, and Fe³⁺ acts as a network former), where polymerization of the SiO₄⁴⁻ network changes during oxidation in atmospheric conditions. For SWFs produced with varying Fe²⁺/Fe³⁺ ratios, the degree of oxidation during subsequent heating influences crystallization and cationic diffusion mechanisms. Our studies have provided important insights into changes in the local environment of Fe (coordination and oxidation state) as well as changes in crystallinity under different heating procedures.

3:30 PM

(PACRIM-S32-010-2025) Revisiting Optical Spectroscopy (Invited)

D. Möncke^{*1}

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UV-Vis optical spectroscopy can provides information on impurities and dopants, not only qualitatively regarding their valency and coordination but also quantitatively. The evaluation of optical spectra can be challenging due to surface or scattering effects, overlapping bands (requiring band deconvolution), and the presence of impurities. Literature is often contradictory and cannot be easily sorted without understanding of ligand field theory and selection rules. A brief introduction on band assignments and speciation of transition metal ions will be followed by examples of spectral changes with optical basicity, temperature (in-situ), and challenging sample geometries. Spectral saturation will be discussed, and information that can be gained from water bands in the IR, the cut off in the UV, where allowed charge transfer (CT) transitions often limit the absorption and may prevent determining the intrinsic band gap via Tauc plots. Just as strong IV CT (intervalence) transitions can indicate clustering of polyvalent ions and often hide the much weaker d-d transitions, while certain absorption bands when matched with a Raman laser can lead to fluorescence and resonance.

4:00 PM

(PACRIM-S32-011-2025) In-situ phase transformation in glasses followed by changes in the electrical properties measured using Electrochemical Impedance Spectroscopy (EIS) (Invited)

N. Elango³; M. Wlochalski²; C. B. Bragatto^{*1}

1. Alfred University, Engineering Department, USA
2. Coe College, USA
3. University of Minnesota Twin Cities, USA

Structural relaxation and crystallization in glasses below the glass transition temperature (T_g) are typically measured ex-situ, which can be slow and to measure the conductivity of glasses during the relaxation and subsequent crystallization, which is related to structural relaxation and crystallization, by following the changes in electrical property in-situ. To test this hypothesis, lithium borate glasses were prepared, and trials were done at high temperatures, between 2 to 10° C below T_g . The T_g and the crystallization temperature were determined using a Differential Scanning Calorimeter (DSC). The EIS instrument was run overnight for 14 to 16 hours at a time, repeatedly measuring impedance across a sample of glass over AC frequencies ranging from 1 Hz to 10⁷ Hz, approximately every 5 minutes. A Python script was used to approximate the equivalent resistance of the glass and calculate conductivity, yielding approximately 300 to 400 conductivity values per test. The experimental data was then to fit the linear changes of the electrical property as a function of time to determine bulk crystal growth rate. Preliminary results validate the technique as a fast and accessible alternative to measure the crystal growth rate in glassy materials below T_g .

4:30 PM

(PACRIM-S32-012-2025) Oxidation Behavior of Laser-assisted Chemical Vapor Deposited SiC Fibers (Invited)

M. Pavel³; K. L. Williams²; R. K. Goduguchinta²; J. Vervlied²; S. Harrison²; G. Thompson^{*1}

1. University of Alabama, Metallurgical & Materials Engineering, USA
2. Free Form Fibers, USA
3. Alabama Materials Institute, USA

Silicon carbide (SiC) fibers have emerged as the dominant strengthening phase used in ceramic matrix composites, which are replacing advanced metal alloys in high-temperature, oxidizing environments. Although the latest generation of polymer precursor derived fibers, such as Hi-Nicalon-S[®] (HNS) are nominally stoichiometric SiC, these fibers still contain an excess of free carbon and oxygen which leads to a degradation in materials performance at elevated temperatures. An alternative method to producing SiC is through laser-assisted chemical vapor deposition (LCVD) where a translating laser facilitates the deposition of SiC out of gaseous, semi-conductor grade precursors. This method yields a significantly purer product which has led to enhanced oxidation resistance. In this work we report that the LCVD fibers exhibit slower oxide growth rates when compared to HNS fibers and behave more like model semi-conductor SiC than polymer derived fibers. This is connected to a detailed characterization of the micro and nanostructure within the LCVD fibers.

Poster Session

Room: Regency A- F

5:30 PM

(GOMD-P001G-2025) Relaxation Behavior of Sodium Aluminosilicate Glasses from Modulated Differential Scanning CalorimetryB. M. Hauke^{*1}; J. C. Mauro¹

1. The Pennsylvania State University, Materials Science and Engineering, USA

Modulated Differential Scanning Calorimetry (MDSC) is a technique that has been used to study the relaxation behavior of many glass families, but the sodium aluminosilicate (NAS) system, which is important for industrial applications, has not received much attention. MDSC is used to measure enthalpy relaxation in various ways and currently has two different analysis techniques, the non-reversing heat flow and the complex heat capacity methods. Here, NAS compositions with ratios of $[Al_2O_3]/[Na_2O]$ from 0-1.42, with SiO_2 kept at about 60 mol% were studied using both analysis methods. The relaxation behavior is then tied to the changing glass structure based on the varying ratios of $[Al_2O_3]/[Na_2O]$.

(GOMD-P002G-2025) Evaluation of mid-wave infrared dispersion properties of chalcogenide glass for GRIN applicationsC. Kosan^{*1}; S. Banker¹; R. Sharma¹; G. Sop Tagne²; M. Kang²; I. Mingareev³; Z. Xu⁴; J. Hu⁴; A. Howe⁵; B. A. Zerbe⁵; S. D. Campbell⁵; D. H. Werner⁵; K. Richardson¹

1. University of Central Florida, CREOL, The College of Optics and Photonics, USA
2. Alfred University, New York State College of Ceramics, USA
3. Florida Institute of Technology, Department of Mechanical and Civil Engineering, USA
4. Massachusetts Institute of Technology, Department of Materials Science and Engineering, USA
5. The Pennsylvania State University, Materials Research Institute, USA

Gradient refractive index (GRIN) optical components are a flexible solution for improving the size, weight, and performance of existing optical systems. For example, planar GRIN lenses have a preferred spatial footprint compared to conventional homogeneous lenses. Additionally, a film can be deposited on a spherical element to correct for chromatic aberration while eliminating the complexity of manufacturing aspherical equivalents. In this work, a multicomponent $GeSe_2-As_2Se_3-PbSe$ chalcogenide glass in bulk and film form-factors were evaluated for their mid-wave infrared optical dispersion. Transmission electron microscopy, energy dispersive spectroscopy, and prism refractometry are used to characterize the glass morphology, crystal microstructure, elemental composition, and multispectral refractive index of the materials and these data are used to model possible optical functional benefits. Because previous studies have revealed properties of the glasses are influenced by melt size, the goal of this work is to examine the sensitivity of this glass's dispersion behavior with melt size and material form factor.

(GOMD-P003UG-2025) Steady-State Nucleation Rate vs Transient Nucleation RateE. Manqueros^{*1}; K. S. Ranasinghe²

1. Kennesaw State University, USA
2. Kennesaw State University, USA

Lithium disilicate was used to reexamine the time-dependent nucleation rate. Using heat treatment times ranging from 1 to 600 hours. The number of nuclei formed in each of the heat treatments were calculated using the DTA method. Data shows the continuous growth of the number of nuclei as the nucleation time increases at a given temperature. Unlike the previously believed steady-state nucleation rate, it is achieved at a higher nucleation time. Our observations

indicate that the transient nucleation rate extended to 600 hours at 450C nucleation temperature. At a nucleation temperature of 440C, the transient nucleation rate was extended to 150 hours. These results indicate that the time-dependent nucleation rates extended to a longer nucleation time before achieving the steady-state nucleation rate.

(GOMD-P004G-2025) Chemical Strengthening Characteristics and Mechanical Properties of Sodium-Alumino borosilicate Glasses with Compositional ChangesJ. Jang^{*1}; K. Park¹; W. Chung¹

1. Kongju National University College of Engineering, Division of Advanced Materials Engineering, Republic of Korea

Sodium alumino-silicate (SAS) glass, commonly used as cover glass for mobile display devices, offers excellent thermal and mechanical properties as well as chemical strengthening capabilities. However, foldable devices require ultra-thin glass (UTG) under <50 um for folding with low radius of curvature which demands high resistance against the bending tensile strength. Previous studies have shown that SAS glass exhibits the best ion-exchange properties for chemical strengthening when the Al_2O_3/Na_2O ratio is 1. Also, the incorporation of B_2O_3 into the glass composition is necessary to lower the Young's modulus. However, study on a glass composition which simultaneously satisfy low Young's modulus and high CS after ion exchange has not been properly carried out. In this study, two series of glasses were fabricated with fixed B_2O_3 content at 15 mol% and SiO_2 content at 55 mol%, respectively. For both glass series, Al_2O_3/Na_2O ratio was fixed at 1 to ensure ion exchange. Various thermal and mechanical properties were analyzed, including Vickers hardness and Young's modulus. Chemical strengthening characteristics were evaluated using FSM. Structural variation depending on the composition was studied by Raman spectroscopy, solid-state NMR, and XPS. Additionally, MD simulations for the glasses were also attempted to validate the experimental results.

(GOMD-P005G-2025) Compositional Study on $SiO_2-Al_2O_3-B_2O_3-Na_2O$ Glasses for Pharmaceutical Vial ApplicationsY. Kim^{*1}; W. Chung¹

1. Kongju National University, Division of Advanced Materials Engineering, Republic of Korea

The recent outbreak of COVID-19 has led to an explosive growth in the bio-pharmaceutical industry, resulting in an increased demand for glass vials used for the packaging, storage, and transport of pharmaceuticals. To prevent drug contamination and degradation as well as breakage during transport, suitable container materials with excellent thermal, chemical, and mechanical durability are essential. Borosilicate glasses, thanks to their low thermal expansion coefficient and high mechanical strength, have been widely used for various pharmaceutical applications such as vials and syringes as a representative of Type I Class B glass. However, a systematic study on the compositional effect on various properties of borosilicate glasses for vial applications has been rarely reported. In this study, a quaternary glass system based on $SiO_2-Al_2O_3-B_2O_3-Na_2O$ was investigated by varying the glass composition. Thermal expansion coefficients and glass transition temperatures were examined by Thermal Mechanical Analysis (TMA). Mechanical property of the glass was monitored by Micro-Vickers hardness tests. Leaching characteristics of the glasses were compared and evaluated using pH titration and ICP-MS analysis. Structural changes depending on the composition were investigated by Raman Spectroscopy, to understand the compositional role on the thermal, mechanical, and chemical properties.

(GOMD-P006G-2025) Revealing Local Environment and Network Topology of ZrO₂-containing Mullite Glasses using Machine Learning Potential

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2. Kyoto Daigaku, Graduate School of Engineering, Japan

Mullite glass (60Al₂O₃-40SiO₂) is one of the notable binary aluminosilicate glasses recognized for their extraordinarily high Vickers hardness and crack resistance compared to conventional glass compositions. Our recent study has demonstrated that the six ternary, xZrO₂-(100-x)·(0.6Al₂O₃-0.4SiO₂) (ZAS) (x=0, 5, 10, 15, 20, 25), glasses with the same ratio of Al₂O₃ to SiO₂ as mullite glass exhibit higher Vickers hardness than mullite glass. While the structure of ZAS glasses has been experimentally investigated, the interplay for network-forming ZrO₂ and Al₂O₃ species has not been fully elucidated due to the limitations of experimental data. In this study, we modeled the accurate glass structures of the ZAS series using machine learning potential (MLP). Ab initio molecular dynamics calculations were performed to collect the training dataset for MLP. As reported in our previous study, we employed a pre-trained model constructed from the large database provided by Meta to model a more realistic glass structure. Then the pre-trained model was fine-tuned with the ZAS glasses and crystals dataset. To confirm the accuracy of newly developed MLP, we compared MD-derived densities and Al coordination numbers with experimental data. The six ternary glasses' local environment and glass network topology were investigated.

(GOMD-P007G-2025) Pressure-Induced Structural Transformations at Different Length Scales in Soda-Lime Silica Glasses

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2. Aalborg University, Department of Chemistry and Bioscience, Denmark

Although soda-lime silica (SLS) glasses are widely used, we still do not fully understand their short-range order (SRO) and medium-range order (MRO) structures. This study examines how pressure affects the structure of simulated SLS glasses with different modifiers to silica ratio. We characterize the SRO by analyzing coordination numbers, Qⁿ speciation, and bond angle distributions. For MRO signatures, we utilize persistent homology and classical ring analysis to capture both chemically and non-chemically bonded rings, as well as voids identified through persistent homology. Our findings reveal that increased pressure leads to densification, causing significant changes in coordination numbers and bond angles in the SRO, alongside alterations in MRO characteristics. By increasing the pressure, we observe that chemically and non-chemically bonded loops and voids have earlier birthtime and deathtime in the persistent diagram. These results emphasize that not only are MRO structures increased in containing modifiers in SLS glasses with higher modifier percentages, but also densification due to increasing the pressure leads to the identification of more loops and voids in persistent homology, showing that MRO signatures such as loops and voids in SLS glasses can be changed through varying pressure and compositions.

(GOMD-P008UG-2025) Four-Coordinated Boron Pairs in Lithium Borate Glasses: Implications for the Borate Anomaly

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2. Coe College, Physics, USA
3. Alfred University, Glass Science, USA

The borate anomaly is characteristic of borate and borosilicate glasses and carries significant implications for technological glasses, due to the associated non-linear changes in the properties. Despite numerous attempts to describe the origin of the anomaly, debate remains prevalent in the literature. Here, a series of lithium borate glasses x Li₂O - (x-1) B₂O₃ were simulated at ambient and high pressures using

molecular dynamics to study the boron anomaly in the glass along with the pressure effects on the structure. Several structural models were used to contextualize the boron structural units and their behavior. This study shows the presence of four-coordinated boron structural unit pairs, as described in P.K. Gupta's random-pair model, and as a result describes a possible origin of the borate anomaly.

(GOMD-P009UG-2025) Molecular Dynamics Simulation Study of Composition Effects on the Diffusion of Calcium-Magnesium-Aluminosilicate Glasses

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The infiltration of calcium-magnesium-aluminosilicate (CMAS) into thermal barrier coatings (TBCs) at elevated temperatures poses a critical challenge to the performance and durability of gas turbines. CMAS primarily originates from environmental contaminants such as sand and volcanic ash, with its composition varying widely, leading to diverse diffusion and melting behavior at high temperatures. In this research, molecular dynamics simulation (MD) was employed to investigate the diffusion of CMAS compositions with varying silica contents, MgO/CaO ratios, and (MgO+CaO)/Al₂O₃ ratios over a temperature range spanning the glass transition temperature (T_g) to the liquidus temperature. The modeling results revealed that the diffusivity of the constituent ions consistently follows the trend Mg²⁺ > Ca²⁺ > Al³⁺ > Si⁴⁺ across all investigated compositions. Silica content was identified as the primary factor affecting diffusivity; higher silica levels significantly reduced diffusivity, especially for Si⁴⁺ and Al³⁺. Additionally, the diffusivity increase with temperature was slower for compositions with higher silica content than those with lower silica content. In contrast to the silica content, variations in MgO/CaO and (MgO+CaO)/Al₂O₃ ratios had a relatively minor impact on diffusivity.

(GOMD-P010-2025) Transitions in silica glass studied by the novel High Temperature Scanning Indentation approach

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The increasing use of oxide glasses in high-tech applications illustrates the demand of novel engineering techniques on nano- and microscale. Due to the high viscosity of oxide glasses at room temperature, shaping operations are usually performed at temperatures close or beyond the point of glass transition T_g, i.e. 1200°C for Fused Silica. Recent micro-pillar-compression results, however, indicate a brittle-to-ductile transition (BDT) to occur at much lower temperatures in the range of 200-400 °C. Due to the experimental complexity, the temperature resolution of micro-pillar-compression experiments is inherently limited. This is where new testing protocols like the "High Temperature Scanning Indentation" (HTSI) can play to their strengths. With a data point recorded every 1-2 °C the HTSI approach allows a quasi-continuous measurement of mechanical properties such as Hardness, Elastic Modulus and the coefficient of strain rate sensitivity with a previously unattainable data density. As an indicator for changes in plastic deformation processes, the changes of the coefficient of strain rate sensitivity with temperature are of particular interest. In this contribution the HTSI approach is applied to pure silica glass as well as soda-lime-silica glass up to temperatures of 600 °C to investigate the point of BDT and T_g in case of soda-lime-silica glass.

(GOMD-P012UG-2025) Scale-Up of a Hard and Crack-Resistant Glass

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Recent advances in glass technology have led to the development of oxide glasses with exceptional hardness and crack initiation resistance. However, scalability remains a critical barrier to their widespread adoption in industrial applications. Glasses within the peraluminous

MgO-Al₂O₃-B₂O₃-SiO₂ system have shown promising results as scalable glasses with high hardness and crack resistance. However, they face challenges related to high liquidus temperatures and low liquidus viscosity. This study aims to address these issues by designing glass compositions with a larger difference between two key temperatures: T(log 3 Poise) and T(liquidus). Achieving this requires compositional fine-tuning and the optimization of processing conditions to prevent devitrification during the cooling of the glass melt, enabling the production of a glass slab with dimensions greater than 100 mm × 100 mm, a Vickers hardness higher than 7 GPa, and a Vickers crack initiation resistance exceeding 1000 gf. By demonstrating the scalability of this advanced glass, the study is expected to contribute to the development of durable, high-performance glass components suitable for structural, optical, and protective applications.

(GOMD-P013G-2025) Hydrothermally Treated Cesium Borosilicate Glass with Enhanced Crack Initiation Resistance and Indent Volume Recovery

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2. Aalborg Universitet Institut for Materialer og Produktion, Denmark

Recent work has found that a hydrated cesium aluminoborate glass shows a dramatic increase in crack initiation resistance (>400N), along with the ability to recover the volume of an induced indent upon storage in a humid atmosphere. This glass has a low chemical durability and stability, and the hydration effect on glass mechanics drastically diminishes when substituting the cesium modifier with other alkali modifiers. Therefore, we here study the effect of hydrothermal treatment of a cesium borosilicate glass with higher chemical durability compared to the cesium aluminoborate glass. We find that hydrothermal treatment of the rigid silica glass structure necessitates both elevated temperatures and higher relative humidity to allow for significant property changes. Still, hydrothermal treatment causes both an increase in crack initiation resistance and a decrease in indent volume, while maintaining the sample's transparency. Thus, these findings shed light on the potential positive effects of using hydrothermal treatment to modify the mechanical properties of oxide glasses.

(GOMD-P014G-2025) Intrinsic limitation of conductivity in depolymerized fast-ion glassy networks

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The electric properties of a model fast-ion electrolyte ((100-x)SiS₂ - xNa₂S) glass is investigated by means of molecular dynamics simulations. These systems appear promising for battery applications and the conductivity is thought to be essentially driven by the concentration of charge carriers (Na) so that the usual amount is found to be between 50% and 80%. We first set up a Buckingham-Coulomb type potential that describes the atomic structure and experimental structure functions (structure factor) in an improved fashion with respect to previous interactions. A systematic investigation of properties with modifier content Na₂S permits to acknowledge an unexpected result which manifests by a near constant of the conductivity upon Na₂S for various isotherms. The analysis indicates that unlike Li-based electrolytes, the diffusivity difference between networks species (Si,S) and ions (Na) is too small so that the contribution to conductivity is essentially driven by the former. The main reason is the reduction of the concentration of network species near 80% of network modifier without any dramatic increase in Na diffusivity, and the emergence of molecular Na₂S in the structure at large modifier content which leads to profound structural changes.

(GOMD-P015-2025) Tailoring Chalcogenide Glasses for Novel Applications

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Among various infrared optical materials, chalcogenide glass is the only amorphous material that is transparent from mid-wave infrared to long-wave infrared, occupying the optical applications of infrared thermal imaging, infrared photonic chip, infrared sensing and remote sensing that other optical glasses cannot enter into. Besides the excellent optical properties including wide transmission range, large linear/nonlinear refractive index, and low thermal coefficient of refractive index, chalcogenide glass also possesses intriguing acoustic-optic, thermoelectric and ionic conduction properties, which are promising for optical, photonic, and energy applications. The R&D of novel chalcogenide glasses and their applications has become one of the research hotspots both in infrared optics and energy fields. Here we would like to present a brief report concerning the recent advances of novel chalcogenide glasses and their applications in our research group @ Ningbo University.

(GOMD-P016UG-2025) Understanding Amorphous GeO₂ Nanoparticle Growth and Stability via Kinetics

A. Kayton*¹; F. Lopez¹; S. Cayo¹; J. F. Destino¹

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As optical technology advances, attention is pulled to the variety of approaches to produce glass alternative to current conventions. Current studies are focused on additive manufacturing (AM) of glass from nanoparticle precursors using silicon dioxide (silica, or SiO₂) or germanium dioxide (germania, or GeO₂) glass formers. The growth chemistry of germania is more complex, and subsequently less understood than silica. To further develop the current understanding of germania particle growth and its potential for AM applications, this project examines the growth kinetics of GeO₂ nanoparticles at varying solutions of pH, with a desire to identify key routes that inhibit crystallization. This study examined pH-adjusted GeO₂ nanoparticle samples that were heated (60 C) over six hours and analyzed in real-time. Nanoparticle growth was quantified using time-dependent dynamic light scattering (DLS) to determine particle diameter and attenuated total reflectance (ATR) Fourier transform infrared spectroscopy (FTIR) was used to determine particle structure. Results indicate a divergence from traditional sigmoidal growth and crystallization trends in strongly acid and basic solutions. Mildly acidic, basic, and neutral solutions produce crystallized nanoparticles within four to six hours of heating, whereas nanoparticles remain amorphous starting at pH 12.0 and below pH 2.0.

(GOMD-P017G-2025) Impact of K and Mg on Nepheline Crystallization in High Level Waste Glasses

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The Hanford site in Washington State houses millions of gallons of high-level radioactive waste (HLW), designated for vitrification into a borosilicate glass waste form. However, upon cooling of the HLW glass melt, nepheline crystallization (NaAlSi₃O₈) can occur, posing a significant challenge to the vitrification process by compromising the chemical durability of the resulting waste form. Consequently, extensive efforts have been made to understanding compositional factors influencing nepheline crystallization, which include concepts such as the optical basicity and ionic field strength. In this work, we will use these concepts as a tool to (1) understand the structural role of K and Mg in [aluminosilicate/borosilicate] glass system, followed by (2) their relation to the kinetics of nepheline crystallization.

(GOMD-P018G-2025) Bromine Addition to Sulfate-containing Hanford Site Low Activity Waste Alumino-Borosilicate Glasses

K. Rodman^{*1}; J. Bussey¹; J. McCloy¹

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Vitrification is accepted as the primary method for immobilizing low activity waste (LAW) at the Hanford Site. However, challenges have emerged in its implementation, including the formation of sulfurous salts within the vitrified melt. The presence of halides is thought to compound this effect due to their affinity for Na. To establish a fundamental understanding of their roles in vitrification, it is beneficial to investigate halides in LAW compositions. The current work examines the relationship between composition and structure of an alumino-borosilicate glass containing sulfate and varying amounts of bromine. Preliminary results indicate NaBr crystallization with as little as 3 mol % Br addition. The NaBr salt contains some Na₂SO₄, demonstrating that Br addition adversely affects sulfate retention. The structural mechanisms underlying bromine incorporation and retention in the glass matrix will be discussed, and comparisons will be drawn with studies on other halides.

(GOMD-P019G-2025) Terahertz Time Domain Spectroscopy of Cermets for Nuclear Waste Immobilization

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2. Alfred University, Inamori School of Engineering, USA

Various nuclear waste forms have been used to immobilize legacy and commercial nuclear wastes for safe long-term geological disposal and isolation around the world. With the world's largest Hanford vitrification plant beginning to operate in Washington state in 2024, large amounts of borosilicate glass will be processed to immobilize low-activity wastes (LAW). However, commercial nuclear waste containing large amounts of metals along with spent fuel and other chemistries need a different waste form for efficient disposal. Ceramic metal composites (cermets) can be used for immobilizing these waste streams into one waste form. We have processed and characterized a series of model systems SS 316-ZrO₂ and SS 316-SiC cermets over ceramic-to-metal ratios of 20-80, 35-50, and 50-50, using spark plasma sintering (SPS) and hot uniaxial pressing (HUP). The temperatures and pressures of processing are 700-900 degrees Celsius and 50 MPa for SPS, and 900-1100 degrees Celsius and 85 MPa for HUP. We have used terahertz time domain spectroscopy (THz-TDS) to record optical and dielectric constants. Ceramic-metal ratio, density, and porosity of these cermets significantly affect the THz properties. We present our results and interpretation, which are useful for nondestructive examination of these waste forms.

(GOMD-P020G-2025) Interionic Effects of F⁻ and PO₄³⁻ and Cation Preference in Simulant Direct-Feed High-Level (DF-HLW) Alumino-Borosilicate Glasses

R. Bergman^{*1}; J. Bussey¹; A. Azeddioui¹; J. McCloy¹

1. Washington State University, School of Mechanical and Materials Engineering, USA

Due to processing nuclear materials, the Hanford site contains 55 million gallons of nuclear waste requiring vitrification to allow for long-term storage. The complexity of these waste streams is driving research on understanding the interactions between the chemical species that form the complex matrix. This project seeks to examine the interactions that occur in waste materials with the numerous anions present. Furthering our understanding of these anions is critical, given the impact they have during waste processing via crystallization or salt formation. Specifically, the role of F⁻ and PO₄³⁻ in simplified direct-feed high level waste (DF-HLW) glass compositions are explored. Two simulated DF-HLW glass series with progressive incorporation of F⁻ and PO₄³⁻ were synthesized, one with mixed Na

and Ca, and one with only Na. Various spectrographic and diffractive techniques were utilized to determine glass characteristics such as structure, density, and T_g. Results show significant interactions between F⁻ and PO₄³⁻, including a higher propensity to crystallize through the formation of fluorapatite (Ca₅(PO₄)₃F). In addition, results show significant differences between the alkali only and mixed alkali-alkaline earth series. These results will help refine the models for Hanford site vitrification as it relates to simultaneously present anions.

(GOMD-P021-2025) Selected transformation of dicalcium phosphate dihydrate (DCPD) to lead-substituted apatite for usage of stabilization of pollutants

E. Ishida^{*1}; M. Tafu¹; T. Toshima¹; Y. Hata²; K. Nagano²; y. Hagino²

1. National Institute of Technology, Toyama College, Japan
2. Fudo Tetra Corp, Japan

In our previous studies, dicalcium phosphate dihydrate (DCPD, CaHPO₄·2H₂O) reacts with fluoride ions to form stable fluorapatite (FAP, Ca₁₀(PO₄)₆F₂). We have been investigating the immobilization of various pollutants in the environment using the DCPD, such as polluted soil in industrial sites. Here, we aim to stabilize lead ions by using the DCPD. Our previous results indicate that the DCPD reacts with lead ions in lower concentrations to form lead-substituted hydroxyapatite (PbHAp, Pb_xCa_{10-x}(PO₄)₆(OH)₂) and hydroxy pyromorphite (HPY, Pb₁₀(PO₄)₆(OH)₂). Formation of the HPY from DCPD remained lead ions in the solution after the reaction. Stabilization of lead ions in wastes is suitable for forming the PbHAp with lower solubility than the HPY. This study aimed to investigate an appropriate method for the selective transformation of the DCPD to the PbHAp in an aqueous solution containing small amounts of lead ions. This presentation describes the results of attempting to selectively transform the DCPD to the PbHAp by nano-hybridizing it with other calcium phosphate particles for the remediation of polluted sites.

(GOMD-P022G-2025) Effects of Rare-Earth Elements on Sulfur Solubility in Borosilicate Glasses for Nuclear Waste Immobilization

S. Kim^{*1}; J. Cho¹; J. McCloy²

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Enhancing sulfur (S) solubility in borosilicate glasses while maintaining durability is critical for the development of advanced glass matrices for nuclear waste immobilization. Phosphorus pentoxide (P₂O₅) has been shown to increase the solubility of sulfur by forming sulfate species; however, its addition often leads to phase separation, resulting in poorly durable phases. To mitigate this issue, this study investigates the structural modifications introduced by incorporating rare-earth elements such as neodymium (Nd) and other lanthanum (Ln). Preliminary analyses suggest that Nd and Ln additions influence the borosilicate network by forming stable rare-earth phosphate complexes, which potentially suppress the formation of undesirable phases. Advanced characterization techniques, including XRD, Raman spectroscopy, NMR, and XAFS, are employed to elucidate the structural role of Nd and Ln in the glass network. The results include increased sulfur solubility and improved durability of the glass matrix. Structural insights from spectroscopic analyses are anticipated to reveal a higher degree of network polymerization facilitated by the rare-earth elements, leading to enhanced chemical durability. These findings will contribute to the design of borosilicate glasses optimized for the immobilization of sulfur-rich nuclear waste streams.

(GOMD-P023G-2025) Ultrafast Laser Welding and Characterization of Glasses and Welded JointsK. Matthies*¹; S. K. Sundaram²

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Welding of glass-on-glass was accomplished using picosecond laser with processing parameters for laser filamentation utilizing a 1064 nm laser, 15 ps pulse duration, and a repetition rate of 155 kHz; along with the laser welding processing utilizing a higher repetition rate of 1000 kHz. The welded joints were characterized using scanning electron microscopy with electron dispersive spectroscopy (SEM EDS) images of microscopic weld lines along with elemental distribution and x-ray fluorescence (XRF) for the composition of the weld lines post-weld. In addition, we used terahertz time domain spectroscopy (THz-TDS) and dual-camera THz scanner to image the joints and report optical and dielectric constants of the glasses and the joints. We will present our results and interpretation to demonstrate non-contact examination of welded glasses for a broad range of applications.

(GOMD-P024G-2025) Terahertz and optical properties of different oxide based glassesH. Kaur*¹; R. Puranik²; S. Prabhu²; S. Kaur¹; N. Verma¹; G. Sharma¹

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Nowadays, terahertz technology is emerging in the field of construction, pharmaceutical, defense, security, communications and material characterization. The glasses are very less explored in literature to design the terahertz components. This study deals with the terahertz properties of different type of oxide families for the applications like terahertz low pass filters, waveguides & substrate for other components. Majorly, this study is focused on sodium germanate, calcium germanate, bismuth borate, bismuth germanate, alkali aluminosilicates and lead aluminosilicates oxyfluoride systems. Using THz-time domain spectroscopy, the refractive indices and dielectric constant of glasses have been calculated. In the literature, the structure terahertz property relationship has been made. To the best of our knowledge, the nonlinear optical and terahertz properties relationship in the glasses has not been studied so far. The linear optical properties have been studied with the help of ellipsometry and UV-Vis Spectroscopy. The nonlinear properties can be explored with Z-scan & Third Harmonic Generation (THG).

(GOMD-P025-2025) Thermal conduction in sodium silicate glasses is governed modal phase changesP. Rasmussen¹; S. S. Sorensen*¹

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Theoretical descriptions of thermal conductivity in glasses are notably more challenging than in crystalline materials, leading to a limited understanding beyond simple glasses like glassy SiO₂. This gap is particularly evident in modified oxide glasses, where additional oxides, such as alkali oxides, disrupt the network structure and alter properties like elasticity and thermal conductivity. Despite their prevalence, the fundamental understanding of heat transfer in modified glasses remains poor. To overcome this the present study investigates sodium silicate glasses [xNa₂O-(100-x)SiO₂], focusing on how increasing Na₂O content influences thermal conductivity. Modal analyses reveal that higher Na₂O levels enhance vibrational localization, distort the modal phases (i.e., acoustic vs optical character), and ultimately lower modal contributions to thermal conductivity. The disordered vibrational phases of sodium ions, compared to the network-forming silicon and oxygen species, are identified as a key factor in the reduced thermal conductivity with increasing Na₂O. These findings provide new insights into glassy heat transfer and the relationship between thermal conduction and vibrational characteristics in glasses.

(GOMD-P026G-2025) The Impact of Anion Ratio on Defect Concentration and the Electrochemical Performance of Sodium Phosphosilicate Mixed Oxy-Sulfide Glass ElectrolytesK. M. Maier*¹; N. Tader¹; A. G. Wakefield²; S. W. Martin¹

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All-solid-state sodium batteries are an attractive option for the future of grid-scale energy storage due to the relative abundance of sodium when compared lithium and reduced risk of fire. To achieve this, novel electrolyte materials, such as glassy solid electrolytes (GSEs) are required. However, the presence of sulfur-defects in these GSEs threatens to undermine their usefulness due to associated reductions in ionic conductivity and stability. Preliminary investigations indicated that sulfur defect concentration increases with increasing oxygen content. However, dilute oxygen doping is required to improve electrochemical stability of GSEs against sodium metal. In this study, seven glasses were synthesized from the series (1-γ)Na₂S + γ{(1-z)[(1-a)SiS₂+aPS_{5/2}]+zNaPO₃} with anion ratio (O/[O+S]) ranging from 0 to 0.226 while glass former ratio (P/[P+Si]) and R-value (Na⁺/[P+Si]) were held constant at 0.274 and 2.5, respectively. Raman and infrared spectroscopy techniques were used to characterize the short-range order structure and sulfur-defect morphology of the GSEs. Differential scanning calorimetry was used to determine the thermal properties and glass transition temperatures. Lastly, the ionic conductivity and cyclic stability were investigated with electrochemical impedance spectroscopy and cyclic voltammetry.

(GOMD-P027-2025) Precision structured glass for PV and other applicationsW. Kuhn*¹

1. Fives Stein, Glass division, France

PV cover glass is widely produced by the rolling process. This imposes structuring of the air side due to the imperfection of the roller surface. Slight structuring has almost no impact on the geometry of the light transmission towards the solar cell surface. However, deeper structures allow for increased light capture, in particular under oblique angles. Ray tracing simulations allow to quantify the improvements. Solar cell yield improvements are estimated. Further applications of structured glass surfaces are of interest for CPV, greenhouse glazing, improved cooling of solar panels... However, a major issue for all these applications arises from the limitations of the conventional rolling process. Only relatively coarse structures can be manufactured. This has drawbacks, regarding the precision of the light ray modulation. Moreover, coarse structures require a higher mean thickness of the glass sheet. A newly developed continuous printing process allows to overcome these limitations. The process can be applied on structureless rolled glass or even on float glass. High shape precision is achieved even for structures <1 mm dimensions. Glass samples were produced on a lab scale and by a pilot installation on a float production line. The produced structures were evaluated by ray-tracing simulations. Precision structures have the potential of great added value to future applications in PV and architectural applications.

(GOMD-P028UG-2025) The Impact of Silicon Ejection on NaPSiSO Glassy Solid ElectrolytesN. Tader*¹; K. M. Maier²; A. G. Wakefield²; S. W. Martin²

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The ejection of silicon in the milling process has been observed in glassy solid electrolytes (GSE) batched with silicon sulfide, leading to silicon inclusions in the glass. These inclusions can negatively impact thermal properties and processability of the GSE, and therefore are a focus of improvement. However, prior work has shown that the NaPSiSO system is capable of re-incorporating excess

silicon additives into the glass network without causing inclusions of elemental silicon. This work sought to determine if silicon ejection occurs in the milling of NaPSiSO precursor powders despite the lack of elemental silicon inclusions observed in NaPSiSO glasses. Samples of milled NaPSiSO powders were removed from the mill pot at various time intervals, and analyzed using Raman spectroscopy to identify the presence of elemental silicon. Glasses were melted from powders milled at various times to determine if ejected silicon has an influence on the resultant glass. The results indicated that silicon ejection does occur in the NaPSiSO system, but at small enough concentrations that the glass network is able to completely reincorporate ejected silicon during melting.

(GOMD-P029UG-2025) Analysis of structure-property relationships of LiPON doped glassy solid electrolytes (GSEs): $58 \text{ Li}_2\text{S} + 42[(1-x) \text{ SiS}_2 + (x) \{(1-y) \text{ LiPO}_3 + (y) \text{ LiPON}\}]$

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Glassy solid electrolytes (GSEs) are a strong contender for the future of solid-state batteries due to their tunable chemistries allowing for high ionic conductivity and electronic insulative ability. It's important to prioritize electrochemical stability to maintain a long lifespan of the GSE without compromising the other desirable properties. In previous research, LiPON has been incorporated to improve the electrochemical stability and ionic conductivity and it was found that increasing LiPON content has a positive and then negative effect on the ionic conductivity. The research was conducted on a limited compositional window, providing insufficient information to determine the structure-property effects with high LiPON incorporation. This research is intended to expand on the series to analyze the effect of LiPON and develop a more comprehensive analysis. Raman spectroscopy is used to analyze the local short range order glass structure, CHNS combustion analysis and X-Ray Photoelectron Spectroscopy are used to quantify the nitrogen species, Electrochemical impedance spectroscopy is used to analyze the ionic conductivity, differential scanning calorimetry is used to analyze the changes in glass transition and crystallization temperatures, and sound velocity measurements are taken to measure the mechanical properties.

(GOMD-P030UG-2025) The Effect of LiCl Doping in the $50 \text{ Li}_2\text{S} + 45 \text{ SiS}_2 + 5 \text{ Li}_{3,48}\text{SiO}_{3,74}$ Glass System

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As global energy demands rise, solid-state batteries (SSBs) are being explored as a safer alternative to lithium-ion batteries due to their reduced risk of thermal runaway. Glassy solid electrolytes (GSEs) are particularly promising due to their high ionic conductivities and tunable chemistries. The $\text{Li}_2\text{S} + \text{SiS}_2 + \text{Li}_{3,48}\text{SiO}_{3,74}$ GSE system is one such solution to make SSBs comparable with the lithium-ion batteries used globally today. For SSBs to meet industry demands, their electrolytes must have an ionic conductivity greater than 1 mS/cm^2 , comparable to current liquid electrolytes. In this work, lithium chloride salt was doped into the glass system to reach higher ionic conductivities and improve cycle stability in SSBs. Raman spectroscopy and Fourier transform infrared spectroscopy were used to analyze the effect the lithium chloride has on the structure of the glass. Electrochemical techniques were used to study how lithium chloride affects the ionic conductivity and performance in a solid-state battery.

(GOMD-P031-2025) Advanced melting technology for low carbon footprint PV glass

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PV glass panels manufacturers claim lifecycle CO₂ footprints as low as $400 \text{ kgCO}_2\text{eq/kWp}$ for c-Si panels, and 220 kg/kWp for thin film panels. The glass production contributes to these footprints with 5% and 12% in function of panel type and design. The glass melting process presents a major part of this 'glass' CO₂ footprint in PV modules. PV glass is today largely manufactured in large, float type melting tanks, with distribution systems towards rolling machines. The standard 'regenerator' design of these melting units leads to specific consumptions of about $5800\text{--}6000 \text{ kJ/kg}$ of melted glass – even for large units with more than 1000 tpd. This presents a high consumption compared clear architectural glass production. We developed an advanced PV glass tank design with regenerative combustion, allowing for a reduction of 800 kJ/kg . A further reduction can be achieved with a high performing oxy-combustion, reaching -25% as recently demonstrated on a mid-size float tank. For a large PV glass tank, oxy-gas consumptions below 4000 kJ/kg are possible. But the most significant reduction is reached by high electrical boosting! The footprint of the combustion can be further reduced from $300 \text{ CO}_2\text{kg/tg}$ to almost $50 \text{ CO}_2\text{kg/t}$ of PV glass – on the basis of green electricity. Significant reductions of the glass CO₂ footprint in PV module production are therefore feasible, with the evolution of the melting technology.

(GOMD-P032UG-2025) Glass-refractory interactions with industrial scaleup of LionGlass

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LionGlass is Penn State's patent-pending group of phosphate-based glass compositions designed to reduce the glass industry's growing carbon footprint. As glassmaking companies have started to reach out about this new environmentally friendly glass, it has become increasingly important to develop a method to determine if there are any compatibility issues between the glass and ceramic refractory materials. Laser Ablation Inductively Coupled Plasma Mass Spectroscopy (LA-ICP-MS) is an advanced way to determine how far the glass diffuses into the refractory material. With the data collected in LA-ICP-MS, diffusion coefficients and elemental activation barriers can be determined based on melting temperature. Results showed that an element's activation barrier decreases with increasing atomic number. This finding indicates that in this glass system, ion size is not the most important factor to be considered, and instead other factors such as molecular structure and charge have more influence in the diffusion process.

(GOMD-P033-2025) Decarbonized glass melting with high TRL tank technology

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In view of the climate crisis, the decarbonation of glass melting processes is a vital priority. Very low CO₂ melting technology must be implemented now – considering the campaign time of the production assets of the glass manufacturers. A wide range of solutions for decarbonation is proposed, covering CCS/CCU, hydrogen combustion, biofuels and electrification. To start with, the application of solutions depends on the cost and availability of the energy carrier. However, whichever technical solution is considered, it will always rely upon the readiness of melting technology. Glass companies are well aware of the risks that arise from significant changes in the tank design, due to the complexity of the melting process. The currently discussed technical solutions are reviewed in the light of their technical maturity. On this basis, a classification of the TRL

level is attempted. Melting tank designs with different TRL levels will be presented. Our full electric or hybrid designs already reach the high TRL levels. The high TRL level of these designs is achieved by thorough integration of the principal melting process requirements, regarding heat fluxes, melt convection and glass quality target. For the design modifications to meet the new requirements, only well proven construction elements are applied to maintain a high TRL level. Results of concept studies, as well as results from tank operation, are presented.

(GOMD-P034-2025) Create low-carbon limes from unused alkaline in washing drainage of returnable glass bottles

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Returnable glass bottles are widely used in beverage bottles. They are recognized as eco-friendly because they are reusable without the remelting process of collected glasses. However, washing the used returnable bottle requires cleaning liquid containing a few percent sodium hydroxide (NaOH). A neutralization process is needed by adding sulfuric acid to the effluent to decrease the pH value and make it suitable for public drainage after washing and rinsing used bottles. We have investigated the recovery of a small amount of NaOH in the washing drainage to low-carbon limes (calcium hydroxide and carbonate) using recycled gypsum powder as calcium resources. Our previous study showed calcium hydroxide was successfully obtained from an aqueous solution containing 1w/v% of the NaOH. This study investigated the combined process of calcium carbonate recovery and the washing drainage's neutralization using recycled gypsum powder. This process was applicable to create low-carbon calcium resources by washing the returnable glass bottle and obtaining the benefit of decreasing the carbon footprint for the glass bottle recycler. This presentation summarizes our achievements in creating low-carbon lime resources from washing drainage of returnable glass bottles and the environmental benefits to the glass bottle industries.

(GOMD-P035UG-2025) Thermal Treatment and Structural Evolution of Hybrid Glass Materials Derived from Nanoparticles

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Nanoparticles have been used as feedstock materials to additively manufacture (AM) variable refractive index freeform optics in compositions inaccessible by conventional melt quench techniques. Germanium and silicon dioxide (a.k.a., germania-silica or GeO₂-SiO₂) glasses exhibit promise for such applications but suffer from several well-known challenges regarding the differing chemical and thermodynamic properties of germania and silica. Thus, the growth of germania-silica nanoparticles and the optimization and ability to heat treat such materials to fully dense glass materials are important. Here, GeO₂-SiO₂ glass materials of varying GeO₂ wt % were examined over the course of the heat treatment process to investigate the role of composition and heat profile on the material microstructure, chemical composition/network structure, and homogeneity. Differential thermal analysis (DTA) was used to determine glass transition and melting temperatures of synthesized materials. From these results, ideal thermal profiles were proposed and applied to replicates of GeO₂-SiO₂ compositions. At various stages of processing, microstructure was probed using scanning electron microscopy (SEM), chemical composition/network structure was probed using Raman spectroscopy, and homogeneity was probed using energy-dispersive X-ray spectroscopic mapping and backscatter electron detection by SEM.

(GOMD-P036UG-2025) Effects of Particle Size and Surface Chemistry on Direct Ink Write Glass Printing

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Glass additive manufacturing (AM), or 3D printing, enables improved precision and compositional control not viable by melt quench techniques. Direct ink writing (DIW) is a glass AM method by which sol-gel-derived silica nanoparticles or commercial fumed silica particles are suspended in a colloid slurry and extruded to print a gel preform that can be consolidated into a fully-dense glass component by ceramic processing. In this presentation, we study how ink composition influences printability (i.e., rheology) and network consolidation (i.e., microstructure and optical transparency). Rheology was modified by varying ink solvents, specifically, the relative ratios of conventional DIW solvents (propylene carbonate and tetraglyme) and silica particle surface area, chemistry, and charge. From these results, the rheology was characterized, indicating polar silica particles achieve a higher solid loading in majority propylene carbonate, and non-polar silica particles disperse best in majority tetraglyme solvent mixtures. Furthermore, greater surface area particles more readily sinter to transparency. This data was used to tune ink formulas for printing applications, with several examples of high-resolution printing (< 200 μm feature size) shown. Results from incorporating polymeric binders and experiments towards understanding limitations to achieving transparency in some particles are also presented.

(GOMD-P037-2025) Literature Review on High Temperature Glass-Ceramic Sealant Research

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Tomorrow's high temperature glass sealants may require temperatures above 800 °C (<https://doi.org/10.1016/j.ijhydene.2017.08.105>). Increasing cation field strength is one avenue for attaining glasses with suitable glass transition temperatures (<https://doi.org/10.1007/s00339-014-8369-4>). Since adding high cation field strength ions tends to raise glass melting temperature, it is useful to assess the impact of a low temperature synthetic approach on performance (<https://doi.org/10.1007/s10853-015-9428-8>). From an operating stability, avoiding crystallization entirely through suitable compositional selection has the advantage of simplicity (<https://doi.org/10.1016/j.ceramint.2019.10.266>). Conversely, compositions using a variety of high field strength cations can be assessed for their impact on crystallization (<https://doi.org/10.1021/acs.inorgchem.0c01567>). Moreover, the impact of various types of structural rearrangement (due to fictive temperature changes)- including crystallization- on relevant properties (such as fracture toughness), is key to device stability (<https://www.sciencedirect.com/science/article/abs/pii/S037877531002241X>). For this, it is advantageous understand which minerals crystallize within a particular glass family (<https://doi.org/10.1016/j.jnucmat.2010.04.021>). If crystallization proves unavoidable, would predicting the "thermodynamic structure" of a fully crystallized system be useful?

(GOMD-P038G-2025) Insights into the dissolution of borosaluminosilicate glasses using solid-state NMR

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The vitrification of radioactive ions in borosilicate glasses has emerged as a viable option for the long-term immobilisation of nuclear waste. However, in a multi-barrier system for radioactive waste disposal, it is necessary to account for the possibility of failure over long time periods. This research focuses on the structural development of the water-glass interface using nuclear magnetic resonance (NMR) spectroscopy to measure changes in the surface layer as a function of glass corrosion. ¹¹B, ²³Na, ²⁹Si and

²⁷Al magic-angle spinning (MAS) and double-resonance NMR are used to infer coordination environments and connectivity relevant to elemental interdiffusion and network reorganization at solid surfaces. These results are interpreted in terms of previously proposed mechanistic steps in glass alteration. The correlation of structural changes with time-dependent mass loss and elemental release into solution provides key constraints to refine long-term predictive models for glass durability. These results will contribute to improved materials and processes for long-term immobilization of radioactive waste.

(GOMD-P039G-2025) Understanding the optical and photoelastic properties of lanthanum borate glasses through spectroscopic investigation

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Lanthanum borate glasses with varied network forming and modifying agents exhibit unique and desirable properties for a variety of applications. However, spectroscopic methods to elucidate the local environment at the lanthanum sites pose spectroscopic challenges. The nuclear magnetic resonance (NMR)-active ¹³⁹La nucleus has a large quadrupole moment which produces lineshapes that can obscure structural information. Additionally, the spectral resolution of the characteristic x-ray photoelectron spectral (XPS) La 3d_{5/2} line is hampered by multiplet splitting, making deconvolution difficult. In this work, the optical properties and chemical structure of glass samples in the Ohara LAH family were characterized with the goal of understanding the wavelength-dependence of their exceptionally high indices of refraction. Compositional and qualitative structural data from XPS and x-ray fluorescence (XRF) are used to complement insight from solid-state multinuclear NMR and Raman spectroscopies. Careful analysis of the spectra and vibrational modes of the network forming cations (²⁹Si, ¹¹B, ³¹P) show an evolving network with increasing lanthanum content. Finally, dispersion of the stress-optic response using the method of Dixon and Cohen is presented, with comparisons drawn to existing local-order dependent models of photoelasticity.

(GOMD-P040G-2025) Structural disorder in Pb- and Zn-bearing silicate glasses: A view from multi-nuclear solid-state NMR spectroscopy

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Lead (Pb) and zinc (Zn) are among the important elements in amorphous oxides with industrial applications (i.e., bioactive glasses and nuclear waste glasses). Knowledge of structures of Pb-Zn-bearing silicate glasses allows us to quantify their advanced functionality and enables inference of efficient enrichment of these elements in ore-forming magmatic melts. Despite the importance, detailed effects of composition on the structures of Pb- and Zn-bearing silicate glasses and melts remain lacking. Here, we explore the effects of varying MO/Na₂O ratios (M=Pb, Zn) on the atomic structures of Pb- and Zn-bearing Na-silicate and Na-aluminosilicate glasses using multi-nuclear solid-state NMR spectroscopy. The bonding configurations around O, Al, and Si are clearly resolved, identifying the roles of Zn and Pb in the glasses. Particularly, a non-linear decrease in the fraction of Na-O-Si with increasing MO content confirms that Zn and Pb mainly act as network modifiers, while Zn could charge-balance Al in Na-free aluminosilicate glasses. Mixing of Na-Zn and Na-Pb deviates from a random distribution, exhibiting chemical ordering, and controlling overall configurational entropy. An increase in Zn and Pb content within the glasses leads to a higher degree of structural disorder, potentially contributing to a more flexible melt structure and enhancing partitioning properties.

(GOMD-P041UG-2025) NMR studies of borosilicate glass alteration related to long-term nuclear waste immobilization

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As the world moves toward carbon-neutral energy, nuclear power is becoming an increasingly prominent source of energy. The associated radioactive waste needs to be sequestered indefinitely to prevent harm to the environment, as some isotopes produced from nuclear reactors remain radioactive for over 1 million years. Vitrification in borosilicate glass is an established technique for nuclear waste storage, however, over very long periods of time, glass waste forms may come into contact with water. Prolonged contact with water causes the formation of a surface alteration layer, which appears to slow down the release of radioactive ions from the glass. More information is needed to understand the structure of the alteration layer, and how its structure impacts its properties. Solid-state NMR of ⁷Li, ¹¹B, ²³Na, ²⁷Al and ²⁹Si are used to understand changes in the short- and medium-range order of the alteration layer with respect to the pristine glass. Results are discussed in terms of the retention of radioactive ions in glasses of different compositions, and implications for long-term immobilization of nuclear waste.

(PACRIM-P001-2025) Development of a Wide-Bandgap Semiconductor Materials Hub Using Process Informatics and AI Technologies

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Developing new materials is a lengthy process, and traditional trial-and-error approaches face limitations in achieving high-performance materials. Single-crystal substrates for semiconductor applications suffer from low reproducibility due to uncontrollable process variables, making statistical methods like design of experiments (DOE) difficult to apply and process optimization time-consuming. Recently, process informatics-based artificial intelligence (AI) technologies have emerged as promising solutions to optimize costly and time-intensive crystal growth processes. This presentation introduces a Korean national project aimed at accelerating the development and improving the quality of SiC and GaN single-crystal substrates, key materials for wide-bandgap (WBG) power semiconductors in next-generation applications like electric vehicles. The study applies process informatics and AI technologies to propose innovative methodologies for developing semiconductor materials and processes, aiming to surpass conventional technologies. The project focuses on building a process-informatics-driven database and AI solutions to optimize single-crystal growth for power semiconductors. By offering productivity-enhanced processes and implementing advanced manufacturing technologies, this study contributes to the advancement of semiconductor material technologies.

(PACRIM-P002-2025) Sonochemically assisted solid-state synthesis of BaZrO₃ powder

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BaZrO₃ has been extensively studied for high-temperature proton conductor. BaZrO₃ powder is typically produced at high temperatures through a solid-state reaction from a mixture of BaCO₃ and ZrO₂ powders. For the solid-state synthesis of oxide powders, the raw materials must be mixed to create a homogeneous mixture with intimate contact between the particles. These mixtures are typically prepared using a ball-mill process. However, collisions between ZrO₂ raw powders and ZrO₂ balls during milling can cause non-stoichiometric Zr contamination and this may affect the properties of the resulting BaZrO₃ ceramics. Here, we present a sonochemical mixing method for contamination-free solid-state synthesis of BaZrO₃ powders. BaCO₃ and ZrO₂ raw powders were mixed using

either the sonochemical or ball-mill method, and then calcined at high temperatures. Detailed structural and electrical characterizations revealed that highly stoichiometric BaZrO₃ powders and the corresponding ceramics could be successfully obtained by adapting the sonochemical mixing process. Our results are not only beneficial for the synthesis of the contamination-free BaZrO₃ powder, but can also be generally applicable to synthesize various contamination-free oxide powders through the solid-state reaction.

(PACRIM-P003-2025) Hydrogen separation and boosting technology using Protonic Ceramic Electrochemical Reactor

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It is expected to be developed an electrochemical device with a proton ceramic conductive electrolyte that can separate only hydrogen from ammonia cracking atmosphere. It is known that BaZr_{0.4}Ce_{0.4}Y_{0.1}Yb_{0.1}O_{3-δ} and BaZr_{0.1}Ce_{0.7}Y_{0.1}Yb_{0.1}O_{3-δ} have high proton conductivity. In this study, using these materials, we investigated the reactivity with Co₃O₄, Fe₂O₃, NiO in the temperature range ≤1450 degree C. In addition, the stability of proton conductor and transition metal oxides under ammonia atmosphere was tested at a temperature range between 400 and 600 degree C.

(PACRIM-P004-2025) Inkjet printing of polysilazane and molybdenum disilicide nanoparticles ceramic coatings for high-temperature applications

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The exceptionally versatile processability of preceramic polymers make them an attractive candidate for the additive manufacturing of ceramic components. This study aimed to develop new composite materials for high temperatures by depositing polysilazane and MoSi₂ nanoparticle inks on silicon wafers using inkjet printing. These coatings display chemical and oxidation resistance and high temperature stability. Additionally, MoSi₂ exhibits electrical conductivity, a property that can be adjusted in the final composite by controlling the volume fraction of MoSi₂. The four-probe method will be employed to control this property. The ink meets inkjet printing specifications for rheological and surface properties. The ink displays Newtonian behavior. The nanoparticles were ball-milled and stabilised to achieve a submicron size and prevent agglomeration. The milling process was controlled by measuring the particle size distribution using dynamic laser scattering. Inkjet-printed thin films and multilayers have formed homogeneous green bodies after UV curing. Subsequently, the thin films were pyrolysed in an inert atmosphere, resulting in the formation of defect-free coatings. The progress of the crosslinking process was investigated in detail using FTIR spectroscopy. The decomposition and pyrolysis processes were studied by means of thermogravimetric analysis.

(PACRIM-P005-2025) Investigation on oxidation behavior of nearly stoichiometric polycrystalline SiC-ZrB₂ fibers doped with ytterbium

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Rare-earth (Re) elements generally play a positive role in modifying the oxidation resistance of SiC ceramics, with the oxidation rate decreasing as the radii of Re³⁺ decrease. In this study, SiC-ZrB₂

fibers and ytterbium-doped SiC-ZrB₂ fibers (SiC-ZrB₂-(Yb)) were produced using a polymer-derived method, and their oxidation behavior in air at 1100 °C to 1500 °C was investigated. Both two types of fibers were near-stoichiometric, but SiC-ZrB₂-(Yb) fibers exhibited better oxidation resistance. The tensile strength retention of SiC-ZrB₂ fibers treated for 1 hour at 1200 °C was 96%, while that of SiC-ZrB₂-(Yb) fibers reached 109%. XRD analysis revealed that small amounts of Yb inhibited the crystallization of SiO₂ oxide layer, maintaining its amorphous structure, which improved the strength of the oxidized SiC-ZrB₂-(Yb) fibers. After 1 hour of treatment at 1500 °C, the tensile strength retention and oxide layer thickness of SiC-ZrB₂ fibers were 42% and 650 nm, respectively, while those of SiC-ZrB₂-(Yb) fibers were 55% and 450 nm. This experimental result suggested that moderate doping with Yb element could strengthen the Si-O bonds and further suppress the oxygen diffusion into the fiber interior, reducing the thickness of the SiO₂ oxide layer. This study provided valuable reference for the application of SiC-ZrB₂-(Yb) fibers in high-temperature oxidation environments.

(PACRIM-P007-2025) Structural characterization of materials for Digital Light Processing of silicon oxycarbide ceramics

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Organosilicon precursors with methacrylate groups in the structure can be processed using additive manufacturing technology by Digital Light Processing (DLP) with the obtaining of 3D elements based on preceramic polymers. Appropriate thermal treatment of the samples will provide the polymer-to-ceramic conversion, which is associated with the transformation of the organosilicon polymer into the final silicon oxycarbide (SiOC) structure. In this research, FT-IR and Raman spectroscopy have been applied to characterize the structure of the processed materials, that is, organosilicon polymers obtained by sol-gel synthesis, photocrosslinked preceramic polymers prepared by the DLP method and SiOC obtained after thermal treatment. The conversion of the polymer into the ceramics has been studied by in situ measurements as a function of temperature. The detailed investigations has also covered the final material, since its physicochemical properties depend not only on the Si:C and Si:O ratios, but also on the content of carbon and its form, as it can be incorporated into the structure or may be a separated phase. 3D structures based on SiOC with specific additives may find applications as catalyst support or as components of scaffolds for tissue engineering. This research was supported by the program "Excellence initiative – research university" for the AGH University of Krakow.

(PACRIM-P008-2025) Structural and functional studies of bioactive PDC layers based on SiMeOC system

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The polymer-derived ceramic is a group of materials obtained by pyrolysis of previously selected macromolecular precursors. This method of fabrication is the main advantage of PDCs because their properties can be easily modified at the stage of synthesis, which contributes to many applications e.g. electronic, corrosion protection, etc. The main representative of PDCs is the silicon oxycarbide which structure can be compared to amorphous silica with partial substitution of O²⁻ by C⁴⁻. This significantly improves the mechanical properties of the material and enhances its bioactivity, thermal and chemical resistance. Also, the potential antibacterial properties could be provided by the introduction of the transition material cations. This study aims to investigate the biological and structural properties of 3 systems: SiOC, SiCuOC and SiZnOC. During the conducted research the preceramic polymer with amine groups was synthesised by sol-gel route and deposited on ASIS 316L steel in the dip-coating processes. After the pyrolysis in an argon atmosphere, the structure and microstructure were examined by FT-IR, Raman and SEM+EDS analyses. The bioactive properties were characterized

by the proliferation rate and cytotoxicity tests. This research was funded by the NCN, grant no. 2019/35/B/ST5/00338 and by the program “Excellence initiative – research university” for the AGH University of Krakow.

(PACRIM-P010-2025) Direct Ink Writing for the fabrication of the geopolymer-based components

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The 19th and 20th centuries, while marked by the benefits of industrial revolutions, also initiated environmental issues persisting today. Anthropogenic climate change is primarily driven by the combustion of fossil fuels and industrial processes, including those in the cement industry. The production of Portland clinker alone accounts for approximately 5% of global CO₂ emissions, prompting the search for material solutions with significantly lower emissions. One promising alternative is the use of geopolymers, whose synthesis produces 4 to 8 times less CO₂ and is less energy intensive. Due to the high applicability of these materials in the construction industry and environmental protection (e.g., immobilization of toxic substances), ongoing efforts focus on developing novel methods for producing geopolymer-based materials. This study employed the scalable Direct Ink Writing (DIW) 3D printing technique to fabricate geopolymer components, from small absorbers to large structures like 3D-printed houses. Key advancements include optimizing raw materials, selecting a liquid medium to ensure proper rheological properties, and refining the DIW process for metakaolin-based geopolymers. Structural and microstructural characterization (e.g., FT-IR, XRD, SEM) validated the results. This research was supported by the “Excellence Initiative – Research University” program at AGH University of Krakow

(PACRIM-P011-2025) Characterization of Low Dielectric Properties of Borosilicate fiber glasses for PCB application at a high frequency of 15 GHz

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Digital technologies continue to expand, particularly in terms of data connectivity and processing rates. Low dielectric glass materials require higher frequency bands. E-glass with 6~8 dielectric constant may cause serious damage to PCB with high power loss. So, low dielectric glass material development is needed for 5G/6G application. In this study, bulk glass samples with composition of xBaO-(14-x)CaO-21B₂O₃-57SiO₂-8Al₂O₃ (x=0.5,1,1.5,2,2.5 and 3mol%) were prepared by conventional melt technique. Each composition was melted in an Pt crucible under atmosphere condition at 1550 °C for 2h. Clear glass with transmittance exceeding 92% were fabricated. The optical, thermal and physical properties, such as dielectric constant, density and glass transition temperature were studied. As the BaO content increased, the glass transition temperature of the glass decreased from 669 °C to 663 °C. The dielectric constant decreased as the content of BaO increased. When BaO content move up to 0.5 mol% and 3 mol%, the dielectric constant increased up to 5.2 and 5.0 at 15GHz. However we succeed in manufacturing less than a 5.2 of low dielectric constant glass. It has been confirmed that the glass with good optical, thermal and dielectric properties can be used as PCB substrate materials.

(PACRIM-P012-2025) Nanowire-Bundled Grain Boundaries in Bi_{0.4}Sb_{1.6}Te₃ Thermoelectric Materials

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Improving thermoelectric material performance is essential for energy harvesting and solid-state cooling applications. This study demonstrated a novel structure of Bi₂Te₃-based thermoelectric materials with ZnO nanowire-bundled grain boundaries, realized via atomic layer deposition (ALD) and subsequent spark plasma sintering (SPS). The ZnO nanowires formed at the interfaces due to the rearrangement of the ALD-grown ZnO ultrathin layer over Bi_{0.4}Sb_{1.6}Te₃ powder, driven by localized heating during the SPS process and the anisotropic nature of ZnO. The nanowire-bundled interfaces enhanced phonon scattering, thereby reducing lattice thermal conductivity while maintaining excellent electronic transport. This structural innovation achieved a high figure-of-merit, $zT_{\max} = 1.74 \pm 0.06$ at 373 K and an average zT of 1.57 over the range of 300–473 K. A thermoelectric module fabricated with 127 p-n pairs achieved a record-high conversion efficiency of 6.57% at a temperature difference of 163 K. These findings highlight the potential of nanowire-bundled interfaces to enhance the thermoelectric material performance and pave the way for scalable next-generation energy conversion technologies.

(PACRIM-P013-2025) How PCSA Supports STEM Outreach with Mini Materials Demo Kits

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The ACerS President’s Council of Student Advisors (PCSA), the student leadership committee within ACerS, has developed K-12 lesson plans and other supporting material for the ACerS Mini Materials Demo Kit, lowering the barrier for teachers or volunteers to bring these materials science activities into the classroom. Teachers may be interested in using the Mini Materials Demo Kits but lack the materials science background to write a full lesson or incorporate the demos into their curriculum. Many active ACerS members are interested in supporting STEM outreach opportunities but may lack the resources to coordinate elaborate activities. The PCSA has created resources to give teachers or volunteers the necessary scientific background, detailed demo instructions, discussion questions, and resources for scaling up activities for larger audiences. We have already introduced many teachers to these resources and are continually expanding our classroom network.

(PACRIM-P014-2025) Fabrication of Ce-Based Defective Oxide Thin Films via Spray Pyrolysis for Electrostriction Application

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Cerium-based defective oxides have garnered attention as potential substitutes for lead-based piezoelectric materials due to their remarkable non-classical giant electrostriction behavior and environmentally friendly nature. This study aims to develop uniform and crack-free Ce-based defective oxide thin films using the spray pyrolysis technique. Ce-Zr-O thin films were synthesized with varying cation ratios of 1:3, 1:1, and 3:1, as well as different precursor volumes of 0.5, 1, 2, 5, 10, and 15 ml, deposited on quartz and sapphire substrates. Scanning Electron Microscopy (SEM) analysis revealed that film uniformity significantly improved with precursor volumes of 10 ml and 15 ml, highlighting the importance of deposition parameters in optimizing thin film quality.

(PACRIM-P015UG-2025) Characterization of ammonia gas adsorption property on various calcium phosphate particles

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Dicalcium phosphate dihydrate (CaHPO₄·2H₂O, DCPD) is used in various applications, such as the starting material of various calcium phosphates and as an abrasive in toothpaste. We have focused on DCPD as a by-product of gelatin production from cow bone and utilize it for various environmental applications. This study aims to apply DCPD to the adsorbent of ammonia, one of the significant malodor gases. Adsorption of the ammonia gas on various calcium phosphate particles was done by mixing calcium phosphates and 20 ppm of ammonia gas in the tedlar sampling bag. Ammonia adsorption amount in a unit-specific surface area was calculated using the result of the specific surface area using the nitrogen gas adsorption method. We found that the DCPD has enhanced adsorption properties of ammonia gas compared to other calcium phosphate, such as hydroxyapatite. We also evaluated the dependence of the crystal face on ammonia adsorption by using conventional DCPD with plate-like and petal-like morphology. We also used crushed granules to reset the crystal orientation. The obtained results suggested that ammonia gas adsorption was in part on specific crystal faces.

(PACRIM-P016-2025) Development and characterization of oxide-carbide ceramic composites for cutting applications

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Ceramic matrix composites (CMCs) are of high interest, mainly due to their high hardness, low abrasion and high chemical resistance, also at elevated temperatures. Their main disadvantage is low fracture toughness which often lead to catastrophic failure during exploitation. Presented work shows that the combination of carbide and oxide phases gives strong synergy effect, resulting materials characterized by both high hardness and fracture toughness. Dense Al₂O₃-ZrO₂-MC composites (where MC can be TiC, WC, WTiC or ZrC) were obtained by SPS. The sintered materials were thoroughly characterized, including assessments of basic physical and mechanical properties, microstructure and phase composition. Finally, the cutting performance of the sintered bodies was investigated. The composite with the addition of tungsten carbide had the best mechanical properties and “duplex” structure with fine grained, homogeneous interpenetrating oxide-carbide phases. This material had relative density near 100%, Young’s modulus of 470 GPa, hardness of 21.5 GPa, good fracture toughness and cutting performance comparable to leading commercial ceramics. This work was carried out within the DuplexCER project: “High performance duplex ceramics for efficient machining of nickel superalloys”, co-funded by National Centre for Research and Development within the M-ERA.NET programme (M-ERA.NET3/2021/82/DuplexCER/2022)

(PACRIM-P017G-2025) Grain design strategy for 3D-printed strong and tough textured ceramics

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Three-dimensional (3D) printing of ceramics offers immense potential for producing complex, high-performance components with tailored properties. However, conventional pressureless sintering, commonly used in ceramic 3D printing, suffers from limited control over atomic diffusion, resulting in textured ceramics with suboptimal mechanical properties compared to pressure-assisted

techniques. This limits the simultaneous enhancement of strength and toughness, a critical challenge for practical applications. Herein, we confirm improved strength and toughness by reducing grain thickness in textured alumina with a “brick and mortar” microstructure, using TiO₂-SiO₂-MgO as the interfacial material. This material was selected from 16 oxide compositions based on a theoretical model predicting superior mechanical properties. The effects of grain thickness, aspect ratio and density on strength and toughness were systematically studied by optimizing sintering conditions. As grain thickness decreases, inherent grain properties improve, stress concentration at the crack tip reduces, and stress distribution broadens, enhancing strength and toughness. The highest flexural strength and fracture toughness were 427.3±56.6 MPa and 5.69±2.06 MPa·m^{0.5}, respectively, at a grain thickness of 1.3±0.4 μm. This research provides a solution to the strength-toughness conflict in 3D-printed textured ceramics with pressureless sintering.

(PACRIM-P018-2025) SPS reactive sintering technology in the production of ultra high temperature borides

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Ultra High Temperature Ceramics are characterised by high melting point, hardness, Young’s modulus, as well as thermal and electrical conductivity, but they are difficult to sinter. This study presents the possibility of using the SPS method to produce tantalum and hafnium borides via reactive sintering. In this work, a method combining synthesis from metal powders (Ta, Hf) and boron and sintering in SPS process was used to produce tantalum and hafnium borides. The precursor powders were investigated by scanning electron microscopy and chemical composition by EDS. Sintering processes were carried out at temperatures 2000°C+2200°C, sintering duration was in a range from 5 to 30 min. During the SPS processes, there was a significant increase in temperature at the reaction temperature, a sudden change in the pressing force and the position of the pressing punch. This is due to the occurrence of an exothermic synthesis reaction and the formation of a new phase. The materials were tested for phase composition by XRD, microstructure by SEM-EDS, apparent density, Young’s modulus, Vickers hardness. Acknowledgement: The study was performed under LIDER XIV Research Project No.LIDER14/0268/2023 entitled “UltraCer project: Innovative PVD targets for ultra high temperature ceramic coatings, reactive sintered using the SPS method” funded by the National Centre for Research and Development of Poland

(PACRIM-P019-2025) Temperature dependence and thermal cycling behavior of elastic properties of fireclay and high-alumina refractories determined by impulse excitation

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The temperature dependence and thermal cycling behavior of elastic properties, e.g. Young’s modulus, is of fundamental importance for the performance of fireclay and high-alumina refractories, which are potential candidates for thermal energy storage. The impulse excitation technique (IET) is ideally suited to determine the temperature dependence and thermal cycling behavior of Young’s modulus. In the present work this is done for siliceous fireclay model materials based on kaolin and quartz and for commercial types of fireclay and high-alumina refractories. Of course, the prediction of elastic properties at high temperature requires not only a knowledge of the porosity and microstructure but also complete information on the solid phase composition, including reliable estimates of the glass phase content. This information, which is in the present work obtained on the basis of X-ray diffraction (project GA25-16482S), is indispensable for the correct interpretation of irreversible changes in elastic properties due to thermal cycling. It shown how the IET can

be used to reveal liquid phase sintering effects and to establish the highest temperature at which these materials can be used without suffering irreversible damage. Systematic IET measurements are supplemented by scanning electron microscopy and mercury porosimetry studies.

(PACRIM-P020G-2025) Activation of volcanic ash as support for FeO_x gliding arc plasma deposition and application in the catalytic oxidation of Rhodamine 6G

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This study reports the chemical activation of volcanic ash (VA) to promote the subsequent deposition of FeO_x nanoparticles through a gliding arc plasma assisted route to obtain an efficient Fenton catalyst for a better degradation of Rhodamine 6G in aqueous solution. Plasma Oxidation of Fe (II) solution within the pores of activated VA was performed, then followed the maturation of crystallites (deposited precipitated) thanks to plasma post-discharge species. The Nitrogen physisorption show that, the acid activation of volcanic ash for 2h (AM-2) using H₂SO₄ solution, followed by gliding arc plasma -assisted hydrolytic precipitation of Iron oxide during 30 min (AM-FeO_x-30/0) significantly decreased the size of agglomerates particles of VA, leading to the increases by two orders the magnitude the total pore volume as well as the specific surface area. Scanning Electron Microscopy and Energy Dispersive X-Ray spectroscopy analyses attested to the incorporation of Fe within the activated volcanic ash framework. Fenton catalytic activity of the different materials was evaluated for degradation of Rhodamine 6 G and revealed degradation degrees of 31, 95, 79, and 80 % respectively for VA, AM-2, AM-FeO_x-0/2 and AM-FeO_x-30/4 in the optimum condition. Recyclability tests confirmed the stable catalytic activity of plasma-supported material after 4 runs.

(PACRIM-P021G-2025) Reinterpreting Portuguese Traditional Red Clay Works with Binder Jetting

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Red clay (RC), an historical ceramic material in the Iberian Peninsula, plays a key role in cultural heritage of Portuguese traditional works. With known production centers in Lisboa, Coimbra and Aveiro, those works allure is attributed to uniqueness like Nisa stone inlaid pottery. Discontinued and substituted by other modern stonewares, there is a serious risk of heritage loss. Additive manufacturing (AM) can help keep alive that cultural heritage by bridging new designs and connecting to the old. Binder jetting (BJ) was employed to explore CAD design and RC relation for the reinterpretation of such works and explore the lack of knowledge of processing complex shapes with those materials by newer technologies. BJ is a powder technology that selectively jets binder and enables 3D layer-by-layer assembly. For that a RC commercial composition was ball milled, sieved, mixed with additives and used in a BJ system to reproduce new designs based on Nisa stone inlaid pottery patterning. The effect of debinding and sintering strategies on the densification of RC were studied. Also, the sintered work was digitally captured to understand the deviations from the CAD model. This work highlights the usefulness of using binder jetting systems to produce unique new pieces in red clay that can capture the remnants of the allure of Portuguese traditional RC works.

(PACRIM-P022-2025) Utilization of radiation technique for synthesis of oxygen-deficient TiO₂ nanoparticles

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Oxygen-deficient titanium oxide (TiO_{2-x}), which shows light absorption in the visible light region, is applied as photocatalysts. The TiO_{2-x} nanoparticles (NPs) are synthesized by hydrothermal method, reduction method, and so on; in the case of hydrothermal method, the TiO₂ NP is reacted with reduction agents under high temperature and high pressure conditions in an aqueous solution, and in the case of reduction method, the TiO₂ NP is reacted with hydrogen and/or carbon as reduction agents at high temperature. In both methods, the particle size of TiO_{2-x} NPs would increase because of the heat treatment at high temperature. It is important to control the particle size in nm-range to retain sufficient large surface area which is one of the most important properties for catalytic performance. We have examined synthesis of TiO_{2-x} NPs from liquid phase with radiation technique. TiO_{2-x} NPs with size of several to 10 nm were obtained by electron beam irradiation to an aqueous solution containing Ti-compounds at room temperature. In the presentation, the relationship between the properties of obtained TiO_{2-x} NPs and irradiation conditions (atmosphere, dose, etc.) will be reported.

(PACRIM-P024-2025) Preparation and Mechanical Properties of Glass-Ceramic Composites with Controlled Amounts of Leucite for Dental Applications

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The aim of this study was to evaluate the mechanical properties of laboratory-prepared dental composites and compare their hardness and fracture toughness with those of commercial dental ceramic materials using the Vickers indentation technique. Glass-ceramic composites with controlled crystal fractions were prepared by mixing and firing powder mixtures of laboratory-synthesized leucite, obtained under hydrothermal conditions, and a glass matrix. One of the most common commercial restorative dental ceramic materials, leucite-based glass-ceramics fabricated using the CAD/CAM system, was selected for comparison with the prepared composites. The results showed that the measurement of hardness and fracture toughness depends on several factors, including the testing conditions (indenter geometry, indentation load, and duration of maximum force), the morphology of the polished surface, the type of crack system developed, the measured indentations, and the empirical equations used to calculate fracture toughness. The Vickers hardness values of the laboratory-prepared leucite composites were found to be very close to those of commercial IPS Empress blocks. The Vickers indentation test was confirmed to be a suitable method for evaluating the fracture toughness of small-sized samples of leucite-based dental composites when low indentation loads were applied.

(PACRIM-P025-2025) New Hydrogel and 3D Printing of Highly Resilient Scaffolds for Esophagus Regeneration

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Esophagus is a multi-layered tissue with multiple cell types. Different tissue engineering techniques have shown limited success in producing multi-strata and evenly stratified esophageal tissue whereas 3D printing is promising for fabricating structurally complicated and functionalized scaffolds for esophagus tissue engineering (E-TE). Hydrogels are commonly used for 3D printing of scaffolds but most of them have poor mechanical properties and low printability, making them unsuitable for bouncy and stiff E-TE scaffolds. In this study, a new photocrosslinkable ink consisting of PVAGMA,

cellulose nanocrystals (CNCs) and β -cyclodextrin microspheres (PVA/CNC/CDMS) was synthesized for making four-layered cylindrical E-TE scaffolds via extrusion 3D printing. GMA-conjugated CDMS was designed to covalently bond to surrounding polymer networks to improve chain interactions between PVAGMA and CNC. Epidermal growth factor and fibroblast growth factor 2 were mixed with inks before 3D printing. Mechanical properties of UV-cured inks and 3D printed scaffolds and in vitro GF release behaviour were investigated. In vitro biological experiments were performed to study cell behaviors on scaffolds. Experiments showed governing effects of H-/covalent bonding and physical crosslinking on properties of the ink and its printability for strong and tough E-TE scaffolds which allowed GF loading and cell seeding.

(PACRIM-P026-2025) Advancing Low-Humidity Operation in PEMFCs via Membrane Surface Modification

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Polymer electrolyte membrane fuel cells (PEMFCs) have emerged as a promising and eco-friendly energy source for portable devices and mobile power systems. However, the commercialization of PEMFCs for high-power operations, such as construction and agricultural machinery, faces challenges related to cost and low-humidity environments. This study introduces a novel approach to address these challenges by utilizing a polymer template for pattern transfer with Nafion membranes. The patterned membrane exhibited increased surface area, leading to superior catalyst activity and improved water management. The increased surface area and three-phase interface improved catalyst efficiency and water generation and discharge, showcasing the potential of utilizing generated water as a valuable resource. The introduction of a cost-effective, patterned membrane not only enhances PEMFC performance but also offers a dual advantage by potentially reducing costs associated with humidification maintenance. Addressing critical issues hindering PEMFC commercialization, our study aims to pave the way for widespread utilization in demanding applications, including construction and agricultural machinery, while simultaneously enhancing their sustainability and economic feasibility.

(PACRIM-P027G-2025) Study on the Aging Effects of Different Relative Humidity on the Properties of Palm Leaf Manuscripts

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The Palm Leaf Manuscripts are a valuable part of world cultural heritage, and understanding how various environmental factors impact its properties is crucial for studying its material characteristics, aging mechanisms, and preventive conservation. This study investigates the long-term aging effects of different relative humidity levels on the physical and chemical properties of palm-leaf manuscripts through accelerated aging experiments. Results indicate that both excessively dry and humid environments significantly affect the manuscript's preservation, posing risks to its longevity. Dry conditions lead to surface cracking, compromising the mechanical strength of the manuscript, while humid conditions foster mold growth, causing marked changes in color, gloss, and moisture absorption. Such changes result in the degradation of key chemical components and further weaken the manuscript's mechanical properties. Samples aged at 50% relative humidity (RH) exhibited no notable deterioration, with all properties remaining stable, suggesting that 50% RH is an optimal humidity condition for preserving palm-leaf manuscripts. This research provides valuable insights into the degradation processes of palm-leaf manuscripts in various environments and offers essential data to support their long-term preservation and preventive conservation.

(PACRIM-P028G-2025) Southeast Asian Origins of Gold-in-Glass Beads from the Luobucuo Lake Site, Tibet: Evidence of Early Maritime Trade between China and Southeast Asia

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Nineteen gold-in-glass beads were unearthed from the Lake Luobucuo site in Tibet. Laser Ablation Inductively Coupled Plasma Atomic Emission Spectroscopy (LA-ICP-AES) analysis reveals that these beads are V-Na-Al glass, with an average alumina content of 6.72%, and were produced using plant ash as flux. Due to their high alumina levels, single-sample t-tests were conducted to compare the chemical composition of the Luobucuo beads with that of Indo-Pacific glass. The results suggest that the beads were most likely produced in Oc Eo, Vietnam, during the 3rd to 6th centuries CE. This conclusion is further supported by Chinese historical records documenting early maritime trade with Funan (an ancient Hinduized kingdom in Southeast Asia) and archaeological evidence of glass production at the Oc Eo site. These beads provide compelling evidence of early maritime trade connections between Southwest China and Southeast Asia.

(PACRIM-P029-2025) Multiphased Al₂O₃-YAG fiber: influence of seeding material and thermal treatment

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Oxide ceramic matrix composites (O-CMC) are important strategic materials and among the different components, the fibers are required to display improved thermo-mechanical properties. To increase creep resistance at high temperatures, fiber composition or microstructure must be finely tuned. The addition of mullite, YAG or ZrO₂ to α -Al₂O₃ showed great results due to their ability to inhibit grain growth and provide their inherent creep resistance to the high-strength alumina. YAG is reported as the most creep-resistant oxide known, has a very good compatibility with alumina up to 1700°C. One of the challenges of NGO fiber development is the understanding of heat treatment parameters (temperature, heating rate, dwell time,) to control the different mechanisms occurring during thermal treatments to obtain the desired ceramic nature (crystal phase) and microstructure (grain size, porosity). Al₂O₃-YAG fiber precursors were prepared by sol-gel method. The effects of Al₂O₃ seeding and sintering parameters on thermal behavior and final properties (crystallization, grain size, densification) were investigated by structural (XRD, FTIR), microstructural (SEM), and thermal (TGA-DTA) analyses. A dense multiphased Al₂O₃-YAG fiber was obtained.

(PACRIM-P030-2025) Near-infrared luminescence enhancement in Nd³⁺ and Er³⁺ doped telluride glasses co-doped with Cr³⁺ ions

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The TeO₂-based glass family attracts significant attention due to its broad range of unique physicochemical properties including low phonon energy, high rare-earth solubility, low melting temperature, high refractive index, good thermal and chemical durability, and exceptional transparency going from visible to mid-infrared spectral region. These glasses represent promising materials for many optoelectronic applications such as solar concentrators, optical amplifiers, lasers or temperature sensors. The tellurite glasses doped with rare-earth metal (Er, Nd) and co-doped with transmission metal (Cr) were prepared by melt-quenching technique with aim to study and understand the energy transfer processes on optical properties. The spectroscopic properties of tellurite glasses doped with Cr³⁺, Er³⁺, Nd³⁺, and co-doped with Cr³⁺/Er³⁺ or Cr³⁺/Nd³⁺ were investigated.

We investigated the effect of chromium ions on the near infrared (NIR) emission of RE ions. In co-doped glasses, the absorbed energy responsible for the broad and intense emission band of Cr³⁺ ions can be efficiently transferred to doped-in RE ions, thus enhancing their NIR emission from the ⁴I_{9/2}, ⁴I_{11/2} in Er³⁺ and ⁴F_{3/2} in Nd³⁺ levels compared to glasses without Cr addition. Moreover, the intense and broad absorption band of Cr³⁺ ions in the UV-VIS region can be exploited for indirect excitation of Er or Nd ions.

(PACRIM-P031-2025) Optimization of Optical and Electrical Properties of Doped ZnO Thin Films Using Machine Learning Models for Advanced Optoelectronic Applications

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This paper presents an innovative approach combining experimentation and Machine Learning modeling to optimize the optical and electrical properties of doped ZnO thin films. Dopants such as Aluminum (Al), Gallium (Ga), and others are used to enhance the electrical conductivity and optical transparency of the films, which are critical for optoelectronic devices such as light-emitting diodes (LEDs), solar cells, and sensors. The study integrates advanced deposition techniques (e.g., sputtering, electron beam evaporation) with Machine Learning algorithms to: Predict the performance of thin films based on fabrication parameters (temperature, dopant type and concentration, deposition conditions). Identify optimal parameter combinations to maximize the desired properties. Minimize experimental trial-and-error cycles through data-driven optimization. The results will include a comparison of the performance of predictive models (neural networks, advanced regression, or random forests) and experimental validation on laboratory-produced samples. This work highlights a promising synergy between advanced materials and artificial intelligence, aligning with PACRIM and GOMD 2025 themes on ceramic and optical technologies.

(PACRIM-P032-2025) Effect of B₂O₃, CaO, and Fe₂O₃ on the solubility of Cr₂O₃ in high-level waste glasses

V. Gervasio*¹; X. Lu¹; N. Bontha¹; T. Jin¹; J. V. Crum¹; N. Lumetta¹; D. Cutforth¹; M. Torres¹; P. Metheny¹; T. Droubay¹; B. J. Riley¹; A. A. Kruger²; J. Vienna¹

1. Pacific Northwest National Laboratory, USA
2. US Department of Energy, Hanford Field Office, USA

Chromium is one of the critical limiting elements in managing the treatment of Hanford nuclear waste, and stabilizing chromium oxide within the glass matrix is essential to avoid issues like salt and crystal formation. One of the factors influencing chromium solubility in the glass matrix is its valence state. In this study, we investigate the redox behavior of chromium in complex borosilicate melts to enhance the efficiency of nuclear waste vitrification. Variables, including temperature, oxygen fugacity, and melt composition, influence the valence states of transition metal ions in the glass. While temperature and oxygen fugacity are well understood, their impacts on multicomponent melts still require further exploration. To achieve this, we examined the optical basicity (OB), a property that reflects the electron donation capacity of glasses, used to predict metal redox states. Conflicting findings have emerged on whether chromium solubility is positively or negatively correlated with OB. In this study, a matrix with 14 glass compositions was designed using a space-filling method. Total Cr₂O₃ and eskolaite contents were measured by electron probe microanalysis, and X-ray diffraction was used to determine Cr solubility in glass.

(PACRIM-P033-2025) Fabrication Process of SiC Matrix Fuel Compacts for High Temperature Gas-Cooled Reactors by Reaction Sintering and Their Properties

K. Yoshida*¹; Y. Fukaya²; M. Goto³; H. Abe⁴; K. Okamoto⁴

1. Institute of Science Tokyo, Japan
2. Japan Atomic Energy Agency (JAEA), Japan
3. University of Fukui, Japan
4. The University of Tokyo, Japan

High Temperature Gas-cooled Reactors (HTGRs) adopting silicon carbide (SiC) instead of conventional graphite for fuel compacts with TRISO fuel particles have been proposed to improve the power density and to enhance the oxidation resistance of the fuel elements in the air ingress accident. To apply SiC as the matrix for fuel compacts, SiC should be dense to retain the fission products inside of the fuel compacts and to increase the thermal conductivity. In this study, the present authors focused on reaction sintering method, which is capable of fabricating dense SiC at lower temperature in a short time, and the fabrication process of the dense SiC matrix fuel compacts by reaction sintering was studied. In addition, characterization and thermal conductivity measurement of the reaction-sintered SiC compacts were conducted.

(PACRIM-P034G-2025) Solid State Reduction of Oxide Mixtures to Achieve High Entropy Alloys: Microstructural Development and Mechanisms

W. Jin*¹; J. McArdle²; M. Watson²; G. Balasubramanian³; A. Kundu⁴; H. M. Chan¹

1. Lehigh University P C Rossin College of Engineering and Applied Science, Materials Science & Engineering, USA
2. University of Canterbury, Chemical and Process Engineering, New Zealand
3. University of New Haven, Mechanical Engineering, USA
4. Lehigh University, Mechanical Engineering & Mechanics, USA

Enhanced reduction of oxide mixtures in dilute hydrogen-argon gas mixtures can be exploited to achieve HEA alloy compositions. Previous work at Lehigh showed that the quaternary Cantor derived HEA (CoFeMnNi) could be successfully processed using this procedure. The enhanced reduction of the manganese oxide can be rationalized due to the increased entropy contribution (ΔS) and negative enthalpy of mixing (ΔH) of the Mn metal in the HEA composition. To further understand this process, binary oxide mixtures that include MnO₂ were reduced under the same reduction conditions as utilized for the CoFeMnNi. The results were analyzed based on microstructure and phase composition. These studies were complemented by in-situ XRD reduction experiments and TGA. Recent work on the processing of the refractory HEA, CrTaVW will also be discussed.

(PACRIM-P035-2025) Thermodynamic prediction and experimental verification of oxide formation and its effect on oxidation behaviors in Al-Mg and Al-Mg-Si alloys

Y. Yoon*¹; N. Kim¹; S. Ha¹; B. Kim¹; H. Lim¹; S. Kim¹

1. Korea Institute of Industrial Technology, Republic of Korea

Al-Mg based alloys are widely used due to their attractive properties such as excellent corrosion resistance, weldability, and formability. In Al-Mg binary system, β -Al₃Mg₂ phase precipitates by eutectic reaction during solidification. However, β -Al₃Mg₂ phase in grain boundaries is preferentially oxidized and strongly affect the oxidation behavior of matrix at high temperatures due to its high concentration of Mg. The enrichment of Mg promotes the formation of MgO and spinel. Therefore, the oxidation of β -Al₃Mg₂ phase can lead to the intergranular oxidation along the grain boundaries. The strengthening mechanisms of Al-Mg alloys can be explained by solid solution strengthening and work hardening. Si addition in Al-Mg alloys induces the formation of eutectic Si and Mg₂Si phase during solidification. The oxide formation can be examined by the

phase diagrams by thermodynamic calculation. Changes in oxidation behavior depending on the type of oxide and compositional variation of alloying elements can be predicted. The co-existence of β - Al_3Mg_2 and $\text{Mg}_2\text{Si}/\text{Si}$ in grain boundaries can affect the oxidation behaviors during heat treatment, melting and casting. The aim of this study is to investigate oxide formation and its effect on oxidation behaviors in Al-Mg and Al-Mg-Si alloys based on phase diagrams and experimental results.

(PACRIM-P036-2025) Influence of Metal Sulfide Precursors on Enhancing Sulfur Tolerance in NH_3 -SCR Catalysts

B. Ye^{*1}; H. Kim¹

1. Korea Institute of Industrial Technology, Republic of Korea

Selective catalytic reduction (SCR) is widely recognized as an effective NO_x removal technology, particularly due to its high efficiency. However, there is a growing demand for low-temperature catalysts to reduce energy consumption, and a significant challenge arises from the rapid deactivation of catalysts in the presence of SO_2 in exhaust gases. To address this issue, we have investigated the use of metal sulfides, which offer enhanced SO_2 resistance, improved dispersion properties, and increased NO_x removal efficiency. In particular, two-dimensional transition metal dichalcogenides and metal sulfides containing elemental sulfur were explored to enhance SO_2 resistance. Among various metal sulfides, WS_2 and MoS_2 , which are commonly used as co-catalysts were selected as precursors for catalyst synthesis via conventional impregnation methods. Additionally, VO_x was nano-dispersed onto the surfaces of these two-dimensional metal sulfides, maintaining thermal stability and preventing sintering even at elevated temperatures, thus enhancing catalytic efficiency. The catalysts were optimized by selecting the optimal coexistence form of sulfide and oxide to improve sulfur resistance, achieved by fine-tuning the sintering temperature of the metal sulfides. Experimental results demonstrate that the developed catalyst exhibits improved efficiency, particularly under conditions where SO_2 is present.

(PACRIM-P037G-2025) In situ X-ray tomographic analysis of terracotta sketches at the Museum Gypsotheca Antonio Canova in Italy

J. Wang^{*1}

1. Università degli Studi di Bologna, Italy

X-ray Computed Tomography (X-CT) is increasingly essential for cultural heritage diagnostics. It allows non-destructive investigation of artifacts without sampling, preserves the integrity of objects while providing three-dimensional insights into their internal structures, and enhanced by modern 3D rendering technologies. Moreover, conservators and restorers are aided by this technique in assessing the condition of artworks as well as in detecting poor restorations and forgeries. This research, a collaboration between the Museum Gypsotheca Antonio Canova in Possagno, Italy, and the University of Bologna, analyzed 34 terracotta sketches by Antonio Canova that require restoration. A transportable inspection system developed by DIFA was employed for preliminary tomographic analysis to characterize their preservation state. The work was conducted in two phases, the first phase involved a diagnostic campaign where 19 terracotta sketches underwent X-ray tomography. This paper presents the findings from the initial phase, focusing on in situ measurements and data processing, including tomographic reconstruction, 3D rendering, and visualization. The outcomes revealed Canova's sculptural techniques, and provided restoration insights into the artifacts, which can help restorers plan effective restoration interventions.

(PACRIM-P038UG-2025) Impact of Processing Parameters on Si Contamination in Oxy-Sulfide GSE: Comparative Analysis of Silicon Contaminated vs. Noncontaminated Glass

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2. Iowa State University of Science and Technology, Materials Science and Engineering, USA

Glassy-state electrolytes are promising candidate electrolytes for future battery technologies. The mixed oxy-sulfide glass [$\text{Li}_2\text{S}+\text{SiS}_2+\text{Li}_{3.48}\text{SiO}_7$] demonstrates the stability in cell contact with NMC 811 cathodes. However, using lab-synthesized SiS_2 introduces silicon contamination into the glass, and the amount of Si contamination is determined by the processing parameters. It is hypothesized that increased milling time and energy input elevate silicon ejection. The amount of silicon contamination correlates to the deterioration in cell performance. Another hypothesis is that unreacted silicon is present within the precursor material (SiS_2). Raman Spectroscopy and X-ray diffraction (XRD) analyses confirm the presence of elemental silicon within the glass and the precursor material (SiS_2). Based on two hypotheses, efforts to reduce milling time and utilize high-purity precursor (SiS_2) from a reliable source minimize silicon ejection, leading to the production of silicon noncontaminated glass. The electrochemical properties of oxy-sulfide glass with silicon-contaminated versus noncontaminated glass are comparatively analyzed.

(PACRIM-P039-2025) Impedance spectroscopy studies on diamond-based nanomaterials and nanostructures

R. Zhang¹; N. Peng²; H. Ye^{*1}

1. University of Leicester, School of Engineering, United Kingdom

2. University of Surrey, Surrey Ion Beam Centre, United Kingdom

Diamond based nanomaterials and nanostructures have gained significant interest across various scientific and industrial fields due to their exceptional electronic, thermal, mechanical properties. This talk delves into the application of impedance spectroscopy as a non-destructive analytical technique to investigate the electrical characteristics and behaviour of these materials and structures at the nanoscale. We will discuss the synthesis and structural characterization of various diamond nanomaterials, including nanodiamonds thin films, powders and electronic devices. The focus will be on understanding their impedance spectra in relation to their intrinsic properties such as grain interiors and grain boundaries, and the influence of factors such as defects, surface modification, and interface. Through detailed impedance measurements, we aim to elucidate the charge transport mechanisms, dielectric properties, and potential interface effects that govern the performance of these diamond-based nanostructures. This study not only enhances the fundamental understanding of diamond nanomaterials but also provides insights into their prospective applications in nanoelectronics devices.

(PACRIM-P040-2025) Carbon Quantum Dots from rice husk for Sustainable Antibacterial Coatings

S. C. Amaral^{*1}; A. Ciccone²; R. E. Galian²; J. Pérez-Prieto²; J. P. Sousa¹

1. International Iberian Nanotechnology Laboratory, Portugal

2. Universitat de Valencia, Instituto de Ciencia Molecular (ICMOL), Spain

Carbon quantum dots (CQDs) have emerged as a versatile class of nanomaterials, owing to their biocompatibility, excellent photostability, high water solubility, and distinctive optical properties. Among their diverse applications, CQDs stand out as promising antimicrobial agents due to their ability to induce bacterial inactivation through various mechanisms, including physical disruption of cell membranes, inhibition of bacterial metabolism, and oxidative stress via reactive oxygen species (ROS) production. With antibiotic resistance recognized as one of the most pressing global health challenges, impacting individuals at all stages of life, the development of alternative antimicrobial strategies is critical. In this study, CQDs

were synthesized from rice husk, leveraging agricultural waste as a renewable precursor to support sustainable nanomaterial production. The incorporation of different dopants (N, S, B) was explored to fine-tune their electronic and optical properties, enhancing ROS generation for superior antimicrobial efficacy. Additionally, surface functional groups were tailored to maximize interactions with microbial cell walls, facilitating membrane rupture. Comprehensive characterization of the synthesized CQDs was performed using UV-Vis spectroscopy, photoluminescence, XPS and TEM, providing detailed insights into their structural and functional properties.

(PACRIM-P041UG-2025) Compositional Exploration of the $\text{Li}_2\text{S} + \text{SiS}_2$ Glass System for Use in Glassy Solid-State Electrolytes

H. Cochran^{*1}; S. J. Leland¹; S. W. Martin¹

1. Iowa State University of Science and Technology, Materials Science and Engineering, USA

Glassy solid-state electrolytes (GSEs) are strong contenders for use in solid-state batteries due to their electrochemical stability, processability, and flexible chemistries. To compete with existing liquid electrolytes, GSEs should have high ionic conductivities ($>1 \text{ ms/cm}^2$). Previous work has shown sulfide chemistries exhibit higher ionic conductivities compared to similar oxide-based systems. Therefore, the $x\text{Li}_2\text{S} + (1-x)\text{SiS}_2$ glass system will be studied. Based on the $\text{Li}_2\text{S}-\text{SiS}_2$ phase diagram, we expect the highest working range (T_x-T_g) to occur at $0.57\text{Li}_2\text{S} + 0.43\text{SiS}_2$ given the low melting temperature eutectic. As the glass redraw process will be used to draw thin film ($<100 \mu\text{m}$) films of glass, a large working range and high thermal stability are desirable. The glass series was synthesized inside a nitrogen glovebox utilizing mechanical mixing and melt quenching. Each glass was thermally investigated using differential scanning calorimetry followed by structural characterization, which was done using Raman spectroscopy and Fourier transform infrared spectroscopy. Lastly, the conductivity was measured at low and high frequencies through a range of temperatures.

(PACRIM-P042G-2025) Investigating Femtosecond Laser Processing of Silica Sand: Crystallization and Impurity Removal

A. Naim^{*1}

1. University of California Davis, Materials Science and Engineering, USA

Investigation was conducted on a raw silica sand with impurities of 306 ppm comprising of Ca, Mg, Al, Ti and elements like Fe, Na, K in trace amounts. The aim was to investigate the effects of direct irradiation of femtosecond pulse laser on SiO_2 . The laser used in this experiment was the Ti:Sapphire laser pulses of 80 fs, wavelength of 820nm and diameter: a laser pulse of 80 MHz at 1.5 eV, an ambient temperature of 298 K. Its been observed in literature study earlier that femtosecond laser irradiation results in amorphization, crystallization, nucleation, amorphization and ablation varies with the increasing laser fluence and decreasing the pulse duration. The laser parameter were carefully designed to acquire desired results of ablation and vaporization of the impurities from the silica sand. A constant ablation threshold fluence on the order of $0.13 \text{ J/mm}^2/\text{s}$ for 80 fs pulse durations was observed for varying time duration of irradiation of laser. The laser treatment resulted in increased crystallinity as well as change in phase from low temperature alpha-quartz phase to high temperature cristobalite.

(PACRIM-P043G-2025) In-situ local probing of domain structures under an applied bias in multi-layered ceramic capacitors

J. Shim^{*2}; W. Kim²; c. Jeon¹; s. lee¹; Y. Shin¹; S. Kim²; Y. Kim²

1. Samsung Electromechanics Research and Development Center, Republic of Korea
2. Sungkyunkwan University College of Engineering, Republic of Korea

Multi-layered ceramic capacitors (MLCCs) are essential passive components, featuring a structure in which internal metal electrodes and dielectric ceramic layers are stacked. They are widely used in electronic devices such as mobile phones and electric vehicles. Traditionally, the capacitance of MLCCs has been analyzed on a macroscopic scale. However, as the thickness of ferroelectric layer and the size of ferroelectric powders continue to decrease, nanoscale studies of ferroelectric layers have become nearly indispensable for understanding underlying capacitance improvement and reliability in MLCCs. While it is widely known that the domain structures influence the capacitance of MLCCs, the relationship between changes in domain structures and corresponding changes in capacitance remains unclear. In this presentation, we performed in-situ observations of domain structures under an applied bias using piezoresponse force microscopy, a mode of atomic force microscopy that explores domain structures and ferroelectricity. We analyzed multi-dimensional domain structures across micrometer-scale areas of the BaTiO_3 layers in MLCCs, revealing a clear correlation between domain structures and capacitance. These findings could provide insight into nanoscale research aimed at improving the performance and reliability of MLCCs.

(PACRIM-P044-2025) Plasma-Treated Nitrogen-Doped Carbon-Supported Pd catalysts for Hydrogen Storage in N-Methylindole

Y. Kim^{*1}; J. Kim¹; D. Lee¹; M. Lee¹

1. Korea Institute of Industrial Technology, Republic of Korea

Liquid organic hydrogen carriers (LOHCs) have emerged as a promising solution for the efficient and safe storage and transport of hydrogen, addressing key challenges in the global transition toward a hydrogen economy. Among LOHC candidates, N-methylindole (NMID) is notable for its high hydrogen storage capacity, thermal stability, and recyclability. However, the practical application of NMID as LOHC is limited by the lack of advanced catalytic systems capable of achieving hydrogenation under mild conditions. Herein, we have studied a novel catalytic approach employing palladium (Pd) nanoparticles supported on nitrogen-doped carbon (N@C) supports prepared via plasma treatment. Plasma treatment introduced nitrogen functionalities onto the carbon surface, enhancing the interaction between Pd and the support and improving catalytic performance during hydrogenation. The prepared catalysts were characterized by X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM), N_2 physisorption, CO chemisorption, and elemental analyzer. The results showed higher hydrogen storage capacity compared to the traditional Pd/C and Pd/ Al_2O_3 catalysts, implying the critical role of nitrogen doping in optimizing the catalytic performance.

Wednesday, May 7, 2025

PacRim S3 - Solid Oxide Fuel Cells and Green Hydrogen Technologies

PACRIM Symposium 3 - Solid Oxide Fuel Cells and Green Hydrogen Technologies I

Room: English Bay

Session Chairs: Hiroyuki Shimada, National Institute of Advanced Industrial Science and Technology (AIST); Sebastian Molin, Gdansk University of Technology

10:20 AM

(PACRIM-S03-001-2025) Protective-conducting composite coatings for SOFC steel interconnects (Invited)

T. Brylewski^{*1}; K. Domaradzki¹; L. Mazur¹; M. Zajusz¹; M. Bik¹; P. Winiarski¹

1. AGH University of Krakow, Faculty of Materials Science and Ceramics, Poland

For a solid oxide fuel cell to operate with high efficiency, its operating temperature needs to be above 873 K. Such conditions, however, can lead to certain issues, including corrosion of metallic interconnects – a fundamental fuel cell component. In these studies, a new $\text{Cu}_{1.3}\text{Mn}_{1.7}\text{O}_4$ (CM)/ $\text{LaNi}_{0.6}\text{Fe}_{0.4}\text{O}_3$ (LNF) composite coating was deposited on the low-chromium ferritic stainless steel. In this system, CM formed the matrix and the LNF perovskite was added as a dispersion phase. Coatings with selected compositions were electrophoretically deposited on metallic substrates and underwent long-term (over 6000 h) oxidation tests in air at 1023 K. The samples were examined by means of XRD, XAS, Confocal Raman Imaging, SEM/EDS and TEM/SAD. A 2-probe 4-point DC method was used for ASR measurements. The addition of LNF to the CM matrix yields a steel/composite coating system that exhibits significantly improved oxidation resistance and electrical properties. It also demonstrates increased stability in the presence of Cr_2O_3 , confirming that CM/LNF can be applied as a material for functional protective-conducting coatings on SOFC interconnects. Acknowledgements: Research project supported by program “Excellence Initiative – Research University for the AGH University of Krakow”, Grant ID 4138 (TB). Funding as part of the National Science Centre (NCN) project No. 2021/41/B/ST8/02187 is also gratefully acknowledged (TB).

10:50 AM

(PACRIM-S03-002-2025) Spray pyrolysis of interconnect protective coatings: processing and properties

S. Molin^{*1}; M. Mehdizade¹

1. Politechnika Gdanska Wydział Elektroniki Telekomunikacji i Informatyki, Department of Functional Materials Engineering, Poland

Spray pyrolysis is an efficient and versatile deposition technique for producing ceramic protective coatings on interconnects in solid oxide cell (SOC) stacks at reduced processing temperatures. This method enables precise control over coating thickness and chemical composition, making it highly suitable for scalable manufacturing. In our work, we focus on the development of Mn-Co and Mn-Cu oxide spinel coatings, which exhibit excellent functional properties such as low corrosion rates and strong chromium retention, critical for enhancing SOC stack longevity. The presentation will explore key factors affecting the coating performance, including precursor selection, deposition parameters, and post-deposition thermal treatments. A comprehensive analysis of the relationship between processing conditions and the resulting microstructural, mechanical, and electrochemical properties of the coatings will also be presented, offering insights into optimizing their application in SOC technologies.

11:10 AM

(PACRIM-S03-003-2025) Tailoring NiCoMn materials for optimal HER performance

C. M. Freitas^{*1}; J. P. Sousa²

1. INL - International Iberian Nanotechnology Laboratory, Kolen'ko Group, Portugal
2. International Iberian Nanotechnology Laboratory, Portugal

The increasing demand for hydrogen as a clean energy carrier drives the growth of efficient water electrolysis catalysts. Pt-based electrocatalysts are usually employed to catalyse HER with very low overpotentials. However, its high cost and low availability continuously prompt the discovery of substitutes that can present comparable catalytic activities. Transition metal catalysts could be considered a good alternative as are more affordable and sustainable. This study aims to use nickel(Ni), cobalt(Co), and manganese(Mn) obtained from battery cathode recycling as electrocatalysts for HER. Although these metals are individually interesting candidates, no reports are found using NiCoMn compounds, especially obtained from battery cathode leaching solutions. In this work, the electrochemical performances of synthesised NiCoMn materials and NiCoMn obtained from cathode recycling were tested for HER in alkaline media. Carbon black was also incorporated in the matrix of ternary transition metal materials to promote synergy between the NiCoMn and this highly conductive material. The detailed electrochemical characterisation revealed that the reduction of the NiCoMn under H_2 flow at 200 °C forms an amorphous/crystalline structure, which exhibits significantly improved electrochemical activity and stability (-0.5 V for 100 h). Additionally, although carbon black decreases the catalyst overpotential, its stability remains unchanged.

11:30 AM

(PACRIM-S03-004-2025) Clean Hydrogen Technologies: Utilization of Ceramics in Production, Distribution and End-Use (Invited)

F. Dogan^{*1}

1. Missouri University of Science and Technology, Dept. of Materials Science and Engineering, USA

Interest in producing and using clean hydrogen has been increasing to address the climate crisis, create economic value, enhance energy security and resilience. Clean hydrogen will play an important role in reducing CO_2 emissions in difficult-to-decarbonize industries, transportation, and the power generation. Hydrogen, as a form of energy storage, can also be utilized to support the expansion of renewable energy. This presentation will address utilization of ceramic materials in production, distribution, and end-use technologies of clean hydrogen as well as emerging demands and potential new opportunities.

PacRim S4 - Polymer-Derived Ceramics/Composites/Nanocomposites as Functional Inorganic Materials

PACRIM Symposium 4 - Pre ceramic polymer chemistry-Structural, chemical and thermal transformations

Room: Plaza C

Session Chair: Aitana Tamayo, Institute of Ceramics and Glass, CSIC

8:00 AM

(PACRIM-S04-024-2025) Development of Processable Polymer Derived Ultra-High Temperature and Compositionally Complex Ceramics and Composites (Invited)

T. Prunyn^{*1}; J. Delcamp¹; M. B. Dickerson¹

1. Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

Demands for materials for extreme environments and high temperatures continue to increase, but there is a limited selection of materials that can withstand these conditions. Of these materials for extreme environments, ultra-high temperature ceramics (UHTCs) have garnered a great deal of interest but are challenging to process into complex components and ceramic matrix composites (CMCs). Pre ceramic polymers (PCPs) are one potential solution towards improving fabrication of CMCs and complex components since they can be processed using numerous techniques (e.g., fiber spinning, composite infiltration, and additive manufacturing) and have their form factor preserved upon conversion to a ceramic. Though PCPs are attractive for creating ceramics and composites, the vast majority of PCPs are silicon-based (e.g., yielding SiC, SiCN, or Si₃N₄ ceramics). In this presentation we will discuss the development of a family of liquid PCPs, referred as Air Force Pre ceramics (AFPCs), that form Group IV, V, and VI UHTCs carbides and nitrides. We will report on various AFPCs and their conversion into UHTC pre ceramic polymers along with some mixtures of AFPCs that yield high-entropy/compositionally complex ceramics. The processing of these AFPCs in carbon fiber-based CMCs will be discussed along with high temperature testing of these composites.

8:30 AM

(PACRIM-S04-025-2025) Novel oxygen-free precursors for Hf-based ultra-high temperature ceramics and composites

Y. Wu^{*1}; W. Han¹; T. Zhao¹

1. Institute of Chemistry, Chinese Academy of Sciences, China

Hf-based ultra-high temperature ceramics and fiber reinforced composites have been widely used in extreme environments. In order to reduce the harmful effects of the carbothermal reduction process on the properties of composites, it is necessary to develop oxygen-free precursors suitable for the precursor infiltration and pyrolysis process. In this work, we report the novel oxygen-free precursors synthesized by a simple amine exchange reaction of hafnium amide. The precursors are liquid at room temperature and do not contain oxygen and silicon in composition. Hf-based ceramics including hafnium carbide and boride are obtained by thermal treatment of the precursors at 1600 °C with a ceramic yield of more than 40%. The oxygen-free characteristics of the precursors is confirmed by the low oxygen content of the pyrolysed product at 900 °C and the low weight loss of the carbothermal reduction process. The production of the precursors has been scaled up to 10 kg, which is convenient for the preparation of ceramic matrix composites by infiltration and pyrolysis process. This work will innovate the toolbox toward novel precursors for Hf-based ceramics and stimulate new ideas from scientists working in the related fields.

8:50 AM

(PACRIM-S04-026-2025) Development of Tailored Polymeric Precursors for Advanced UHTC Fabrication via the PIP Method

J. So^{*1}; K. Lee¹; S. kim¹; S. Lee¹

1. Korea Institute of Materials Science, Republic of Korea

Ultra-high-temperature ceramics (UHTCs) are vital materials in aerospace and defense due to their exceptional heat and ablation resistance. However, their extremely high melting points, exceeding 2000°C, create challenges in shaping and sintering, necessitating effective densification methods. One promising technique is the polymer infiltration and pyrolysis (PIP) method. This process involves introducing a low-viscosity polymeric precursor into a matrix and converting it into ceramics through high-temperature pyrolysis, enabling the densification of various ceramics and near-net shape fabrication. The success of the PIP method relies on using liquid polymer precursors with low viscosity for efficient matrix infiltration and high yield for effective ceramization. Our research group has extensively studied the PIP process and developed tailored synthetic strategies to create suitable ceramic precursors. Specifically, we focus on precursors for producing ZrO₂, ZrC, and SiC. In this presentation, we will share our precursor synthesis methods and examine how applying these precursors through the PIP process impacts UHTC properties, highlighting advancements in their fabrication and practical application.

9:10 AM

(PACRIM-S04-027-2025) High-pressure synthesis, mechanical properties and oxidation behavior of polymer-derived boron-containing α/β -Si₃N₄/Si ceramics

W. Li^{*1}

1. The University of Alabama at Birmingham, Department of Mechanical and Materials Engineering, USA

The preparation of dense additive-free Si₃N₄-based ceramics has attracted great attention due to the achievable improvements in high-temperature mechanical properties. In this work, advanced dense amorphous SiBN and α/β -Si₃N₄/Si monoliths without using sintering additives were prepared by high pressure-high temperature technique using polymer-derived amorphous Si₃N₄ and SiBN powders as raw materials. The crystallization behavior and phase transformation of the polymer-derived amorphous samples were studied in the temperature range from 1000 °C to 1800 °C. The results demonstrate that the incorporation of boron in the Si₃N₄ matrix suppresses phase transformation from α -Si₃N₄ to β -Si₃N₄. Furthermore, the mechanical properties of the as-prepared samples were measured and the maximum hardness and fracture toughness of boron-rich SiBN samples reached up to 14.8 GPa and 7.96 MPa•m^{1/2}, respectively. In addition, the oxidation behavior of the obtained samples was investigated at 1000 °C and 1400 °C. The results show that the incorporation of boron significantly improves the oxidation resistance of the samples. This work provides a guidance for the synthesis of amorphous SiBN and boron-containing α/β -Si₃N₄-based ceramics with excellent mechanical properties and oxidation resistance.

PACRIM Symposium 4 - Forming technologies of preceramic polymers including 3D-printing

Room: Plaza C

Session Chair: Shotaro Tada, Nagoya Institute of Technology

9:30 AM

(PACRIM-S04-028-2025) Formulation of Preceramic Polymers for Photocuring and 3D Printing (Invited)

H. Yazdani Sarvestani¹; T. Lacelle³; A. Kulkarni¹; Y. Martinez-Rubi³; A. Robitaille²; B. Ashrafi¹; M. Jakubinek^{*3}

1. National Research Council Canada, Aerospace, Canada
2. Defence Research and Development Canada, Valcartier Research Centre, Canada
3. National Research Council Canada, Division of Emerging Technologies, Canada

Preceramic polymers address many of the shaping constraints in traditional ceramics processing, and enable near-net-shape manufacturing of using polymer processing methods. Of particular recent interest for producing novel, complex, highly customized geometries is the use of preceramic polymers in 3D printing methods based on photopolymerization, such as stereolithography and digital light processing. In general, PCPs require modification – additives to control the polymerization – in order to produce well-defined geometries by these methods. Here we describe the formulation of commercial polysiloxane PCPs to produce UV-curable preceramics optimized for 3D printing of low density lattice geometries. The resulting green parts are pyrolyzed at high temperature and assessed in compression tests as well as for their temperature stability and composition. The combination of PCPs with polymer additive manufacturing, enables the definition of complex and customized ceramic shapes, offering a promising route to produce tough, strong, lightweight ceramic components.

10:00 AM

(PACRIM-S04-029-2025) Characterization of shaped articles made from polycarbosilane and their deformation characteristics during heat treatment

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1. Korea Institute of Ceramic Engineering and Technology, Emerging Materials R&D Division, Republic of Korea
2. Korea Institute of Ceramic Engineering and Technology, Republic of Korea

Polycarbosilane, a precursor for SiC, is primarily used in fiber production or as a matrix material for ceramic matrix composites (CMCs). Its applications are also expanding into 3D SiC printing technology with recent advancements in additive manufacturing. However, a significant limitation in the development of polycarbosilane is that it undergoes shrinkage deformation due to weight loss during the pyrolysis process. In this study, we analyze the shaped and cured polycarbosilane products, discussing how these characteristics affect high-temperature deformation. Polycarbosilane, like other polymer materials, undergoes thermal expansion, and the causes of deformation can vary depending on the temperature range of heat treatment. Additionally, this deformation exhibits different behaviors based on the curing conditions. Therefore, the shrinkage behavior of the cured polycarbosilane product was examined by altering the heat treatment conditions to align with the characteristics of the final cured product.

10:20 AM

(PACRIM-S04-030-2025) Preparation and Processing of Silicon based Polymer-Derived Ceramic Precursors

Y. Lu^{*1}; H. Chen¹; X. Hu¹

1. Nanyang Technological University, Singapore

Ceramics have found many enabling and promising applications in a broad field of modern industries due to their high mechanical strength and hardness, resistance to temperature and wear and corrosion. Polymer-derived ceramic (PDC) is an alternative to conventional ceramic synthesis and of great interests to researchers. Compared to ceramic powders, preceramic polymers (PCPs) as PDC precursors are easier shaping and processing and have lower ceramic conversion temperature. Various strategies of preparing of PCPs have been investigated and reported. For instance, polycarbosilane as a SiC precursor can be simply approached by Yajima route. Processing technologies such as electrospinning and casting are also readily applicable to PCPs, resulting in facile fabrication of ceramic fibers and films that are difficult to obtain by powder processing. Moreover, additive manufacturing (AM) also enables fabrication of complex ceramic structures with PCPs. Based on our experiences on AM processing of high-performance thermoset and glassy carbon, we formulated PCP resins and developed AM processed SiOC consequently. Recently, we investigate the modification of PDC precursor to obtain electrospun fibers with higher ceramic yield. Our results find that PCPs are crucially promising candidates for achieving high-performance ceramic products and are applicable for processing with various fabrication methods.

PacRim S6 - Dielectric Ceramics for Microwave and Submillimeter-Wave Applications

PACRIM Symposium 6 - Materials for Microwave and Millimeter-Wave Applications

Room: Balmoral

Session Chairs: Michael Lanagan, Penn State University; Rick Ubc, Boise State University

8:00 AM

(PACRIM-S06-020-2025) The Structure and Microwave Properties of Mg₄Nb₂O₉ Ceramic with addition SrTiO₃

C. Lei^{*1}; Y. Chen¹; Y. Wu²; K. Feng³

1. Chinese Culture University, Department of Chemical & Materials Engineering, Taiwan
2. National Taipei University of Technology, Department of Materials and Mineral Resources Engineering, Taiwan
3. Ming Chi University of Technology, Department of Mechanical Engineering, Taiwan

In this work, we synthesize the Mg₄Nb₂O₉ ceramics by the mixed oxide method with SrTiO₃ additive, to investigate the structure and microwave properties of this mixture. The Mg₄Nb₂O₉ ceramics is decomposed by additive SrTiO₃, because the Nb-ion of Mg₄Nb₂O₉ ceramics is dissolving into SrTiO₃, replacing Ti-ion site and forming the Sr₂NbO₃ structure, then the excess MgO becomes second phase. The SEM images are observed two types grains: the larger Mg₄Nb₂O₉ grains and smaller Sr₂NbO₃ grains, and the grain size was growth with sintering temperature increasing. The room temperatures Raman spectrum is only observed the Mg₄Nb₂O₉ phonon modes without Sr₂NbO₃ phonon modes. The Qxf-values of Mg₄Nb₂O₉ and SrTiO₃ mixture is decreasing with additive increasing; but the K-values of samples are larger increasing with high-K SrTiO₃ additive increasing. The microwave dielectric property can be enhanced by increasing sintering due to low porosity.

8:20 AM

(PACRIM-S06-021-2025) Oxygen deviation drives the formation of 1:1 ordering in Ba(Mg_{1/3}Nb_{2/3})O₃ Ceramics revealed by iDPC-STEM

L. Zhang^{*1}; M. Fu²

1. Northwestern Polytechnical University, Materials Science and Engineering, China
2. Northwestern Polytechnical University, China

The regulation of ordered domains is essential for perovskite materials. Conventionally, doping, non-stoichiometric compositions, or prolonged thermal treatments have been widely used to regulate the growth and type of ordered domains. However, those approaches may potentially alter the chemical composition or yielding limited efficacy. In this study, we applied pressure during the sintering process to effectively induce atomic reorganization, resulting in the formation of 1:1 ordering within the 1:2 system of Ba-based ceramics. Microscopic characterization further revealed that 1:1 ordered domains preferentially nucleate and grow at the antiphase domain boundaries of the 1:2 ordered domains, forming substructures and subsequently growing in a defined manner. Moreover, iDPC quantitative analysis demonstrated that 1:1 ordering is not solely determined by the arrangement of Mg²⁺ and Nb⁵⁺, but is also influenced by the deformation of oxygen octahedra (oxygen ion deviation). The oxygen ion deviation along the $\langle 110 \rangle_c // \langle 1-10 \rangle_H$ direction exhibits a positive correlation with the 1:1 ordering of local ions. These findings contribute to a more profound comprehension of the ordered domain structures and phase transition characteristics, offering theoretical guidance for the further regulation of perovskite domain structures.

8:40 AM

(PACRIM-S06-022-2025) High Tunability and Low Loss in Layered Perovskite Dielectrics through Intrinsic Elimination of Oxygen Vacancies

H. Zhang^{*1}; H. Gidden¹; T. Saunders¹; N. Liu¹; V. Aurullo-Peters²; X. Xu³; M. Palma³; M. Reece²; I. Abrahams³; H. Yan²; Y. Hao¹

1. Queen Mary University of London, School of Electronic Engineering and Computer Science, United Kingdom
2. Queen Mary University of London, School of Engineering and Materials Science, United Kingdom
3. Queen Mary University of London Faculty of Science and Engineering, United Kingdom

Dielectric materials with moderate dielectric permittivity, high tunability and low loss are critical in modern communication technology. However, high tunability is often associated with high loss and high dielectric permittivity. Here, a novel material, textured Sr₂(Ta_{1-x}Nb_x)₂O₇ (STN), with a layered perovskite structure, has been designed to break this correlation. These materials exhibit low dielectric loss associated with oxygen vacancy elimination through the creation of stacking faults in the layered structure, as evidenced by transmission electron microscopy. A modification of the Vendik model was used to fit the thermal dependence of their relative dielectric permittivity, which included an oxygen defect parameter as an indicator of the oxygen defect concentration. The high tunability is attributed to the presence of local polar nano-clusters just above the Curie point. A 2-step spark plasma sintering method was employed to prepare grain-oriented ceramics with optimised properties. A near optimum maximum tunability of 72% at room temperature was obtained for a textured Sr₂Ta_{1.88}Nb_{0.12}O₇ ceramic, with moderate dielectric permittivity ($\epsilon' \sim 520$) and a dielectric loss of less than 1%.

9:00 AM

(PACRIM-S06-023-2025) Observation of high out-of-plane tunability and low loss in Ruddlesden-Popper phase films

V. St. George^{*2}; F. Bergmann²; M. Barone¹; A. Ross⁴; Z. Tian³; S. Freed²; M. Papac²; D. Schlom¹; N. Orloff²

1. Cornell University, Department of Materials Science and Engineering, USA
2. NIST, Communications Technology Laboratory, USA
3. University of California, Berkeley, USA
4. The Pennsylvania State University, USA

Microwave circuits like tunable filters and phase shifters rely on high tunability and low loss dielectrics. About a decade ago, scientists observed a record-breaking combination of high in-plane tunability and low loss in strained Ruddlesden-Popper phase Ba_xSr_{1-x}TiO₃ thin films at microwave frequencies. However, most voltage-tunable devices employ out-of-plane geometries, hindering the implementation of Ruddlesden-Popper films in microwave circuits. Still, theory predicts that engineering strainless Ruddlesden-Popper phase Ba_xSr_{1-x}TiO₃ with a high barium content should result in high out-of-plane tunability. Here, we report on measuring this high out-of-plane tunability in Ruddlesden-Popper phase Ba_xSr_{1-x}TiO₃ thin films and show that we can engineer the Ruddlesden-Popper phase to result in low dielectric loss at microwave frequencies. This result shows that Ruddlesden-Popper phase dielectrics can indeed be tunable out-of-plane while retaining their low dielectric loss. Our observations set a new benchmark for low loss out-of-plane tunable microwave dielectrics.

PACRIM Symposium 6 - Domain Structures/Engineering

Room: Balmoral

Session Chairs: Rick Ubic, Boise State University; Michael Lanagan, Penn State University

10:20 AM

(PACRIM-S06-024-2025) Domain interface structure analysis and dielectric properties regulation of non-stoichiometric Ba(Mg_{1/3+x}Nb_{2/3})O_{3+x} microwave dielectric ceramics

Y. Liu^{*1}; M. Fu¹; X. Ma¹

1. Northwestern Polytechnical University, China

In this study, the effects of cationic ordering and ordered domains on the microwave dielectric properties of 1:2 ordered Ba(Mg_{1/3}Nb_{2/3})O₃ complex perovskite ceramics were systematically investigated. Ba(Mg_{1/3+x}Nb_{2/3})O_{3+x} ceramics were successfully prepared using solid-state reaction method, and all ceramics were synthesized as ordered structure with space group P-3m1. The uniform distribution of ordered domains are significantly regulated by non-stoichiometry. The ordered domains are composed of sub-micron ordered domains and nano domains. Submicron ordered domains are separated by anti-phase domain boundaries, which contain 5-10 atomic layers of disorder. The interior of nanodomains is composed of disordered and twin domains. There is a transition zone at the twin domain interface, where Mg : Nb ≈ 1 : 1. Imbalance in composition and charge leads to octahedral distortion. This distortion and charge imbalance may be the reason why the dielectric loss of nanodomains is greater than that of inverse domain boundaries. Non-stoichiometric regulation of the microstructure uniformity of Ba(Mg_{1/3}Nb_{2/3})O₃ ceramics improves the quality factor. The important findings of this study can provide effective references for the microstructure characterization and properties control of ordered perovskite microwave dielectric ceramics.

10:40 AM

(PACRIM-S06-025-2025) Determination of Domain Structures in Ca-based Perovskite Ceramics with Pseudo-cubic StructureX. Ma*¹

1. Northwestern Polytechnical University, China

Domain structures and configuration of domain walls in $\text{Ca}_{1-0.3x}\text{La}_{0.2x}(\text{Mg}_{1/3}\text{Nb}_{2/3})_{1-x}\text{O}_3$ ($0 < x < 1$) ceramics have been investigated by X-ray diffractometry (XRD), electron backscattered diffractometry (EBSD), Transmission Kikuchi diffraction (TKD) and transmission electron microscopy (TEM). Tilting experiments by TEM meet the demand of edge-on condition, thus two basic types of domain structures have been identified as {101} reflection twin and 90° rotation twin along [010] direction. Moreover, {121} reflection twin usually exists in high temperature phase of Ca-based perovskite ceramics also unexpectedly appear in the as-sintered samples forming a zig-zag like interface. A possible model of domain configuration at the {121} reflection twin boundary has been constructed to illustrate such abnormal phenomenon.

11:00 AM

(PACRIM-S06-026-2025) Effect of microstructure and microwave dielectric properties in nonstoichiometric 1:1 ordered $\text{Nd}(\text{Mg}_{1/2+x}\text{Ti}_{1/2})\text{O}_{3+x}$ perovskite ceramicsM. Fu*¹

1. Northwestern Polytechnical University, China

The structural and microstructural characteristics at different scales have a significant impact on the dielectric loss of microwave dielectric ceramics. This study takes 1:1 ordered $\text{Nd}(\text{Mg}_{1/2}\text{Ti}_{1/2})\text{O}_3$ ceramics with ultra-low dielectric loss as the research object, and systematically investigates the effects of grain size, chemical defects, B-site cation ordering type, and ordered domains on their microwave dielectric properties. With the increase of Mg^{2+} content, $Q \times f$ value first increases and then decreases, and reaches the maximum value at $x = 0.01$. The optimal microwave dielectric properties are: $\epsilon_r = 26.5$, $Q \times f = 70000$ GHz, $\tau_f = -55.4$ ppm/°C.

PacRim S12 - Eng Ceramics and Ceramic Matrix Composites - Processing/Design/Applications**PACRIM Symposium 12 - Novel sintering and microstructure control IV**

Room: Plaza B

Session Chair: Kevin Plucknett, Dalhousie University

8:00 AM

(PACRIM-S12-022-2025) Micromechanical characterization of room-temperature plasticity in oxide ceramics (Invited)H. Masuda*¹

1. The University of Tokyo, Department of Materials Engineering, Japan

The brittle nature of ceramics has been the thick barrier against their potential applications in many industries. The brittleness of ceramics is mostly attributed to the limited plasticity, which is associated with poor mobility of dislocations. The engineering of dislocation characteristics is of great importance to enhance the plasticity and finally to overcome the brittleness. However, only limited methodologies have conventionally been available to evaluate plastic behaviors of ceramics below their ductile-to-brittle transition temperatures. In recent years, micromechanical testing such as nanoindentation and micropillar compression has attracted attention as a technology to characterize plastic behaviors of brittle materials even at room temperature. We have also characterized small-scale plasticity of oxide ceramics such as Y_2O_3 -stabilized ZrO_2 , Al_2O_3 , and SrTiO_3 to

evaluate the impacts of orientations and grain boundaries on their strength and ductility through micromechanical testing combined with electron microscopy observation and numerical simulation. These works revealed that room-temperature plasticity of oxide ceramics exhibited strong anisotropy due to dislocation activities, whereas grain boundaries insignificantly affected the local hardness as compared with metallic materials. Their physical mechanisms would be discussed in the presentation.

PACRIM Symposium 12 - Novel sintering and microstructure control V

Room: Plaza B

Session Chair: Kevin Plucknett, Dalhousie University

8:30 AM

(PACRIM-S12-023-2025) Elucidation of initial low-temperature degradation mechanism of 3 mol% Y_2O_3 stabilized ZrO_2 ceramics by using microcantilever bending tests (Invited)T. Takahashi*¹; K. Niregi¹; t. yahagi¹; T. Ohji¹; J. Tatami²

1. Chiho Dokuritsu Gyosei Hojin Kanagawa Kenritsu Sangyo Gijutsu Sogo Kenkyujo, Japan
2. Yokohama National University, Japan
3. Yokohama Kokuritsu Daigaku, Japan

The initial degradation of the surface of 3 mol% Y_2O_3 stabilized ZrO_2 ceramics (3Y-TZP) exposed into a hydrothermal environment was investigated using the microcantilever bending tests. The samples with different distribution of Y within grains were prepared by sintering at different temperatures. Hydrothermal treatment was carried out at 150 °C for up to 20 h. Microcantilever beam specimens were fabricated in the area free of cracks and pores on the surface of the samples. The bending strength near the surface decreased after just 1 h of hydrothermal treatment, regardless of the sintering temperature. The propagation path of cracks on the surface of the specimens before hydrothermal treatment differed depending on the sintering temperature of the sample. This is thought to be related to the formation of nanoscale inhomogeneous structures within the grains during sintering. After degradation, cracks propagated preferentially along grain boundaries, regardless of the sintering temperature of the sample or the progress of the $t \rightarrow m$ phase transformation. These results suggest the existence of a new degradation process of “grain boundary degradation” prior to grain boundary crack initiation, which has been understood to be the first cause of the degradation.

PACRIM Symposium 12 - Novel sintering and microstructure control VI

Room: Plaza B

Session Chair: Kevin Plucknett, Dalhousie University

9:00 AM

(PACRIM-S12-024-2025) Process Parameter Effects on the Wear Response of Al_2O_3 Ceramics Produced Using Digital Light Projection Additive Manufacturing (Invited)A. David¹; G. Boubnova¹; M. Amegadzie¹; K. P. Plucknett*¹

1. Dalhousie University, Mechanical Engineering, Canada

Digital light processing (DLP) is a ‘layer-by-layer’ vat photo polymerisation (VPP) approach for additive manufacturing (AM). In the present work, DLP has been used for manufacturing alumina (Al_2O_3) based ceramics to investigate their reciprocating wear behaviour. The influence of both the printed layer thickness (varied from 10 to 75 μm) and the build inclination angle (varied from 0 to 90° in 15° increments) have been assessed for the DLP processed Al_2O_3 . After pre-conditioning and burnout steps, the Al_2O_3 samples were sintered in air (typically 1650 °C for 2 h). Wear rates were measured sliding against $\beta\text{-Si}_3\text{N}_4$ counter face spheres,

with tests conducted at a frequency of 5 Hz, for a maximum duration of 60 minutes. The reciprocating wear tests were performed at room temperature (22 ± 2 °C), with applied loads of up to 80 N, applied normal to the surface being evaluated. This work highlights the impacts of the printing parameters on the measured coefficients of friction, specific wear rates, and microstructural damage. These studies highlight the important design criteria that need to be considered when utilising AM methods for production of advanced ceramic wear components.

9:30 AM

(PACRIM-S12-025-2025) Tribological behavior of plasma sprayed bimodal microstructured Al_2O_3 -YSZ-CNT composite coatings

S. Ponnareddy*¹; A. Kumar²; M. K. Singh²; K. Balani¹

1. Indian Institute of Technology Kanpur, Materials Science and Engineering, India
2. Indian Institute of Technology Kanpur, Mechanical Engineering, India

Plasma-sprayed Al_2O_3 -YSZ ceramic boast superior wear resistance, but their brittleness indicates the need for further improvement. Bimodal microstructure coatings are a promising solution because they combine the strength from fully melted regions with the toughness from partially melted regions, for arresting crack propagation. The current study has developed plasma sprayed bimodal microstructure coatings using conventional Al_2O_3 ($\mu\text{-Al}_2\text{O}_3$) powders and nano Al_2O_3 reinforced with nano YSZ (3/8 mol%) with CNTs reinforcements. Microstructural analysis of Al_2O_3 YSZ- CNT coatings revealed bimodal microstructured coatings with fully melted regions and partially melted nano-structured region (NR). Nano reinforcements of YSZ & CNT toughness, while CNTs contribute to improved toughness and lubrication effects. Nano hardens increased from approximately 12 GPa to 17.8 GPa. Additionally, composite coatings demonstrated improved reliability (Weibull modulus) of 9, compared to 5.6 ($\mu\text{-Al}_2\text{O}_3$). Tribological studies of plasma sprayed coatings against WC surfaces demonstrated a coefficient of friction ranging from 0.5 to 0.8. Microstructural analysis of the wear track revealed adhesive wear with significant plastic deformation. The study concludes that Al_2O_3 -YSZ-CNT bimodal composite coatings outperform $\mu\text{-Al}_2\text{O}_3$, making them a promising candidate for wear resistance application.

9:50 AM

(PACRIM-S12-033-2025) Thermal Conductivity Measurement of Heat-Dissipating Filler Particles Using Frequency-Domain Thermoreflectance Microscopy

T. Uchiyama*¹; S. Yabumoto¹; D. Hayashi¹; T. Ota¹

1. ScienceEdge Inc., Japan

Thermal interface materials (TIMs) are composed of heat-dissipating filler particles, typically less than several tens of micrometers in size. These fillers include single crystals, polycrystals, and sintered fine particles. Since the mean free path (MFP) of thermal conduction phonons is constrained by the particle size and structure, the thermal conductivity of the fillers is expected to differ from that of bulk materials. However, the small size of these particles poses a challenge for measurement using conventional methods. To address this, we developed a frequency-domain thermoreflectance (FDTR) microscope capable of localized laser heating with a micro-spot focus, enabling the thermal conductivity measurement of individual filler particles such as Al_2O_3 single-crystal particles, AlN polycrystalline particles, and sintered AlN particles. Our findings reveal that the phonon MFP is indeed limited by the size of the constituent particles, while the sintering interfaces between particles do not act as significant barriers to diffusive heat transport.

10:10 AM

(PACRIM-S12-034-2025) Development of Solid-State Li-ion and Metal-Air Batteries (Invited)

R. Liu*¹

1. National Taiwan University, Department of Chemistry, Taiwan

To reach carbon neutrality before 2050, 80% of fossil fuels will be replaced by renewable energy to decrease CO_2 emissions. In energy substitution, energy storage devices, such as Li-ion batteries, are widely used in the smart grid and electric cars. After 30 years of development, the energy density of Li-ion batteries reaches 300 mAh kg^{-1} . Solid-state Li-ion batteries are studied intensively for a high energy density of 500 mAh kg^{-1} before 2030. In a solid-state battery, solid-state electrolyte is essential in improving electrochemical performance. In this report, a development on solid-state electrolytes will be introduced. Different rechargeable metal-air batteries have caught much attention as one of the most intriguing methods that could simultaneously address carbon dioxide-related environmental concerns and ever-increasing sustainable energy storage demands. We will also introduce these types of batteries and give prospects compared to solid-state Li-ion batteries.

10:40 AM

(PACRIM-S12-035-2025) A new, affordable clay-based ceramic membrane for oil-water emulsion separation

Y. Manawi*¹

1. Hamad Bin Khalifa University Qatar Environment & Energy Research Institute, Qatar

This study introduces a cost-effective ceramic membrane made from halloysite nanotubular (HNT) clay, addressing the high cost of ceramic membranes caused by expensive raw materials and energy-intensive sintering. Fabricated using a die press method and sintered at lower temperatures than commercial membranes, the membrane's properties were evaluated for chemical composition, surface characteristics, hydrophilicity, durability, oil rejection, and antifouling performance. The optimized composition (halloysite: Al_2O_3 : starch at 60:25:15 wt.%) resulted in a pore size of 230 nm, 62.4% porosity, and 1040 LMH/bar water permeability. It exhibited superhydrophilic and underwater superoleophobic properties. Oil-water separation tests at oil concentrations of 724 and 1014 mg/L achieved over 99% oil rejection. The first filtration cycle showed a 54% higher flux recovery ratio (FRR) for the lower concentration, while the second cycle had a 30% higher FRR for the higher concentration, likely due to oil film formation reducing penetration. Tests with real produced water from gas extraction confirmed its suitability for pre-treatment before reverse osmosis. The results highlight the potential of this low-cost HNT-based ceramic membrane as a viable alternative for oily wastewater treatment, offering economic and environmental benefits.

PacRim S13 - Functional Defects in Ceramic Materials

PACRIM Symposium 13 - Characterization and applications of defect-induced emergent phenomena

Room: Grouse

Session Chair: Candace Chan, Arizona State University

8:30 AM

(PACRIM-S13-005-2025) Effect of rare earth oxides on the thermal stability of $\text{Mn}_{0.76}\text{Fe}_{0.87}\text{Co}_{1.07}\text{Zn}_{0.3}\text{O}_4$ NTC ceramics under high temperature nitrogen atmosphere (Invited)

S. Liang^{*1}

1. Ningxia University, China

In this study, La_2O_3 and Y_2O_3 were utilized as a rare earth oxide dopant to synthesize $x\text{R}_2\text{O}_3\text{-Mn}_{0.76}\text{Fe}_{0.87}\text{Co}_{1.07}\text{Zn}_{0.3}\text{O}_4$ ($x = 0.0025, 0.005, 0.01, 0.02$) NTC materials via solid-state sintering. The effect of high-temperature N_2 annealing on the electrical properties of these materials were investigated. Results indicated that after nitrogen annealing at 750 °C for 4 hours, the variation rates of resistivity (ρ_{25}) and material constant ($B_{25/50}$) significantly decreased with increasing La doping. For the undoped sample, the $\Delta\rho_{25}$ was 176% and the $\Delta B_{25/50}$ was 6%. For the La-doped sample with $x = 0.01$, the $\Delta\rho_{25}$ was reduced to 8% and the $\Delta B_{25/50}$ to 1%, demonstrating improved stability. This improvement is attributed to the preferential aggregation of La at grain boundaries, filling gaps and forming R-O bonds that hinder oxygen vacancy migration. Impedance spectroscopy analysis revealed a decreased intensity of the grain boundary relaxation peak with rare earth elements, suggesting fewer defects within the grains post-annealing. Similar results were obtained when Y doping was used instead of La doping.

9:00 AM

(PACRIM-S13-006-2025) Functional Defects in Advanced Ceramics Fabricated by Selective Laser Sintering (Invited)

B. Cui^{*1}; L. Trinh¹; X. Zhang¹; F. Wang¹; L. Wadle¹; H. Dong¹; Y. Lu¹

1. University of Nebraska-Lincoln, USA

Direct selective laser sintering (SLS) process is a novel and promising approach for additive manufacturing of various ceramic materials such as BaTiO_3 and compositionally complex carbides. Without polymer binders or resins, a dense ceramic layer could be formed with a thickness of several hundred micrometers in which pores or microcracks are absent. The SLS process may induce ultrafast densification, metastable phase transformation, and extraordinary defects. For example, a Ti-rich secondary phase was distributed at grain boundaries of the SLSed hexagonal BaTiO_3 , while cellular structures with element segregation and dislocations on cell boundaries were observed in SLSed $(\text{Zr},\text{Nb},\text{Ta},\text{Ti},\text{W})\text{C}$. This talk will discuss the new phenomenon and fundamental questions related to the defect formation during SLS of advanced ceramics.

PACRIM Symposium 13 - Defects for energy, thermal, mechanical, and electronic applications II

Room: Grouse

Session Chair: Munekazu Motoyama, Kyushu University, Kyushu Daigaku, Fukuoka, Fukuoka Prefecture, JP, academic

10:20 AM

(PACRIM-S13-007-2025) The effect of light illumination on the dislocation behavior in inorganic semiconductors (Invited)

A. Nakamura^{*1}

1. Osaka Daigaku, Department of Mechanical Science and Bioengineering, Japan

Inorganic semiconductors are essential to modern technologies, such as power electronics and integrated circuits. However, their application in advanced fields has been limited due to their limited plasticity. In contrast, our research has shown that external light environment plays an important role in controlling the plasticity at room temperature. ZnS single crystals exhibit brittle properties under normal light environments, but in complete darkness they show surprising plasticity mediated by the glide and multiplication of dislocations. Furthermore, creep deformation behaviors of the ZnS crystals have shown that the mobility of dislocations changes by more than three orders of magnitude depending on the presence or absence of light. The cause of these phenomena is believed to be that in the presence of light, the atomic bonding state with local electronic structure at the dislocation core changes due to the electrostatic interaction between the photo-excited carriers caused by the internal photoelectric effect and the structural charge of individual dislocations, resulting in a change in the mobility of the dislocation, thus limiting the plasticity. These findings have broken the conventional wisdom that inorganic materials are brittle and easily fractured at room temperature, and have led to new possibilities for the processing and application of various ceramic materials.

10:50 AM

(PACRIM-S13-008-2025) Photo-plasticity of semiconductors: Controlling dislocation motion using illumination

Y. Zou^{*1}

1. University of Toronto, Canada

The hardening effect under illumination has been discovered in semiconductors for several decades, known as photo-plastic effect. It is widely believed that this effect arises from the reduction in dislocation mobility caused by light. However, dislocation dynamics under illumination is poorly understood due to the lack of direct evidence. In this study, we provide both experimental evidence and atomic simulations for reduced dislocation mobility in semiconductors under UV light. By combining photo-nanoindentation, transmission electron microscopy (TEM), and atomic simulations, we visualized dislocation distribution in both darkness and under illumination. Our results show that dislocations move shorter distances under light compared to darkness. Molecular dynamics (MD) simulations, utilizing machine learning potentials, reveal that photoexcitation increases the Peierls stress and decreases dislocation motion, which consistent with experimental findings. These results offer direct evidence of reduced dislocation mobility under illumination and atomic-scale insights into the dislocation dynamics under illumination.

11:10 AM

(PACRIM-S13-009-2025) Ceramic coating for passive daytime radiative cooling applications

K. Banerjee^{*1}; Z. Wu¹; Y. Tang¹; H. Wang¹; H. Yan¹

1. Queen Mary University of London, School of Engineering and Materials Science, United Kingdom

The cooling of buildings during the daytime is related to energy cost and CO₂ emissions. The wide usage of air conditioners consumes a huge amount of power and generates greenhouse gases. The coating of passive daytime radiative cooling (PDRC) materials on buildings can help to cool down the indoor temperature. The working principle of PDRC materials depends on the less absorption of sunlight and emission of long-wave infrared radiation to the cold space (3 K). Although thin film and multilayer-based PDRC materials are reported for cooling applications, the development of a cost-effective PDRC layer with large scalability and selective long-wave infrared radiation emission is challenging. In this work, we reported a low-cost composite of SiO₂ and a glass mixture for PDRC applications. The slurry of the composite was painted on the commercial bricks and cooling performance was tested. Considering the wavelength of Si-O bond vibration, the SiO₂ is selected to attain high emission in the atmospheric transparent window. In addition, the combination effects of porous microstructure, and the high band gap of this coating layer are highly beneficial for the scattering of sun rays and limiting the absorption. The selective emission of the composite-designed PDRC material in the wavelength region of 8-13 μm, with solar reflectance of 80 % of the coating assists in reducing the temperature up to 5 °C.

PacRim S14 - Advanced Structural Ceramics and CMCs for Ultra Extreme Environments

PACRIM Symposium 14 - Advanced Structural Ceramics and CMCs for Ultra Extreme I

Room: Cypress

Session Chairs: Theresa Davey, Bangor University;
Samuel Humphry-Baker, Imperial College London

10:20 AM

(PACRIM-S14-001-2025) Crystal plasticity and strengthening of rock salt carbides from the atomic level to the micro-scale (Invited)

T. Csanádi^{*1}; J. Koltai²; Z. Dankházi²; Y. Ravikumar¹; A. Kovalčíková¹; M. Reece³

1. Institute of Materials Research, Slovak Academy of Sciences, Slovakia
2. Eotvos Lorand Tudományegyetem Természettudományi Kar, Hungary
3. Queen Mary University of London, School of Engineering and Materials Science, United Kingdom

The mutual enhancement of strength and plasticity is a great challenge in hard and brittle materials. This phenomenon has been investigated in rock salt carbides, including (Hf-Ta-Zr-Nb)C high-entropy carbide and monocarbides such as TaC and HfC, using various experimental and computational methods. Different crystallographic facets were subjected to nanoindentation and micropillar compression to determine strength/hardness and slip activation of grains. Critical resolved shear stress (crss) values corresponding to the {110}<1-10> and {111}<1-10> slip systems were calculated for both ideal and dislocation-containing crystals by first-principles density functional theory. Micropillar compression, combined with other techniques (SEM, EBSD, TEM), revealed that the crss is the lowest on the {110} glide plane with significantly enhanced value (~2.8 GPa) for (Hf-Ta-Zr-Nb)C compared to the component carbides (1.4-1.8 GPa). Still, there is a possibility to activate the {111} in specific cases. Simulated crss values correlate with experiments and make it possible to describe the experimental

orientation-dependence hardness and slip activation using finite element simulations. Thus, nanoindentation is suggested to be a quick and efficient tool to assess the grain strength and to search for the activation of {111}<1-10> systems which endow rock salt carbides with improved plasticity.

10:50 AM

(PACRIM-S14-002-2025) Developing Anisotropic Microstructures in UHTCs for New Thermal Protection Systems (Invited)

C. Tallon^{*1}

1. Virginia Polytechnic Institute and State University, Materials Science and Engineering, USA

One of the most extreme scenarios for any material class is associated with the reentry conditions of that hypersonic vehicles have to withstand: huge heat fluxes and soaring temperatures, extensive thermal gradients, stagnation pressures and ruthless oxidative environments, etc. Ultra-High Temperature Ceramics (UHTCs) are a significant part of the equation to solve the problem of material selection component survivability for these vehicles. There has been a remarkable development over the past 20 years for UHTCs in their state-of-art manufacturing and microstructural design, although most of the solutions still revolves around isotropic microstructures. More recent advances in manufacturing have paved the way for exploring different UHTC microstructures that could lead to other heat management strategies. In this talk, innovative colloidal processing approaches to develop anisotropic microstructures in UHTCs will be discussed: including aligned porosity, textured microstructures and high aspect ratio building blocks. The microstructures will be discussed for small and large, complex geometries. This anisotropy has the potential to allow the tailoring of the thermomechanical response in different directions within the same component, and enable innovative active and passive cooling strategies. This also opens the door to different type of applications beyond hypersonics for these materials.

PacRim S15 - Porous Ceramics - From Innovative Processing to Advanced Industrial applications

PACRIM Symposium 15 - Porous Ceramics: From Innovative Processing to Advanced Industrial applications II

Room: Seymour

Session Chair: Tobias Fey, Friedrich-Alexander University Erlangen-Nürnberg

8:00 AM

(PACRIM-S15-003-2025) Composite materials with cross-scale cellular and porous structure and their application in heat conversion processes (Invited)

F. Scheffler^{*1}; U. Betke²; M. Scheffler²

1. Otto-von-Guericke-Universität Magdeburg, Inst for Chemistry, Germany
2. University of Magdeburg, Inst for Materials and Joining Technology, Germany

Mankind faces unprecedented challenges, particularly with regard to reducing emissions, conserving energy, and saving resources. The demand for thermal energy, both as process heat and for space heating, represents a significant share of energy consumption. One way to reduce the associated demand for primary energy in this context is the use of waste heat or renewable heat sources. This requires suitable active materials for efficient heat conversion and storage. The utilization of low-temperature heat and/or waste heat can be achieved with the help of microporous adsorbents such as zeolites and metal-organic frameworks (MOFs), which, however, need to be properly supported. The first part of this contribution

provides an overview of the combination of macroporous support structures with microporous adsorbents, with a focus on ceramic foams as supports. In the second part, options for increasing the share of microporous components on such macroporous supports are discussed, and, finally, a perspective on existing and potential applications of such material combinations in heat conversion is provided.

8:30 AM

(PACRIM-S15-004-2025) From Timeless Japanese Wood Joinery to Advanced Ceramic Joint Interlocking

P. Hoffmann^{*1}; L. Wahl¹; S. Funk¹; T. Fey²

1. FAU Erlangen-Nürnberg, Institute of Glass and Ceramics, Germany
2. Friedrich-Alexander University Erlangen-Nürnberg, Department Material Science and Engineering, Germany

Efficiency, adaptability, and sustainability are key factors in developing high-performance architected materials. While monolithic ceramics are limited, hybrid structures with multiple components offer enhanced functionality. We investigated modular, interlocking ceramic structures with inherent stability, consisting of detachable and replaceable building blocks. Inspired by Japanese Wood Joining WJ, we developed innovative interlocking joints without bonding phases, meeting requirements for self-supporting structures in demanding applications like high temperatures. To address ceramics' brittleness, we applied principles of Topological Interlocking TI, localising fracture propagation through modularity, a significant advantage over monolithic structures. We introduce a novel hybrid approach, Ceramic Joint Interlocking CJI, combining WJ's self-supporting strength with TI's modularity. Using low-pressure ceramic injection moulding, we fabricated intricate interlocking ceramic components with multiple joints that assemble without external forces. Mechanical performance was evaluated through deflection measurements. This novel approach enables modular, reusable, and inherently stable ceramic structures, presenting the potential for durable, flexible, high-performance applications.

8:50 AM

(PACRIM-S15-005-2025) Combination of Freeze Casting and Gelcasting to obtain porous ceramics

I. Klösel^{*1}; T. Fey¹

1. Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Materials Science and Engineering, Germany

Well-established techniques for tailoring the microstructure and enhancing the mechanical and thermal properties of porous ceramics are freeze casting and gelcasting, which offer a wide range of technological applications requiring lightweight materials with high permeability such as thermal insulation, filtration, catalysis or biomedical implants. By combining these conventional techniques, it is possible to utilise the advantages of both methods. While the freeze casting approach enables the formation of highly directional and interconnected pore structures by freezing a ceramic slurry and subsequent sublimation of the solvent, the gelcasting approach ensures mechanical strength by using a polymer gel to solidify the ceramic network prior to sintering. In this study, alumina (Al_2O_3) foams with different ceramic contents of the suspensions are prepared using the gelcasting process and agarose as gelling agent, which are then frozen and freeze-dried. The influence of the drying time of the gelled foam before freezing and the water content of the suspension on the porosity development is investigated. The mechanical and thermal properties as well as the microstructure are also analysed.

9:10 AM

(PACRIM-S15-006-2025) Lightweight and high-strength textured fibrous Si_3N_4 3D scaffold seeded with $\beta\text{-Si}_3\text{N}_4$ particles prepared via freeze casting

J. Yang^{*1}; Q. Zhi¹; B. Wang¹

1. Xi'an Jiaotong University, State Key Laboratory for Mechanical Behavior of Materials, China

Highly porous Si_3N_4 ceramics with unidirectionally aligned pore channels are gaining significant attention across various fields due to their outstanding functional capabilities. Herein, we design and fabricate a novel $\beta\text{-Si}_3\text{N}_4$ scaffold composed of directionally aligned lamellar walls with a textured microstructure by directionally freeze casting of $\alpha\text{-Si}_3\text{N}_4$ suspensions with fine elongated $\beta\text{-Si}_3\text{N}_4$ seeds addition, followed by liquid phase sintering. During the sintering, the scaffold exhibited anisotropic shrinkage, and fibrous $\beta\text{-Si}_3\text{N}_4$ grains were synthesized through epitaxial growth on the seeds preferentially oriented or the nuclei originated from $\alpha\text{-Si}_3\text{N}_4$ powders, resulting in the grains aligned parallel to lamellar walls and bridged the walls. Seed additions of 7 to 15 wt% were beneficial for the optimized distribution of the two types of $\beta\text{-Si}_3\text{N}_4$ grains, which contributed to the excellent resistance to buckling-induced fracture for the walls. Compared with other unidirectional porous Si_3N_4 prepared by freeze-casting in the literature, the Si_3N_4 scaffold exhibited outstanding compressive strength, ranging from 2.8 to 22.0 MPa, as the porosity decreased from 94.4 % to 88.0 % and the density increased from 175 to 365 mg/cm^3 .

9:30 AM

(PACRIM-S15-007-2025) Automating the Future: High-Throughput Production of Porous Alumina Ceramics

E. Wolf^{*1}; K. G. Webber¹; T. Fey¹

1. Friedrich-Alexander-Universität Erlangen-Nürnberg, Institute of glass and ceramics, Germany

The high-throughput (HT) method is characterized by an automated sample preparation and analysis coupled with AI-driven data evaluation. While it is already well established in the pharmaceutical and chemical fields, its application in materials science, especially in ceramics research, remains limited. Key areas in ceramics research that would greatly benefit from the use of HT processing are the analysis of phase diagrams or the evaluation of the complicated relationship between microstructure and properties in porous ceramics. We present the first step toward automated processing of porous ceramics by the sacrificial templating method, using an automatic powder dispensing robot to improve accuracy and reduce manual work. Porous alumina ceramics with varying porosities (0 - 50 vol%), pore geometries (spherical and fibrous) and pore sizes (10 - 150 μm) were successfully fabricated using different organic pore formers. Precise dosing enabled fine tuning of porosities, resulting in highly tunable mechanical properties. The microstructure was analyzed using $\mu\text{-CT}$ technique, characterizing the shape, connectivity and size of the pores. Our results highlight the significant potential of high-throughput methods in advancing porous ceramic research, offering opportunities for increased efficiency and precision in material characterization and development.

PACRIM Symposium 15 - Porous Ceramics: From Innovative Processing to Advanced Industrial applications I

Room: Seymour

Session Chairs: Patrizia Hoffmann, Friedrich-Alexander-Universität
Erlangen-Nürnberg; Tobias Fey, Friedrich-Alexander University
Erlangen-Nürnberg

10:20 AM

(PACRIM-S15-001-2025) Deformation Control for Optimizing Kelvin Cell Architecture

S. Funk¹; T. Fey*¹

1. Friedrich-Alexander University Erlangen-Nürnberg, Department
Material Science and Engineering, Germany

The mechanical performance of porous and cellular structures is closely correlated with their micro- and macro geometric design. The impact of architectural variations on the remaining physical properties, in particular strength, stiffness, and load distribution, is of critical importance. An optimized architectural design can result in a significant enhancement of these properties. This study examined the effects of stretching or compressing Kelvin cells with a 45° angle along the z-axis, resulting in architectures with variations of controlled deformation angles between 15° and 60°. The Kelvin cell Al₂O₃ structures were designed, 3D-printed, and sintered at 1600°C. It was found that depending on the deformation angle, the anisotropic volumetric shrinkage from 45° could be compensated for in order to achieve a non-deformed structure. The results of the compression tests supported by FEM-simulations indicate that variations in the deformation angles significantly affected the mechanical properties. This investigation highlights the potential for optimizing cellular structures in order to achieve specific mechanical properties, which can be readily achieved through the precision of the VPP process.

10:40 AM

(PACRIM-S15-002-2025) Preparations and Characterizations of Reticulated Porous Ceramics for Environmental and Military applications

J. Ha*¹; H. Lee¹; J. Lee¹; I. Song¹

1. Korea Institute of Materials Science, Republic of Korea

Porous ceramics have garnered increasing attention in various research fields due to their exceptional thermal and chemical resistance, which surpasses that of porous metals and polymers. Among the diverse types of porous ceramics, reticulated porous ceramics show significant industrial promise because of their low density and high permeability. Despite these advantages, their applications in environmental fields (e.g., filtration) and military contexts (e.g., radar absorption) remain limited. This is primarily due to the relatively low compressive strength of reticulated porous ceramics compared to other porous ceramic types. Consequently, this study aims to enhance the compressive strength of reticulated porous ceramics by optimizing process parameters such as the solid loading level, particle size, and the incorporation of additives into ceramic slurry samples. The characteristics examined in this study include pore features (density, size, and structure), sintering behavior (linear shrinkage), mechanical properties (compressive strength), and dielectric properties (breakdown strength).

PacRim S16 - Advanced Powder Processing and Manufacturing Technologies

PACRIM Symposium 16 - Novel synthesis of powder and granulation technology

Room: Stanley

Session Chair: Yuki Yamaguchi, National Institute of Advanced
Industrial Science and Technology (AIST)

8:00 AM

(PACRIM-S16-001-2025) On the Large-Scale Combustion Synthesis of SiC Aerogels (Invited)

L. Han¹; H. Li¹; Y. Li¹; J. Li*¹

1. Technical Institute of Physics and Chemistry, China

Ceramic aerogels have been identified as a potentially valuable material for thermal insulation and protection in harsh environments. However, current synthesis methods are not yet energy-, time- and cost-effective for large-scale production and applications, particularly for non-oxide ceramic aerogels. Here we reported a new way to synthesize SiC aerogels within seconds and over liter scale, with a demonstrated throughput of ~16 L min⁻¹ in a typical lab experiment. The key lies in renovated combustion synthesis and properly chosen catalyst which leads to a volumetric expansion rate from powders to aerogels of over 1,000%. The obtained SiC aerogels have high porosity (≥99.6%), low density (~12 mg cm⁻³), low thermal conductivity (0.027 W m⁻¹ K⁻¹), and high compressibility, and remain flexible over a wide temperature range (-196 to 1100 °C). The combustion synthesis is self-sustainable and requires minimal energy input. The cost of the product is estimated to be \$0.7 L⁻¹, making it a highly cost-effective solution. Our invention provides a practical pathway for large-scale applications of ceramic aerogels and calls for a rethinking of self-propagation high temperature synthesis in a one-step conversion from raw chemicals to bulk products.

8:30 AM

(PACRIM-S16-002-2025) Graphene coating by mechanical treatment on water resistance of aluminium nitride particles for spray freeze granulation drying of aqueous slurry (Invited)

J. Tatami*¹; R. Yamazaki¹; M. Iijima¹; N. Kondo³; S. Kawaguchi²

1. Yokohama National University, Japan

2. PRECI Co., Ltd., Japan

3. National Institute of Advanced Industrial Science and Technology, Japan

In order to give water resistance to aluminum nitride particles for preparation of ceramics using aqueous slurry, graphene coating by mechanical treatment on the particles was investigated. Graphene coating was carried out on the surface of the fine aluminum nitride particles which was obtained by mechanical treatment of mixed powder of graphene and aluminum nitride in a compression and shear field. The graphene-coated aluminum nitride particles showed excellent water resistance, since the pH value of the aqueous suspension did not change and aluminum hydroxide was not detected even after stirring for long time. The relative density of the aluminum nitride ceramics obtained with the composite particles was high, and their secondary phase was also found to be yttrium aluminate having less oxygen than those prepared without graphene coating, due to suppressed hydrolysis.

9:00 AM

(PACRIM-S16-003-2025) Spray freeze granulation drying using non-aqueous slurries for fabricating homogeneous silicon nitride ceramicsR. Yamazaki¹; J. Tatami²; M. Iijima¹; S. Kawaguchi³; N. Kondo⁴

1. Yokohama-shi, Graduate School of Environment and Information Sciences, Japan
2. Yokohama National University, Japan
3. PRECI Co., Ltd., Japan
4. Sangyo Gijutsu Sogo Kenkyujo Chubu Center, Japan

The application of spray freeze granulation drying technique to the fabrication of nitride ceramics is expected to improve the properties such as the strength of sintered bodies. However, it is rarely applied because aqueous slurries are used in the granulation method. In this study, we prepared silicon nitride slurries with solvents mixed tert-butyl alcohol and cyclohexane to ratios of 0:100, 20:80, 40:60, 80:20, 100:0, instead of water. In situ observation of these freezing behaviors of the slurries with optical coherence tomography, which enables to visualize the internal structure without destruction, showed that the use of mixed solvents with eutectic compositions resulted in homogeneous freezing and the production of freeze-dried bodies without coarse pores. The granules produced from this slurry by spray freeze granulation drying were spherical and soft with no significant segregation of particles or organic matter inside. In addition, the green bodies made from the granules were sintered, yielding silicon nitride ceramics with homogeneous internal structure and high strength.

9:20 AM

(PACRIM-S16-004-2025) Freeze-granulation of suspension or solution: innovative processes for MOX fuel fabricationL. Ramond¹; F. La Lumia¹; F. Lebreton¹; G. Bernard-granger¹; C. Pagnoux²

1. Commissariat à l'énergie atomique et aux énergies alternatives Marcoule, CEA/DES/ISEC/DMRC, Université de Montpellier, France
2. Institut de Recherche sur les Ceramiques, France

The current industrial manufacture of UO_2 - PuO_2 MOX fuel pellets is carried out by a dry route process, through steps involving fine powders (grinding, mixing and pressing). In order to limit powder dissemination and to improve the processability (flowability and pressability) of the UO_2 - PuO_2 powder mixture, innovative wet-route processes are investigated to form granulated powders. Freeze granulation have been developed and performed at CEA both on a concentrated, water-based powder suspension and on a nitric solution containing U and/or Pu cations. The suspension or solution is atomized into small droplets that are instantly frozen in liquid nitrogen. The resulting frozen granules are then freeze-dried to sublimate the ice and yield a dry granulated powder. Granules properties can be controlled through the suspension/solution formulation and the atomization conditions. In the case of the freeze granulation of a solution, a calcination step is also necessary to convert the granules from nitrate to oxides. After pressing and sintering, MOX pellets were characterized (density, microstructure, U/Pu homogeneity...). For both suspensions and solutions, the good pressability leads to the formation of dense ($D_{rel} > 95\%$) and homogenous pellets by uniaxial pressing and sintering. The freeze granulation of U/Pu nitric solutions provides a remarkably homogeneous distribution of U/Pu elements.

9:40 AM

(PACRIM-S16-005-2025) Fabrication of C12A7 with various anion encapsulationK. Takiishi¹; J. Song²; M. Watanabe²; M. Inada²; T. Ishihara²

1. Kyushu Daigaku Kogakubu Daigakuin Kogakufu, Japan
2. Kyushu Daigaku, Japan

$\text{C12A7}:\text{OH}^-$ has a cage-like crystal structure and encapsulates hydroxide ions within the cage to compensate the positive charge of the cage. The hydroxide ions in the cage can be substituted for other anions and electrons, which provides various properties

express depending on anion species. We have successfully synthesized C12A7 from hydrogarnet precursor prepared by liquid phase method. In addition, we succeeded to synthesize C12A7 with the substitution of Al site with Si. In this study, the effect of anion substitution in C12A7 was investigated. C12A7 was obtained by heat treatment of hydrogarnet with SiO_2 and CaF_2 . The lattice constant of non-Si doped C12A7 with CaF_2 decrease indicating that OH^- in mayenite was replaced to F^- . On the other hand, the lattice constant of Si doped C12A7 was smaller than that of non-Si doped C12A7 ; however, that did not change regardless of addition CaF_2 . Substitution of Al sites with Si increased the amount of fluoride ions, which are encapsulated anions. These results suggest that C12A7 can be used as an ion storage material.

PACRIM Symposium 16 - Novel forming and sintering technology

Room: Stanley

Session Chairs: Junichi Tatami, Yokohama National University

10:20 AM

(PACRIM-S16-006-2025) Advanced Powder Processing: From Flash Sintering to Ultrafast Sintering without Electric Currents in Specimens (Invited)J. Luo¹

1. University of California San Diego, USA

In this talk, I will first review a series of mechanistic studies of flash sintering using ZnO as the model system [see a perspective: Scripta Mater. 146:260 (2018)]. In 2015, we reported that flash sintering generally starts as a thermal runaway. In 2017, we furthered suggest ultrahigh heating rates enable ultrafast sintering by demonstrating that similar densification rates can be achieved via (1) flash sintering and (2) rapid thermal annealing (intense infrared heating without an electric field) with similar heating rates of ~ 200 K/s. Subsequently, general ultrafast sintering methods, enabled by the same under-lying mechanism, were demonstrated in collaborative studies led by Professor Liangbing Hu, e.g., ultrafast high-temperature sintering [Science 368:521 (2020)] and atmospheric-pressure plasma sintering. Two ultrafast reactive sintering schemes have also been developed to synthesize and fully densify high-entropy metal diborides in ~ 2 minutes with or without electric currents in the specimens. We also develop two-step flash sintering to densify ceramics with suppressed grain growth. Our on-going exploration of a new ultrafast sintering scheme will also be discussed (unpublished results).

10:50 AM

(PACRIM-S16-007-2025) Study on the 3D printing of zirconia and silicon nitride by stereolithography (Invited)J. Zhang¹

1. Shanghai Institute of Ceramics Chinese Academy of Sciences, China

Stereolithography is an attractive technique for the fabrication of complex-shaped ceramic components with high dimensional accuracy. The materials used in stereolithography are the blend of photocurable monomer, resin, ceramic powders and photoinitiator etc, which can be solidified under a certain amount of radiation. Presently, alumina, silica and zirconia powder have been successfully prepared by stereolithography method with high accuracy. However, there are still quite a lot problems in term of solid loading, the curable thickness and printing accuracy that need to be well resolved. In this study, two ceramic powder were studied for Stereolithography. The dispersion of ceramic powder in photocurable resin and the slurries properties were intensively investigated. The selection of dispersant, and the slurry properties were studied based on the adsorption, FTIR, rheological and contact angle etc. measurements. The factors that influence the curable thickness and the printing accuracy were investigated. The binder removal,

sintering and the final properties of the ceramics were also characterized. Finally, the optimized composition, the processing parameter for the development of high performance ceramics through stereolithography were presented.

11:20 AM

(PACRIM-S16-008-2025) Fabrication of MgO bulk ceramics with dispersed nitride phosphor particles by reaction sintering with cold isostatic pressing (Invited)

T. Takahashi¹; J. Tatami²

1. Chiho Dokuritsu Gyosei Hojin Kanagawa Kenritsu Sangyo Gijutsu Sogo Kenkyujo, Japan
2. Yokohama National University, Japan

For wavelength conversion materials for high-power LEDs, a wide range of fluorescent wavelengths, high thermal conductivity, and translucency are required. For example, if the temperature of the component is less than 200 °C, the required thermal conductivity is approximately 10 Wm⁻¹K⁻¹. All-ceramic phosphors exhibit high thermal conductivity, but densification by high-temperature sintering is an issue, and they have been limited to a few phosphors. In this study, MgO bulk ceramics with a thermal conductivity of 10 Wm⁻¹K⁻¹ were fabricated using the reaction sintering with cold isostatic pressing (RS-CIP) method. In this method, molding and sintering are performed separately using a 1 GPa hydrostatic press. This improves the homogeneity and filling of the particle assembly structure in the compact, which forms the basis of the microstructure, and achieves high densification without heating with a minimum amount of solvent added. Furthermore, a red phosphor material was fabricated by densifying MgO with a nitride phosphor (CaAlSiN₃:Eu²⁺, CASN) particles that degrades and changes when heated to several hundred °C, and it was confirmed that the material has the same luminescent properties as the raw CASN powder and can be excited by blue laser light.

PacRim S17 - Additive Manufacturing of Ceramics and Composites

PACRIM Symposium 17 - Additive Manufacturing of Ceramics and Composites I

Room: Prince of Wales

Session Chairs: Chao Ma, Arizona State University;

Trent Allen, Tethon 3D

10:20 AM

(PACRIM-S17-001-2025) Additive Manufacturing of Textured Ceramics (Invited)

C. Ma^{*1}

1. Arizona State University, USA

Ceramic additive manufacturing holds great potential to transform various industrial applications. Binder jetting has unique advantages over other AM processes, such as the capability to produce parts of large sizes and complex geometries. In this work, textured ceramics were successfully obtained using binder jetting for the first time, demonstrating aligned grains and directionally tailored properties. The templated grain growth approach was employed. A mixture of alumina nanoplatelets and nanoparticles was used as the feedstock powder: the nanoplatelets served as templates for epitaxial grain growth during sintering while the nanoparticles were consumed by the grain growth. After producing green samples through binder jetting, debinding, calcination, and sintering were performed. With the Archimedes method, it was found that the bulk density of the sintered samples with alumina nanoplatelets was lower than that without them. Scanning electron microscopy and X-ray diffraction results showed that morphological and crystallographic textures were achieved in the sintered samples containing alumina nanoplatelets. The flexural testing results indicated that the textured

structure led to an improvement in the flexural strength, despite the lower bulk density of the textured samples. This work demonstrates that binder jetting can effectively produce textured ceramics with customized properties along desired directions.

10:50 AM

(PACRIM-S17-002-2025) Tomorrow's additive manufactured ceramic materials look nothing like they do today (Invited)

T. Allen^{*1}

1. Tethon 3D, USA

Additive manufacturing (AM) of ceramics is entering a new era of customization, where materials are no longer defined by standard formulations like alumina but are instead tailored to the unique demands of each application. This study highlights the transformative role of data-driven approaches in optimizing powder formulations, resin chemistries, and sintering parameters to achieve unparalleled material performance. Through predictive modeling manufacturers can design ceramic materials with specific mechanical, thermal, or optical properties, ensuring a perfect match for industries such as aerospace, healthcare, and energy. By integrating process data with advanced characterization techniques, this approach minimizes trial-and-error and accelerates innovation. This paradigm shift from one-size-fits-all materials to application-specific designs positions ceramic AM as a highly versatile and efficient manufacturing technology for tomorrow's challenges.

11:20 AM

(PACRIM-S17-003-2025) 3D printing buildability response of hybrid copper mine tailings geopolymer and cement material

A. Ventura¹; M. Plata¹; K. Baladad¹; E. d. Magdaluyo^{*1}

1. University of the Philippines Diliman, Department of Mining, Metallurgical and Materials Engineering, Philippines

This study investigates the 3D printing buildability of a sustainable hybrid geopolymer-cement material incorporating 22.5% copper mine tailings by total solid mass. Activation was achieved with 1M potassium hydroxide (KOH) to support both geopolymerization and cement hydration. A Taguchi L9 design of experiments assessed buildability through variations in plasticizer content (0%, 1%, and 3%) and solid-to-liquid ratios (0.24, 0.25, 0.26) to optimize shape retention. Hollow cylinders (60 mm diameter, 16 mm height) were printed at 20 mm/s, with a layer height of 2 mm and a 7.6 mm nozzle. Results showed that 1% plasticizer provided optimal shape retention of the 3D print samples; 0% plasticizer resulted in inadequate extrusion and adhesion, while 3% led to excessive flow and widening at the base layer. Deformation observed in the lower layers was due to compression from additional layers, indicating the need for parameter adjustments, such as print speed and extruder pressure. Surface morphology, chemical bonding, and compositional analyses further supported the printability potential of copper tailings-based hybrid geopolymers for sustainable materials.

11:40 AM

(PACRIM-S17-004-2025) Design concepts for strong and damage tolerance 3D-printing alumina-based multi-material components

R. Bermejo^{*1}; J. Schlacher¹; S. Nohut²; M. Schwentenwein²

1. Montanuniversitat Leoben, Materials Science, Austria
2. Lithoz GmbH, Austria

The potential of the Lithography-based Ceramic Manufacturing (LCM) technology to design novel alumina-based ceramic systems is explored. The first approach demonstrates the use of the LCM technology to print alumina-based ceramic parts with superior strength. The combination of alumina (outer regions) with alumina-zirconia (ZTA) layers introduces compressive residual stresses in the surface layers. A characteristic biaxial strength as high as 1 GPa is measured on the alumina-based multilayers. The second approach shows the effectiveness of the multi-material design to enhance the thermal

shock resistance of 3D-printed alumina-based ceramics. In this damage tolerant design, the alumina layers are embedded between ZTA-layer regions. The corresponding tailored compressive residual stresses in the embedded alumina layer regions act as an effective barrier to crack propagation, providing a minimum strength for the architecture. The retained strength after thermal shock of the multi-material ceramic is significantly higher than that of the monoliths, owed to the crack arrest capability of the embedded layers. In the last step, the feasibility of designing and printing a more-complex shaped component with tailored residual stresses is represented, which may open new application fields in the future.

PacRim S20 - Advanced Functional Materials for Clean Energy Solutions

PACRIM Symposium 20 - Advanced synthesis and characterization of photovoltaic materials

Room: Georgia A

Session Chairs: Lionel Vayssieres, Xi'an Jiaotong University; Soham Mukherjee, Uppsala Universitet

8:00 AM

(PACRIM-S20-006-2025) External Magnetic Fields in Molecular and Materials Transformations (Invited)

T. Fischer*¹; S. Mathur¹

1. University of Cologne, Institute of Inorganic and Materials Chemistry, Germany

External stimuli like magnetic and electric fields are mainly used to probe molecular and materials properties, but their application in materials synthesis or molecular transformation is often limited to niche applications. Here we discuss the use of external magnetic fields in chemical vapor deposition (CVD) of functional thin films using molecular single-source precursors. CVD in general has emerged as a versatile technique for fabrication of thin films and coatings with a wide range of mechanical, electrochemical, electrical, tribological and optical properties, where precursor/substrate characteristics, flow rate, temperature, and pressure are the conventional process-control parameters, influencing the deposition characteristics. With the introduction of external magnetic fields, new process spaces emerge to modulate the CVD process independent of the conventional process-control parameters. On the other hand, molecular transformations are also directly influenced by external magnetic, which enable alternate reaction pathways for the activation of small molecules for hydrogen production, and ammonia synthesis. This talk will provide an overview of different external field assisted CVD methods and provide examples on the alternate process parameter space for functional thin-films as heterogeneous catalysts in (photo)electrocatalytic small molecule activation.

8:30 AM

(PACRIM-S20-007-2025) Mechanical properties and instability of halide perovskite single crystals

Y. Zou*¹

1. University of Toronto, Canada

Organic-inorganic halide perovskites (OIHPs) are promising materials for LEDs and X-ray detectors, but their instability in radiation environments restricts their practical application. Here we use both electron beam from SEM and synchrotron X-ray beam from light source to investigate the radiation-induced instability of two types of OIHP single crystals, FAPbBr₃ and MAPbBr₃. There are distinct cracking patterns on the crystal surfaces under electron beam and composition changes under X-ray beam. We propose a mechanism based on energy conversions from volume strain caused by the organic component volatilization to crack formation. In addition, we test the Young's modulus and hardness to study the effects

of beam radiations on their mechanical performance. This work provides valuable insights into the stability and mechanical reliability of OIHP single crystals under external radiations for the first time.

8:50 AM

(PACRIM-S20-008-2025) Antimony selenide based thin film photovoltaic solar cells (Invited)

G. Liang¹; S. Chen¹; G. Chen¹; Y. Luo²; M. Cathelinaud²; H. MA²; X. Zhang*²

1. Shenzhen University, College of Physics and Optoelectronic Engineering, China
2. Universite de Rennes, Chemistry, France

Antimony selenide (Sb₂Se₃) is an emerging semiconductor material with interesting chemical and physical properties, including high stability, non-toxicity, an optimal bandgap as well as a high absorption coefficient for solar energy harvesting. The performance of Sb₂Se₃-based thin film solar cells has been recently boosted to higher than 10%. Current challenges in Sb₂Se₃-based devices can be categorized into three main aspects. First, the strong anisotropic nature of Sb₂Se₃ thin films raises the question of achieving preferentially oriented large-grain growth to facilitate charge carrier transport. Second, the material suffers from inherently low carrier concentrations and high defect density. Finally, reducing carrier recombination losses at both the front and back interfaces remains critical to improving overall carrier transport efficiency. These issues have been addressed by using different strategies. Promising improvements in both band alignment and surface passivation for enhancing the efficiency of these solar cells will be discussed.

9:20 AM

(PACRIM-S20-009-2025) The local chemical environment of sulfur atoms: how to probe solar devices made of Cu(In,Ga)(S,Se)₂ and other things (Invited)

C. Heske*¹

1. University of Nevada Las Vegas, Chemistry & Biochemistry, USA

This presentation will demonstrate the unique capabilities of cutting-edge x-ray spectroscopy methods (in particular element-specific soft x-ray emission spectroscopy, XES) to derive important insights into solar devices (solar water splitting and photovoltaics) from the viewpoint of sulfur. The presentation will include results from lab-based x-ray and UV photoelectron spectroscopy, inverse photoelectron spectroscopy, and x-ray-excited Auger electron spectroscopy, complemented by XES and soft x-ray absorption spectroscopy using high-brilliance synchrotron radiation. A particularly powerful approach is their resonant combination, Resonant Inelastic soft X-ray Scattering (RIXS), best displayed in a "RIXS map". The presentation will present recently developed instrumentation for studying electronic and chemical properties, buried layers and materials in situ and operando environments (focusing on the novel X-SPEC beamline and its unique endstations at the KIT Light Source in Karlsruhe, Germany). Then, we will discuss the impact of sulfur on the electronic properties (such as the level alignment) at surfaces and interfaces, and how to go about learning more about local chemical bonding (hybridization) in the vicinity of sulfur atoms, using a large variety of compounds as examples – sulfides, sulfates, and, in particular, chalcopyrites.

PACRIM Symposium 20 - Advanced synthesis and characterization of lanthanide materials

Room: Georgia A

Session Chairs: Thomas Fischer, University of Cologne;
Gunnar Westin, Uppsala University

10:20 AM

(PACRIM-S20-010-2025) Luminescent Rare Earth Doped Nanoparticles: Advancing Renewable Energy Solutions? (Invited)

F. Vetrone*¹

1. INRS, Université du Québec, Centre Énergie, Matériaux et Télécommunications, Canada

Luminescent rare earth doped nanoparticles are currently being studied for applications in clean and renewable energy solutions. Since their discovery, these nanomaterials have vastly matured, progressing from the basic understanding of the photophysical properties governing their nanoscale luminescence, to their use in the study of a number of fundamental properties and ultimately to a plethora of applications. This interest stems primarily from the ability to stimulate these luminescent nanoparticles with near-infrared (NIR) light as well as their diverse emission wavelengths spanning the UV to the NIR. Therefore, with a single NIR excitation wavelength, it is possible to observe anti-Stokes emission, known as upconversion, or single photon (Stokes) NIR emission. Here, we present our work on the synthesis and surface functionalization of various NIR excited (and emitting) core/shell rare earth doped nanostructures/nanoplatfoms and demonstrate how their various emissions could be harnessed for diverse applications including alternative energy. Moreover, we investigate how these functional nanoparticles could be rendered even more versatile through rational combination with other NIR excited optical nanostructures.

10:50 AM

(PACRIM-S20-011-2025) Microwave-Driven Materials Chemistry: Tuning the Properties of Lanthanide-Doped Nanostructures (Invited)

E. Hemmer*¹

1. University of Ottawa, Chemistry and Biomolecular Sciences, Canada

The remarkable optical properties of the lanthanides (Ln) make Ln-based materials ideal for applications ranging from biomedicine to optoelectronics and energy conversion technology. Lanthanide-based nanoparticles based on NaLnF_4 are commonly synthesized by the thermal decomposition of metal precursors in high-boiling-point solvents, based on convectional heating. Microwave reactors can improve reproducibility as offering better control over a reaction environment, more homogeneous heat distribution yields narrow size distributions, and rapid heating to the desired temperature shortens reaction times. Targeting applications in optoelectronics, photochemistry, and energy conversion, boosting the efficiency of lanthanide-based nanomaterials is key. In addition, some lanthanides have outstanding magnetic properties. For instance, we recently demonstrated for the first time the single-molecule magnet (SMM)-like behavior for Ln-based NPs. Alternatively, host materials such as $\text{Gd}_2\text{O}_2\text{S}$ have been proposed as nano-scintillators. In all of these cases, structural control is crucial to establish and understand structure-property relationships in the emerging class of Ln-based nanomaterials. This presentation will shed light on the synthesis of upconverting and near-infrared emitting nanoparticles, exploring the microwave-assisted strategy and the properties of NaLnF_4 and related materials.

11:20 AM

(PACRIM-S20-012-2025) Defect engineering – Molecule like europium clusters in ZnO (Invited)

G. Westin*¹

1. Uppsala University, Sweden

Doped semiconductor oxides are highest importance for renewable energy conversion and electronics. Crystal quality, size, connectivity, and surface structure along with the dopants electronic state, coordination and distribution are all pivotal for the properties and crucially dependent on the synthesis parameters. Here, Eu-doped ZnO nano-crystalline sponges with up to 33% Eu in ZnO are presented. The high doping levels found in the rich literature has spurred debate as the comparatively very large and aliovalent Eu^{3+} dopant ions should not fit in the h-ZnO lattice. A study using TG/DSC, XRD, XPS, IR- and Raman spectroscopy, EXAFS, SEM,(S)TEM/ED/DF/EELS/EDX/ePDF, and DFT proved that the Eu-ions were actually present in the 10 nm sized ZnO nano-crystals. Their presence did not change the h-ZnO unit cell-volume or yield XRD peaks assignable to Eu-oxide. EXAFS, XRD and DFT showed the ZnO:5% Eu crystals to contain Eu-oxide clusters with 4-8 Eu-ions without much disturbance of the ZnO matrix. Some changes were discerned in the IR and Raman spectra from 10 to 20% Eu indicating structure changes. A detailed HR-(S)TEM study of the 5 and 20%Eu samples, including ePDF allowing for spatial investigation of metal-ion coordination revealed that besides the Eu-doped ZnO crystals, there was a 5-10 Å layer of an Eu-rich phase.

11:50 AM

(PACRIM-S20-013-2025) Synthesis Strategies for Tunable Amorphous-Crystalline Metal-Organic Framework Nanohybrids

W. Zhang¹; N. Pinna*¹

1. Humboldt-Universität zu Berlin, Department of Chemistry, Germany

Metal-organic frameworks (MOFs) with encapsulated nanoparticles enjoy a vastly expanded application potential in catalysis, filtration, and sensing. The selection of particular modified core nanoparticles has yielded partial successes in overcoming lattice mismatch. However, restrictions on the choice of nanoparticles not only limit the diversity, but also affect the properties of the hybrid materials. Here, we show a versatile synthesis strategy using a representative set of MOFs and nanoparticle cores that are fine-tuned to incorporate from single to hundreds of cores in mono-, bi-, tri- and quaternary composites. This method does not require the presence of any specific surface structures or functionalities on the pre-formed cores. Our key point is to regulate the diffusion rate of base vapors that deprotonate organic linkers and trigger the controlled MOF-growth and encapsulation of nanoparticles. Furthermore, by mimicking the Stöber method to silica, we have extended the approach to amorphous metal organic frameworks colloids and coatings. The interplay between the amorphous phase formation and its crystallization allows to engineering novel hierarchical materials with tunable properties for applications ranging from catalysis, sensing to energy storage and conversion.

PacRim S21 - Cultural Heritage of the Pacific Rim

PACRIM Symposium 21 - Cultural Heritage of the Pacific Rim IV

Room: English Bay

Session Chair: Christina Bisulca, Detroit Institute of Arts

8:00 AM

(PACRIM-S21-027-2025) Degradation of cellulose acetate films during ageing

L. Liu*¹

1. Fuzhou University, China

Cellulose acetate (CA) was widely used by the film industry as well as by artists to create fine and decorative art. CA films plasticized with different content of diethyl phthalate (DEP) and triphenyl phosphate (TPP) were aged in different conditions for the study of the degradation markers and the plasticizer loss by means of optical microscope (OM), scanning electron microscope (SEM), X-ray diffraction (XRD), Gel Permeation Chromatography (GPC), Fourier-transform Infrared Spectroscopy (FTIR), Thermogravimetric Analysis (TG) and Thermogravimetric Analysis combined with Fourier-transform Infrared Spectroscopy (TG-FTIR). Degradation markers, such as changing of appearance, decreasing of molecular weight and changing of crystallinity were observed in ageing samples. At the same time, plasticizer loss of ageing samples appeared but differs among different ageing condition. In perspective, this systematic approach can be extended to the study of CA artefacts and other degradation conditions that would affect the deterioration pathway.

8:20 AM

(PACRIM-S21-028-2025) Study of the Lacquering Materials and Techniques in East Zhou, Qin and Han Dynasties

Y. Fu*¹; S. Wei²

1. University of Science and Technology Beijing, Institute for Cultural Heritage and History of Science & Technology, China
2. University of Science and Technology Beijing, China

Lacquerwares are the precious cultural relics in China. To study the materials and techniques used for making lacquerwares in different period of times is significant for people to understand the development and inheritance of the techniques. In this study, archaeological lacquerwares including lacquer wine sets, lacquer wooden sword, lacquer umbrella, lacquer screen etc. from Eastern Zhou to Qin and Han dynasties were studied. Multi-techniques, including pyrolysis gas chromatography/mass spectrometry, Fourier transform infrared spectroscopy, scanning electron microscopy and energy dispersive spectrometry, Raman spectroscopy and X-ray diffraction were conducted for the characterization of the complex lacquering materials and techniques. The results show not only urushiol but also laccol were detected in Chinese lacquerwares. Oils, mastic resin, pine resin, blood, clay, bone ash, cinnabar, soot and iron black were found as additives, respectively. Different lacquering techniques such as Youshi, Yuanqi and Caoqi crafts, and various ground layer making techniques including ash mixed with lacquer, ash mixed with blood and ash mixed with oil were also revealed during the period. The study can definitely enrich people's understanding of the lacquering materials and craft in the past.

8:40 AM

(PACRIM-S21-029-2025) Innovative machine learning algorithms for prediction and classification of archaeological metals

F. Armetta¹; M. Saladino*¹

1. Università degli Studi di Palermo, STEBICEF, Italy

Machine learning and artificial intelligence have shown the powerful impact of data analysis in identifying key variables for object classification or result prediction. The cultural heritage field has also benefited, and the MML-ARCH project aims to develop predictive models using machine learning to analyze archaeological and physico-chemical data, offering innovative diagnostics for cultural heritage. Data is collected through advanced non-invasive techniques to preserve artifacts. Algorithms identify correlations between archaeological and material data, creating predictive models for future studies. Study objects include coins and arrowheads from Western Sicily, with algorithms analyzing diverse variables from various substrates and techniques. Acknowledgements: Project MML-ARCH - "Metodologie di machine learning applicate all'archeometria: una nuova frontiera per l'interpretazione materica dei Beni Culturali", Programma "CHANGES Cultural Heritage Active Innovation for Sustainable Society" CUP B53C22003890006 - Codice Identificativo PE_00000020, finanziato dall'Unione Europea - Next Generation EU sui fondi PNRR MUR - M4C2 - Investimento 1.3 "Partnership estesi a Università, centri di ricerca, imprese e finanziamento progetti di ricerca".

PacRim S23 - Advanced Processing and Manufacturing Technologies for Ceramics

PACRIM Symposium 23 - Novel forming technologies, 3D printing, near-net shaping

Room: Georgia B

Session Chairs: Xu Wang, Northwestern Polytechnical University; Koji Morita, National Institute for Materials Science (NIMS)

8:30 AM

(PACRIM-S23-018-2025) A Novel Approach of Fabricating Monodispersed Spherical Refractory Powders for Laser Additive Manufacturing (Invited)

N. Nomura*¹; Z. Zhou¹; W. Zhou¹

1. Tohoku Daigaku, Graduate School of Engineering, Department of Materials Processing, Japan

Refractory metals or ceramics with superior mechanical and functional properties at elevated temperatures are in high demand in the automobile and aerospace industries. Unfortunately, manufacturing refractory materials with complex structures using traditional methods remains challenging. Laser additive manufacturing (AM) is considered as a potential alternative. However, it is difficult to fabricate refractory AM powders because of their high melting points or complex compositions. To address this challenge, freeze-dry pulsed orifice ejection method (FD-POEM) has been developed. Refractory MoSiBTiC alloys, ZrO₂- and SrTiO₃-based ceramics were selected as examples for demonstrating the application potential of FD-POEM. Elemental powders were first dispersed in water to form a uniform high-concentration slurry, which was then extruded through an orifice by diaphragm vibration and froze instantly in liquid nitrogen. After a freeze-drying process, spherical FD-POEM powders were obtained successfully. The relationship among FD-POEM powder features, melting behaviors, and comprehensive properties of AM builds was investigated. The findings of this study demonstrate that the integration of FD-POEM with AM paves the way for designing advanced refractory materials with high structural flexibility and excellent performance characteristics.

9:10 AM

(PACRIM-S23-019-2025) Tuning the properties of hybrid glasses through processing (Invited)

M. M. Smedskjaer^{*1}; S. Mollick¹; F. Cao¹; S. S. Sørensen¹

1. Aalborg University, Department of Chemistry and Bioscience, Denmark

Metal-organic or hybrid glasses are a recently discovered chemical family of glasses. They offer unique features, such as combining nano-porosity (as is typical for metal-organic framework crystals) with lack of grain boundaries (as is typical for glasses). The advantage of melt-quenching to produce glass materials lies in its ease of processing, allowing the formation of glasses in various shapes, but it has so far been challenging to prepare large, defect-free hybrid glasses. Focusing on zeolitic imidazolate frameworks (ZIFs), we here report on how processing can be used to tune their properties and functionalities for novel applications. For example, we show how hydrothermal treatment and co-melting with halide salts can be used to continuously tune the degree of network polymerization. In turn, this can be used to vary their melting and glass transition temperatures and thus improve the sample quality and size. We also show how ZIF-oxide composite glasses can be formed and used to functionalize the nanoporous ZIF glass structure. The resulting materials show promise within water softening applications. Overall, these findings could be important for enabling the next generation of functional, tunable hybrid glasses.

9:40 AM

(PACRIM-S23-020-2025) Fabricating Luminescent Glass and Ceramics Derived from Mesoporous Powders by Spark Plasma Sintering

B. Zhou^{*1}; L. Wang²; W. Jiang¹

1. Donghua University, Institute of Functional Materials, China
2. Donghua University, College of Materials Science and Technology, China

Due to the attractive properties as excellent thermal and chemical resistance, high transparency, high thermal conductivity, and great fiber-drawing ability, transparent glass/ceramic is probably an ideal matrix for light converter. Luminescent glasses/ceramics with different properties have been widely used in lighting fields. However, the high temperature required to prepare transparent glass/ceramic by conventional methods is an obstacle for controllable synthesis and well protection of the embedded materials. This report introduces a novel, facile route for the preparation of stable monolithic glass/ceramic-based luminescent materials, which can be widely used to introduce temperature-sensitive functional materials, by Spark Plasma Sintering (SPS). Furthermore, the research progress and superiority of SPS technology used to develop the light-emitting glass/ceramic containing nanocrystals, bismuth ions, and phosphors. Owing to the fast sintering procedure of SPS with relatively low temperature, the size, shape, surface topography, and optical properties of the dopants in luminescent glass/ceramic are found to be similar to those of untreated counterparts, which means that the sensitive dopants can be completely protected.

PACRIM Symposium 23 - Joining, integration, and machining technologies

Room: Georgia B

Session Chairs: Morten Smedskjaer, Aalborg University;
Naoyuki Nomura, Tohoku Daigaku

10:20 AM

(PACRIM-S23-021-2025) Defect-mediated mechanical behaviors of oxide ceramics subjected to flash processing (Invited)

H. Masuda^{*1}

1. The University of Tokyo, Department of Materials Engineering, Japan

Flash processing in strong electric fields enables rapid densification of oxide green compacts even at low furnace temperatures and in short time. This enhanced sinterability in electric fields is possibly attributed to the promotion of rate-controlling diffusional kinetics. Extensive studies have been dedicated to the potential contributions of field-induced defects to the enhanced diffusion. Recently, we have found anelastic behaviors of transition metal oxides, such as Y_2O_3 -stabilized ZrO_2 and rutile TiO_2 , subjected to AC flash processing. This anelasticity was characterized by rate-dependent elastic softening, as revealed through nanoindentation experiments at room temperature. This suggests that unusual point defects with considerable ionic mobility were induced by flash processing. In this presentation, the physical mechanisms of defect-mediated mechanical behaviors and potential extension to the enhanced diffusion would be discussed based on our recent studies of anelasticity and defect characterization among transition metal oxides subjected to flash processing.

10:50 AM

(PACRIM-S23-022-2025) Effect of interfacial structure on the preferred orientation and phase distribution of alumina-based eutectic ceramics (Invited)

X. Wang^{*1}; Q. Hu²

1. Northwestern Polytechnical University, China
2. Shanghai Jiao Tong University, School of Materials Science and Engineering, China

The directionally solidified eutectics, such as $Al_2O_3/Y_3Al_5O_{12}$ (YAG), and $Al_2O_3/YAG/ZrO_2$ have received considerable attentions because of its good oxidation resistance, microstructure stability, creep resistance and outstanding high-temperature (close to the melting point) mechanical properties. Thus, they are supposed as one of the most promising structural materials in a new generation gas turbines operating at 1923 K. In the present work, we prepared single crystal of $Al_2O_3/YAG/ZrO_2$ ternary eutectic by an optical floating zone furnace. The crystallography, interfacial structure and phase distribution were investigated. It is found that that the distribution of ZrO_2 was mainly dominated by the minimization of the interfacial strain energy. Therefore, to improve their mechanical properties, ZrO_2 were then redistributed by tuning the interfacial mismatch by high-entropy YAG. The results shows that the ZrO_2 was distributed more uniformly and dispersedly, and the preferred orientations were also changed. As a result, mechanical performance including hardness, elastic modulus, and fracture toughness had been greatly improved because of the refined microstructure, tailored interfacial structure, and homogeneous distribution of ZrO_2 caused by the introduction of the high entropy ($5Re_{0.2}$)AG.

PacRim S24 - Solid-State Optical Materials and Luminescence Properties

PACRIM Symposium 24 - Solid-State Optical Materials and Luminescence Properties

Room: Prince of Wales

Session Chair: Marcelo Nalin, Institute of Chemistry and Chemical Technology, Mongolian Academy of Sciences

8:00 AM

(PACRIM-S24-018-2025) Machine Learning-Driven Design of Phosphors with Activators Exhibiting Tunable Oxidation States (Invited)

F. Massuyeau¹; E. Glais¹; H. Yuan¹; R. Gautier^{*1}

1. Institut des Matériaux de Nantes Jean Rouxel, France

Designing photoluminescent materials with tailored properties is a challenging task, as minor changes in chemistry or crystal structure can significantly impact their optical behavior. The complexity is further amplified by the presence of low-concentration dopants or defects and the interplay of phenomena such as reabsorption and energy transfer, making it difficult to predict optical properties prior to synthesis and characterization. To address this challenge, we employ machine learning to accelerate the discovery of white-light-emitting materials for solid-state lighting applications. This presentation will highlight several families of doped materials, including $(\text{CaMg})_x(\text{NaSc})_{1-x}\text{Si}_2\text{O}_6:\text{Eu}$, $\text{Li}_2\text{BaSiO}_4:\text{Eu,Ce}$ and $\text{Ca}_{14}\text{Zn}_6\text{Ga}_{10}\text{O}_{35}:\text{Mn,Tm}$. These materials exhibit a range of broad and narrowband emissions with high photoluminescence quantum yields. Machine learning tools were utilized to identify critical experimental parameters, enabling the design of phosphors with targeted photoemission characteristics.

8:30 AM

(PACRIM-S24-019-2025) Thermal, structural and low-temperature spectroscopic properties of laser ceramics based on yttrium-aluminum garnet heavily doped with neodymium ions (Invited)

D. Hreniak^{*1}

1. Institute of Low Temperature and Structure Research, Division of Optical Spectroscopy, Poland

The current development of laser materials technology can be determined, in a broad sense, by the goal of increasing their power and efficiency. For common applications, the economic aspect is also important. Both of these criteria are addressed by new high optical quality ceramic laser materials doped with rare earth ions. For future applications, including those involving space applications, it is also important to understand the spectroscopic properties of these materials at low temperatures. This paper presents the results of optical and thermal studies of yttrium-aluminum garnet (YAG) optical ceramics doped with Nd^{3+} ions at concentrations higher than the YAG: Nd^{3+} single crystals. The result of the studies presented in this work is the investigation of the spectroscopic properties of YAG ceramics doped in the range of 1-4 % at. in the wide range of temperature (5 -330 K). In addition, X-ray diffraction, thermoluminescence and Raman measurements were performed to investigate the effect of doping on structural stresses and the formation of possible defects. The effect of these defects on the formation of centers leading to the capturing of excitation energy in traps was also determined, and identified and analyzed by thermoluminescence measurements over a wide temperature range.

9:00 AM

(PACRIM-S24-020-2025) Synthesis of Novel Luminescent Materials via Glass Crystallization Techniques (Invited)

A. J. Fernández Carrión^{*1}; V. Castaing⁴; A. Becerro Nieto⁴; M. Pitcher³; M. Allix²

1. Universidad de Sevilla, Química Inorgánica & Instituto de Ciencia de los Materiales de Sevilla, Spain
2. CNRS (CEMHTI), France
3. Centre National de la Recherche Scientifique, France
4. Consejo Superior de Investigaciones Científicas, Instituto de Ciencia de los Materiales de Sevilla, Spain

Nowadays, both indoor and outdoor lighting consumes a significant amount of energy, being the conventional lighting devices extremely inefficient. The quest for advanced luminescent materials has led to the exploration of innovative synthesis techniques that enhance material properties and energy efficiency. This study introduces a novel approach to synthesizing luminescent materials through a glass crystallization route, aimed at applications in lighting technology. By employing a controlled crystallization process from a glass matrix, we have developed a series of luminescent materials, some of them transparent within the visible range, that exhibit unique optical properties. This method allows for the precise doping of activator ions into host lattice sites, significantly enhancing the luminescence efficiency and color purity.

9:30 AM

(PACRIM-S24-021-2025) Development of RF magnetron co-sputtered amorphous Ge-Bi-Se chalcogenide films for photonic applications

A. Viswanathan⁵; J. Gutwirth⁵; Y. Ghandaoui¹; A. Hammouti²; T. Halenkovic⁵; S. Slang⁵; M. Pavlista⁵; S. Pechev³; J. Guin⁴; L. Deniel²; L. Bodiou²; M. Alouini²; J. Charrier²; P. Nemeč⁵; V. Nazabal^{*1}

1. CNRS-University of Rennes 1, ISCR, France
2. Institut Fonctions Optiques pour les Technologies de l'Information, France
3. Institut de Chimie de la Matière Condensée de Bordeaux, France
4. Univ Rennes CNRS, Physics Institute Rennes, France
5. University of Pardubice, Czechia

RF magnetron co-sputtered amorphous Ge-Bi-Se films were fabricated using polycrystalline GeSe_2 and Bi_2Se_3 targets. Their structural, linear, and non-linear optical properties were studied to understand compositional influence for future photonic applications. A broader Ge-Bi-Se amorphous region with a noticeably high Bismuth atomic percentage is observed using this deposition method compare to conventional glass synthesis. The structural characteristics of the co-sputtered films were analyzed using Raman spectroscopy where increasing bismuth concentration shifted all vibrational bands to the lower energy side with reduced intensity. A decrease in optical bandgap energy values and the corresponding increase in refractive index value n at telecommunication wavelength indicate the strong influence of bismuth on optical properties of films. Third-order nonlinear optical parameters were calculated from linear parameters using semi-empirical equations and Sheik-Bahae formalism in order to allow their prediction according to the film composition and taking into account the wavelength of use. Following these simulations, which enabled the selection of interesting compositions in terms of ONL applications, this work also focused on demonstrating the feasibility of manufacturing ridge waveguides from these GeBiSe co-sputtered films.

PacRim S27 - International Symposium of Fundamental and Frontier Sciences of Ceramics

PACRIM Symposium 27 - International Symposium of Fundamental and Frontier Sciences of Ceramics IV

Room: Cypress

Session Chair: Ricardo Castro, Lehigh University

8:00 AM

(PACRIM-S27-021-2025) Hard-to-sinter oxide ceramics: are there easier ways how to sinter them? (Invited)

A. Talimian²; A. Najafzadekhoe²; M. Michálková¹; K. Maca³; D. Galusek^{*2}

1. IIC SAS, Joint Glass centre, Slovakia
2. Trencianska Univerzita Alexandra Dubceka v Trencine, Centre for functional and surface-functionalized glass, Slovakia
3. Brno University of Technology, Czechia

Most oxide ceramics, especially those where transparency is desired, are notoriously hard to sinter, and usually require high sintering temperatures and long sintering times or, alternatively, the use of pressure assisted sintering. The latter usually uses graphite supplements, posing a high risk of carbon contamination that impairs transparency. Present contribution summarises our efforts in developing new ways of preparing translucent and transparent polycrystalline ceramics, or ceramics with specific (such as eutectic-like) microstructures by a suitable combination of various approaches ranging from the use of unconventional sintering additives, specific precursor (including glass) powders, and optimized sintering regimes both with and without applied pressure. The efforts are documented by successful sintering of a range of various materials, from fine-grained yttria, through amorphous and polycrystalline yttrium aluminium garnet (YAG) and $MgAl_2O_4$, to materials with eutectic-like microstructure in the system Al_2O_3 - Y_2O_3 - (ZrO_2) .

8:30 AM

(PACRIM-S27-022-2025) Achieving Superhardness and Enhanced Toughness in High-Entropy Boride-Based Composites by Tailoring Their Multi-Scale Microstructures (Invited)

J. Zou^{*1}

1. Wuhan University of Technology, China

Unlike strong yet tough high entropy alloys, high entropy ceramics normally exhibit good hardness but poor strength and fracture toughness. To overcome this obstacle, B_4C - $(Zr_{0.2}Hf_{0.2}Nb_{0.2}Ta_{0.2}Ti_{0.2})B_2$ composites with a unique hierarchical microstructure are designed and prepared by boronizing reaction sintering of dual-phase multicomponent carbides. In the as-obtained composites, massive platelet-like aggregations assembled by core-rim structured $(Zr_{0.2}Hf_{0.2}Nb_{0.2}Ta_{0.2}Ti_{0.2})B_2$ fine grains are distributed randomly in the B_4C matrix. Such special microstructure makes B_4C - $(Zr_{0.2}Hf_{0.2}Nb_{0.2}Ta_{0.2}Ti_{0.2})B_2$ composites exhibit excellent mechanical properties. More importantly, during producing indents, homogenization of core-rim structured $(Zr_{0.2}Hf_{0.2}Nb_{0.2}Ta_{0.2}Ti_{0.2})B_2$ alongside more difficult lattice glides caused by short-range ordering and rough glide planes containing different-dimension transition metal atoms cooperatively induce increased indentation volume work and consequently unparalleled Vickers hardness, which is confirmed by in-depth transmission electron microscopy characterization. This work gives a new inspiration to design high performance high-entropy ceramics via multi-scale microstructure tailoring and composition tuning.

9:00 AM

(PACRIM-S27-023-2025) Dopant effects on grain boundary plane distributions in alumina (Invited)

A. Erlacher¹; M. Stuer^{*1}

1. Swiss Federal Laboratories for Materials Science and Technology, Empa, Switzerland

Over the last decades, the emergence and establishment of advanced rapid sintering methods has significantly enhanced the exploration of the two-dimensional density-grain size parametric space. Favoring densification over grain growth, these sintering techniques enabled rapid progress in fields such as non-cubic transparent ceramics, where birefringence renders optical properties highly sensitive to grain size. The same rapid sintering methods offer opportunities in ceramic microstructure engineering beyond the density-grain size paradigm: the ability to achieve full densification in minutes – or even seconds – allows development of heat treatments specifically tailored to advanced microstructural design, and in particular grain boundary engineering. In this study, abnormal grain growth is employed as a proxy indicator for the occurrence of complexion transitions in grain boundaries. Changes in grain boundary plane distributions before, during, and after abnormal grain growth are studied to elucidate how various doping strategies and associated complexion transitions influence the statistical occurrence of specific grain boundary planes. Given the significance of grain boundaries in critical macroscopic properties, the work aims to demonstrate how rapid sintering techniques can be effectively harnessed for advanced materials property engineering and ceramic performance optimization.

PacRim S29 - Progress in High-Entropy Materials

PACRIM Symposium 29 - Multiscale modeling and simulations

Room: Plaza A

Session Chairs: Dilpuneet Aidhy, Clemson University; Michael Widom, Carnegie Mellon University

8:00 AM

(PACRIM-S29-017-2025) Disordered enthalpy-entropy descriptor for high-entropy ceramics discovery (Invited)

S. Curtarolo^{*1}; H. Eckert¹; S. Divilov¹

1. Duke University, Materials Science, Electrical Engineering and Physics, USA

Disordered multicomponent systems have been studied for the last two decades for their revolutionary properties. Resilient compositions can be stabilized by maximizing entropy (configurational/vibrational) of (near) equimolar mixtures. The search for new systems is mostly performed with trial-and-error techniques, as effective computational discovery is challenged by configurational immensity: the synthesizability of high-entropy ceramics is typically assessed using ideal entropy along with the formation enthalpies from density functional theory or with simplified descriptors or machine learning methods. Vibrations — even if they may have significant impact on phase stability — are drastically approximated to reduce the computational cost, or often avoided with the hope of them being negligible, due to the technical difficulties posed in calculating them for disordered systems. In this presentation I will address many of the problems in the discovery of disordered systems, offer some data-based effective solutions, and discuss the avenues opened by the latter, especially for plasmonic-hyperbolic applications.

8:40 AM

(PACRIM-S29-018-2025) Ab Initio Design of High-Entropy Thermal/Environmental Barrier Coatings (Invited)S. Hao¹; R. Oleksak¹; Ö. Doğan¹; M. Gao*¹

1. National Energy Technology Laboratory, USA

Next generation thermal/environmental barrier coatings (TEBC) require carefully balancing various properties including phase stability, thermal conductivity, coefficient of thermal expansion (CTE), mechanical properties, and resistance against hot corrosion and water vapor recession. This work mainly focuses on rapid design of cost-effective high entropy rare-earth disilicates and aluminum garnets to protect SiC-based ceramic matrix composites and nickel-based superalloys in the hot section of gas turbine engines using density functional theory methods. Our calculations identify several low-cost high entropy TEBC exhibiting ultralow thermal conductivity at 1500 K and desirable CTE while maintaining good mechanical properties, including $\text{Er}_{1/2}\text{Y}_{3/4}\text{Yb}_{3/4}\text{Si}_2\text{O}_7$, $\text{Gd}_{1/4}\text{Er}_{1/4}\text{Y}_{3/4}\text{Yb}_{3/4}\text{Si}_2\text{O}_7$, $\text{Eu}_{1/4}\text{Er}_{1/4}\text{Y}_{3/4}\text{Yb}_{3/4}\text{Si}_2\text{O}_7$, and $(\text{Y}_{1/4}\text{Gd}_{1/4}\text{Er}_{1/4}\text{Yb}_{1/4})_3\text{Al}_5\text{O}_{12}$. This work also aims to gain fundamental understanding of oxygen diffusion in model disilicates. Minimizing oxidizer (such as water vapor and oxygen) permeability through the EBC layer can significantly decrease the growth rate of thermally grown oxide and extend the service life of the coating system. Oxygen diffusion mechanisms including formation energy of defects under varying oxygen conditions and defect migration energy barriers will be presented.

9:10 AM

(PACRIM-S29-019-2025) High-throughput DFT Simulations of High Entropy Perovskite Using Neural Network Potential (Invited)G. Liu¹; S. Yang¹; Y. Zhong*¹

1. Worcester Polytechnic Institute, Mechanical and Materials Engineering, USA

LaCoO₃-based perovskite shows promise as a solid oxide cell (SOC) air electrode material. To enhance its performance, researchers typically incorporate dopants to improve stability and oxygen ionic conductivity, properties that can be calculated via first-principles simulations. However, the vast number of potential dopants, concentrations, and combinations renders such calculations computationally intractable using conventional potentials from VASP. This study presents a novel high-throughput approach leveraging neural network potential (NNP) developed by Matlantis to optimize dopant configurations in LaCoO₃. We systematically investigate the effects of 20 distinct dopant elements, encompassing both A-site (Mg, Ca, Sr, Ba, Ce, Pr, Nd, Sm, Gd) and B-site (Sc, Ti, V, Cr, Mn, Fe, Ni, Cu, Zn, Al, Ga) substitutions, on the material's stability and oxygen ionic conductivity. Especially, the high entropy perovskite based on LaCoO₃ has been systematically investigated. Our methodology demonstrates a significant advancement in the computational exploration of doped perovskites and high entropy perovskite, offering a more efficient alternative to conventional calculations. The findings provide valuable insights for future SOC development.

9:40 AM

(PACRIM-S29-020-2025) First-principles study of the order-disorder transition in the AlCrTiV high entropy alloy (Invited)M. Widom*¹

1. Carnegie Mellon University, USA

The AlCrTiV high entropy alloy undergoes an order-disorder transition from body centered cubic (Strukturbericht A2) at high temperatures to the CsCl structure (B2) at intermediate temperatures. We model this transition using first principles Monte Carlo/molecular dynamics simulations. Simulation results yield the temperature-dependent energy, entropy, heat capacity, occupancy fluctuations, and diffraction patterns. The contribution of chemical disorder to the entropy is calculated on the basis of point and pair

cluster frequencies. The simulated structures exhibit compensated ferrimagnetism, and the Fermi level lies in a pseudogap. Sensitivity to the exchange-correlation functional is discussed.

10:30 AM

(PACRIM-S29-021-2025) High temperature dislocation glide mechanisms in refractory multi-principal element alloys (Invited)I. Beyerlein*¹

1. University of California System, Santa Barbara, USA

In recent years, refractory multi-principal element alloys (RMPEAs), both single phase and multi-phase materials containing nano-precipitates, have been introduced with the promise of unusual or unprecedented properties. These high-performance alloys exhibit far greater compositional and microstructural complexities at the scale of a dislocation than those of traditional ones, warranting study of the underlying dislocation dynamics. In this talk, we will describe recent developments of a 3D computational materials technique designed to predict discrete dislocation pathways at elevated temperatures in these complex systems. With application to RMPEAs, we will present temperature dependent glide mechanisms deployed by dislocations in RMPEAs and discuss how they are distinct from the pure metal constituents. The analysis finds that the screw dislocation glide mechanisms transition twice, and each transition is accompanied by a change in glide line morphology and mobility. Predicted changes in critical glide stress and mobility with temperature can help in understanding why RMPEAs exhibit unique and favorable high-temperature mechanical behavior.

11:00 AM

(PACRIM-S29-022-2025) Electronic density of states as the descriptor of elastic bond strength, ductility, and local lattice distortion in BCC refractory alloys (Invited)D. Pant¹; D. Aidhy*¹

1. Clemson University, Materials Science and Engineering, USA

Generally, while density functional theory (DFT) is instrumental in developing fundamental understanding of materials, there is a significant gap that relates electronic structure to the mechanical properties in metallic alloys. We show that the electronic occupancy at the Fermi level, $N(E_f)$, derived from electronic density of states, is a key descriptor of alloy strength and ductility. Our calculations demonstrate that lower $N(E_f)$ is indicative of stronger bonds with higher stiffness, resulting in increased elastic constants. Further, the presence of high bond stiffness suggests a covalent bond character, which contributes to directional bonding and resistance to deformation, leading to higher bulk (B) and shear (G) moduli. Consequently, $N(E_f)$ is found to be strongly correlated with alloy ductility. We also show that local lattice distortion is only partially dependent on the atomic radii difference; instead the atomic bond stiffnesses play a much stronger role. These results advance the understanding on the role of electronic structure to explain mechanical properties of alloys.

11:30 AM

(PACRIM-S29-023-2025) Tuning Structure and Properties in High-Entropy Materials through Disorder (Invited)C. M. Rost*²; G. Niclescu¹; G. R. Bejger²; J. Barber²; S. Ayyagari³; M. Webb⁴; L. Min³; S. Almishal³; N. Alem³; J. Heron⁴; Z. Mao³; J. Maria³

1. James Madison University, USA

2. Virginia Polytechnic Institute and State University, Materials Science & Engineering, USA

3. The Pennsylvania State University, USA

4. University of Michigan, USA

Disorder plays a pivotal role in defining the properties of materials, especially in high-entropy oxides (HEOs), where extensive disorder creates opportunities for new discoveries. This work focuses on synthesizing and characterizing novel HEOs in powder, thin film, and single-crystal forms to investigate how compositional disorder drives

structural evolution and functional properties. For thin-film HEOs, we observe a structural transition from rocksalt to spinel phases under varying oxygen partial pressures. In single-crystal HEO spinels, high-temperature magnetization, neutron scattering, and synchrotron-based techniques reveal distinct ferrimagnetic transitions at elevated temperatures, dependent on composition. Additionally, in high-entropy perovskite oxides (HEPO), B-site disorder is shown to modulate the time stability of remanent polarization. Techniques such as transmission electron microscopy (TEM) and X-ray absorption fine structure (XAFS) enable detailed probing of nanoscale structural variations. This study emphasizes how lattice distortions in high-entropy phases significantly influence material behavior, offering valuable insights into the interplay between disorder and properties. These findings advance our understanding of HEOs and pave the way for their application in functional materials.

PacRim S31 - On the design & dev of next generation nanolayered (3D and 2D) structural & func mtl

PACRIM Symposium 31 - Next-generation nanolayered structural/functional materials I

Room: Oxford

Session Chairs: Michael Naguib, Tulane University;
Vadym Mochalin, Missouri University of Science and Technology

8:00 AM

(PACRIM-S31-001-2025) Synthesis of 2D Functional Ceramics and their Hybrids for Energy Applications (Invited)

M. Naguib*¹

1. Tulane University, Physics and Engineering Physics, USA

Two-dimensional (2D) materials exhibit unique properties compared to their three-dimensional (3D) counterparts due to their morphology and high surface area. Most 2D materials are ceramics, and among them, MXenes (2D transition metal carbides and nitrides) are one of the fastest-growing families, valued for their diverse compositional space and functionalities. Transition metal carbo-chalcogenides (TMCCs) are a novel class combining the carbide core of MXenes with the chalcogenide surface of transition metal dichalcogenides (TMDCs). These materials resemble MXenes but feature a chalcogen-terminated surface. TMCCs are synthesized via a simple solid-state method, avoiding the hazardous etching processes required for MXene synthesis. This scalable approach allows for the production of tens of grams in the lab without acids. We pioneered the synthesis of the first TMCC members, Nb₂S₂C and Ta₂S₂C, and their solid solutions, using liquid exfoliation. This presentation will highlight advancements in the synthesis of MXenes, their hybrids, and multi-layer TMCCs, as well as their exfoliation into 2D sheets. We will also discuss the potential of these functional 2D ceramics and their hybrids for energy and environmental applications, including batteries, supercapacitors, electrocatalysis, and radioactive iodine capture.

8:30 AM

(PACRIM-S31-002-2025) Let's talk A: MAX phases with exotic A-elements (Invited)

C. Birkel*¹

1. Arizona State University, USA

The number of MAX phases has increased tremendously over the last decade which has been driven by reports on interesting magnetic behavior of Cr- and Mn-based MAX phase thin films as well as using MAX phases as precursors for 2D MXenes. More than 350 members are known, which include ternary compounds and (single-, double-site) solid solutions. The vast majority of MAX phase works are on compounds with group 13 and 14 A-elements, e.g. Al, Ga, Si, however,

the chemical diversity is much greater and goes far beyond these elements. In this talk, I would like to discuss our work on MAX phases with "exotic", meaning less common, A-elements. This includes P- and As-containing MAX phases, such as V₂PC and V₂AsC, as well as new A-site solid solution MAX phases, e.g. M₂(Ga/Ge)C (M = Cr, V). I will also show a new MAX phase that contains an entirely unexpected element on its A-site. Aside from their synthesis and structural science, I will discuss the oxidation behavior of some of these phases. We synthesize our materials by classical and non-conventional (microwave heating) solid-state reactions and sol gel-based approaches. All products are carefully characterized by numerous diffraction (lab and synchrotron X-rays), microscopy, spectroscopy (lab and hard-X-ray photoelectron spectroscopy) and thermal analysis techniques.

9:00 AM

(PACRIM-S31-003-2025) Order-Disorder in Multi-Transition Metal MAX phases and MXenes (Invited)

B. C. Wyatt¹; B. Anasori*¹

1. Purdue University, Materials Engineering, USA

The family of two-dimensional (2D) transition metal carbides and nitrides, known as MXenes, is one of the largest 2D material families, with over eighty synthesized compositions. MXenes are primarily synthesized through the top-down selective etching of their precursor MAX phases. Consequently, the design of new MXene compositions depends on the synthesis of novel MAX phases. In 2021, a new research area emerged within MAX/MXenes: high-entropy MAX and MXene phases, making MXenes one of the first 2D materials to enter the field of high-entropy research. In these phases, four or more transition metals are combined as solid solutions within the 2D atomic planes. In this talk, I will present a systematic study of over 36 multi-transition-metal MAX/MXene phases, incorporating different numbers and types of transition metals in the M layers. Specifically, we study MAX and MXene phases with 2, 4, 5, 6, 7, 8, and 9 transition metals from groups 4 to 6 of the periodic table. The goal is to understand the influence of entropy versus enthalpy on the formation of these phases. By combining various elements and analyzing the atomic layer-by-layer composition of the MAX phases, we determine how many transition metals are required to form fully disordered high-entropy MAX phases. Additionally, we demonstrate how to synthesize novel high-entropy MXenes from these phases and explore some of their properties.

9:30 AM

(PACRIM-S31-004-2025) Reactivity and applications of 2D Transition Metal Carbides (MXenes) (Invited)

V. Mochalin*¹

1. Missouri University of Science and Technology, USA

A large family of two-dimensional transition metal carbides and nitrides (MXenes) raises interest for many applications due to their high electrical conductivity, mechanical properties, potentially tunable electronic structure, nonlinear optical properties, and the ability to be manufactured in the thin film state. However, their chemistry that is key to development of these applications, still remains poorly understood. In this presentation we will discuss recent progress in understanding fundamental MXene chemistry and harnessing it for suppressing unwanted reactions and prolonging stability of these materials, thereby improving their performance in applications. For example, suppressing oxidation and hydrolysis at high pH was demonstrated as an effective way to prolong shelf-life and stability of MXene aqueous colloids. Use of polyphosphate also has been shown to improve chemical stability of MXene aqueous colloids. Other selected examples illustrating connections between understanding MXene chemistry and development of their applications will also be considered.

Thursday, May 8, 2025

PacRim S1 - Environmental barrier coatings for high-performance ceramics

PACRIM Symposium 1 - Environmental barrier coatings for high-performance ceramics I

Room: Oxford

Session Chair: Eeshani Godbole, GE Aerospace Inc

10:20 AM

(PACRIM-S01-001-2025) Environmental Barrier Coatings Applied by Axial Plasma Spraying (Invited)

N. Markocsan^{*1}

1. University West, Dept. of Engineering Science, Sweden

Ceramic Matrix Composites (CMCs) are prime candidates for replacing metallic parts, in the hottest sections of the next-generation gas turbine engines. In order to prevent surface recession in the presence of steam and other corrosive gases inside engines, CMCs are typically protected using Environmental Barrier Coatings (EBCs). EBCs can be applied by thermal spraying and usually consist of a silicon bond coat and a rare earth disilicate topcoat. A promising topcoat material currently drawing attention is ytterbium disilicate (YbDS). In this work YbDS topcoats were developed by atmospheric and suspension plasma spray (APS and SPS respectively) using axial feedstock feeding. The impact of process parameters on the microstructure and functional performance of the YbDS coatings has been comprehensively investigated. Main focus was on phase composition, crystallinity, porosity, erosion and thermal cycling. Process parameters such as carrier gas flow rate, enthalpy, and stand-off distance were found to have a significant effect on the coating's microstructure and properties.

10:50 AM

(PACRIM-S01-002-2025) Tailoring Microstructure and Phase Constitution of Ytterbium Disilicate Environmental Barrier Coatings Manufactured by Atmospheric Plasma Spraying (Invited)

J. Zhang^{*1}, H. Wang², Z. Luo¹, J. Wang¹

1. Institute of Metal Research Chinese Academy of Sciences, Shenyang National Laboratory for Materials Science, China
2. Liaoning Academy of Materials, Institute of Coating Technology for Hydrogen Gas Turbines, China

Environmental barrier coatings (EBCs) are needed to protect SiCf/SiC ceramics from degradation advanced modern gas turbines. Ytterbium disilicate, in recent studies, has been considered as a promising EBC candidate. In the current report, insights gained through fundamental research on process-stoichiometry-phase-structure-property linkages of Yb₂Si₂O₇ agglomerated feedstocks is focused with varied manufacturing parameters for atmospheric plasma spraying (APS). The evolution of different EBC chemistries along with deliberate variations in process conditions to provide a framework for fundamental description of the deposition process and post-spray thermal treatments. Together with discussion on coating performance with combined steam and CMAS exposures.

11:20 AM

(PACRIM-S01-003-2025) Design and Synthesis of Innovative Sol-Gel Coatings for Metal Substrates and Future CMC. Applications in High-Temperature Environments for Aeronautics

B. Toury^{*1}; L. Lager²; J. Delfosse³; S. Benayoun²; S. Senani - de Monredon³

1. Universite Claude Bernard Lyon 1, France
2. Ecole Centrale de Lyon, France
3. Safran SA, France

Environmental barrier coatings (EBCs) are essential for protecting ceramic matrix composites (CMCs) in high-temperature environments, particularly in the context of next-generation aircraft engines. Extending this technology to metallic substrates, such as titanium alloys, offers an opportunity to enhance their high-temperature performance while laying the groundwork for future adaptation to CMCs. By studying EBCs on metals, we can explore the sol-gel process to get protective coatings that are directly transferable to CMC applications. In this study, we designed and synthesized a high-temperature anti-oxidizing coating using a sol-gel process, initially focusing on metallic substrates. This approach enables the direct deposition of sol onto complex-shaped substrates, with precise control over the coating's stoichiometry. The morphology of the coatings was examined using SEM, while additional characterizations by XPS, solid-state NMR, and thermal analyses provided insights into the mechanisms occurring during the curing treatment. Initial oxidation tests demonstrated the potential applications of these coatings. This work not only addresses the challenges faced by metals in high-temperature environments but also provides a foundation for extending such coatings to protect CMCs in future aeronautic applications.

11:40 AM

(PACRIM-S01-004-2025) Oxygen activity in composite mullite-Si sintered pellets

A. Setlur^{*1}; J. Wan¹; C. Henderson¹; R. Davis¹

1. GE Research, USA

Advancements in fuel efficiency and new fuels in next generation aircraft engines will demand higher operating temperatures of SiC ceramic matrix components that exceed the melting point of Si bondcoat or oxygen barrier layer of current generation environmental barrier coatings (EBCs) by ~150°F with EBC surface temperatures ~3000°F (1650°C). A composite mullite bondcoat with second phase oxygen getters has been developed for use in such high temperature EBC systems. These bondcoats with Si & SiC inclusions have demonstrated performance to provide effective protection of SiC-SiC CMC substrates. Oxidant permeability is one factor in high temperature EBC oxidation life and depends on defect transport (e.g. oxygen vacancies, metal vacancies, oxygen interstitials) under a chemical potential gradient. Understanding oxygen activity in model systems will give fundamental insight towards EBC material system improvements and component lifetime. We study a mullite-Si sintered pellet representative of composite mullite-Si bondcoats & use Cr³⁺ luminescence from Cr contamination to evaluate oxygen activity in mullite-Si composites after exposure at 2700°F-1 atm O₂ for 100-2000 hrs. The data is analyzed based on thermodynamic stability of Cr³⁺ from assessments of Cr₂O₃/CrO stability and data from slag and glass literature to gauge oxygen activity. Implications for oxygen transport in these mullite-Si composite pellets are discussed.

PacRim S2 - Frontier of modeling and Design of Ceramics and composites

PACRIM Symposium 2 - Modeling Surfaces, interfaces, defects, amorphous matter

Room: Balmoral

Session Chairs: Dilpuneet Aidhy, Clemson University;

Eva Zarkadoula, Oak Ridge National Lab

8:00 AM

(PACRIM-S02-001-2025) A Computational Framework for Analyzing Complex Interfaces: From First-Principles to Machine Learning, with a Case Study on LaCoO₃/La₂NiO₄ (Invited)

G. Liu¹; S. Yang¹; Y. Zhong^{*1}

1. Worcester Polytechnic Institute, Mechanical and Materials Engineering, USA

Perovskite oxides are essential materials widely used as electrodes in solid oxide fuel cells (SOFCs) and solid oxide electrolysis cells (SOECs), where interfaces critically influence performance. Investigating these complex interfaces typically relies on computational methods such as first-principles calculations, which provide high accuracy but are constrained by the computational resources required for large supercells and detailed physical potentials. This work introduces a streamlined computational framework to analyze interfaces, exemplified by the LaCoO₃/La₂NiO₄ interface. Lattice matching algorithms were applied to construct interface models, while machine learning-based interatomic potentials accelerated simulations. Key factors influencing interface stability, such as geometry, size, and thickness, were systematically examined. Active learning strategies enabled exploration of interfacial orientations and compositions, facilitating predictive modeling of interface stability. By integrating machine learning, this framework reduces computational costs while offering critical insights into interface properties. It serves as a practical guide for optimizing SOFC and SOEC interfaces, advancing materials development for enhanced performance.

8:30 AM

(PACRIM-S02-002-2025) Computational Insights into the Grain Boundaries and Interfaces Present in Yttria Stabilized Zirconia Used in Solid Oxide Fuel Cells (Invited)

J. C. Madrid¹; K. K. Ghuman^{*1}

1. Institut National de la Recherche Scientifique, Énergie Matériaux Télécommunications, Canada

The ability to manipulate and harness inherent disorder in materials - whether due to finite-dimensional defects like vacancies, dopants, and grain boundaries, or complete atomic randomness as seen in amorphous materials - can drive innovation in the design of energy materials. This talk explores recent computational progress in understanding the behaviors of polycrystalline materials used in Solid Oxide Fuel Cells (SOFCs), focusing on their optimization for next-generation devices. Materials used in SOFCs are typically polycrystalline, exhibiting variations in grain sizes, orientations, dopant segregation, and defect distribution, often with a high density of grain boundaries and interfaces that significantly impact their performance, particularly in terms of ionic conductivity. I will present our latest findings concerning the microstructural and ionic behaviors observed at grain boundaries and interfaces within Yttria Stabilized Zirconia (YSZ) used in SOFCs. Through integrating classical and quantum simulations, our work has developed realistic models of these materials, providing explanations for observed experimental phenomena. Finally, challenges in assessing the cumulative impact of microstructural defects and the role of advanced computational tools in overcoming them will also be discussed.

9:00 AM

(PACRIM-S02-003-2025) Impact of quantum structures of dislocation cores on peculiar mechanical properties in inorganic semiconductor crystals (Invited)

K. Matsunaga^{*1}

1. Nagoya University, Materials Physics, Japan

Semiconductor crystals tend to fail in a brittle manner at low temperatures against external applied stresses. It has been considered their brittleness arises from their complicated crystal structures and strong ionic/covalent bonds. However, our research group found out that ZnS single crystals, one of II-VI group semiconductors, undergo extraordinarily large plastic deformation even at room temperature when deformed in complete darkness. Glide dislocations with a high density on the {111} planes were introduced in the samples deformed in darkness. In contrast, such multiplication of glide dislocations was not observed in light illumination, leading to brittle mechanical behavior of ZnS. In order to clarify effects of light illumination on dislocation mobility, DFT calculations of the glide dislocations were performed. It was found that specific electronic and atomic structures localized at the dislocation cores are formed depending on the absence or the presence of excess carriers that would be excited by external light. Peierls potentials of the glide dislocations were also evaluated, and it turned out that the presence of excess carriers can strongly affect glide-motion resistance of the dislocations in ZnS. Similar experimental and theoretical investigations were also performed for GaP, and the results were compared with those in ZnS.

9:30 AM

(PACRIM-S02-004-2025) DFT-based calculations of equilibrium point-defect concentrations in semiconductors and ceramics (Invited)

T. Ogawa^{*1}

1. Ippan Zaidan Hojin Fine Ceramics Center, Nanostructures Research Laboratory, Japan

Formation energies of point defects, including vacancies, interstitial atoms, and substitutional impurities, in crystalline solids with a band gap, are typically evaluated through density functional theory (DFT) calculations with corrections for charged defects. These formation energies are essential for estimating point-defect concentrations under thermal equilibrium (constant temperature and chemical potentials) by optimizing the Fermi level to satisfy the charge neutrality condition. However, relating the obtained concentrations as a function of chemical potentials to the experimental behaviors is not an easy task, because atomic fraction is typically controlled during synthesis. To address this, we developed a framework based on the constant-N approach, which determines the concentrations as a function of the number of atoms or atomic fractions via the Legendre transformation. In this paper, we present the details of this framework and demonstrates through examples which includes semiconductors for thermoelectricity and fluoride-ion and proton conductors as ionic conductors.

PACRIM Symposium 2 - Machine Learning and Artificial Intelligence in Materials Modeling

Room: Balmoral

Session Chairs: Giacomo Giorgi, The University of Perugia

10:20 AM

(PACRIM-S02-006-2025) Unified Moment Tensor Potential for Silicon and Silica: Bridging Crystalline and Amorphous States (Invited)

L. Béland^{*1}; K. Zongo²; H. Sun¹; N. Mousseau³; C. Ouellet-Plamondon²

1. Queen's University, Mechanical & Materials Engineering, Canada
2. ETS-Montreal, Canada
3. Université de Montréal, Canada

Silicon and silica are central to technologies ranging from semiconductors to silicate-based materials, but modeling these systems poses challenges due to their complex charge-transfer interactions. This talk will focus on a unified moment tensor potential (MTP) developed to describe silicon, oxygen, and silica across crystalline, interfacial, and disordered states. Trained on a comprehensive ab initio database, this MTP achieves high accuracy in predicting structural and dynamic properties while offering computational efficiency. A secondary focus will explore the application of this MTP in conjunction with the Activation Relaxation Technique (ARTn) to generate amorphous silica structures. This combined approach successfully creates amorphous systems devoid of coordination defects, providing an example of how the potential can be applied to study disordered phases. By emphasizing the capabilities and flexibility of the MTP, this presentation will demonstrate its potential for advancing simulations of complex materials, with a brief discussion on how it can complement advanced structural preparation methods like ARTn. This work highlights progress in developing machine learning-based potentials to unify the modeling of disparate material phases.

10:50 AM

(PACRIM-S02-007-2025) Thermal conductivity analysis of polymer-derived composite via image-based structure reconstruction, computational homogenization and machine learning

M. Fathidoost^{*1}; Y. Yang¹; B. Xu¹

1. Technische Universität Darmstadt, Mechanics of Functional Materials Division, Institute of Materials Science, Germany

The thermal behavior of polymer-derived ceramic composites is influenced by the structural and interface characteristics, making the establishment of structure-property relationships (SPR) essential for designing advanced materials with tailored properties. However, identifying accurate microstructural descriptors and generating training data presents significant challenges. The study addresses these issues by employing machine learning (ML) techniques on microstructure and thermal conductivity data derived from physical simulations, validated with experimental results. Microstructures are reconstructed from SEM images, and the diffuse interface method is used to interpolate phase and interface properties, enabling efficient handling of complex microstructures. This integrated approach highlights the potential of ML to overcome traditional limitations, providing a pathway to optimize and predict composite properties. Principal Component Analysis (PCA) reduced the 2-point statistics to represent the microstructures, serving as inputs to the ML model. Physical simulations provided thermal conductivity values as outputs. The trained model demonstrated high accuracy, supporting sensitivity analysis and inverse material design.

11:10 AM

(PACRIM-S02-017-2025) Atomistic Modeling of Ion Beam Irradiation: Insights into Ion-Matter Interactions for Material Modification (Invited)

E. Zarkadoula^{*1}

1. Oak Ridge National Laboratory, Center for Nanophase Materials Science, USA

The ion beam modification of materials is a critical area of research where highly energetic ions are used to induce significant changes in microstructure, phase stability, and mechanical, optical and electronic properties. Ion-matter interactions are governed by complex, multi-scale processes, requiring a fundamental understanding to predict and control a material's response to radiation. Molecular dynamics (MD) simulations are a useful tool for investigating ion-matter interactions and radiation damage processes, gaining insights into mechanisms at timescales often inaccessible by experiments, and linking processes at the atomic level to observations at larger scales. In this presentation, I will discuss atomistic modeling approaches to ion beam irradiation and material modification. I will explore different regimes of ion-matter interactions and different damage processes and provide insights from modeling and experiment. Results from MD simulations and the thermal spike model will be presented and key mechanisms driving material modifications will be highlighted. Additionally, I will discuss current limitations and ongoing efforts in predicting the response of different materials to energetic ion beams. Work was supported by the Center for Nanophase Materials Sciences, a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory.

PacRim S3 - Solid Oxide Fuel Cells and Green Hydrogen Technologies

PACRIM Symposium 3 - Solid Oxide Fuel Cells and Green Hydrogen Technologies II

Room: English Bay

Session Chairs: Hiroyuki Shimada, National Institute of Advanced Industrial Science and Technology (AIST); Kevin Huang, University of South Carolina

8:00 AM

(PACRIM-S03-005-2025) Study of oxygen surface exchanges and oxygen diffusion through mixed ionic-electronic conductors by semi-permeation method (Invited)

P. Geffroy^{*1}

1. IRCER CNRS, Ceramic processes, France

The understanding of oxygen transport mechanisms through mixed ionic-electronic conductors (MIEC) is of great interest for the development of electrochemical devices at high temperature, and for energy conversion applications. Modeling the electrical charge transport process through an MIEC is an important challenge for improving oxygen transport membranes (OTM), solid oxide fuel cells (SOFC), or electrolyzers (SOEC). This work is focused also on evaluating the oxygen exchange kinetics at the surface of MIEC close and far to equilibrium, specifically the identification the relationship between oxygen flux and the driving force, for which there is none or few data in the literature. This approach is a great importance for the determination of two coefficients — the oxygen diffusion coefficient and the surface exchange coefficient, which are obviously key parameters for the electrochemical performance of a material. The determination of these coefficients can be largely impacted by the experimental measurement conditions. This work shows that it is possible to determine the two coefficients for mixed ionic-electronic conductors, with suitable accuracy, by the oxygen semi-permeation method. Finally, this method gives a better understanding of the oxygen exchange kinetics at the surface of MIEC, either near and far from the equilibrium.

8:30 AM

(PACRIM-S03-006-2025) Materials for Intermediate Temperature Solid Oxide Cells (Invited)

K. Huang*¹

1. University of South Carolina, Mechanical Engineering, USA

High-efficiency and high-rate productions of energy and hydrogen via high-temperature solid oxide cells are of vital importance to the realization of a clean and sustainable energy future. High-temperature solid oxide cell (SOC) technology is thermodynamically and kinetically advantageous over internal combustion engines for power generation and low-temperature electrolytic cells for hydrogen production. However, the commercial development of SOC technology is severely challenged by poor durability, largely attributed to the high operating temperature that triggers a wide range of materials degradation mechanisms. Therefore, reducing the operating temperature of SOC from the current 750°C to 600-650°C, for example, is highly preferable to improve durability by mitigating or even completely shutting down the degradation mechanisms. Here in this presentation, materials options to enable the reduced operating temperature for SOCs are thoroughly discussed from a viewpoint of material properties. Several examples of cell materials well positioned for intermediate-temperature SOC applications are illustrated. Future research directions in materials development for SOC technology are also suggested.

9:00 AM

(PACRIM-S03-008-2025) Innovative approaches to obtain c-axis-oriented apatite-type Lanthanum silicate electrolyte

C. Bourguès*¹; L. Arbelaez¹; P. Geffroy¹; A. Aimable¹; K. Fukuda²; E. Bechade¹

1. Institut de Recherche sur les Ceramiques, France
2. Nagoya Kogyo Daigaku, Department of Environmental and Materials Engineering, Japan

The texturing of polycrystalline ceramics enable the possibility to strength selectively some keys properties by reducing the non-constructive influence of random grain orientation. Lanthanum silicate oxyapatites (LSO) have drawn attention as substitute material for Zr-based electrolytes in SOFC fuel cells, due to their exceptional ionic transport properties at low operating temperature. These materials are known to exhibit anisotropic behavior along c-axis direction which provides preferential pathways for ion migration, allowing higher oxygen ions mobility, maximizing the overall ionic conductivity. An approach using the reactive diffusion technique between layers of La₂SiO₅ and SiO₂ compounds has been pushed forward to obtain a highly oriented LSO layer. The impact of the multilayers configuration and additional annealing step on the chemical composition, microstructure, and electrochemical properties of LSO was investigated. The resulting materials exhibit significantly higher ionic conductivity compared to the literature, offering a real breakthrough for improving SOFC performances and evidences the importance to texture the LSO electrolyte. Beside, alternative synthesis approaches have been engaged to produce anisotropic morphology of LSO feedstock susceptible to be oriented by innovative processes as a preliminary step to move toward a realistic fabrication of a full fuel cell.

9:20 AM

(PACRIM-S03-009-2025) Structural and Electrochemical Properties of Praseodymium Oxide as a High-Performance Oxygen Electrode for Low-temperature Solid Oxide Cells

B. Lemieszek*¹; A. Maximenko²; M. Struzik³; M. Malys³; M. I. Asghar⁴; P. Z. Jasinski¹; S. Molin¹

1. Politechnika Gdanska Wydział Elektroniki Telekomunikacji i Informatyki, Department of Functional Materials Engineering, Poland
2. Uniwersytet Jagiellonski w Krakowie, Poland
3. Politechnika Warszawska, Poland
4. Tampereen korkeakouluuyhteisossa, Finland

Praseodymium oxide (PrOx) presents a highly promising alternative to conventional cobalt-based materials, such as LSC or LSCF, for oxygen electrode applications in SOCs. This material is characterised by a broad range of stoichiometries, deviating from conventional models based on randomly dispersed isolated point defects. The structural characterisation of the material was conducted using techniques such as X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS), alongside measurements of its electrical conductivity. Electrochemical analysis revealed exceptionally low polarization resistance values, measured at 0.021 Ωcm² at 600 °C and 0.254 Ωcm² at 500 °C. These values, which are rarely observed at such relatively low temperatures, were achieved through a simple spin-coating technique. This method also enabled precise determination and control of the optimal electrode thickness. Detailed impedance analysis using Distribution of Relaxation Times (DRT) provided a deeper understanding of the physicochemical mechanisms occurring at the electrode, as well as insights into the factors limiting the reaction. Furthermore, the study investigated the impact of external factors, such as humidity, on the overall efficiency of the oxygen electrode. We also determined the long-term stability of the cells under a range of conditions.

PACRIM Symposium 3 - Solid Oxide Fuel Cells and Green Hydrogen Technologies III

Room: English Bay

Session Chairs: Leonard Kwati, Kyushu Daigaku Carbon Neutral Energy Kokusai Kenkyujo; Kevin Huang, University of South Carolina

10:20 AM

(PACRIM-S03-010-2025) Electrochemical Performance of Ru Doped SFM Perovskite Electrode Materials for Solid Oxide Electrolysis cells

S. An*¹

1. Inner Mongolia University of Science and Technology School of Materials and Metallurgy, Department of Metallurgical Engineering, China

Sr_{1.95}Fe_{1.5}Mo_{0.4}Ru_{0.1}O_{6.8} electrode materials were synthesized through B-site doping of Ru element. The phase characterization revealed that both SFMRu and SFM possess a cubic perovskite structure. In CO₂ atmosphere, the electrical conductivity of SFMRu exhibited slightly higher than that of SFM material, while demonstrating 2-3 times improvement in chemical diffusion coefficient and surface oxygen exchange coefficient relative to SFM. The SFMRu electrode exhibits higher CO₂ adsorption capacity due to the increase of oxygen vacancies and the elevating of surface adsorbed oxygen resulting from enhanced spillover of lattice oxygen at elevated temperatures. Consequently, the CO₂ electrolysis performance of the SFMRu electrolytic cells surpassed that of the SFM cells with a remarkable current density increase by 157% at 800 °C and 1.5 V (2130 mA cm⁻²). Furthermore, excellent CO yield and Faraday efficiency were achieved by the electrolytic cell using SFMRu as an electrode material along with its superior stability in constant-current electrolysis mode.

10:40 AM

(PACRIM-S03-011-2025) Mesoscale Simulations of Solid Oxide Electrolysis Cells with Synthetic Structures (Invited)P. Jayapragasam³; Y. Shoukry¹; K. Huang²; X. Jin^{*1}

1. The University of Texas at Dallas School of Economic Political and Policy Sciences, Mechanical Engineering, USA
2. University of South Carolina, Mechanical Engineering, USA
3. National Renewable Energy Laboratory, USA

Solid oxide electrolysis cells (SOECs) are valued for their role in hydrogen production and as energy storage solutions, particularly with renewable energy sources. Traditionally, SOECs' complex microstructures are analyzed using focused ion beam-scanning electron microscopy and energy dispersive X-ray spectroscopy. This conventional method is labor-intensive and time-consuming, limiting high-throughput analysis and hindering advancements in SOEC technology. To address these challenges, this study utilizes DREAM 3D, an open-source software for generating synthetic microstructures, focusing on the half-cell configuration that includes the O₂-Electrode and Electrolyte with a buffer layer. We developed a detailed 3D numerical model to study the transport dynamics of oxygen vacancies, holes, and electrons, and to explore the interactions between the triple phase boundary (3PB) and double phase boundary (2PB). Additionally, a perturbed model under DC bias was implemented to monitor the impedance evolution of the oxygen electrode during extended operational tests. This approach enhances our understanding of electrochemical and mechanical coupling in SOECs, aiding experimentalists in interpreting complex data, particularly when mechanical effects like delamination are challenging to quantify directly.

11:10 AM

(PACRIM-S03-012-2025) Automatic & Autonomous Solution For New Generation SOFCA. Huang^{*1}

1. MTI Corporation, Technical Department, USA

Automatic and autonomous equipment is critical for exploring new generation Solid Oxide Fuel Cells (SOFC) with a low working temperature and high efficiency. Reliable data collection and analysis with high throughput is most important for AI-driven SOFC material discovery. We will introduce how to achieve autonomous dosing of multi-source solids, uniform mixing, pellet press, and high temperature sintering, which accelerates materials discovery by 16 to 32 times. Our system is also able to combine with different characterization instruments including split fuel cells and electrochemical stations.

11:30 AM

(PACRIM-S03-013-2025) Effect of BaO/Al₂O₃ ratio on crystallization and properties of glass ceramic sealantsJ. Begos^{*1}; A. F. Laplace¹; G. Delaizir²

1. Commissariat à l'énergie atomique et aux énergies alternatives Marcoule, University of Montpellier, CEA/DES/ISEC/DPME/LFCM, France
2. Institut de Recherche sur les Ceramiques, Université de Limoges, UMR CNRS 7315, France

Hydrogen production by high-temperature steam electrolysis is achieved using complex structures such as Solid Oxide Cells (SOC) stacks. Ensuring the sealing of this metallic/ceramic multilayer is still challenging. Sealing solution needs to meet several specific properties (thermomechanical, chemical and electrical). Glasses and glass-ceramics have been identified as suitable candidates for this such application. This work consists in the study of glass sealants for high-temperature electrolyzers (HTE) currently developed at CEA France. Samples in the BaO-SiO₂-Al₂O₃-B₂O₃-MgO glass system have been studied and s. Several glasses with different BaO/Al₂O₃ contentsratio have been synthesizedelaborated. These glasses have been thermally heat-treated in order to assess their microstructural evolution in HTE working temperature range (~700-900°C). After thermal treatments, glass-ceramic samples have been obtained and.

They have been characterized by Scanning Electron Microscope – Energy Dispersive Spectroscopy (SEM-EDS) and X-Rays Diffraction (XRD) to get insights into the nature and fractionproportion of both crystalline and residual amorphous phases. This work shows a significant modification of the crystallization behavior with the composition and the thermal treatment duration. Effect of the sample microstructure over Coefficient of Thermal Expansion (CTE) is also reported.

PacRim S4 - Polymer-Derived Ceramics/ Composites/Nanocomposites as Functional Inorganic Materials**PACRIM Symposium 4 - Detailed characterization of PDC and hybrids**

Room: Plaza C

Session Chair: Qingbo Wen, Central South University

8:00 AM

(PACRIM-S04-032-2025) Probing structure of PDCs with solid-state NMR: an overview of possibilities (Invited)C. Gervais^{*1}

1. Sorbonne Universite, LCMCP, France

The production of ceramics from polymeric precursors allows both the elaboration of precursors with varied architectures and thus of ceramic materials with completely new structures, and also the production of shaped materials including hybrid composites. The overall process for the formation of PDCs consists in the preparation of the pre-ceramic polymers, their cross-linking and ceramization. Considering these synthesis steps, a better understanding of the systems at all stages is relevant since it is essential to characterise in detail the structural transformations occurring to understand polymer-ceramic relationships and optimize the polymer architecture for the target material. Solid-state Nuclear Magnetic Resonance (NMR) appears to be a particularly well adapted characterisation technique since it allows not only to investigate the local environment of nuclei but also the longer range connectivities between nuclei. Screening a large range of systems, the relevant nuclei that can be probed will be presented with their advantages and drawbacks, as well as the main NMR sequences that can be used to obtain as much structural information as possible. In particular, it will be shown how an appropriate combination of solid state NMR techniques can be used to deal with the lack of sensitivity of some isotopes or a lack of resolution of the spectra due to the quadrupolar character of the nuclei.

8:30 AM

(PACRIM-S04-033-2025) Frustrated Lewis Pair Functionalization of Precursor-Derived Ceramic for Small Molecule Activation (Invited)S. Tada^{*1}

1. Indian Institute of Technology Madras, Department of Metallurgical and Materials Engineering, India

Small molecule activation by heterogeneous catalysts offers promising pathways for transforming small molecules, such as H₂ and CO₂, into valuable products. Recent efforts have focused on achieving high catalytic activity using earth-abundant elements, including transition metals (TMs) and main-group elements. Notably, the replacement of rare and expensive TMs in catalysis has been driven by the discovery of unique reactions mediated by main-group elements. Frustrated Lewis pairs (FLPs), consisting of a Lewis acid (LA) and a Lewis base (LB), can act as small molecule activation sites by preventing the classical LA-LB dative bond formation due to steric hindrance. FLPs exhibit a distinctive “push-pull” effect, efficiently enabling the activation of various small molecules and

revealing unexpected catalytic properties. Although molecular FLPs are widely studied, extending this concept to solid-state materials has gained significant attention in recent years. Herein, we report on the hydrogen activation capability of Si-based non-oxide ceramics (Si_xN, where X = Al or B) synthesized via a polymer-derived ceramic (PDC) route, as well as the FLP functionalization of organic-inorganic framework synthesized by supramolecular precursors. Our findings demonstrate the potential of these materials to expand the applicability of FLP-based catalysis in heterogeneous systems.

9:00 AM

(PACRIM-S04-034-2025) Polymer-Derived Ceramics: Probing Structure Through Infrared and Raman Spectroscopy

P. Jelen^{*1}; M. Bik¹; J. Marchewka¹; M. T. Sitarz¹

1. Akademia Gorniczko-Hutnicza im Stanislaw Staszica w Krakowie, Poland

Polymer derived ceramics include silicon-based ceramic materials e.g. carbides, oxycarbides, oxynitrides. They are characterized by high thermal, chemical and oxidation resistance. These materials are obtained by the pyrolysis of preceramic precursors, like organosilicon polymers which makes it possible to design materials for specific applications especially with the proper addition of cationic modifications (e.g. boron, copper, iron). Among these, silicon oxycarbides (SiOC) are the most interesting. They possess the amorphous silica structure where part of oxygen atoms is replaced by carbon atoms. The primary analytical tool for PDC-based materials is X-ray diffraction. It is a well-established method, but one that has its limitations like the inability to identify amorphous phases in the material. The seemingly simple and versatile method of FT-IR and Raman spectroscopy, which is a complementary method, provide great opportunities to study chemical bonds in PDC materials. The biggest advantage is the non-destructive nature and the ability to measure amorphous materials. These measurements allow for the precise determination of nanometric layers, or inclusions, which, combined with chemical imaging methods, provides an inside to the chemical structure of PDC materials. This research was supported by the "Excellence Initiative – Research University" program at AGH University of Krakow

PACRIM Symposium 4 - Development of porous architectures spanning single and multiple length scales

Room: Plaza C

Session Chair: Zhaou Yu, Xiamen University

9:20 AM

(PACRIM-S04-035-2025) Hierarchically porous polymer-derived SiOC monoliths for chemical conversion and adsorption (Invited)

T. Konegger^{*1}; K. Rauchenwald¹; T. Felsberger¹; J. Eßmeister¹; K. Föttinger²

1. TU Wien, Institute of Chemical Technologies and Analytics, Austria
2. Technische Universität Wien Institut für Materialchemie, Austria

The implementation of polymer-derived ceramic materials containing porosity spanning several length scales has gained increasing attention in recent years owing to the global need for more sustainable industrial processes requiring novel material concepts. Here, significant progress has been made possible by revolutionary processing techniques and structuring approaches providing monolithic parts of varying complexity. In this contribution, we highlight the potential of monolithic, hierarchically porous polysiloxane-derived SiOC materials for prospective applications in the fields of chemical conversion processes, particularly CO₂ utilization, as well as for adsorption applications in water purification. After highlighting different approaches to generate hierarchical pore structures into SiOC monoliths by processing variants such as light-based additive manufacturing coupled with polymerization-induced phase separation, or solidification templating using binary solvent systems, two distinct use cases will highlight the applicability of the material systems. The first use case involves the use of Ni-functionalized SiOC monoliths in CO₂

methanation, while the second use case assesses the suitability of SiOC for the removal of organic contaminants from water. In both cases, hierarchically porous SiOC monoliths provide promising performance and potential for further fields of application.

9:50 AM

(PACRIM-S04-037-2025) Nitrogen-doped carbon/CoFe nanoparticle/CoN composite with hierarchical meso-macro pores as an electrocatalyst for the oxygen reduction reaction

Y. Sugahara^{*1}; Y. Li¹; N. Ebato¹; Y. Guo¹; Y. Yamauchi²

1. Waseda University, Japan
2. Nagoya University, Department of Materials Process Engineering, Japan

Polydopamine was assembled with two soft-template Pluronic triblock polymers, F-127 and P-123, doped with trivalent cobalt and iron ions and the resultant precursor was pyrolyzed to obtain nitrogen-doped carbon containing CoFe alloy, Co and CoN with hierarchical meso-macro pores. F-127 and P-123 were mixed and trimethylbenzene was added for increasing the micelle size. A cobalt complex and iron salt were added to the solution and dopamine was mixed. Dopamine was polymerized by adding aqueous ammonia to obtain the precursor, which was pyrolyzed under nitrogen atmosphere. The obtained product consisted of spheres with the size of about 200 nm. CoFe nanoparticles were observed in the spheres. X-ray photoelectron spectroscopy revealed the presence of C-C (284.8 296 eV), C-N (286.1 eV), and C=O (288.4 eV) bonds. The product excellent a remarkable catalytic activity for oxygen reduction reaction (ORR) in both alkali (half-wave potential: 0.943 V vs. RHE) and acid (half-wave potential: 0.811 V vs. RHE) media. While nitrogen-doped carbon with hierarchical meso-macropores provided abundant sites for accommodating active metal species, the bimetallic CoFe nanoparticles had abundant active catalytic sites for ORR.

PACRIM Symposium 4 - Fundamental processing-microstructure-properties relationships

Room: Plaza C

Session Chair: Michael Jakubinek, National Research Council Canada Emerging Technologies Division

10:25 AM

(PACRIM-S04-038-2025) Fabrication of Simple and Complex Shaped Ultra-High Temperature Ceramic Matrix Composites and Their Performance in Relevant Environments (Invited)

D. Sciti^{*3}; A. Vinci³; L. Zoli³; A. Airoidi¹; M. De Stefano Fumo²; A. M. Caporale¹

1. Politecnico di Milano, Italy
2. Centro Italiano Ricerche Aerospaziali, Italy
3. Consiglio Nazionale delle Ricerche, ISSMC, Italy

Thermal protection materials for space vehicles must endure extreme temperatures, chemical environments, and rapid thermal changes. UHTCMCs (ultra-high temperature ceramic matrix composites) combine UHTC-rich matrices with carbon fibers, improving damage tolerance and ablation resistance above 2000°C. In this talk we show the recent advancements in the manufacturing of UHTCMCs with simple and complex shapes and their mechanical and environmental testing. Fibre reinforcement has been shown to improve the damage tolerance at room and elevated temperature. Optimized microstructures and textures led to exceptional ablation/erosion resistance beyond 2000°C in arc jet and in rocket nozzles. The latest studies include the production of prototypes with leading-edge profiles tested in a hypersonic plasma wind tunnel. Two manufacturing approaches were evaluated: machined composites from sintered manufactures and near-net shape prototypes via polymer infiltration and pyrolysis. Tests in the Scirocco plasma wind tunnel at CIRA revealed distinct thermal behaviors due to different manufacturing methods. Microstructural analyses and mechanical tests were conducted to assess oxidation and strength degradation from these extreme conditions.

10:55 AM

(PACRIM-S04-039-2025) Single-source precursor synthesis of novel Si(Hf, Ta, B)CN-based ceramic nanocomposites and their behavior in harsh environmentsM. Boroojerdi^{*1}; J. Bernauer¹; S. Kredel¹; R. Riedel¹; E. Ionescu²

1. Technische Universität Darmstadt Fachbereich Material- und Geowissenschaften, Germany
2. Fraunhofer-Einrichtung für Wertstoffkreislaufe und Ressourcenstrategie IWKS, Germany

In the present work, Si(Hf, Ta, B)CN-based polymer-derived ceramic nanocomposites were synthesized via a single-source precursor route through the chemical modification of a commercially available polysilazane (i.e., Durazane 1800) with molecular hafnium, tantalum, and boron compounds. The successful modification of the polysilazane was confirmed by nuclear magnetic resonance (NMR) and infrared (IR) spectroscopy. Cross-linking and shaping of the preceramic polymers was achieved via warm pressing. Subsequent pyrolysis at 1000 °C in an inert gas atmosphere delivered dense monolithic samples which were studied with respect to their microstructure, phase composition as well as mechanical properties. Moreover, coefficients of thermal expansion, thermal conductivity, and the high-temperature oxidation behavior of the prepared samples were analyzed. The obtained results highlight Si(Hf, Ta, B)CN-based ceramic nanocomposites as a promising alternative to conventional thermal barrier coatings (TBCs), offering superior thermal stability, durability, and efficiency in extreme environments. "This study was financially supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under project GRK 2561."

PacRim S10 - Ceramics of Tomorrow for Green Energy and Cleaner Environment**PACRIM Symposium 10 - Ceramics of Tomorrow for Green Energy and Cleaner Environment I**

Room: Georgia B

Session Chairs: Eva Hemmer, University of Ottawa;
Scott Misture, Alfred University

8:00 AM

(PACRIM-S10-001-2025) Carbon Nanomaterials - A Sustainable Pathway to Green Energy Solutions (Invited)R. Naccache^{*1}

1. Concordia University, Chemistry and Biochemistry, Canada

Carbon nanomaterials have garnered significant interest owing to their versatile properties with a vast potential in sensing and imaging applications, in optoelectronics, Catalysis, as well as energy conversion. Their ultra-compact size, low cytotoxicity, low photo-bleaching/bleinking, tunable photoluminescence, combined with simple, environmentally friendly and low-cost synthesis, makes them ideal and cost-efficient candidates for study. In this work, we discuss the synthesis of carbon nanomaterials via a myriad of techniques including solvent mediated and solid-state bottom-up synthesis methods, with simple organic precursors. We focus our efforts on tailoring their physico-chemical and optical properties and exploit them in order to design multifunctional materials for environmental and clean energy applications namely in decontamination of waters from pesticides, organic molecules and other emerging contaminants, as well as the conversion of refined and waste oils to biofuels via chemical or light-mediated approaches. We also investigate the potential to prepare these nanosized dots from waste materials as we prioritize sustainability without compromising function and performance in environmental and clean energy applications.

8:30 AM

(PACRIM-S10-002-2025) Hydrogen Sensors for Hydrogen Economy (Invited)O. K. Varghese^{*2}; D. Waligo²; M. Paulose¹

1. University of Houston, Department of Physics, USA
2. University of Houston, Department of Physics and Texas Center for Superconductivity, USA

The impending paradigm shift in the energy sector behooves the researchers to develop supporting technologies concurrently. For example, hydrogen is increasingly used as an energy vector and the technology development for its detection is important not only for the safety of people and facilities but also for a clean environment. Hydrogen is not a greenhouse gas and this is often highlighted as its most desirable property. Nevertheless, it poses environmental risks as an indirect greenhouse gas, primarily by extending the atmospheric lifetime of methane. Therefore, the hydrogen leaks into the atmosphere, even at low concentrations, should be promptly detected and prevented. We have recently developed a novel material exhibiting ultra-high sensitivity to hydrogen. The chemical sensor fabricated using the material has the potential to detect low-concentration hydrogen selectively in industrial and domestic environments at room temperature. This presentation is aimed at discussing the details of this work.

9:00 AM

(PACRIM-S10-003-2025) Role of Innovative Materials Engineering for Advancing the Clean Energy and Smart Agriculture Technologies (Invited)G. Selopal^{*1}; S. Madhu¹; U. Sohail¹; S. Singh¹; M. Chinna¹

1. Dalhousie University, Department of Engineering/ Faculty of Agriculture, Canada

As the world moves towards a sustainable future, advanced materials engineering plays a key role in revolutionizing clean energy and smart agriculture. In particular, colloidal quantum dots (QDs) are widely used as building blocks for clean energy and smart agriculture technologies due to their remarkable size/shape/composition-controlled optoelectronic properties associated with the "quantum confinement" effect. However, the performance of QDs-based devices is still lower than the expected theoretical value, mainly associated with slow charge injection/transfer rate from QDs to scavengers and fast non-radiative carrier recombination within the QDs and QDs/metal oxide/electrolyte interface. Surface engineering of QDs is an effective approach to address these challenges. In this talk, the advanced surface engineering of colloidal QDs with different shell materials and layer thicknesses, as well as interface optimization, will be discussed. A detailed discussion on the effect of different shell thicknesses, compositions, and interfacial layers of core/shell QDs on the optoelectronic properties compared to the control QDs will be discussed. Finally, the application of optimized colloidal QDs for clean energy technologies such as photovoltaics, green hydrogen production and smart agriculture technologies will be presented, and possible future directions will be discussed.

9:30 AM

(PACRIM-S10-004-2025) Enhancement of photocatalytic activity using defect engineering by controlling stoichiometry in LaTiO₂N inverse opal photonic crystalT. Maekawa^{*1}; N. Tateishi¹; Y. Ikeda¹; H. Fukuma¹; G. I. Waterhouse²; K. Murai¹; T. Moriga¹

1. Tokushima Daigaku, Japan
2. The University of Auckland, New Zealand

In this research, polycrystalline LaTiO₂N inverse opal (IO) photonic crystal photocatalysts with different macropore diameters were synthesized using polymethyl methacrylate (PMMA) and polystyrene (PS) colloidal crystals as sacrificial templates. The photonic bandgaps (PBGs) in LaTiO₂N IO powder redshifted as increasing macropore diameter, in accordance with the modified Bragg's law equation. Owing to polycrystalline properties, the PBGs position in

LaTiO₂N IO showed angular independence in response to changes in the incident angle of light. LaTiO₂N IO powders have demonstrated the ability to modulate their color through structural coloration derived from PBGs, indicating potential applications as pigments. By adjusting the La/Ti ratio in LaTiO₂N IO, the number of defects generated during nitridation can be controlled. This is due to the fact that the excessive lanthanum oxide acts as a protector, suppressing the production of reduced titanium species. The photocatalytic activity in La/Ti = 1.05 for the degradation of tetracycline was maximized. This study represents the first report to combine photonic crystal engineering and defect engineering in composite metal oxynitride powders, providing insights into their optical properties.

10:10 AM

(PACRIM-S10-005-2025) Functional Nanocomposites of Ceramics and 2D Materials for Water Nanofiltration, Purification and Diagnostics (Invited)

G. Fanchini*¹

1. University of Western Ontario, Physics and Astronomy, Canada

In this talk, we review our development of next-generation membranes for water nanofiltration, purification and diagnostics based on nanoporous 2D materials and colloidal ceramics fillers. We present a fabrication process in which graphene flakes are utilized to fabricate a continuous membrane in which leaks between juxtaposed flakes are sealed by colloidal ceramics, in a treatment that precedes opening of the pores through graphene. Copper nanoparticles are subsequently deposited on the flakes of this 2D material, and their etching ensures the opening of nanopores (5-50 nm) without compromising the membrane continuity, which is ensured by the ceramic phase that makes these nanofilters leak-free. Our nanofiltration system combines the advantages of graphene membranes, suitable to differential pressures as low as ~10 KPa, with those of graphene oxide, offering scalability over large areas. We show that our membranes offer superior retention of cation impurities, including Mn(II) and Fe(II). In the last part of our talk, we present how this technology can be combined with sorbents and semiconducting 2D materials such as MoS₂ for improved water purification combined to chemiresistive diagnostics. Collectively, our work demonstrates the outstanding capabilities of nanocomposite materials in water filtration.

10:40 AM

(PACRIM-S10-006-2025) Synthesis of mesoporous silica from geothermal water and the application for environmental purification (Invited)

Y. Watanabe*¹

1. Hosei Daigaku Rikogakubu Daigakuin Rikogaku Kenkyuka, Japan

Mesoporous silica was successfully synthesized for the first time using geothermal water from the Onuma Geothermal Power Plant, in Akita Prefecture, Japan. Cetyltrimethylammonium bromide (CTAB) reacted with the geothermal water, which had a total silicic acid concentration of 475 mg/L (SiO₂), at pH 7.0, pH 8.2 and pH 9.0 for 30 min at a temperature of 90 °C. Through calcination of the resulting precipitate at 550 °C, mesoporous silica with a pore size of about 2.8 nm and a specific surface area of more than 800 m²/g was formed. The total silicic acid concentration in the solution, after formation of the mesoporous precipitates, was reduced to less than 280 mg/L. This indicates efficient recovery of supersaturated silicic acid from the geothermal water. The monosilicic acid in the geothermal water plays an important role in the formation of mesoporous silica. Production of mesoporous silica by our method will contribute to the prevention of silica scale formation in the piping systems. This mesoporous silica contains a small amount of aluminum in the structure, which is useful as an ion exchanger for ammonium ion.

11:10 AM

(PACRIM-S10-007-2025) Understanding the impact of TiO₂ microstructure on the photocatalytic conversion of polystyrene nanoplastics into valuable organic products

C. Canovi*¹; C. Siligardi¹; E. Cedillo-González¹

1. University of Modena and Reggio Emilia, Department of Engineering “Enzo Ferrari”, Italy

The urgent need to mitigate plastic pollution drives research into developing advanced ceramic materials for sustainable environmental remediation. Nanoplastics (NPs) are a global issue due to their persistence, bioaccumulation, and harm to ecosystems and human health. This study investigates the correlation between the microstructure of TiO₂ and the photocatalytic efficiency in converting water-dispersed polystyrene (PS) NPs into valuable products using UV light. Three different TiO₂ microstructures (spheres, “raspberries” and rods) were synthesized by varying HCl concentration in hydrothermal processing at 150°C. Chemical and structural characterization showed that all TiO₂ samples consist of rutile-phase. Photocatalytic tests were combined with scavenger studies to elucidate the conversion mechanism. It was found that “raspberries” and spheres-shaped microstructure presented the highest conversion because their morphology traps NPs into their surface while their high surface area increases the interaction of PS with the oxidant hydroxyl radicals adsorbed in the surface of TiO₂. Compared to commercial TiO₂, the new microstructures achieved superior conversion, demonstrating higher efficiency. This study concludes that microstructure is key in enhancing photocatalytic conversion of these non-conventional, non-water-soluble contaminants.

11:30 AM

(PACRIM-S10-008-2025) Magnetic-Field-Stimulated Efficient Photocatalytic N₂ Fixation over Defective BaTiO₃ Perovskites

M. Feng*¹

1. Jilin Normal University, Key Laboratory of Functional Materials Physics and Chemistry of the Ministry of Education, China

Efficient coupling solar energy conversion and N₂ fixation by photocatalysis has been shown promising potentials. However, the unsatisfied yield rate of NH₃ curbs its forward application. Defective typical perovskite, BaTiO₃, shows remarkable activity under an applied magnetic field for photocatalytic N₂ fixation with an NH₃ yield rate exceeding 1.93 mg L⁻¹ h⁻¹. Through steered surface spin states and oxygen vacancies, the electromagnetic synergistic effect between the internal electric field and an external magnetic field is stimulated. X-ray absorption spectroscopy and density functional theory calculations reveal the regulation of electronic and magnetic properties through manipulation of oxygen vacancies and inducement of Lorentz force and spin selectivity effect. The electromagnetic effect suppresses the recombination of photoexcited carriers in semiconducting nanomaterials, which acts synergistically to promote N₂ adsorption and activation while facilitating fast charge separation under UV-vis irradiation.

11:50 AM

(PACRIM-S10-021-2025) Hybrid multiscale ceramics enhanced mechanical behaviour and energy applications (Invited)

D. Giuntini*¹

1. Eindhoven University of Technology, Mechanical Engineering, Netherlands

[See page 154 for abstract](#)

PacRim S12 - Eng Ceramics and Ceramic Matrix Composites - Processing/Design/Applications

PACRIM Symposium 12 - Processing-microstructure-mechanical properties correlation I

Room: Plaza B

Session Chairs: Zbigniew Pedzich, AGH University of Krakow; Junichi Tatami, Yokohama National University

8:00 AM

(PACRIM-S12-026-2025) Bending strength and cyclic fatigue of grain boundary in high thermal conductivity silicon nitride ceramics (Invited)

J. Tatami^{*1}; K. Matsuura¹; M. Iijima¹; K. Matsui¹; T. Takahashi²; T. Yahagi²; H. Nakano³; T. Ohji¹

1. Yokohama National University, Japan
2. Kanagawa Institute of Industrial Science and Technology, Japan
3. Toyohashi University of Technology, Japan

The bending strength of the grain boundaries in the Si_3N_4 ceramics with high thermal conductivity, which was measured using micro-cantilever beam specimens, depended on the added rare earth ions. The Si_3N_4 ceramics prepared by adding Lu^{3+} , which has the smallest ionic radius among rare earth ions, showed the highest grain boundary strength. The grain boundary strength at the surface where cyclic loading was applied using a spherical indenter was degraded compared to before indentation. Considering the large number of dislocations observed near the cyclically loaded surface, the reason for the strength degradation of the grain boundaries due to cyclic loading can be attributed to stress concentration caused by dislocation pile-ups.

8:30 AM

(PACRIM-S12-027-2025) Manufacturing of titanium boride basing UHTC composites by reactive sintering utilizing different titanium precursors (Invited)

Z. Pedzich^{*1}; D. Koziem¹; A. Wilmanski¹; W. Banas¹; A. Wojteczko¹; P. Tatarko²; D. Salamon³

1. AGH University of Krakow, Department of Ceramics and Refractory Materials, Poland
2. Institute of Inorganic Chemistry, Slovak Academy of Sciences, Department of Ceramics, Slovakia
3. Montanuniversitat Leoben, Austria

The production of UHTC composites based on TiB_2 by reaction sintering can be a very good method for reducing the temperature of synthesis of finished dense elements, the operating temperatures of which reach even 1800 C, in conditions even 700 degrees lower. As a source of boron in such materials, boron carbide B_4C is usually used. The source of titanium can be many more chemical compounds. The simplest solution is to use metallic titanium, but this does not ultimately provide a material with good properties. The skillful selection of precursors from the group of intermetallic compounds in the Ti-Si (TiSi , TiSi_2 , Ti_3Si_3), Ti-Al (TiAl , Ti_3Al , TiAl_3) or even MAX phases (Ti_3SiC_2 , Ti_2AlC) systems allows for precise control of the type and kinetics of reactions occurring during sintering and temperature of this process. This approach allows for the optimization of the phase composition and the final microstructure of composites, ensuring very good mechanical and thermal parameters. The paper presents materials obtained using different precursors. Their mechanical and thermal properties were compared, as well as their performance in oxidation tests performed using a torch at a 1800 C. Work was supported by the Polish State Ministry of Science and Higher Education by the program Excellence Initiative-Research University for the AGH University of Krakow, grant ID 9886.

9:00 AM

(PACRIM-S12-028-2025) Secondary phases reinforced carbide and boride ceramics: Effect of silicon carbide and graphite platelets on mechanical and tribological properties (Invited)

A. Kovalčíková^{*2}; P. Tatarko¹; R. Sedláček²; Z. Chlup³; D. Medved²; E. Mudra²; J. Dusza²

1. Institute of Inorganic Chemistry, Slovak Academy of Sciences, Department of Ceramics, Slovakia
2. Institute of Materials Research, Slovak Academy of Sciences, Division of Ceramic and Non-Metallic Systems, Slovakia
3. Institute of physics of materials Czech Academy of Sciences, Czechia

An understanding of the relation of material composition with mechanical characteristics is necessary to meet requirements of friction and wear for tribological applications. The main focus is on the development of wear-resistant components working at extreme conditions. The role of GPLs with different size and morphology up to 10 wt. % and/or SiC up to 25 wt. % on densification, microstructural development, mechanical properties and tribological behavior of brittle titanium diboride ceramics was studied. Instrumented hardness, bending strength, chevron -notched fracture toughness, ball on flat tribological tests, SEM/FIB microscopy, and Raman spectroscopy were used for the testing and characterization of the investigated composites. According to the results for optimal strength and fracture toughness, the amount of GPLs and SiC additive should be 2 wt. % and 20 wt. %, respectively. Increasing amount of GPLs has also positive influence on wear of the composites due to the observed wear mechanisms. Achieved results of tested mechanical properties were compared with carbide based ceramic composites. Acknowledgements: This work was supported by the Slovak Research and Development Agency under the contracts APVV-21-0402, APVV-22-0493, and by the project of Slovak Academy of Sciences IMPULZ IM-2022-67.

9:30 AM

(PACRIM-S12-029-2025) Confocal laser fluorescence microscopy for in-situ observation of particle motion in highly concentrated slurries (Invited)

M. Uematsu^{*1}; T. Kimura¹

1. Japan Fine Ceramics Center, Japan

The molding process using high-concentration ceramic slurries is widely used in producing engineering ceramics. Properties such as particle size distribution, viscosity, and dispersion state of the slurry influence the microstructure of the green body and the performance of the final product. Understanding slurry properties in relation to the ceramic microstructure is essential. These properties affect particle packing behavior during molding, and understanding particle motion helps predict it. However, high-concentration slurries of fine particles often exhibit nonlinear flow behaviors, such as thixotropy, and how particles move in these slurries is not fully understood. Furthermore, the internal structure of the slurry changes during molding, making it difficult to predict local structural variations. To better understand particle motion, a transparent slurry was developed to visualize the internal structure directly. The slurry was made from a transparent raw powder material and a liquid with the same refractive index, minimizing light scattering at the powder-liquid interface and allowing visible light to pass through. By dissolving a fluorescent agent and observing the slurry with a confocal fluorescence microscope, real-time cross-sectional images of the slurry's interior were captured, and continuous scanning revealed structural changes.

10:20 AM

(PACRIM-S12-030-2025) Structure, mechanical properties and thermal stability of TiNbVTaZrHf-N coatings deposited by reactive sputtering

F. Lofaj^{*1}; L. Kvetkova¹; P. Hviscova¹; M. Mikula²; T. Roch²; T. Fiantok²

1. Institute of Materials Research of SAS, Division of ceramics and non-metallic materials, Slovakia
2. Univerzita Komenskeho v Bratislave Fakulta matematiky fyziky a informatiky, Slovakia

The work investigates the structure, phase, chemical compositions, mechanical properties, and thermal stability of the TiNbVTaZrHf-N_x coating system which is among the promising candidates for applications in extreme conditions. Two series of coatings with nitrogen concentrations from 0 at% to 50 at% were deposited in a hysteresis-free regime by reactive DC magnetron sputtering and reactive High Target Utilization Sputtering (HiTUS), respectively. All nitride coatings formed homogeneous solid solutions with nanocrystalline and textured structures. DFT calculations confirmed the stability of such solid solutions and a transition from bcc toward fcc structure above certain nitrogen concentrations. Coating stoichiometry correlated with the changes in the indentation hardness and indentation modulus. The highest hardness in DCMS coatings of H_{IT} ~ 40 GPa and indentation modulus E_{IT} ~ 490 GPa were slightly higher than in the HiTUS coatings. H_{IT}/E_{IT} and limited pillar split measurements suggested these coatings exhibit brittle behavior with the fracture toughness only around 1 MPa.m^{1/2}. The investigations of thermal stability in a vacuum revealed that the loss of nitrogen starts above 1200°C and occurs via bubble formation along the boundaries between columnar grains.

10:40 AM *Moved to poster session*

(PACRIM-S12-031-2025) Processing and properties of damage tolerant reactively sintered high-entropy diboride ceramic composites reinforced with SiC

R. Sedláč^{*1}; T. Csanádi¹; M. Hrubovčáková¹; I. Shepa¹; L. Daková¹; A. Kovalčíková¹; Z. Chlup²; Z. Fogarassy³

1. Institute of Materials Research, Slovak Academy of Sciences, Division of Ceramic and Non-Metallic Systems, Slovakia
2. Institute of Physics of Materials, Czech Academy of Sciences, Czechia
3. Institute of Technical Physics and Materials Science, Centre for Energy Research, Hungary

A detailed systematic study investigates the influence of the sintering parameters on microstructure development and mechanical properties of (Hf-Ta-Zr-Nb-Ti)B₂-SiC high-entropy diboride ceramics, synthesized by reactive SPS technology. Composites were produced based on in-situ solid state reaction during the densification process of equimolar precursor transition metal carbides of HfC, TaC, ZrC, NbC, and TiC, along with the corresponding amounts of B₄C and Si. The reactive sintering conditions were optimised, the temperature varied from 1650 to 2100 °C, and dwell time from 5 to 20 mins. Microstructural characterisation was performed by SEM and TEM with EDS, and phase composition by XRD. Mechanical properties, such as nano/micro/macro hardness, fracture toughness, bending strength, and elastic modulus were measured. The combination of in-situ reaction and SPS resulted in the prepared high-entropy ceramics exhibiting significant densification and exceptional values of fracture toughness (4.71±0.16 MPa.m^{1/2}) and bending strength (655.12±48.24 MPa). The relationship between microstructural development and basic mechanical properties has an important role in the further development of these perspective materials. Acknowledgment: "Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00746."

PACRIM Symposium 12 - Processing-microstructure-mechanical properties correlation II

Room: Plaza B

Session Chairs: Zbigniew Pedzich, AGH University of Krakow; Junichi Tatami, Yokohama National University

11:00 AM

(PACRIM-S12-036-2025) Enhanced densification and dielectric properties in BaTiO₃ through a cold-sintering pre-treatment, minimizing secondary phases

S. Jeon^{*1}; A. Ullah¹; H. Palneedi¹

1. Changwon National University, Republic of Korea

The cold sintering process (CSP) is now a well-known technique to densify ceramic materials at extremely low temperatures. This study utilized the CSP as a pre-treatment to densify BaTiO₃ before traditional sintering (TS) at high temperatures. With CSP pre-treatment at 225 °C followed by TS at 1000 °C (CSP + TS), a high relative density (96.86 %TD) was achieved with an average grain size of 1.52 μm. In contrast, poor outcomes of 60.56 %TD and 0.29 μm were obtained in the same BaTiO₃ sample without CSP pre-treatment, highlighting the benefits of this approach. The significant improvement in density of the CSP + TS sample was evident over a wide temperature range (900-1200 °C), resulting in superior dielectric properties compared to the TS samples due to the synergistic effect of proper grain size without abnormal grain growth. In addition, the enhanced dielectric performance was attributed to reduction of harmful secondary phases such as BaCO₃ and Ba₂TiO₄. This study demonstrates an advantageous processing route for BaTiO₃ using the CSP pre-treatment.

PacRim S13 - Functional Defects in Ceramic Materials

PACRIM Symposium 13 - Defect engineering in electrochemical energy materials

Room: Grouse

Session Chair: Eric Gabriel, Boise State University

9:00 AM

(PACRIM-S13-010-2025) Influence of Interlayer Cation Ordering on Na Transport in P2-Type Na_{0.67-x}Li_yNi_{0.33-z}Mn_{0.67+z}O₂ for Sodium-Ion Batteries

E. Gabriel^{*1}; Z. Wang²; V. V. Singh²; K. Graff¹; J. Liu³; C. Koroni¹; D. Hou¹; D. Schwartz¹; C. Li³; J. Liu⁴; X. Guo⁴; N. C. Osti³; S. Ong²; H. Xiong¹

1. Boise State University, Materials Science and Engineering, USA
2. University of California San Diego, Department of NanoEngineering, USA
3. Oak Ridge National Laboratory, Neutron Scattering Division, USA
4. Washington State University, Department of Chemistry, USA

P2-type Na_{2/3}Ni_{1/3}Mn_{2/3}O₂ (PNNMO) has desirable electrochemical properties as a positive electrode for sodium ion batteries. PNNMO exhibits intralayer transition metal ordering of Ni and Mn and intralayer Na⁺/vacancy ordering. Na⁺/vacancy ordering may impede fast Na⁺ transport and can be affected by the transition metal ordering. We show by neutron/X-ray diffraction and density functional theory calculations that Li doping (Na_{2/3}Li_{0.05}Ni_{1/3}Mn_{2/3}O₂, LFN5) promotes ABC-type interplanar Ni/Mn ordering without disrupting the Na⁺/vacancy ordering and creates low-energy Li-Mn coordinated diffusion pathways. A structure model is developed to quantify the intralayer cation mixing and interlayer cationic stacking fault densities. Quasielastic neutron scattering reveals that the Na⁺ diffusivity in LFN5 is enhanced compared to PNNMO, increasing its capacity at high current. Na_{2/3}Ni_{1/4}Mn_{3/4}O₂ (NM13) lacks Na⁺/vacancy ordering and has comparable diffusivity to LFN5 but has the smallest capacity at a high current. The high site energy of Mn-Mn coordinated Na compared to Ni-Mn, and higher density of Mn-Mn coordinated Na⁺

sites in NM13 disrupts the low-energy diffusion pathways. These results suggest that the interlayer ordering can be tuned through the control of composition, which has an equal or greater impact on Na⁺ diffusion than the Na⁺/vacancy ordering.

9:20 AM

(PACRIM-S13-011-2025) Copper-Alloy Fluorides as Cathode Active Materials for All-Solid-State Fluoride Batteries

M. Motoyama^{*1}; T. Nakagawa²; K. Sakurai²; T. Nakatani³; H. Kiuchi³; Z. Ogumi³; T. Abe³

1. Kyushu University, Kyushu Daigaku, Fukuoka, Fukuoka Prefecture, JP, academic, Kyushu University Platform of Inter-/Transdisciplinary Energy Research, Japan
2. Kabushiki Kaisha Honda Gijutsu Kenkyujo, Japan
3. Kyoto Daigaku, Japan

Fluoride batteries are promising due to their potential for achieving greater energy densities than lithium-ion batteries.¹ The cathode and anode active materials in fluoride batteries are typically metal fluorides (e.g., CuF₂, AlF₃). However, these materials suffer from low electrical conductivity and F⁻ conductivity. To address this limitation, doping metal cations into metal fluorides to introduce atomic defects and enhance F⁻ diffusivity within electrode active materials has emerged as a promising approach. Previously, we demonstrated that the Cu_{0.72}Ni_{0.38} alloy serves as a superior cathode active material compared to pure Cu and pure Ni.² Despite this advantage, the mechanism underlying the lower overpotential of NiF₂ defluorination in Cu_{0.72}Ni_{0.38} cathodes compared to pure Ni cathodes remains unclear. To elucidate this mechanism, we conducted operando hard X-ray photoelectron spectroscopy measurements on Cu_{0.72}Ni_{0.38} cathode films. These measurements aimed to provide insights into the charge/discharge reaction mechanisms of Cu_{0.72}Ni_{0.38} cathode films. Acknowledgments This paper is based on the results obtained from projects JPNP16001 and JPNP21006, commissioned by the New Energy and Industrial Technology Development Organization (NEDO). References 1. Gschwind et al., J. Fluor. Chem., 182, 76 (2016). 2. Motoyama et al., ACS Appl. Mater. Interfaces, 16, 53631 (2024).

9:40 AM

(PACRIM-S13-012-2025) Microstructural and Electrochemical Improvements in Garnet Solid Electrolytes Prepared via Reactive Sintering from Doped Pyrochlore Precursors

J. Guo¹; C. K. Chan^{*1}

1. Arizona State University, Materials Science and Engineering; School for Engineering of Matter, Transport and Energy, USA

Garnet-type Li₇La₃Zr₂O₁₂ (LLZO) is a promising ceramic electrolyte for all-solid-state batteries because of its high electrochemical stability and ionic conductivity. We show that doped pyrochlore (La₂Zr₂O₇) can serve as precursor for LLZO, a process we call “pyrochlore-to-garnet” (P2G). For Ta-doped LLZO (LLZTO), dense LLZTO is directly obtained via reactive sintering of the multi-doped pyrochlore with LiOH and displays high relative density and ionic conductivity 0.4-0.7 mS/cm using only 2 h sintering at 1100 deg C. Investigation of the synthesis parameters shows that liquid phase sintering is important for achieving high pellet densities. Galvanostatic Li stripping measurements show that P2G LLZTO can withstand higher critical current densities and displays less Li deposition along the grain boundaries compared to SSR LLZTO. The improved cycling behavior in P2G LLZTO could be from the smaller grain sizes, more homogenous current density at the interfaces and different grain boundary properties. Advanced characterization methods reveal more insights on the microstructural features and functional defects that could give rise to the improved electrochemical properties. This work shows the P2G method is a promising and versatile alternate method for the synthesis and processing of many kinds of garnet solid-electrolyte materials.

PacRim S14 - Advanced Structural Ceramics and CMCs for Ultra Extreme Environments

PACRIM Symposium 14 - Advanced Structural Ceramics and CMCs for Ultra Extreme II

Room: Cypress

Session Chairs: Christopher Weinberger, Colorado State University; Yinglu Tang, Technische Universiteit Delft

8:00 AM

(PACRIM-S14-004-2025) A design of UHTCs and refractory compositionally complex ceramics used at above 2000°C by using calculation thermodynamics (Invited)

Y. Arai^{*1}; R. Tsuruoka¹; A. Tada¹; R. Inoue¹; Y. Kogo¹

1. Tokyo University of Science, Japan

Ceramic materials containing 5 or more ultra-high temperature ceramics are recognized as refractory compositionally complex ceramics (RCCCs) or refractory high-entropy ceramics (RHECs). UHTCs, RCCCs and fiber reinforced their composites have been considered as potential candidates for heat resistance materials such as components for re-entry vehicles and hypersonic vehicles exposed in oxidizing atmosphere at above 2000°C. In this harsh environment, SiC is a key additive to form SiO₂ scale on their surface, which act as a barrier for oxygen diffusion. However, SiC reacts with oxygen to form gaseous SiO instead of SiO₂ scale and formed SiO₂ begins to decompose at above 2000°C. Thus, a new strategy for the design of heat resistance materials available at above 2000°C is required. In this presentation, a design guideline for UHTCs, RCCCs and their composites exposed at above 2000°C in oxidizing atmosphere will be proposed. To predict complex reaction during material process and formed compounds, material process with the combination of calculation phase diagram (CALPHAD) is also proposed. Some important conditions for material using extreme environment will be discussed in terms of reaction and recession during exposure.

8:30 AM

(PACRIM-S14-005-2025) Compositionally complex carbide ceramics: a perspective on irradiation damage (Invited)

B. Cui^{*1}; L. Trinh¹; F. Wang¹; L. Wadle¹; Y. Lu¹; K. Bawane²; K. Hattar³; Z. Hua²; L. Malakkal²; L. He⁴

1. University of Nebraska-Lincoln, USA
2. Idaho National Laboratory, USA
3. University of Tennessee, Knoxville, USA
4. NC State University, USA

Extensive experimental and computational studies have demonstrated outstanding physical and chemical properties of the novel materials of compositionally complex carbides (CCC), enabling their promising applications in advanced fission and fusion energy systems. This presentation provides a comprehensive overview of radiation damage behavior reported in the literature to understand the fundamental mechanisms related to the impact of multi-principal metal components on phase stability, irradiation-induced defect clusters, irradiation hardening, and thermal conductivity of compositionally complex carbides. Several future research directions are recommended to critically evaluate the feasibility of designing and developing new ceramic materials for extreme environments using the transformative “multi-principal component” concept. Compared to the existing materials for nuclear applications including stainless steels, nickel alloys, ZrC, SiC, and potentially high-entropy alloys, as well as certain other compositionally complex ceramic families, CCC appear to be more resistant to amorphization, growth of irradiation defect clusters, and void swelling.

9:00 AM

(PACRIM-S14-006-2025) Engineering hexagonal shielding materials for radiation tolerance (Invited)

S. A. Humphry-Baker^{*1}; M. Harada¹; K. Bakkar¹; J. Davidson¹; S. Uthayasekaran¹; T. Zagyva¹

1. Imperial College London, Materials, United Kingdom

Due to their outstanding neutron attenuation properties, WC and WB₂ are leading candidates for compact nuclear reactors, where they must withstand radiation doses approaching 100 dpa, producing extensive point defects and transmuted helium. This will induce lattice swelling, which, if not properly controlled can cause component fracture. In this presentation lattice swelling is characterised as a function of irradiation dose and temperature, and microstructures tailored for improved swelling resistance. Irradiations were performed using helium and tungsten ions at DCF in the UK, up to 10 dpa and 750 °C. The irradiated materials were characterised using grazing-incidence X-ray diffraction and transmission electron microscopy. We find that WB₂ is highly sensitive to electronic stopping of helium ions, with amorphisation being caused at the relatively low displacement damage region (~1 dpa), even at 300 °C. In both materials, there is a monotonic decrease in defect concentration and lattice swelling with increasing temperature. The swelling is anisotropic in both materials, with a greater expansion in the c-axis vs. the a-axis. Such anisotropy causes strain localisation at the grain boundaries, leading to spontaneous cracking in some samples. Microstructures with improved radiation damage resistance are engineered, e.g. with refined grain structures and/or more radiation tolerant W:B stoichiometries.

9:30 AM

(PACRIM-S14-007-2025) The role of chemistry and processing on the hardness of transition metal carbides and nitrides

B. Watkins¹; A. Stubbers²; G. Thompson²; C. R. Weinberger^{*1}

1. Colorado State University, Department of Mechanical Engineering, USA
2. University of Alabama, Alabama Materials Institute, USA

The mechanical properties of the transition metal carbide/nitrides are dependent on the nonmetal content as well as the transition metal. The hardness of the group IVB carbides decrease monotonically with loss of carbon while the group VB carbides and IVB nitrides show a rise in hardness with carbon loss. Uniquely, TaC shows a in hardness and its variation with carbon content. Despite the large number of theories posed to explain different aspects of these trends, there is no theory proposed to date that explains these trends. In this talk, we provide the first comprehensive theory that can explain these trends. We combine density functional theory, a Peierls Nabarro model of dislocation motion, and models of indentation plasticity and fracture to simulate hardness trends across materials. These results demonstrate that the anomalous hardness can be attributed to changing dislocation mobility and its competition with fracture.

10:50 AM

(PACRIM-S14-009-2025) Paralineer Oxidation Kinetics and Passivation Mechanisms of SPS-Sintered ZrC Ultra-High Temperature Ceramic (UHTC) (Invited)

Y. Lin¹; H. Brouwer²; V. Popovich²; Y. Tang^{*1}

1. Technische Universiteit Delft, Aerospace Engineering, Netherlands
2. Technische Universiteit Delft Faculteit Mechanical Engineering, Netherlands

ZrC Ultra-High Temperature Ceramic (UHTC) is a promising material for extreme environmental applications. However, its susceptibility to oxidation at elevated temperatures remains a major issue. Despite existing studies on ZrC oxidation, there remains literature controversy on the oxidation rate and activation energy of ZrC. To address these questions, the present work fabricated highly dense and high-purity monolithic ZrC UHTC via two step spark plasma sintering (SPS). The oxygen pressure-temperature-time (P-T-t) dependent oxidation kinetics on monolithic SPS-sintered ZrC UHTC was reported for the first time. The P-T-t dependent

paralineer oxidation kinetics and passivation mechanism of highly densified SPS-sintered ZrC were revealed in the range of oxygen pressure 2–21% O₂ (2–21 kPa), temperature 600–1000 °C (873–1273 K) and isothermal hold up to 10800 s (3 hr). The results indicate that the SPS-sintered ZrC ceramic exhibits three-stage oxidation, namely parabolic, intermediate and linear oxidation. The dependence of oxygen pressure, temperature and elapsed time on parabolic, intermediate and linear oxidation region and the 3D P-T-t space for each oxidation stage are discovered. Furthermore, the conditions to maintain the ZrC UHTC passivation capability are unraveled.

11:20 AM

(PACRIM-S14-010-2025) Effect of gaseous environmental conditions on the atomic composition of ceramic materials during heat treatment of organometallic polymer precursors (Invited)

Y. Lee^{*1}

1. Korea Institute of Ceramic Engineering and Technology, Republic of Korea

Non-oxide ceramics are used in high-temperature and extreme environments because of their properties, which include high thermal stability, exceptional mechanical strength, and resistance to oxidation. However, traditional sintering methods are often energy-intensive and face challenges in controlling the microstructure effectively. To address these issues, polymer-derived ceramic (PDC) technology has been developed for manufacturing ceramics such as silicon carbide (SiC), boron carbide (B₄C), and silicon nitride (Si₃N₄). Polymer precursors are transformed into ceramics through a heat treatment; however, achieving a stoichiometric composition during this process can be challenging. For instance, polycarbosilane, which is a precursor for silicon carbide (SiC), can sometimes incorporate unwanted oxygen. Additionally, excessive carbon prevents the growth of SiC crystals and may lead to graphitization in an isolated state. In organometallic compounds, metals tend to be more stable when coordinated with nitrogen (M-N) than when bonded to carbon (M-C). However, nitrogen is lost more quickly than carbon during heat treatment. This study discusses the impact of the gas environment on converting amine-based organometallic polymer precursors into either nitride (AlN) or carbide (HfC) ceramics.

PacRim S15 - Porous Ceramics - From Innovative Processing to Advanced Industrial applications

PACRIM Symposium 15 - Porous Ceramics: From Innovative Processing to Advanced Industrial applications III

Room: Seymour

Session Chairs: Edwyn Wolf, Friedrich-Alexander-Universität Erlangen-Nürnberg; Isabella Klösel, Friedrich-Alexander-Universität Erlangen-Nürnberg

8:00 AM

(PACRIM-S15-008-2025) Hierarchical Structured Composites with Multiple Porosity (Invited)

W. Schwieger^{*1}; F. Scheffler²; M. Hartmann³

1. Friedrich-Alexander-Universität Erlangen-Nürnberg, Chemical and Biochemical Engineering, Germany
2. Lehrstuhl für Technische Chemie Otto-von-Guericke-Universität, Lehrstuhl für Technische Chemie, Germany
3. Friedrich-Alexander-Universität Erlangen-Nürnberg Technische Fakultät, Erlangen Center for Interface Research and Catalysis (ECRC), Germany

Hierarchical structured zeolite containing composites based on different materials, e.g. porous glasses, ceramic foams and /or metal based structured monoliths as the one, supporting component, and different zeolitic materials as the second component are prepared,

characterized and tested in different applications, e.g. as catalysts. Such materials combine both, the stability, strength and e.g. porosity on the one side provided by the support and the activity and selectivity on the other side provided by the zeolitic component. Thus, this might be interesting materials for technical applications, like adsorptive and/or catalytic processes. Starting with a historical overview of zeolite-based composites, the development from the glass/zeolite based composites via the foam based/zeolite materials to the metal/zeolite based structured reactors with the advantage of the resulting hierarchical organized porosity and optimized heat transfer properties will be demonstrated. The advantages of such hierarchical structured material especially for catalytic applications will be shown for few example reactions in this paper.

8:30 AM

(PACRIM-S15-009-2025) Surface modification of silica porous materials for environmental purification

M. Inada^{*1}

1. Kyushu Daigaku, Japan

Li_4SiO_4 is one of the CO_2 capture materials at high temperatures. To enhance the CO_2 capture ability, a large surface area is effective. However, it is hard to synthesize the Li_4SiO_4 porous materials due to high covalent bonding of itself. In addition, thermal decomposition occurs at high temperature. Mesoporous silica is useful as adsorbent and catalyst support, which is desired to be developed as a free-standing body, not as a powder. In this study, we tried to modify the surface of silica (SiO_2) porous glass with Li_4SiO_4 for CO_2 capture and with mesoporous silica for water purification.

8:50 AM

(PACRIM-S15-010-2025) High-temperature stability of aluminosilicate glass particle pellets and its dependence on chemical composition

P. Jensen^{*1}; L. Skovby¹; M. Solvang²; L. Belmonte²; Q. Zheng³; Y. Yue¹

1. Aalborg Universitet, Department of Chemistry and Bioscience, Denmark
2. ROCKWOOL A/S, Denmark
3. Qilu University of Technology, China

Stone wool is a commonly used material for fire-safe thermal insulation. Fire safety stems from the high-temperature stability (HTS) of stone wool. HTS is attributed to stone wool's special physical characteristics, including high glass transition temperature and strong crystallization tendency compared to glass wool and organic wool. This study explored the HTS of aluminosilicate glass particles as an analogue for stone wool fibres as an efficient and cost-effective pathway for optimizing stone wool properties for fire safety. Using lab-synthesised glass particle pellets and stone wool fibres, we investigated the influence of specific surface area (SSA) and chemical composition on HTS. Our results demonstrate an inverse negative correlation between SSA and HTS but a positive correlation between SSA and iron oxidation, a process favourable for HTS. Glass particle pellets were utilized to study the influence of $\text{MgO}/(\text{MgO}+\text{CaO})$ and $\text{MgO}/(\text{MgO}+\text{FeO})$ molar ratios on HTS. It was found that increasing $\text{MgO}/(\text{MgO}+\text{CaO})$ enhanced HTS, lowered glass stability, and reduced shrinking rates, whereas increasing $\text{MgO}/(\text{MgO}+\text{FeO})$ increased HTS and lowered the glass stability. Both series exhibited a residual glassy phase after crystallisation, which underwent viscous deformation at higher temperatures, significantly reducing the final collapse temperature.

PacRim S16 - Advanced Powder Processing and Manufacturing Technologies

PACRIM Symposium 16 - Novel material recycling and energy-saving process

Room: Stanley

Session Chairs: Satoshi Tanaka, Nagaoka University of Technology; Takuma Takahashi, Chiho Dokuritsu Gyosei Hojin Kanagawa Kenritsu Sangyo Gijutsu Sogo Kenkyujo

8:20 AM

(PACRIM-S16-009-2025) Near-room temperature fabrication of perovskite oxide ceramics via acid-base chemical densification and a recycling process of ceramic components (Invited)

Y. Yamaguchi^{*1}; H. Sumi¹

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

We have developed a new technology called acid-base chemical densification (ABCD) process, which can be used as a low-energy ceramic manufacturing process. This is a method for producing bulk ceramics that uses conventional oxide particle synthesis reactions. It is possible to produce BaZrO_3 with a relative density of over 90% at temperatures below 150 °C. In addition, we have found that by slightly changing the conditions of the chemical reaction conducted to densify the bulk ceramics, it is possible to disaggregate it into fine particles. This method of converting bulk ceramic materials into fine particles is a very simple process that involves treating the materials in a hydrothermal environment at a temperature below 200 °C or less. In addition, when a ceramic-metal composite is treated by this method, it is possible to recover the metal components without dissolving them. Therefore, it is considered that this conversion method from bulk to fine particles can be used as a recycling process that can efficiently separate ceramics and metal materials.

8:50 AM

(PACRIM-S16-010-2025) Selective debonding of polymer adhesives with functional particles by external stimuli (Invited)

M. Inutsuka^{*1}; C. Tokoro¹

1. Waseda University, Japan

Polymer adhesives, such as hot-melt adhesives (thermoplastic polymers) and epoxy resins (thermosetting polymers), are widely used to bond ceramics, metals, polymers and other materials, and assemble them to products. For the recycling of used products, debonding and disassembling method for the polymer adhesives is significant. In this study, we aim to achieve highly selective debonding of the polymeric adhesives using external stimuli, such as electrical pulsed discharge and microwave irradiation. The addition of conductive particles such as carbon black (CB) and silver (Ag) nanoparticles can decrease the breakdown voltage of the polymer adhesives, resulting in introducing explosive discharge by the application of electrical pulse inside the adhesive. We also prepared well-dispersed Ag particles with surface modification, and the aggregation structure of the Ag particle and its contribution to the pulsed discharge debonding were examined by experiments and simulations. We also found that microwave irradiation with a power of 100 W increased the temperature of the model polymer with a CB content of 3 wt% to above 200 °C. The increased temperature can lead to softening and debonding of the thermoplastic polymer adhesives. These debonding techniques with external stimuli can contribute to material separation and recycling using less energy than conventional methods.

9:20 AM

(PACRIM-S16-011-2025) Selective removal of Cr compounds from electric arc furnace slag by air classification

M. Koide^{*1}; K. Oyama²; Y. Takaya³; C. Tokoro¹

1. Waseda Daigaku, Japan
2. Kyushu Daigaku, Japan
3. Tokyo Daigaku, Japan

Electric arc furnace slag is a byproduct of steel scrap refining. It must be effectively used as a recycled resource because of its enormous production volume. Assuming that cement raw materials take advantage of calcium (Ca) compounds, one of the main components of furnace slag, there is a risk that chromium (Cr) in the slag will be oxidized to hexavalent during the cement manufacturing process. Therefore, a preliminary treatment to reduce the Cr content in the slag is required. In this study, we attempted to separate Cr from slag by air classification based on differences in particle size and specific gravity. Classification experiments were performed on oxidizing and reducing slags produced during the refining processes using an elbow jet air classifier. As a pre-treatment, the oxidizing slag was ground, but the reducing slag was already in powder form, we used it without grinding. The results showed that the Cr concentrations were similar among all fractions in the oxidizing slag. However, the Cr concentrations of the reducing slag were higher in the coarse powder fraction, whereas Ca tended to be concentrated in the fine powder fraction. Air classification with an elbow jet air classifier was found to be effective in reducing the Cr content from reducing slag, suggesting that it could be used in the raw material production process of cement.

9:40 AM

(PACRIM-S16-012-2025) Energizing mechanism through epoxy adhesive by adding conductive Ag nanoparticles for Pulsed discharge

K. Matsuo^{*1}; M. Inutsuka²; T. Koita⁴; S. Yamashita⁵; Y. Okada⁵; T. Saito⁶; M. Kubo⁶; H. Kamiya³; C. Tokoro³

1. Waseda University, Waseda Daigaku, Shinjuku, Tokyo, JP, academic, School of Creative Science and Engineering, Japan
2. Waseda Daigaku, Waseda Center for a Carbon Neutral Society, Japan
3. Waseda University, Japan
4. Waseda Daigaku Riko Gakujutsuin, Japan
5. Tokyo Noko Daigaku, Japan
6. Tohoku Daigaku, Japan

The demand of various metal/non-metal composite materials is increasing, especially in the automobile industry. Polymer adhesives such as epoxy resin are often used to bond these materials strongly. In terms of resource recycling, however, end-of-life composite materials should be disassembled in each material. Thus, debonding method for the polymer adhesives is required. Previously, we proposed a quick and low-cost method for dismantling the polymer adhesive using an electric pulsed discharge. In this method, an electric pulse with high voltage was applied to the sample over a short time, then an explosive discharge inside the adhesive layer causes the rapid expansion of gas, resulting in the dismantling of the adhesion. We reported the addition of conductive carbon black into the epoxy adhesive can control the discharge position inside the adhesive, resulting in successful separation. Nevertheless, we have not achieved fine controlling of the dispersion and aggregation of particles in the adhesive, and the mechanism of the dismantling by pulsed discharge has not been clarified. In this study, we used Ag nanoparticle as the conductive filler, whose aggregation structure can be controlled by surface modification with ligand molecules. The revealed the aggregation structure of the Ag particles, electric properties and dismantling behavior of the adhesive by Pulsed discharge.

PACRIM Symposium 16 - Characterization and evaluation of particle and powder

Room: Stanley

Session Chairs: Jingxian Zhang, Shanghai Institute of Ceramics Chinese Academy of Sciences; Manabu Inutsuka, Waseda university

10:20 AM

(PACRIM-S16-013-2025) Evaluation of the distribution and origin of process-related large defects in sintered ceramics in multiscale observations (Invited)

S. Tanaka^{*1}

1. Nagaoka University of Technology, Materials Science and Technology, Japan

In order to truly understand the process of manufacturing ceramics, it is necessary to observe a large volume of samples. This is because just as the strength distribution of ceramics varies to some extent, the distribution of defects also varies from place to place. In other words, multi-scale observation at a certain volume, from the particle level to the sub-millimeter level, is important. Advances in micro-focus computer microtomography (μ -CT) have made it possible to observe defects in three-dimensional non-destructive evaluation, but evaluation large volumes are still not enough. By using transmission observation technology using near-infrared light, we are able to obtain defect information contained in large volumes. On the other hand, the details of the observed defects are clarified by using a field emission-scanning electron microscopy. In this presentation, we will introduce the results of research conducted during the process from green to sintered body using alumina ceramics as a model. Defects at the interface of the granules remain for some time after the start of sintering. Not all defects remained, but the coarse defects surrounded by the four granules remained. In another example, we also showed that adding zirconia into alumina makes the growth rate of defects slow.

10:50 AM

(PACRIM-S16-014-2025) Visualization of drying behavior of aqueous silica slurries with different organic additives by in-situ OCT observation

H. Kuroda^{*1}; J. Tatami¹; M. Iijima¹; T. Takahashi²

1. Yokohama National University, Japan
2. Chiho Dokuritsu Gyosei Hojin Kanagawa Kenritsu Sangyo Gijutsu Sogo Kenkyujo, Japan

In order to clarify the effect of the organic additives in slurries on the change in internal structure, it was visualized using optical coherence tomography. In this study, three types of aqueous silica slurries with polyethyleneimine as a dispersant and PVA with different saponification degree (99, 81 and 65%) were prepared by ball milling. The slurries were formed into sheets and observed for internal structural changes during the drying process while heated by infrared heater. In the initial stage of drying, particles agglomerated from the surface towards bottom, and the particle concentration in the agglomerated areas increased as the degree of saponification of PVA increases. This is due to differences in the distribution of ζ potential and the thickness of the adsorption layer, caused by the PVA adsorbed on the particle surface. In the middle stage of drying, agglomerated areas also developed lateral direction in the lower part of the slurry, and agglomerated areas locally deformed simultaneously. Deformability of the agglomerated areas depended on the particle concentration of the agglomerated area and thickness of the adsorption layer. The relative density of the dried body depended on the particle concentration in the agglomerated area in the initial stage and deformability of the agglomerated area in the middle stage.

11:10 AM

(PACRIM-S16-015-2025) mmWave/Sub-THz Low Loss Materials Measurement with Latest Commercially Available Fixtures (Invited)S. Phommakesone*¹

1. Keysight Technologies Inc, USA

The trend of many industries such as beyond 5G, military communications, autonomous vehicles, data center is moving into mmWave / Sub-THz frequency range; there is an increased demand for the highest level of raw materials performance. To achieve faster time to market, reduce cost and meet the performance requirement the designers need to use material that has low dielectric properties in both Dk and Df. The Dk and Df effects how signal propagate through the substrate, transmission line, or devices. At the mmWave/Sub-THz frequency range, the propagation properties of the materials being used start to play a critical role in the overall performance. Materials property is a last place to think that is the cause or limitation of the performance. However, the fact is everything starts with raw materials. Without knowing the reliable material measurement solutions commercially available today, manufacturers are forced to extrapolate materials data from low frequencies to high frequencies, which can lead to mistakes that can have potentially devastating costs. This presentation will share what are currently available today. And share best measurement practices and sample preparation.

PacRim S17 - Additive Manufacturing of Ceramics and Composites**PACRIM Symposium 17 - Additive Manufacturing of Ceramics and Composites II**

Room: Prince of Wales

Session Chairs: Shenqiang Ren, University of Maryland;

Chang-Jun Bae, Korea Institute of Materials Science

8:00 AM

(PACRIM-S17-005-2025) AI-assisted Parametric Modeling of Extrusion-based Additive Manufacturing for Li-ion battery (Invited)Y. Li¹; B. Gao¹; C. Bae*¹

1. Korea Institute of Materials Science, Division of Nano Materials Research, Republic of Korea

Structural cathodes fabricated by extrusion-based additive manufacturing enable faster Li-ion transport owing to reduced tortuosity and increased specific area. However, predictive guidelines for printed feature accuracy considering material properties and process parameters remain limited. Herein, an AI-assisted parametric modeling framework is proposed to optimize the geometric accuracy of printed features. Machine learning algorithms trained on experimental data were employed to refine geometry predictions based on ink rheology, viscosity, and viscoelasticity. This approach highlights the critical role of internal friction between lithium cobalt oxide and Super P nanoparticles in ensuring printability. AI-enabled optimization of printing parameters, particularly under the thinning mode, facilitated the tailoring of L/N ratios for high-resolution structural electrode fabrication. Additionally, fluid dynamics combined with the Darcy-Weisbach equation was integrated into an AI-enhanced predictive model to calculate flow rates and pressure drops, achieving high agreement with experimental results. This study establishes AI-driven guidelines for extrusion-based electrode printing, advancing the design and performance of lithium-ion batteries.

8:30 AM

(PACRIM-S17-006-2025) Process Investigation and Performance Optimization of Binder Jetting for Complex Ceramics (Invited)Q. Wei*¹; W. Zhao¹

1. Huazhong University of Science and Technology, China

In the past 20 years, ceramic binder jet additive manufacturing technology has become a revolutionary method to fabricate complex ceramic components, especially in aerospace, biomedical, electronic information and many other key areas to show significant application potential and value. This report introduces some achievements of the Center for Additive Manufacturing of Huazhong University of Science and Technology (HUST) in the field of binder jetting of ceramic materials from the aspects of equipment hardware-software system-material process. It focuses on the research progress of Y₂O₃, A₂O₃, SiC and other ceramic materials in terms of raw material optimization, binder design, printing parameter improvement and post-processing enhancement. Through the “coating - activation” two-step method to successfully solve the nano-granulation Y₂O₃ powder can not be printed through the binder jet problem; through the CuO enhancement of A₂O₃ ceramics can be prepared to flexural strength of 101MPa; through the independent research and development of carbon black ink can greatly improve the density of SiC more than 99% and strength of 320MPa.

9:00 AM

(PACRIM-S17-007-2025) Robust Thermomechanical Sintering Simulation of 3D-Printed Objects with Various Internal Lattice Filling Structures (Invited)C. Manière*¹; J. Diatta²; S. Marinel¹1. Laboratoire de Cristallographie et Sciences des Matériaux, France
2. Université Assane SECK de Ziguinchor, Senegal

The majority of 3D-printed components feature a bioinspired infill design, consisting of a dense outer shell and internal lattice structures. This approach enhances the strength-to-weight ratio while improving print quality and reducing manufacturing time. However, simulating the sintering of these intricate porous structures poses significant challenges due to their high degrees of freedom, often resulting in computational instabilities and prolonged simulation durations. Despite the prevalence of lattice-filled parts, no comprehensive method currently exists for modeling their sintering behavior. This study introduces a continuum-based approach to address these challenges, enabling efficient and accurate simulation of real parts and their lattice behavior in a fraction of the sintering time. The methodology employs a sub-model to calculate the effective thermal conductivity and sintering moduli of lattice structures with varying porosities, which are then used to simulate sintering and heating in the lattice regions. An advanced thermomechanical simulation integrates these parameters to predict sintering with high precision, incorporating thermal gradients, deformations, and anisotropy that influence the final part's dimensions. The method is demonstrated on honeycomb lattices, highlighting its robustness and efficiency for practical applications.

9:30 AM

(PACRIM-S17-008-2025) Pre-ceramic Molecular Precursor Derived Ceramics For Extreme Environments (Invited)S. Ren*¹

1. University of Maryland, USA

Compositionally complex ceramics provide a significant advantage over traditional ceramics when it comes to operating in extreme environments, their high-temperature stability, highly distorted lattices and unique metallic, covalent, and ionic bonding. However, unlocking the full potential of such complex composition ceramics is impeded by the limited availability of pre-ceramic polymers and an Edisonian approach to its pyrolysis. In this talk, I will report the synthesis of compositionally complex ceramics with excellent

high-temperature stability using a preceramic molecular approach based on the crosslinking of transition metal salts with the short-chain silicon monomers. Molecular monomers allow for precise control over the dispersion of transition metals at the atomic level and the formation of dense, pore-free ceramics. We crosslinked transition metal elements from groups 4-6 with preceramic monomers, resulting in compositionally complex ceramics with a lower pyrolysis temperature in a shorter time span. Furthermore, the speed and scalability of the ceramic formation enables rapid screening of different compositions as oxidative barrier coatings on metals or other intricate structures. This could enable rapid discovery of novel thermal protective ceramics that can be utilized for a broad range of applications taking place under extreme conditions.

10:20 AM

(PACRIM-S17-009-2025) Fundamental Understanding of Thermal Debinding of 3D Printed Ceramic Body: Numerical Simulation and Experimental Verification

B. Gao^{*1}; Y. Li¹; H. Son¹; C. Bae¹

1. Korea Institute of Materials Science, Republic of Korea

Thermal debinding is a critical and delicate process for ceramic industry, especially for next-generation additive manufacturing technology. However, the current strategy of binder burning is time & energy-consuming. Here, we investigated the dynamic temperature evolution, binder distribution and mass transport through combining the theoretical simulation, experimental analysis, and non-destructive monitoring technology. Theoretical simulation provides the spatial and temporal evolution of temperature and binder based on 1-order reaction process. Experimental results demonstrate a controllable of debinding degree proportional to the heat absorption adjusted by the heating rate and isothermal stages. Micro-CT observations quantify the binder distribution, gradient of which results from higher heating rate generating an interface between binder-rich and binder-free region. This study provides insights into the dynamic process of binder burning, which is critical for obtaining a safe burned ceramic body.

10:40 AM

(PACRIM-S17-010-2025) Magnetically assisted 3D printing of functional materials (Invited)

H. Le Ferrand^{*1}

1. Nanyang Technological University, Singapore

Composites and ceramics with locally controlled microstructure exhibit outstanding properties. However, their fabrication in 3D shapes using automated and controlled processes is still challenging. Here, this is addressed using magnetic fields with 3D printing. The inks are composed of magnetically-functionalized microplatelets dispersed in water with some additives. The ink is extruded continuously to build structures with any possible orientation of the microplatelets. The microplatelets can be made of alumina and turned into a strong an anisotropic, crack-free ceramic after sintering at 1600 C in air. The microplatelets can also be made of graphite and turned into a strong, electrically and thermally conductive composite after sintering in reducing atmosphere at 1400 C. These composites, with the locally tailored microstructure and the 3D shapes, offer the capability to create cheap, customizable, and effective electromagnetic shielding materials for electronic packaging applications. The design of a new automated machine is required for this process. The machine comprises a stage, 10 motors to rotate the rotating magnet around the nozzle and an extrusion nozzle fixed on a 3 axis cartesian gantry. Given the stage of only 5 cm diameter, the equipment has potential for printing small items such as electronic devices and components, jewellery, dental implants.

11:10 AM

(PACRIM-S17-012-2025) Charge-discharge properties of tin-iron-soda-silicate glass anode for oxide all-solid-state sodium battery prepared by laser irradiation process

F. Sato^{*1}; T. Honma¹

1. Nagaoka University of Technology, Department of Materials Science and Bioengineering, Japan

In this study, we investigated the formation of the interface between a tin-iron-soda-silicate glass anode (55SnO-15Na₂O-6.75 Fe₂O₃-23.25SiO₂) and a solid electrolyte ceramic, along with the charge-discharge properties of the joined glassy anode and solid electrolyte in an oxide-based all-solid-state sodium ion batteries using laser-based additive manufacturing technology. Using a screen-printing method, a composite paste comprising the anode active material and solid electrolyte Na₃Zr₂Si₂PO₁₂ was prepared and applied to the solid electrolyte. Laser irradiation at a wavelength of 1064 nm, a power of 3 W, and a scanning speed of 100 mm/s was employed to form the interface between the anode and solid electrolyte. An all-solid-state half-cell was fabricated, and charge-discharge tests were conducted at 25°C with a current density of 35 mA/g. The tests yielded a reversible charge-discharge curve around 100 mAh/g. Notably, the glassy anode operated without the addition of an electronic conductive agent, suggesting that the metallic components in the glass inherently provide sufficient electron conduction. This study represents the first demonstration of an all-solid-state battery operating through laser-processed interface formation, highlighting the significant potential of oxide-based ASSBs utilizing glassy anodes.

PacRim S20 - Advanced Functional Materials for Clean Energy Solutions

PACRIM Symposium 20 - Advanced synthesis and characterization of solar / electric fuel materials I

Room: Georgia A

Session Chairs: Flavio de Souza, Federal University of ABC;

Ooman Vargese, University of Houston

8:00 AM

(PACRIM-S20-014-2025) On Efficient Materials & Devices for Solar SeaWater Splitting (Invited)

L. Vayssieres^{*1}

1. Xi'an Jiaotong University, IRCRE, China

The cost and scarcity of fuels, high pollution levels, and major environmental disasters are critical challenges we are facing due to fossil fuels-based economies. These challenges could be addressed by implementing sustainable green inexpensive energy sources. The combination of advanced synthesis, quantum technologies and characterization such as operando spectroscopies is the key to large-scale fabrication of highly efficient stable devices for clean sustainable societies based on hydrogen economy. Our strategy is to fabricate earth-abundant oriented arrays of quantum rods and dots of high purity by aqueous synthesis at low temperature without surfactant and controlled dimensionalities and surface chemistry with miminiband for high visible-light conversion, bandgaps and band edges optimized for stability and operating at neutral pH and low-to-no bias. The in-depth investigation of their size-dependent interfacial electronic structure and electrical properties provide better structure-efficiency relationships for a cost-effective and sustainable generation of hydrogen from the 2 most abundant geographically-balanced free resources on earth, i.e. the sun and seawater. An overview is presented for native and doped oxide, nitride, sulfide, and hybrid, their photoelectrochemical and electronic structure characterization at synchrotron facilities, and charge dynamics, dopant, plasmonic, and thermal processing effects.

8:30 AM

(PACRIM-S20-015-2025) Materials Tuning of Visible-light Responsive Peroxo-modified Titanate Nanotube via Ion Doping (Invited)H. Yasunari¹; Y. Kondo²; H. Park¹; H. Nishida¹; Y. Seo¹; S. Chou¹; T. Goto¹; T. Sekino^{*1}

1. Osaka University, SANKEN (The Institute of Scientific and Industrial Research), Japan
2. Osaka University, Japan

Titanate (titania) nanotubes (TNTs) have received much attention as promising photocatalysts because of their high specific surface area with nanometer-scale structures of wide bandgap oxides and resultant superior photocatalytic properties compared to conventional titanium dioxides. We have demonstrated that the introduction of peroxo ligands into TNTs (PTNTs) significantly reduces the band gap energy and imparts visible light responsivity. In this study, we developed the bottom-up process of PTNTs synthesis to further improve their photocatalytic activities, combining the introduction of peroxo ligands with transition metal addition such as Ni and Cu. Powder X-ray diffraction analysis of as-synthesized samples shows that all the Ni-added PTNTs (Ni-PTNTs) had similar crystal structures to that of the previously reported PTNTs, regardless of the amount of Ni added. The field emission scanning electron microscopy analysis exhibits that the both PTNTs and Ni-PTNTs had nanotubular structures. Detailed crystallographic, nanostructural and photocatalytic properties of the metal-added PTNTs will be discussed.

9:00 AM

(PACRIM-S20-016-2025) Molecular precursor route to heterogeneous nanocatalystsS. Mishra^{*1}

1. University of Lyon1, Institut de Recherches sur l'Environnement et la Catalyse de Lyon (IRCELYON), France

Nanometric heterogeneous catalysts enjoy tremendous advantages over the conventional catalysts due to their versatility in size, structure, morphology and composition, each contributing to their unique catalytic properties and activity. Owing to the number of advantages they offer, soft chemical routes such as sol-gel processes or metal-organic decomposition are very promising for the elaboration of nanomaterials. Surprisingly, such 'bottom-up' synthesis with precision at the atomic/molecular level, which offers many advantages such as control over their size, shape and nanostructuring, high surface area, homogeneous doping of active catalysts on support, etc., remains much less utilized for the synthesis of heterogeneous catalysts, probably because it requires expertise in areas which have traditionally been not closely connected. This presentation will describe 'bottom-up' synthesis of inorganic nanocatalysts with a special emphasis placed on the design 'single-source' precursors with appropriate properties for a clean, low-temperature conversion into nanomaterials with minimum undesired residues. Different catalytic applications of the obtained nanomaterials will be described.

9:30 AM

(PACRIM-S20-017-2025) Splitting of CH₄ and CO₂ Using Advanced Functional Materials (Invited)O. K. Varghese^{*1}; D. Waligo¹; M. Paulose²; L. Schaffer¹

1. University of Houston, Department of Physics and Texas Center for Superconductivity, USA
2. University of Houston, Department of Physics, USA

As the hydrogen economy is on the horizon, there is an urgent need to develop cleaner options for hydrogen production. Hydrogen is currently produced primarily from fossil fuels, especially via steam methane reforming. These are high-temperature processes with intense CO₂ emission. Solar photocatalytic and photoelectrochemical

processes offer green pathways for converting methane to hydrogen and reducing CO₂. We have studied these processes by applying nanostructured ceramic semiconductors as photocatalysts. This presentation provides the details of these experiments and associated optical simulation studies.

PACRIM Symposium 20 - Advanced synthesis and characterization of solar and electric fuel materials II

Room: Georgia A

Session Chairs: Lionel Vayssieres, Xi'an Jiaotong University; Bruce Koel, Princeton University

10:20 AM

(PACRIM-S20-018-2025) Advanced Architectures for Solar-Driven Water Splitting and CO₂ Reduction (Invited)R. Solarska^{*1}

1. Uniwersytet Warszawski, Centre of New Technology, Poland

The development of efficient and stable photocathodes for photoelectrochemical (PEC) CO₂ reduction and hydrogen evolution is vital for sustainable energy technologies. Copper(I) oxide (Cu₂O) is a promising material for PEC CO₂ reduction, but its low catalytic efficiency and poor stability hinder its practical use. In this study, we investigate two approaches to improve the performance of Cu₂O-based photocathodes. First, we introduce a Cu₂O/Zn₂(OH)₈Cl₂ (ZHC) heterostructure, which enhances CO₂ reduction by improving CO* adsorption, leading to the formation of multi-carbon products, including methanol, ethanol, propylene, and butadiene. This photocathode operates at 0.78 V vs. RHE, with a current density of -1.2 mA/cm². Density functional theory (DFT) calculations reveal that this heterostructure enhances CO₂ adsorption, promoting the formation of C₂ products. Secondly, we optimize CuO:Zn nanostructures to mitigate photocorrosion, doubling the photocurrent compared to pure CuO. This CuO:Zn thin film exhibits a cathodic photocurrent of 4 mA/cm² and a quantum efficiency of 35%. These findings offer valuable insights into the design of high-performance copper-based photocathodes, advancing the development of efficient solar-driven energy solutions for both CO₂ reduction and hydrogen production.

10:50 AM

(PACRIM-S20-019-2025) Hematite Photoelectrode Synthesis for Scalable Photoelectrochemical Devices: A Cost-Effective Approach with Improved Performance (Invited)F. L. de Souza^{*1}

1. Centro Nacional de Pesquisa em Energia e Materiais, CNPEM, Brazil

The challenge of scaling photoelectrochemical (PEC) devices for efficient solar energy conversion and green hydrogen production requires robust and cost-effective manufacturing approaches. This study presents a novel polymeric precursor solution for synthesizing hematite photoelectrodes, enabling the production of homogeneous ultra-thin films (~125 nm) with areas reaching up to 200 cm² at reduced costs. While initial PEC devices demonstrated promise, a significant photocurrent drop was observed as the photoelectrode area increased. To address this, we modified the precursor solution by incorporating Hf⁴⁺, which improved the morphology and adherence of the photoelectrodes. This tailored synthesis technique enabled interface-specific doping, enhancing film conductivity and mitigating photocurrent decline in larger electrode areas. As a result, we achieved an impressive homogeneous photocurrent of 1.6 mA cm⁻² at 1.45 V across a 15.75 m² electrode area, utilizing less than 70 µg of active photoelectrode material. Moreover, our preliminary cost analysis suggests that this low-energy fabrication method represents a significant advancement in green hydrogen production, paving the way for sustainable and efficient technologies in renewable energy.

PacRim S28 - Joining and Integration of Ceramics for Enabling Complex Components and Adv Apps

PACRIM Symposium 28 - Joining and Integration of Ceramics for Enabling Complex Components and Adv Apps I

Room: Seymour

Session Chair: Heloisa Ramlow, Swiss Federal Laboratories for Materials Science and Technology

10:20 AM

(PACRIM-S28-001-2025) Enhanced hydrothermal corrosion resistance of SiC/SiC joints with CaO-Modified Y_2O_3 - Al_2O_3 - SiO_2 Glass Under PWR Conditions

S. Yang*¹

1. Northwestern Polytechnical University School of Materials Science and Engineering, China

Y_2O_3 - Al_2O_3 - SiO_2 (YAS) glass interlayers are widely used for joining SiC/SiC composites due to their thermal and mechanical compatibility. However, YAS joints exhibit poor hydrothermal corrosion resistance under pressurized water reactor (PWR) conditions, limiting their long-term application. To address this, we incorporated CaO into the YAS glass system, improving its thermal stability and chemical durability by reducing the polymerization of the glass network and promoting the formation of stable crystalline phases. The CaO-modified YAS (CYAS) joints achieved shear strengths of ~57.1 MPa at room temperature and ~15.8 MPa at 1200 °C, meeting requirements for accident situations. They also exhibited excellent air tightness under 15 MPa pressure for 72 hours without leakage. Hydrothermal corrosion tests revealed a significantly reduced corrosion rate for CYAS (~0.16 mg/cm²/day) compared to YAS (~2.7 mg/cm²/day). The CYAS joints maintained structural integrity after 25 days, with shear strength retained at ~26.1 MPa, while YAS joints degraded to ~6.3 MPa within 15 days. The incorporation of CaO effectively enhanced the high-temperature mechanical performance, air tightness, and hydrothermal corrosion resistance of the joints, establishing CYAS glass as a promising material for advanced SiC/SiC composite cladding applications in PWR environments.

10:40 AM

(PACRIM-S28-002-2025) Low-Temperature Direct Bonding of Silicate Glasses Using NH_3 Plasma Activation

S. Nagai*¹; K. Nakao¹; Y. Hayashi¹

1. AGC Kabushiki Kaisha, Japan

A direct bonding technique is used to fabricate optical devices as it can integrate glass materials without adhesive. To date, several surface-activation methods have been proposed to achieve the direct bonding of silica glass at low-temperature annealing. However, achieving sufficient bonding strength is still difficult in some multi-composition glasses such as aluminosilicate glass. To overcome the limitations of glass composition, we must clarify the mechanism of bonding reaction in detail. This study investigated the bonding strength of various silicate glasses after several plasma treatments. Silica, aluminosilicate and borosilicate glass wafers were prepared. Each wafer was modified with NH_3 or H_2O plasma treatment, then contacted and annealed at 200°C. The NH_3 plasma and H_2O plasma introduced Si-NH₂ and Si-OH groups, respectively. The bonding strength of glasses was improved the most by NH_3 plasma. The strength improvement was highest for silica glass, followed by borosilicate and aluminosilicate glasses. Surface characterizations revealed that the strength improvement is related to the number of

Si-NH₂ consumed at the interface, which was correlated to the SiO₂ content in the silicate glasses. Based on the unveiled mechanisms, we proposed a novel bonding method for aluminosilicate glass using a combination of wet chemical treatment and NH_3 plasma.

PacRim S29 - Progress in High-Entropy Materials

PACRIM Symposium 29 - Thermodynamic, kinetic, physical, and environmental properties I

Room: Plaza A

Session Chairs: Elizabeth Opila, University of Virginia;

Jing Liu, University of Alberta

8:00 AM

(PACRIM-S29-024-2025) Exploring High Entropy Materials for Advanced Technologies (Invited)

Y. Zhang*¹

1. Queen's University, Mechanical and Materials Engineering, Canada

Substitutional disorder in high-entropy materials (HEMs) gives rise to diverse and tunable bonding environments, not typically possible in conventional materials. Extreme conditions, such as high temperature, high current, high pressure, and high radiation environments, can push materials from thermal equilibrium to far-from-equilibrium and pose unique challenges in predicting their performance. Despite the potential of HEMs, there is a lack of systematic studies on the relationship between composition, structure, and properties. Substitution disorder is expected to modify defect dynamics and energy dissipation processes, yet understanding the underlying mechanisms is still in its early stages. The chemical disorder in HEMs and the associated physical properties under both equilibrium and non-equilibrium conditions remain largely unexplored. To reveal the atomic and electronic structure responsible for variations in material properties, detailed characterization of elemental distribution, electronic structures, lattice distortions, corresponding scattering mechanisms, and associated energy transfer is crucial in determining the contributions and impacts of various alloying elements. Understanding how chemical disorder in HEMs can be utilized to tailor physical properties, enhance or control energy transport, and improve irradiation tolerance is vital for advanced technological applications.

8:40 AM

(PACRIM-S29-025-2025) Development of High Entropy Ceramic Materials for Nuclear Waste Management (Invited)

M. Lee¹; H. Seong¹; S. Lee¹; H. Ryu*¹

1. Korea Advanced Institute of Science and Technology, Republic of Korea

The development of advanced materials for the adsorption and immobilization of radioactive elements is crucial for effective nuclear waste management. High entropy ceramic materials have emerged as promising candidates due to their compositional flexibility, enabling superior adsorption and immobilization properties. However, the vast compositional space of these materials poses a significant challenge, making conventional trial-and-error approaches impractical. This study employs a machine learning-assisted experimental framework to identify and develop high entropy ceramic materials tailored for the adsorption and immobilization of cesium (Cs) and iodine ions. Using high-throughput virtual screening, high entropy MXene, layered double hydroxides (LDHs), and hollandite systems were synthesized with minimal experimental effort. The high entropy MXene and LDH systems exhibited outstanding aqueous adsorption capacities for Cs and iodate ions, respectively. Furthermore,

high entropy hollandite achieved the highest Cs loading among the systems and demonstrated cold immobilization capabilities, significantly reducing volatile Cs loss during high-temperature sintering. This work highlights the potential of machine learning-assisted discovery to accelerate the development of high entropy ceramic materials, providing innovative and efficient solutions for nuclear waste management.

9:10 AM

(PACRIM-S29-026-2025) Xenotime Rare Earth Orthophosphates as EBC Candidate Materials (Invited)

I. Hawthorne¹; W. Riffe¹; P. E. Hopkins²; E. J. Opila^{*1}

1. University of Virginia, Materials Science and Engineering, USA
2. University of Virginia, USA

Rare earth (RE) orthophosphates with the tetragonal xenotime structure are potential candidates for environmental barrier coatings (EBCs) on SiC-based hot-section turbine engine components. Naturally occurring xenotime minerals contain yttrium, gadolinium, dysprosium, erbium, and ytterbium, consistent with the overall RE abundance in the earth's crust. In this study, orthophosphates of each of these five individual REs, a synthetic mineral, and an equimolar composition were synthesized. Among these compositions, GdPO₄ takes on the monoclinic monazite structure while all others had the xenotime structure. Advantages of using xenotime minerals as precursors for EBCs include lower costs and less environmental impact due to elimination of the RE separation process, as well as lower thermal conductivities expected from multicomponent rare earth compounds. Properties relevant for EBCs were characterized experimentally. Results showed reduced thermal conductivity of the synthetic xenotime relative to the individual tetragonal orthophosphates. Thermal expansion coefficients of the tetragonal phases were slightly larger than SiC exhibiting an anisotropy of about 13%. Steam stability was improved compared to state-of-the-art Yb₂Si₂O₇ and showed some preferential volatility of REPO₄ constituents. Preliminary CMAS resistance studies show improvement relative to RE disilicates, but variability in results is not yet understood.

9:40 AM

(PACRIM-S29-027-2025) Exploring Thermally Grown Complex Concentrated Oxides on AlCrTiVNi₅ Alloy for Enhanced High-Temperature Performance (Invited)

J. Liu^{*1}; H. Sun¹; H. Zhang¹

1. University of Alberta, Chemical and Materials Engineering, Canada

High-temperature (HT) applications demand oxide scales that grow slowly and adhere well to the surface. The concept of complex concentrated alloys (CCAs) has now been applied to oxide systems, leading to the development of thermally grown complex concentrated oxides (TG-CCOs). This study explores TG-CCOs formed on a newly designed AlCrTiVNi₅ alloy, selected for its unique blend of FCC/BCC stabilizers, negative mixing enthalpies, high oxidation potential, and low diffusion coefficients. We investigated the TG-CCOs developed on this alloy at 1000°C to assess their suitability for HT applications. Our analysis highlights the alloy's corrosion resistance and structural stability in challenging HT environments. Notably, the TG-CCOs exhibited excellent thermodynamic stability, with enhanced corrosion resistance in a Na₂SO₄/NaCl mixture at 900°C. Characterization results reveal notable transformations in the oxide scale's crystal structure and composition, shifting from rock-salt to corundum phases under corrosive conditions. Density functional theory calculations and lattice distortion assessments indicate these structural transitions improve coating durability. This work demonstrates the potential of TG-CCOs as robust protective coatings for the power generation sector, providing critical insights for designing high-entropy oxides that endure extreme environments.

10:30 AM

(PACRIM-S29-028-2025) Novel transparent high-entropy sesquioxide ceramics with high physicochemical plasma etching resistance

Y. Shin¹; S. Ham¹; H. Kim¹; M. Kim¹; J. Ko¹; J. Lee¹; Y. Park¹; H. Ma^{*1}

1. Korea Institute of Materials Science, Republic of Korea

High-entropy ceramics exhibit novel intrinsic properties and have been explored for a wide range of applications, including thermal insulators, energy storage, and optical materials. However, both their resistance to plasma etching and potential applications in the semiconductor industry remain underexplored. The semiconductor industry recently has faced increasing demands for further miniaturization of line widths and the achievement of high aspect ratios in wafer fabrication. The etching processes impact both the chips and the ceramic components involved. There is consequently a critical need to develop materials that exhibit excellent resistance to plasma etching while minimizing the generation of contaminant particles. In the present study, we successfully fabricated single phase high-entropy sesquioxides with minimized residual pores in their microstructure. We conducted a comprehensive structural analysis of them. We also evaluated their plasma etching resistance, and they exhibited an etching rate as low as 8 nm/h. The surface roughness changes were also minimized after an erosion process. These high-entropy ceramics, with their excellent etching resistance and ability to prevent contaminant generation, have the potential to significantly improve the production yield of semiconductor wafers. Furthermore, high optical transparency was also achieved.

11:00 AM

(PACRIM-S29-029-2025) Design of Novel Materials Using Machine Learning (Invited)

S. Fensin^{*1}; H. Ozdemir²; J. Callanan¹; M. Htoon¹; B. Lovato¹; J. Valdez¹; J. Cooley¹

1. Los Alamos National Laboratory, USA
2. Koc Universitesi Muhendislik Fakultesi, Turkey

Our goal is to realize the long-standing challenge of Materials by Design given a set of required and desired properties, and other constraints (e.g. cost of manufacturability), utilize artificial intelligence and machine learning (AI/ML) to identify promising candidate materials, specifically compositions and processing conditions. As part of this goal, available literature data on material testing of high entropy alloys (HEAs) was collected and supplemented with theoretical properties like difference in atomic radius (dr), valence electron concentration (VEC). These data were used to train a machine learning model that then predicted novel material compositions with a good combination of yield strength and ductility. These compositions were manufactured using arc melting and their microstructure and mechanical properties measured. This work showed that the experimental data matched well with the prediction when there was no elemental segregation. While this specific example is investigating collection of data on a handful of composition, we are continuing to develop methodologies (automated testing) to perform high-throughput experiments. This development is needed to collect enough data to train ML models.

PacRim S31 - On the design & dev of next generation nanolayered (3D and 2D) structural & func mtl

PACRIM Symposium 31 - Next-generation nanolayered structural/functional materials II

Room: Oxford

Session Chairs: Surojit Gupta, University of North Dakota;
Babak Anasori, Purdue University

8:00 AM

(PACRIM-S31-007-2025) Synthesis of Nanoscale Ag-Intercalated Muscovite Mesocrystal

C. Sung^{*1}; Y. Chu²

1. National Yang Ming Chiao Tung University, Department of Materials Science and Engineering, Taiwan
2. National Tsing Hua University, Department of Materials Science and Engineering, Taiwan

Nanostructured materials have attracted significant interest for their potential in functional applications, particularly plasmonics. This study demonstrates a 3D mesocrystal system formed by intercalating silver nanoparticles (Ag NPs) within the layers of artificial muscovite, a 2D ceramic material. The layered muscovite structure provides a nanometer-scale cavity with an internal pressure of approximately 0.1 GPa, which effectively confines the growth direction and the size of Ag NPs. Through hydrothermal method and vacuum annealing, Ag NPs were successfully synthesized with an average size of 82 nm, and a coverage exceeding 40% was obtained, while the ideal maximum coverage is 50 %. X-ray diffraction (XRD) results confirmed an epitaxial relationship between Ag (111) and muscovite (001). Furthermore, the Laue diffraction result and cross-sectional TEM analysis revealed that the nanoparticles demonstrate characteristics similar to those of single crystals. This unique structural design enhances the plasmonic properties of the material, making it well-suited for surface-enhanced Raman scattering (SERS) applications. Using probe molecules Rhodamine 6G (R6G) and Crystal Violet (CV), the SERS performance of the Ag/muscovite mesocrystal system demonstrated detection limits as low as 10^{-6} M and 10^{-7} M, respectively. These results highlight the potential of this material as a reliable SERS substrate for detection.

8:20 AM

(PACRIM-S31-008-2025) Synthesis and Oxidation Behavior of MAX Phase-Based Coatings Produced by Magnetron Sputtering for High-Temperature Applications

R. Anton^{*2}; K. Beck¹; E. Wiesner²; S. Boubtane²; M. Galetz¹; U. Schulz²; N. Laska²

1. DECHEMA Forschungsinstitut, Germany
2. Deutsches Zentrum für Luft- und Raumfahrt DLR, Germany

In this study, Ti_2AlC , and Ti_2AlN MAX phase coatings were synthesized using direct current (DC) magnetron sputtering and reactive sputtering techniques. Ti_2AlC coatings were produced using three pure elemental targets (Ti, Al, and C), while Ti_2AlN was deposited using Ti and Al targets with nitrogen as a reactive gas. All coatings exhibited X-ray amorphous, dense columnar structures post-deposition. Analytical techniques such as GDOES, EDS, and XRD were employed to refine composition, and high-temperature XRD was used to study crystallization and phase stability under vacuum and laboratory air atmosphere. Oxidation behavior was evaluated on inert substrates and high temperature lightweight materials such as γ -TiAl and SiC at two temperature regimes: 800 °C and 1200 °C. The formation of a protective α - Al_2O_3 oxide layer, critical for oxidation resistance, was observed. Ti_2AlC demonstrated superior stability, with minimal interdiffusion and strong coating adhesion on γ -TiAl substrates. The Ti_2AlN MAX phase coating on SiC, showed the

formation of a protective α - Al_2O_3 layer, but degradation due to the interdiffusion of Si and C from the substrate into the coating. By applying an interlayer of AlN the interdiffusion could be prohibited.

8:40 AM

(PACRIM-S31-009-2025) On the design and manufacturing of MAX and MAB phases

S. Gupta^{*1}

1. University of North Dakota, Mechanical Engineering, USA

MAX and MAB phases have emerged as an important class of materials for different types of high performance applications. In order to commercialize these materials, it is pertinent to develop novel manufacturing practices for rapid commercialization. In this presentation, I will review some of the recent development in the manufacturing of these materials. More particularly, I will review the usage of salt encapsulation, particle size engineering, and precursor design for enhancing the commercialization process.

9:00 AM

(PACRIM-S31-010-2025) Designing Bio-mimetic Multifunctional Core-shell Fiber aerogels

A. Isari^{*1}; M. Arjmand¹

1. The University of British Columbia, School of Engineering, Canada

The development of multifunctional materials for thermal insulation and electromagnetic interference (EMI) shielding has been constrained by limitations such as fragility and low processability in traditional aerogels. Inspired by the core-shell structure of Canadian goose feathers, this study presents a novel biomimetic approach to fabricating core-shell fiber aerogels. These fibers feature a conductive MXene core encapsulated in a polyimide shell, produced using a coaxial wet-spinning process. The porous MXene core provides high electrical conductivity, enabling efficient EMI shielding, while the polyimide shell ensures mechanical robustness, hydrophobicity, and stability under extreme conditions. The fibers achieve optimal thermal insulation and shielding performance with a hierarchical architecture. The porous shell reduces impedance mismatch, enhancing absorption-dominant EMI shielding with a total shielding effectiveness (SET) of ~55 dB and an absorption coefficient of 0.74 in the X-band frequency range. Thermal testing demonstrates superior heat dissipation, with the fibers maintaining low surface temperatures and thermal stability up to 400°C. In a nutshell, this study highlights the adaptability of the fabrication process, allowing precise control over pore size, shell thickness, and structural morphology through the modulation of coagulation bath composition.

9:20 AM

(PACRIM-S31-011-2025) Exotic Photothermal Properties in Ti-based MXenes for Optoelectronics

S. Ippolito^{*1}; F. Urban¹; P. Samori²; J. E. Spanier¹; Y. Gogotsi¹

1. Drexel University College of Engineering, Materials science and engineering, USA
2. Universite de Strasbourg, France

We investigate the photothermal properties of Ti-based MXenes, $Ti_3C_2T_x$ and Ti_2CT_x , as well as their potential use for optoelectronic applications. We compare their electrical response upon laser irradiation along with their photothermal behavior by changing the environmental conditions, pressure and/or temperature (T). We observe two clearly distinct behaviors: $Ti_3C_2T_x$ shows a negative response upon laser irradiation (i.e., current decreases), while Ti_2CT_x exhibits a positive response (i.e., current increases). This is due to the different Resistance (R) vs. T trend recorded for the two systems, with $Ti_3C_2T_x$ showing $dR/dT > 0$, unlike Ti_2CT_x with $dR/dT < 0$. Moreover, different kinetics have been observed for the two MXenes: $Ti_3C_2T_x$ exhibits a symmetric and fast current rise and decay (≈ 10 s), while Ti_2CT_x presents a striking asymmetric and much slower kinetics during the current rise (≈ 10 s) and decay ($\approx 10^4$ s). Such exotic photothermal

kinetics is strongly affected by the operating conditions and can be fine-tuned by exposing the devices to different atmospheres (Air vs. Ultra-High Vacuum) and T (from 100 K to 350 K). Our work highlights the effects of stoichiometry in Ti-based MXenes optoelectronic devices, with emphasis on their photothermal characteristics. Particularly, the exotic photothermal kinetics recorded for Ti_2CT_x might pave the way for its use in multi-stimuli memory and neuromorphic devices.

9:40 AM

(PACRIM-S31-012-2025) Bio-mimetic, knittable Multifunctional Core-shell Fiber aerogels

A. Isari*¹

1. The University of British Columbia, School of Engineering, Canada

The development of multifunctional materials for thermal insulation and EMI shielding has been constrained by limitations such as fragility and low processability in traditional aerogels. Inspired by the core-shell structure of goose feathers, this study presents a novel biomimetic approach to fabricating fiber aerogels. These fibers feature a conductive MXene core encapsulated in a polyimide shell, produced using a coaxial wet-spinning process. The porous MXene core provides high electrical conductivity, enabling efficient EMI shielding, while the polyimide shell ensures mechanical robustness, hydrophobicity, and stability under extreme conditions. With a hierarchical architecture, the fibers achieve optimal thermal insulation and shielding performance. The porous shell reduces impedance mismatch, enhancing absorption-dominant EMI shielding with a total shielding effectiveness (SET) of ~55 dB and an absorption coefficient of 0.74 in the X-band frequency range. Thermal testing demonstrates superior heat dissipation, with the fibers maintaining low surface temperatures and thermal stability up to 400°C, outperforming traditional materials like Kevlar and cellulose paper. This study highlights the adaptability of the fabrication process, allowing precise control over pore size, shell thickness, and structural morphology through the modulation of coagulation bath composition.

PacRim S1 - Environmental barrier coatings for high-performance ceramics

PACRIM Symposium 1 - Environmental barrier coatings for high-performance ceramics II

Room: Oxford

Session Chair: Anant Setlur, GE Global Research

1:15 PM

(PACRIM-S01-005-2025) Sealing systems in aeroengines and their environmental challenges (Invited)

S. Schrufer*¹

1. Rolls-Royce Deutschland Ltd und Co KG, Materials Engineering, Germany

In aeroengines, sealing systems both in the compressor and the turbine play an important role to minimize tip clearances, reduce leakage and increase efficiency. In the compressor, the ceramic drum liners have an abrasive nature ensuring sealing against static nickel vanes, while the abradable casing liners are made of a metal phase, a self-lubricating non-metal phase and a polymer for porosity generation (and run against Ni or Ti blades). The temperatures are moderate, and oxidation or corrosion is observed depending on running conditions and environmental factors. In the turbine, the Rolls-Royce solution for a sealing system in shroudless turbines is a double layer system on the static component consisting of a zirconia interlayer and a spinel abradable top layer. Those sealing systems need to show good abradability, high temperature stability and thermo-mechanical resistance. Additionally, strategies to increase the CMAS resistance are required to increase the component life. The present work gives an overview of the performance and the challenges of these sealing systems in small and medium engines.

1:45 PM

(PACRIM-S01-006-2025) Steam oxidation of ytterbium silicate environmental barrier coatings produced using electrophoretic deposition and air plasma spray (Invited)

P. Xiao*¹

1. The University of Manchester, Department of Materials, United Kingdom

Electrophoretic deposition (EPD) were used to produce ytterbium silicate environmental barrier coatings (EBCs) on SiC and Si bond coat with uniform coatings with control microstructure. The EBCs produced via EPD and that from air plasma spray (APS) were exposed to steam environments at high temperature. Then they were examined with use electron microscopy for microstructure characterisation, indentation for mechanical characterisation and Raman spectroscopy for residual stress measurements. There have been significant difference in microstructure evolution, TGO growth and TGO/EBC interface in EBCs produced with use of APS and EPD respectively. These findings indicate the degradation and failure mechanisms of APS EBCs and underscore the potential of EPD technique to produce $Yb_2Si_2O_7$ EBCs with enhanced performance.

2:15 PM

(PACRIM-S01-007-2025) Oxidation mechanism of modified silicon/ytterbium disilicate environmental barrier coatings

K. Lee*¹; J. Stuckner¹; A. Garg¹; R. I. Webster¹; L. Wilson¹

1. NASA Glenn Research Center, USA

Environmental barrier coatings (EBCs) are an enabler for SiC/SiC ceramic matrix composites (CMCs) in gas turbines. One of the most critical EBC failure modes is steam oxidation-induced failure. Long steam oxidation life, therefore, is a key to the reliability of CMC components. The chemistry of EBC and underlying CMC substrate has significant impact on the steam oxidation life of the current state-of-the-art EBC (Gen 2 EBC: Si/Yb₂Si₂O₇). NASA has developed chemically modified Gen 2 EBCs (Mod Gen 2 EBCs) that reduce the parabolic steam oxidation rate constant of Gen 2 EBC by more than tenfold. Key variables that control the oxidation of Mod Gen 2 EBCs include EBC chemistry, CMC chemistry, and post-EBC fabrication heat treatment. Aluminum and boron in the SiO₂ oxide scale are two key elements having an overarching influence on EBC oxidation kinetics. Complex interactions among EBC variables dictate the concentration of aluminum and boron in the SiO₂ oxide scale and thus the EBC oxidation kinetics. This paper will discuss the mechanism behind the correlation between EBC variables and oxidation kinetics.

PACRIM Symposium 1 - Environmental barrier coatings for high-performance ceramics III

Room: Oxford

Session Chair: Anant Setlur, GE Global Research

3:30 PM

(PACRIM-S01-008-2025) High temperature coatings for SiC_f/SiC composite (Invited)

J. Wang*¹

1. Institute of Metal Research Chinese Academy of Sciences, Advanced Ceramics and Composites Division, China

SiC_f/SiC composite are emerging material for aviation engine hot-section components. Environmental barrier coating (EBC) can protect SiC_f/SiC components against harsh thermal and chemical attacks in combustion environment. Advanced rare earth silicate EBCs provide reliable protections up to a surface temperature of 1350°C. However, the present EBCs demonstrate limited capability of corrosion resistances to hot steam and molten CaO-MgO-Al₂O₃-SiO₂ (CMAS) deposit at higher temperatures, as well as the phase instability and amorphization during coating fabrication. To address these critical challenges, new strategies are adopted to design new EBCs

through multilevel optimizations, including both the multi-RE-component (or high entropy) modification and microstructure/phase regulation. The advancements of new high temperature coatings support the applications of SiC_f/SiC composite.

4:00 PM

(PACRIM-S01-009-2025) CMAS degradation of Ytterbium disilicate coatings: Texture evolution of apatite phase with exposure time at high temperature

E. B. Owusu^{*1}; A. R. Romero²; B. Zhang¹; O. Gavaldà-Diaz⁴; N. Neate³; K. Voisey¹

1. University of Nottingham, Mechanical, Materials and Manufacturing, United Kingdom
2. Tecnalia, Basque Research and Technology Alliance (BRTA), Mikeletegi Pasealekua 2, Spain
3. University of Nottingham Nanoscale and Microscale Research Centre, United Kingdom
4. Department of Materials, Royal School of Mines, Imperial College London, United Kingdom

Ytterbium disilicate (YbDS) has properties, like high temperature phase stability and coefficient of thermal expansion that matches that of silicon-based ceramic matrix composites, expected of materials for environmental barrier coatings. For YbDS to be fully endorsed as the ideal candidate material for EBCs, it must withstand steam and calcium-magnesium-aluminum-silicate (CMAS) corrosion. YbDS coatings react with CMAS to form a dense interaction layer of ytterbium disilicate and apatite phases that slows further CMAS infiltration. In this research, we manufactured YbDS coatings using suspension plasma spray technique and explored the structural integrity of the interaction layer by exposing them to CMAS at 1350 °C for 0.5 h, 12 h, 48 h and 96 h. SEM analysis on the coatings after exposure for 0.5 h and 12 h showed interaction depths of 159 μm and 284 μm, and complete infiltrations after 48 h and 96 h respectively. XRD analysis revealed that the intensity of the apatite peaks for {200} and {102} decreased relative to {211} with increase in exposure times up to 48 h but increased again after 96 h exposure which indicates a change in crystallographic texture. The preferred orientation of the apatite phase with exposure times may have contributed to the inability of the interaction layer to retard further CMAS infiltration over the entire duration.

PacRim S2 - Frontier of modeling and Design of Ceramics and composites

PACRIM Symposium 2 - Modeling insights into physical properties

Room: Balmoral

Session Chairs: Kulbir Ghuman, Institut National de la Recherche Scientifique; Takafumi Ogawa, Japan Fine Ceramics Center

1:15 PM

(PACRIM-S02-008-2025) Unraveling Photoplasticity in ZnS: Enhanced Peierls Stress under Photoexcitation (Invited)

Q. An^{*1}

1. Iowa State University, Materials Science and Engineering, USA

Semiconductors, vital components in electronics and solar panels, are inherently brittle and susceptible to damage. When exposed to light, their mechanical properties can change, becoming either harder or softer—a phenomenon known as photoplasticity. Although this effect has been known since 1957, its underlying mechanisms remain poorly understood. In this presentation, we delve into the mechanisms driving photoplasticity in zinc sulfide (ZnS) using an advanced computational framework that integrates density functional theory (DFT), constrained DFT (CDFT), and machine learning force fields (ML-FF). Specifically, we investigate the behavior of dislocations, focusing on core reconstruction, the

Peierls barrier, Peierls stress, and dislocation dynamics under both ground-state (dark) and photoexcited (illuminated) conditions. Our findings show that photoexcitation significantly increases the Peierls stress by reducing strain concentration at the dislocation core, facilitating a transition from ductile to brittle behavior under light exposure. Remarkably, this occurs without significant alterations to the dislocation core structure. These results provide a deeper atomic-scale understanding of photoplasticity in ZnS and highlight the accuracy and efficiency of combining CDFT with ML-FF to study complex material responses to photoexcitation.

1:45 PM

(PACRIM-S02-009-2025) Electronic and Optical Features of 2D and quasi-2D halide Pb-free Perovskites (Invited)

G. Giorgi^{*1}; M. Palummo²; K. Yamashita³

1. The University of Perugia, Department of Civil & Environmental Engineering, Italy
2. Università degli Studi di Roma Tor Vergata, Department of Physics and INFN, Italy
3. Yokohama Shiritsu Daigaku, Quantum Chemistry Division, Japan

Halide perovskites (HPs) represent the big thing in photovoltaics of the last decades. After the very first work of Miyasaka et al. astonishing conversion efficiencies have been indeed reported when exploiting such compounds in solar devices. Some issues anyway still prevent HP implementation in mass production devices. One of them is the presence of a short-chain (hydrophilic) organic cation in HP chemical formula (the archetypal compound is MAPbI₃, MA=CH₃NH₃⁺) which speeds up the degradability of the material. Still related to the formula, the presence of Pb raises concern about the possible dispersion of a toxic element in the environment. To overcome these issues, two possible alternatives have been suggested. One is based on the dimensional reduction of the 3D bulk HP: replacing the short- with a long-chain (hydrophobic) ensures a net stabilization of the final device. The second is based on the reduction of Pb concentration, replacing it with Sn²⁺ (or Ge²⁺) or with two metals with +1/+3 oxidation state. Here, I show results about optoelectronic features of 2D/3D and pure 2D HPs obtained by means of a many-body perturbation theory approach (GW+BSE). Finally, I discuss the structural and electronic features of the interfaces naturally occurring between Ge- and Ge/Sn-terminated HPs and germania, showing similarities and differences between crystalline and amorphous GeO₂ at such interfaces.

2:15 PM

(PACRIM-S02-010-2025) Oxygen vacancy formation energetics in MgO-based high entropy oxides from DFT and experimental validation (Invited)

O. Opetubo¹; T. Shen¹; R. Bordia¹; D. Aidhy^{*1}

1. Clemson University, Materials Science and Engineering, USA

In contrast to single or double cation based oxides, high entropy oxides (HEOs) consist of equi- or near equimolar concentration of multiple cations randomly distributed on a crystal lattice. The random distribution causes a wide diversity of nearest-neighbor environments around oxygen atoms. Consequently, a range of bonding environments and oxygen vacancy formation energies are observed. We investigate oxygen vacancy formation energies in Mg(ZnCoNiCu)O-based HEO using density functional theory (DFT). We find that vacancy formation energy trends are controlled by cation valence charge. We explicitly determine the effect of all cations on the formation energies. In addition, we quantify the inherent and the vacancy-induced lattice distortion in HEOs. Experimentally, a series of binary, ternary, quaternary and quinary HEOs are synthesized using a simple and scalable polymeric steric entrapment method. By annealing in inert environment, oxygen vacancies are analyzed by XPS and TGA. The experimental observations agree with our DFT calculations. This understanding contributes to oxygen vacancy transport useful in microstructure evolution and electrochemical applications.

2:45 PM

(PACRIM-S02-011-2025) Designing the ion-exchange process for metastable phases: a case of ternary wurtzite-type-related oxidesI. Suzuki^{*1}; M. Kita²; K. Washizu¹; T. Omata¹

1. Tohoku University, IMRAM, Japan
2. Toyama National College of Technology, Japan

Ion exchange phenomena, where ions in solids are topotactically replaced by other ions, have been known for decades. Since the 1980s, their application in material exploration has been actively pursued. In the 21st century, ion exchange reactions have enabled the synthesis of novel metastable oxides that cannot be obtained through conventional high-temperature reactions (e.g., $\beta\text{-NaGaO}_2 + \text{CuCl} \rightarrow \beta\text{-CuGaO}_2 + \text{NaCl}$). Such ion exchange reactions proceed when the free energy change $\Delta G (= \Delta H - T\Delta S)$ of the overall reaction is negative, while they do not occur when ΔG is positive. Interestingly, the reaction progress is governed solely by the overall ΔG , meaning that even if the precursor and target phase are fixed, ΔG (and thus the reaction feasibility) can be controlled by changing the ion source. However, due to the limited thermodynamic data available for relevant compounds, there have been few examples of designing ion exchange reactions from a thermodynamic perspective. In this study, we screened the feasibility of ion exchange reactions based on ΔH values obtained from first-principles calculations and explored previously unachievable ion exchange routes.

PACRIM Symposium 2 - Modeling mechanical behavior at various scales

Room: Balmoral

Session Chair: Qi An, Iowa State University

3:30 PM

(PACRIM-S02-012-2025) Data Analytics-Enabled Phase Field Modeling of Microstructurally Complex Materials (Invited)R. Garcia^{*1}

1. Purdue University, Materials Engineering, USA

The modern development of advanced materials demands: 1) the formulation of methodologies that provide an accurate description of the materials that integrate these devices at each length scale; 2) the systematic and mindful coarse-graining of lower length scale methodologies into higher length scale descriptions, and 3) the establishment of meaningful databases that enable the development of insight to understand and then engineer advanced, reliable, next generation devices. Here, by defining a thermodynamically consistent representation of materials that spatially resolves the multiphysical fields that results from formally considering microstructural features such as grain size, crystallographic texture, grain boundaries, particle size, and porosity, the time-dependent behavior is analyzed. Progress towards directly integrating the physical contributions of each individual phase by starting from scattered thermodynamic data, and microscopy images, thermodynamically consistent phase field models are parameterized to describe the equilibrium and microstructural evolution of materials. Applications of the developed portfolio of methodologies is demonstrated for ceramic-ceramic interfaces, such as LiFePO_4 and LiCoO_2 systems, metal-ceramic interfaces, such as CoCu-BaTiO_3 VAN structures, and metal-metal interfaces, such as those observed in textured Al-thin films.

4:00 PM

(PACRIM-S02-013-2025) From Theory to Practice: Modeling Microscopic Chemical and Physical Phenomena using Macroscopic Computational Fluid Dynamics for Glass ManufacturingK. Kirchner^{*1}; J. Lotter¹; T. van Lier¹; S. Cooper¹

1. CelSian, USA

To manufacture superior commercial product quality, an accurate predictor of both microscopic and macroscopic phenomena is of paramount importance. Often computational toolsets narrow a research project to a particular length-scale, even though factors influencing product performance span the microscopic atomic features of the material as well as the macroscopic processing conditions and environmental parameters of the plant. Computational fluid dynamics (CFD) is a numerical analysis approach that routinely quantifies macroscopic glass flow patterns, temperature gradients, and energy balances. More recently, a CelSian commercially-available CFD software has expanded capabilities to include models for critical microscopic glass chemical and physical phenomena. This presentation will highlight practical applications where such software has been strategically implemented to enhance quality in glass plants as well as reveal new understanding of the fundamental glass science driving structure-property-performance relationships. Current developments have unlocked new ways to couple detailed redox chemistry with bubble growth, sand dissolution, and coloration. We will show how academic and industrial research amongst each length-scale can come together to reveal practical implications directly in glass mass manufacturing facilities.

PacRim S3 - Solid Oxide Fuel Cells and Green Hydrogen Technologies**PACRIM Symposium 3 - Solid Oxide Fuel Cells and Green Hydrogen Technologies IV**

Room: English Bay

Session Chairs: Kevin Huang, University of South Carolina; Toshio Suzuki, Precision Combustion, Inc.

1:15 PM

(PACRIM-S03-014-2025) Development of high-performance protonic ceramic cells for highly efficient applications (Invited)H. Shimada^{*1}; M. Fujioka¹; K. Watanabe¹; S. Aman¹; M. Momai¹; Y. Yamaguchi¹; K. Nomura¹; Y. Mizutani¹

1. National Institute of Advanced Industrial Science and Technology (AIST), Japan

Protonic ceramic cells (PCCs) are an electrochemical device capable of highly efficient energy-conversion. PCCs can be employed for various applications such as fuel cells for power generation and electrolyzers for hydrogen production. Achieving higher performance and durability will facilitate their commercialization. To improve PCC performance, we investigated a by-layered electrolyte structure with highly durable $\text{Ba}(\text{Zr},\text{Yb})\text{O}_{3-\delta}$ and high proton conductive $\text{Ba}(\text{Zr},\text{Ce},\text{Y},\text{Yb})\text{O}_{3-\delta}$. We report on the structural characterization results and electrochemical performance in both fuel cell and electrolysis modes of the bi-layered electrolyte PCCs. In addition, we report the recent progress of the PCC development in AIST, including the cell fabrication processes, the analysis and evaluation techniques, durability test results.

1:45 PM

(PACRIM-S03-015-2025) Proton solubility in perovskite-type fuel cell air electrodes: a first-principles modeling perspective (Invited)

C. Fisher^{*1}; A. Taguchi¹; T. Ogawa¹; A. Kuwabara¹

1. Japan Fine Ceramics Center, Japan

Developing mixed-conducting oxides for use as air electrodes in protonic ceramic fuel cells is one strategy for increasing cell efficiency, as this should provide a greater reaction surface area for oxygen reduction. Because of their complex chemistry, however, few studies have examined proton solubility in these materials directly, and hence little is known about their propensity for high proton conductivity. To help identify promising candidate materials, we performed first-principles calculations of 3d transition metal oxide perovskites $LnMO_3$ (Ln = lanthanide; M = transition metal) and found that proton incorporation (hydration) becomes less favorable as the number of 3d electrons increases. In contrast, electronic conductivity, as assessed from band structure plots and effective masses, generally increases. Our results suggest that good mixed proton-hole conducting oxides are likely to be obtained using transition metals from the middle of the period (M = Mn, Fe, Co) together with La or slightly smaller lanthanide ions. Acknowledgment: This work was performed as part of the Development of Ultra-High Efficiency Protonic Ceramic Fuel Cell Devices project (JPNP20003), commissioned by the New Energy and Industrial Technology Development Organization.

2:15 PM

(PACRIM-S03-016-2025) Oxygen permeability and PCFC cathode performance of Ba-Co-Fe-Y based mixed conductive perovskite oxides (Invited)

I. Kagomiya¹; M. Alam^{*1}; T. Kato¹; K. Watanabe²; H. Shimada²; H. Sumi²; Y. Mizutani²

1. Nagoya Kogyo Daigaku, Japan

2. Sangyo Gijutsu Sogo Kenkyujo Chubu Center, Japan

Proton-conducting ceramic fuel cells (PCFCs) have a potential achieving high power generation efficiency (~70%) in the mid-temperature range (500-600°C). However, a significant decrease in PCFC cathode performance in the middle temperature range obstructs the high efficiency. The main reason for this problem is that the dissociation of oxygen molecules at the cathode is a rate-limiting step in the mid-temperature range. To overcome the problem, we consider mixed conductive oxides with higher oxygen permeability as the cathode candidates because the high permeability means that the faster O_2 dissociation and higher oxide ion conductivity. With the point of view, this study particularly focuses on Ba-Co-Fe-Y based perovskites as the cathode candidates, which show a high oxygen permeability in mixed conductive oxides. This study investigated effects of other elemental doping (Mg, Ti, Ni, Zn, Zr) in $BaCo_{0.4}Fe_{0.4}Y_{0.2}O_{3-d}$ on oxygen permeabilities and the cathode performance. As results, Mg- and Ni-doped samples showed higher oxygen permeability among the prepared samples. The PCFC single cells with cathodes Mg- and Ni-doped samples showed lower polarization resistance, contributing to higher maximum power densities. Thus we suppose that the higher oxygen permeability results in the lower polarization resistances for the cathodes.

2:45 PM

(PACRIM-S03-017-2025) Processing and Challenges Scaling-up protonic membranes for electrochemical cells (Invited)

L. Kwati^{*1}; R. Kunaiev²; I. Povstugar³; J. Otomo⁴; S. Yamate⁴;

W. A. Meulenber⁵; T. Ishihara⁶; H. Matsumoto¹

1. Kyushu Daigaku Carbon Neutral Energy Kokusai Kenkyujo, Center for Energy System Design (CESD), Japan

2. Graduate School of Engineering, Kyushu University, Fukuoka, Japan, Japan

3. Central Institute of Engineering, Electronics and Analytics 3 (ZEA 3), Forschungszentrum Jülich, Germany

4. Institute of Science Tokyo, Department of Transdisciplinary Science and Engineering, School of Environment and Society, Japan

5. Forschungszentrum Jülich Institut für Energie- und Klimaforschung, IEK-1 Membranes, Germany

6. Kyushu University, International Institute for Carbon-Neutral Energy Research, Japan

As global energy demands and environmental challenges arise, the pursuit of sustainable and efficient energy conversion and storage systems has become a central focus of scientific research. Ceramic proton-conducting solid oxide electrolyzers and fuel cells represent the future of sustainable energy. Despite considerable interest in these technologies, skepticism regarding their scalability and commercialization persists due to challenges in producing large-area, defect-free protonic ceramic electrolytes with consistent performance. This paper presents our recent efforts on the challenges and scalable fabrication of chemically homogeneous proton-conducting half-cells measuring 5×5 and 10×10 cm², using $SrZr_{0.4}Ce_{0.4}Y_{0.1}O_{3-d}$; NiO as an interlayer, which significantly enhances electrolyte densification at 1300 °C. The as-fabricated half-cell demonstrates active interdiffusion of strontium and barium between the electrode and electrolyte layers, resulting in a mixed phase that boosts performance and scalability. Atom probe tomography was utilized to gain insights into the local atomic-scale chemistry of the electrolyte grain boundaries, given their importance in overall conductivity and device performance. These results are discussed alongside techno-economic analysis on PCFC production and stack costs.

PACRIM Symposium 3 - Solid Oxide Fuel Cells and Green Hydrogen Technologies V

Room: English Bay

Session Chairs: Sebastian Molin, Gdansk University of Technology;

Fatih Dogan, Missouri University of Science and Technology

3:30 PM

(PACRIM-S03-019-2025) Advanced, Reversible Solid Oxide Cells

T. Suzuki^{*1}; M. Dewa¹; N. Cameron¹; C. Junaedi¹; S. Roychoudhury¹

1. Precision Combustion, Inc., USA

Reversible solid oxide fuel cells (R-SOFC) is a key technology for the emerging clean and sustainable energy as well as industrial decarbonization. Precision Combustion, Inc. (PCI), with the support from National Aeronautics and Space Administration (NASA), has been developing a solid oxide cell that allows reversible enable both highly efficient power generation and energy-efficient production of H_2 at intermediate temperatures. The technology is based on PCI's novel cell architecture and materials as well as progressive ceramic processing techniques to enable coefficient of thermal expansion matched architecture that allows fast transients. The focus of our development is to obtain R-SOFC systems with significant reduction in size, weight, energy consumption (electrolysis mode) and improved fuel utilization (fuel cell mode). The new cell architecture presents several advantages over conventional approaches including high gravimetric and volumetric power density, simplified stack structure, and rapid thermal cycle tolerance for fast start-up and shutdown. In this

paper, we will present results from preliminary performance characterization of the lab-scale, advanced solid oxide cells in both SOFC and SOEC mode. Performance evaluation under pressurized condition and trade analysis of different operational modes for aerospace and terrestrial applications will also be presented.

3:50 PM

(PACRIM-S03-020-2025) Electrochemical reactions of ammonia formation and decomposition in protonic ceramic electrolysis cells

J. Otomo^{*1}; M. Okazaki¹

1. Institute of Science Tokyo, Department of Transdisciplinary Science and Engineering, School of Environment and Society, Japan

Electrochemical reactions of ammonia formation and decomposition were investigated using protonic ceramic electrolysis cells (PCECs) with barium cerate- and barium zirconate-based proton conducting electrolytes. Ammonia is a promising energy carrier because of its high energy density and easy liquefaction, and the electrochemical synthesis of ammonia with PCECs can provide an efficient energy conversion process for ammonia production with steam electrolysis ($N_2 + 3H_2O \rightarrow 2NH_3 + 1.5O_2$). In this study, reaction kinetic analyses with Fe- and Ni-based catalysts were performed at around 500°C. The ammonia formation rate was improved by the electrochemical promotion of catalysis (EPOC), and it was determined by the forward reaction, i.e. ammonia formation, and the backward reaction, i.e. ammonia decomposition. To design an efficient system for ammonia production, we discussed the reaction kinetics and relevant mechanisms. On the other hand, the ammonia decomposition reaction can be applied to obtain pure hydrogen by using PCECs as well, in which the ammonia decomposition reaction proceeds at the anode, and subsequent proton pumping produces pure hydrogen at the cathode. Thus, this study discussed the reaction kinetics of ammonia decomposition as well as ammonia formation to provide a strategy for designing new efficient systems with ammonia as an energy carrier.

4:10 PM

(PACRIM-S03-021-2025) Development of cathode for protonic ceramic fuel cell using Yb-doped barium zirconate

Y. Okuyama^{*1}; T. Nishiya¹

1. Miyazaki Daigaku Kogakubu Daigakuin Kogaku Kenkyuka, Japan

The Ni anode-supported protonic ceramic fuel cell using $BaZr_{0.8}Yb_{0.2}O_{3-\delta}$ and $BaZr_{0.3}Yb_{0.2}Co_{0.5}O_{3-\delta}$ as electrolyte and cathode, respectively were constructed and power density was investigated, with the high power output (497 mWcm^{-2} at 600°C) obtained. To clarify the elementary reaction of cathode impedance component in proton-conducting ceramic fuel cells, proton/deuteron isotope effects on electrode resistance were measured in the OCV and polarized states. DRT analysis of the cell impedance showed that the electrode impedance of PCFC could be separated into five component. The isotope effect of the impedance was investigated by replacing the anode gas from H_2O-H_2 to D_2O-D_2 , and the isotope effect was observed in the two components on the high frequency under OCV, indicating that it is attributable to the anodic reaction. On the other hand, no isotope effects were observed in the three high-frequency components under OCV, but isotope effects were observed in the lowest-frequency component under bias (0.6 V). This component is considered to be the component attributed to the water vapor formation reaction and was found to have the highest resistance among the impedance components of the cathode.

PacRim S5 - Geopolymers - Low Energy and Environmentally Friendly/Scalable Ceramics

PACRIM Symposium 5 - Geopolymers - Low Energy and Environmentally Friendly, Scalable Ceramics

Room: Stanley

Session Chair: Yaman Boluk, University of Alberta

1:15 PM

(PACRIM-S05-001-2025) Production and performance of hybrid copper mine tailings-based geopolymer cement composite (Invited)

E. d. Magdaluyo^{*1}; K. Baladad¹; D. Quinagoran¹; J. Narvaez¹; J. Cruz¹; D. Tungpalan¹

1. University of the Philippines, Philippines

This study investigates the performance of hybrid geopolymer cement mortar blocks produced using copper mine tailings sourced from Marinduque, Philippines, as one of the precursors. Mortar specimens containing 7.5%, 15%, 22.5%, and 30% mine tailings by weight were prepared using NaOH, KOH and $Ca(OH)_2$ as alkaline activators at concentrations of 1M and 3M. The mechanical properties of the samples were evaluated through unconfined compression tests, while the crystalline and phase composition, surface morphology, and chemical bonding of the fabricated samples were also examined. Static leaching tests were conducted to assess the mobility of contaminants, particularly heavy metals, in the geopolymer samples. Results from the unconfined compression tests indicate that the majority of the fabricated samples, with strength values ranging from 24.22 MPa to 53.99 MPa, meet the ASTM C150 strength requirements. The leaching test analyses suggest effective encapsulation and immobilization of metals utilizing the fabricated hybrid geopolymer cement composite materials.

1:45 PM

(PACRIM-S05-002-2025) Synthesis and Characterization of Waste-Based Geopolymer Binders for Radiation Shielding Applications (Invited)

R. F. Florez^{*1}; S. Restrepo-Arcila²; C. H. Giraldo³; H. A. Colorado L.²

1. Canadian Nuclear Laboratories, Advanced Reactors Chemistry and Materials, Canada

2. Universidad de Antioquia, Colombia

3. Missouri University of Science and Technology, Nuclear Engineering, USA

This work studied the synthesis and characterization of two novel of geopolymeric composites derived from spent Zn-C battery powder, steel dust, and construction demolition waste (CDW). Formulations with battery waste powder and steel dust replacements ranging from 5 to 40 wt% were mixed with CDW and activated using mixture of potassium silicate and sodium hydroxide. The resulting paste were heat cured at 80°C for 24h. The geopolymer composites were analyzed via XRD and SEM to assess their phase composition, densification behavior, and microstructure. The mechanical properties were also evaluated by compression tests. Additionally, the gamma ray shielding effectiveness of the geopolymers was determined experimentally by transmission experiments with ^{137}Cs and ^{60}Co sources. Moreover, the variation of the main gamma-ray attenuation parameters of the composites with photon energy was evaluated theoretically. The results indicated the addition of battery waste to the CDW-based geopolymers led to low degree of compactness and reduced performance in the mechanical and shielding properties. On the contrary, geopolymers produced with Steel dust and CDW exhibited enhancement in their mechanical and shielding properties compared to the control sample. The outcomes of this investigation provide foundations for the design of new geopolymers for radiation shielding applications.

2:15 PM

(PACRIM-S05-003-2025) Pilot Scale Production and Field Testing of Low CO₂ Emission Construction Material at the University of Alberta Campus (Invited)

Y. Boluk^{*1}; V. Bindiganavile¹; J. Goncalves¹; H. Sajid¹; M. Gül²

1. University of Alberta, Civil and Environmental Engineering, Canada
2. University of Alberta, Canada

Greenhouse gas emissions are at the center stage worldwide, and efforts are ongoing to achieve net-zero emissions by 2050. Geopolymers, recognized as a promising choice, offer significantly lower greenhouse emissions, energy consumption, and carbon footprint. In contrast to Portland cement, one ton of aluminosilicate precursor in a geopolymer system contributes a mere 0.184 tons of CO₂, representing an 80% reduction in carbon emissions. However, it's important to note that building materials made out of geopolymers must not only meet or exceed the strength of Portland cement concrete but also be prepared within a precise setting time and possess workable rheology, presenting a significant challenge in their use. We are scaling up the production of our developed low-carbon emission cement Geopolymer with additive Dry Water (GP-DW) and field tests on the Campus. Ultra-low greenhouse gas emitter cementitious material geopolymers are not new, however, commercial applications have not materialized because of the difficulty of controlling their performance characteristics. We solved this problem by developing a GP-DW system. The dry water is physically in powder form but contains 92% water. We will produce our GP-DW at the pilot scale and precast. The prepared pavement will be tested for durability during six months under real environmental conditions.

2:45 PM

(PACRIM-S05-004-2025) Enhancing Cement Sustainability through the Use of Porous Supplemental Cementitious Materials

J. M. Rimsza^{*1}; M. Mills¹; A. Tuinukuafe¹

1. Sandia National Laboratories, USA

Cement and concrete production account for approximately 5% of global carbon emissions, primarily due to the high processing temperatures and CO₂ off-gassing during calcination. The use of supplemental cementitious materials (SCMs) has gained traction to reduce the amount of cement clinker in concrete, thereby lowering its carbon footprint. In addition to industrial by-products like silica fume and fly ash, mined nanoporous aluminosilicate minerals known as zeolites can also be utilized as SCMs. The incorporation of zeolites not only modifies the properties of the resulting cement-zeolite composite due to their structural characteristics but also due to their high silica content and the introduction of charge-balancing cations (H⁺, Na⁺, Ca²⁺). This study evaluates the integration of sodium mordenite (Na-MOR) into ordinary portland cement, focusing on its impact on mineralogy and structure. Furthermore, carbonation experiments on the cement-zeolite composite were conducted to assess the potential for passive mineralization as an ambient carbon sink. The findings aim to inform the application of porous SCMs as an effective carbon mitigation strategy. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2025-00535A

PacRim S10 - Ceramics of Tomorrow for Green Energy and Cleaner Environment

PACRIM Symposium 10 - Ceramics of Tomorrow for Green Energy and Cleaner Environment II

Room: Georgia B

Session Chairs: Oomman Varghese, University of Houston;
Gunnar Westin, Uppsala University

1:15 PM

(PACRIM-S10-012-2025) Microwave-Assisted Synthesis as New Route to Bright Rare-Earth-Based Ceramic Materials (Invited)

E. Hemmer^{*1}

1. University of Ottawa, Chemistry and Biomolecular Sciences, Canada

The remarkable optical properties of the rare-earth (RE) make RE-based materials ideal for applications ranging from biomedicine to optoelectronics and energy conversion technology. This is due to the unique electronic properties of the RE elements allowing for upconversion, i.e., the emission of UV-visible light under near-infrared excitation. Upconverting nanoparticles (UCNPs) based on sodium rare-earth fluorides (NaREF_n) are commonly synthesized by the thermal decomposition of metal precursors in high-boiling-point solvents, based on convective heating. Microwave reactors can improve reproducibility as offering better control over a reaction environment, more homogeneous heat distribution yields narrow size distributions, and rapid heating to the desired temperature shortens reaction times from hours to minutes. Targeting applications in optoelectronics, photochemistry, and energy conversion, boosting the efficiency of upconverters is key. This presentation will shed light on the microwave-assisted synthesis of core/(multi) shell UCNPs and highlight pros and cons of this strategy towards the design of small-yet-bright upconverters, whereas special attention will be paid to their architecture-dependent optical properties.

1:45 PM

(PACRIM-S10-010-2025) Complex semiconductor structures built from Ångström to microstructure (Invited)

G. Westin^{*1}

1. Uppsala University, Sweden

Doped oxide semiconductors offer low cost and environmentally benign materials for use in photo-assisted fuel synthesis, solar-cells, and sensors. Crystal quality, surface, size and connectivity, as well as dopant electronic state, coordination and distribution are all determining the material properties and are crucially dependent on the synthesis parameters. In addition to doping, ultra-thin homogeneous or heterogeneous films may be added for improved properties or added functionality. Solution based synthesis offer efficient routes to complex thin- and ultra-thin films, nano-sponges, and nano-particles. Such solution based routes using either reactive metal alkoxides or salt-based routes will be presented in some detail connecting synthesis parameters with target material structure and properties. The possibility of extending the doping range much beyond the thermodynamic stability will be shown, as well as the possibility to obtain dopant metal-ion oxide clusters within semiconductor crystals, virtually without disturbance of the hosting semiconductor structure. This opens avenues for materials design. Finally, efficient processes to thin- and ultra-thin films of different composition and complexities will be shown. Such processes are better suited than e.g. ALD to produce complex composition thin- and ultra-thin coatings.

2:15 PM

(PACRIM-S10-011-2025) From MXene to Oxide: Nanoscale Materials Transformation for Advances in Energy Storage (Invited)E. Pomerantseva*¹

1. Drexel University, Materials Science and Engineering, USA

Two-dimensional (2D) transition metal carbides (MXenes) have emerged as promising precursors for the synthesis of electrochemically active oxides with advanced properties as electrodes in energy storage devices. In this presentation, we will discuss a solution-based transformation process involving the reaction of MXene nanoflakes with hydrogen peroxide, followed by hydrothermal treatment. The atomic-scale reactions that occur during this transformation process drive the reorganization of the MXene structure into product oxides, allowing for the control of defects and interfaces. This capability is critical for enhancing the electrochemical charge storage properties of the resulting materials. Additionally, the properties of MXene-derived oxides can be further tuned to meet specific performance targets through the addition of chemically pre-intercalated ions in the synthesis mixture. In this talk, we will present examples of enhanced electrochemical stabilization achieved through the chemical preintercalation of stabilizing ions, the control of morphology, and the formation of heterointerfaces. Given the chemical versatility of MXenes, the strategies for introducing preintercalated ions, dopants, and heterointerfaces are broadly applicable to a wide range of MXene-derived oxides, offering significant potential for improving performance across various energy storage technologies.

2:45 PM

(PACRIM-S10-009-2025) Catalytic Performance of Magnetic Field-Assisted Chemical Vapor Deposition Synthesized CoFe_2O_4 Thin Films: Electrochemical Ammonia Synthesis (Invited)T. Karimpour¹; T. Fischer¹; S. Mathur*¹

1. Universitat zu Koln, Institute of Inorganic and Materials Chemistry, Germany

Ammonia assumes a significant role in the realms of agriculture and the forthcoming era of carbon-neutral energy provision.^{1,2} The electrocatalytic reduction of nitrate to ammonia (NO_3RR) stands as an appealing prospect for both nitrate elimination and ammonia synthesis.³ Herein, $[\text{Co}\{\text{Fe}(\text{O}^i\text{Bu})_4\}_2]$ and $[\text{Fe}\{\text{Fe}(\text{O}^i\text{Bu})_4\}_2]$ complexes were synthesized and employed as single-source precursors for the production of CoFe_2O_4 and Fe_3O_4 thin films via magnetic field-assisted chemical vapor deposition. Our finding illuminates the superior catalytic efficacy of CoFe_2O_4 thin films, underscoring the pivotal role of cobalt as an active metal in electrochemical NO_3RR . The application of an external magnetic field significantly enhanced the phase purity of the resulting crystalline cobalt ferrite films, and consequently improved their catalytic activity. The ammonia production rate achieved with our catalytic system was determined to be $1617 \mu\text{g}\cdot\text{h}^{-1}\cdot\text{cm}^{-2}_{\text{cat}}$, accompanied by a notable maximum Faradaic efficiency of 87.9%. To delve into the influence of cobalt in NO_3RR , we conducted extensive investigations into the catalytic performance of spinel structures using DFT calculation. Our results corroborate our experimental findings and underscore the profound impact of cobalt as the primary active metal for NO_3RR .

3:30 PM

(PACRIM-S10-013-2025) Tuning nanostructures of 2-D metal oxide nanosheets (Invited)S. T. Mixture*¹

1. Alfred University, MSE, USA

Vanadate, titanate, niobate, perovskite and related layered oxides and the 2-D nanosheets derived from layered oxides, are of interest for electrochemical, photochemical and sensor materials. Synthesis of these materials is often challenging, and exfoliation, electrochemical deposition and solution chemical methods are often used. The talk will cover a range of synthesis approaches, including exfoliation

using various organic amines and will show the resulting structures of the materials from the atomic to the micrometer scale. Extensive electron microscopy, diffraction, spectroscopy and total scattering studies provide a picture of the high surface area materials, and electrochemical studies in various electrolytes provides a view into surface vs. intercalative mechanisms during operation. Assimilation of the studies demonstrates that a key process parameter is electrostatic self-assembly, which defines the extent to which the nanosheets restack, and consequently the device properties.

4:00 PM

(PACRIM-S10-014-2025) Computational Insights into the interfaces and grain boundaries present in LLTO (Invited)J. C. Madrid¹; K. K. Ghuman*¹

1. Institut National de la Recherche Scientifique, Énergie Matériaux Télécommunications, Canada

Meeting the escalating energy demands of electric vehicles and portable devices necessitates high-energy rechargeable batteries. Among various inorganic materials garnering attention in solid-state battery systems, Li-La-Ti-O (LLTO) stands out as a promising candidate as it exhibits high bulk Li ion conductivity, excellent high voltage stability, and remarkable hardness, which mitigates dendrite formation. Consequently, there have been several efforts to improve their conductivity. Literature suggests that the low conductivity of LLTO is due to grain boundaries (GBs), while conversely, LLTO conductivity increases in the presence of TiO_2 . Both effects, the negative impact of GBs and the positive influence of TiO_2 lack a satisfactory explanation, prompting us to perform a comprehensive Molecular Dynamics investigation. Our study involved a detailed analysis of symmetric and mixed LLTO GBs and LLTO/ TiO_2 interfaces under diverse conditions. This exploration has yielded intriguing insights into the complex interplay of these factors. In this presentation, I will share our results and discuss the migration mechanisms of Li-ion within the elaborate microstructures of LLTO. These findings not only shed light on the mysterious phenomena of LLTO conductivity but also offer valuable perspectives for designing and optimizing solid-state batteries, shaping the future of energy storage applications.

4:30 PM

(PACRIM-S10-015-2025) Hydrothermal conversion to pollucite and the hydroxyapatite coating for the fixation of radioactive cesium ionsE. Uehara*¹; L. Tong¹; A. Maki¹; M. Iwama¹; K. Komazawa¹; K. Tamura²; Y. Watanabe¹1. Hosei Daigaku Rikogakubu Daigakuin Rikogaku Kenkyuka, Japan
2. Busshitsu Zairyo Kenkyu Kiko, Japan

As a result of the Great East Japan Earthquake of March 2011, radioactive cesium (^{137}Cs), which has a long half-life of about 30 years, was released into the environment around the Fukushima Dai-ichi nuclear power plant. The consequences of this disaster required methods for the recovery and fixation of ^{137}Cs . One of the methods used to recover the ^{137}Cs is cation exchange using MOR-type zeolite, mordenite. The reason for using this method is that mordenite has high Cs^+ selectivity. However, in a high cation concentration, some Cs^+ ions in the large pores, may be released by cation exchange. The ANA-type zeolite, pollucite (POL), has pores of 0.28 nm diameters, which are smaller than the diameter of Cs^+ ions. POL is synthesized by an alkaline hydrothermal treatment of natural zeolites such as clinoptilolite, mordenite, and chabazite. This hydrothermal conversion is useful for the fixation of Cs^+ . In the present study, the conversion of mordenite, which has been exchanged with radioactive Cs^+ to produce POL by hydrothermal treatment was investigated. In addition, a coating of hydroxyapatite, which has a low solubility, was applied to pollucite surfaces to provide a multiple protective barrier.

4:50 PM

(PACRIM-S10-016-2025) Synthesis, dielectric study and energy storage characteristics of Nb₂O₅ added BaTiO₃ based electroceramics

S. Ahmad*¹

1. Islamia College Peshawar, Physics/ Centre for material sciences, Pakistan

Relaxor ferroelectrics materials display themselves to be potential candidates for many everyday electronic applications including energy storage, and pulse power capacitors because of their highly unique characteristics. Ba_{0.98}Bi_{0.02}Ti_{0.98}Mg_{0.01}Ce_{0.0103}+xwt% Nb₂O₅ (x=0, 05) ceramics using commercial grade raw materials through solid state processing technique. The phase, microstructure dielectric and energy storage properties have been investigated. The XRD analysis revealed single perovskite phase with orthorhombic crystal is obtained for x=0 composition while perovskite phase having cubic crystal symmetry for the 05wt% Nb₂O₅ added composition. A normal ferroelectric nature is obtained for the Pure and transformed to relaxor nature upon addition 05wt% Nb₂O₅ ceramics. The average grain size has been observed to decrease via Nb₂O₅ addition and a dense microstructure with an average grain size ~1.2 μm is obtained for 05wt% Nb₂O₅ sample. High ε_r~2600 with tanδ<0.02 at 1 kHz accompanied by a Wrec ~1.68 J/cm³, η~70 at an electric field ~ 231 kV/cm is obtained for 5wt% Nb₂O₅ sample at room temperature.

5:10 PM

(PACRIM-S10-017-2025) Ceramic Materials for Thermophotovoltaic Optical Emitters (Invited)

M. Leite*¹

1. UC Davis, Materials Science and Engineering, USA

Thermophotovoltaics (TPV) entail a cutting-edge route for converting heat into usable electricity through a clean energy paradigm. Yet, to date, a very limited number of materials have been investigated and tested for the optical emitters. Using a material screening approach that considers both the optical properties and the thermochemical stability of >2,800 material combinations with melting point >2,000 °C, we have identified optimized options for a bilayer optical emitter design. In this talk I will discuss our findings encompassing ceramic materials and which combinations can enable power conversion efficiency > 50%. We also quantify and decouple the effects of cell bandgap and power of emitter in our numerical analysis. We quantify the response of some down selected bilayers, such as B4C/AlN, using in situ, high-temperature optical measurements. Overall, our approach can be expanded to other energy harvesting applications that involve multiple stacks of the ceramic materials as well as complex structures (beyond thin films).

PacRim S14 - Advanced Structural Ceramics and CMCs for Ultra Extreme Environments

PACRIM Symposium 14 - Advanced Structural Ceramics and CMCs for Ultra Extreme III

Room: Cypress

Session Chairs: Tamás Csanádi, Institute of Materials Research, Slovak Academy of Sciences; Carolina Tallon, Virginia Tech

1:15 PM

(PACRIM-S14-011-2025) Oxidation of Refractory Metal Carbides in Molecular and Atomic Oxygen (Invited)

C. Stephens¹; S. Donaldson¹; M. Richwine¹; C. Recupero¹; E. J. Opila*¹

1. University of Virginia, Materials Science and Engineering, USA

Refractory metal carbides are candidates for ultra-high temperature hypersonic vehicle leading edge applications. The hypersonic vehicle leading edges are exposed to dissociated oxygen in addition to ultra-high temperatures. In this presentation, a novel cost-effective

microplasma resistive heating system capable of ultra-high temperature oxidation in molecular oxygen (MO) as well as atomic oxygen (AO) was used to elucidate the oxidation mechanisms of TaC, ZrC, and HfC in conditions relevant to hypersonic flight. Oxidation was conducted at temperatures of 1300 to 1600°C for times up to seven minutes in 1% O₂ balance argon with and without oxygen dissociation. Exposures of TaC in AO-containing environments resulted in more rapid carbide grain boundary attack. Exposures of ZrC and HfC resulted in a dense inner layer of ZrO₂ or HfO₂ + finely dispersed nanocarbon and an outer layer of porous ZrO₂ or HfO₂. AO exposures reduced the stability of the carbon in the inner oxide layer. In all cases, oxidation kinetics in AO-containing environments were more rapid. Implications of these results for use of metal carbides as leading edge materials will be discussed.

1:45 PM

(PACRIM-S14-012-2025) Oxidation resistance of UHTCMCs fabricated by Liquid Silicon Infiltration and Sintering

A. Vinci*¹; L. Zoli¹; M. Friess²; D. Sciti¹

1. CNR - ISSMC, Italy

2. DLR - German Aerospace Center, Institute of Structures and Design, Germany

In this study, carbon fibre reinforced ZrB₂/SiC composites were fabricated using two distinct processes: Liquid Silicon Infiltration (LSI) and Sintering via SPS. The microstructures of the composites were compared, revealing that both techniques produced a homogeneous dispersion of the ceramic matrix around the fibres. The sintered composites exhibited a more uniform, albeit less dense, microstructure, while the LSI composites were fully dense but showed occasional uninfilted spots between the fibre bundles. The oxidation resistance in air of both composites was evaluated at 1650°C, with exposure times ranging from 1 to 15 min. The oxidation behaviour of both materials was similar at short exposure times, with the formation of an outer silica layer. However, significant differences were observed for longer exposure times. The LSI composites experienced severe degradation, likely due to oxidation of residual silicon and weakening of the ceramic matrix. In contrast, the sintered composites demonstrated only a slight thickening of the oxide scale. This comparison highlights the different oxidation resistance mechanisms and performance of UHTCMCs processed by LSI and sintering, offering insights into the advantages of LSI as a less demanding processing route but also showing its limitations for prolonged exposure to extreme environments.

2:05 PM

(PACRIM-S14-013-2025) Prediction and Understanding of Thermal Transport in Crystalline Materials at Ultra-High Temperatures (Invited)

T. Feng*¹

1. The University of Utah, Mechanical Engineering, USA

The development of many next-generation technologies such as hypersonic aircraft and re-entry vehicles, higher-efficiency gas turbine systems, has been pushing the working environment to ultra-high temperatures (e.g., 1000 - 3000 K). However, there is still not a good understanding or accurate prediction of thermal transport at ultra-high temperatures due to the complexity of heat carrier transport at extreme temperatures. We may find that the carrier transport is very different than what we thought at ultra-high temperatures. In this talk, I will review our recent progress on thermal transport prediction at ultra-high temperatures. The heat transport mechanisms that are found to be important at ultra-high temperatures include (1) the higher order phonon scattering, (2) the temperature softening effect on anharmonic interatomic force constant and phonon scattering cross-section, (3) diffusion contributions, and (4) radiation contributions. The significance of each component is heavily material-dependent. Without losing generality, we will cover example materials including ultra-high

temperature ceramics (e.g., ZrC, HfC), thermal barrier coating materials (e.g., $\text{La}_2\text{Zr}_2\text{O}_7$, $\text{Sm}_2\text{Zr}_2\text{O}_7$), ceramics (e.g., SiC, Al_2O_3), and nuclear fuel (UO_2). Through validation against experimental data, we will show the accuracy of the predictions.

2:35 PM

(PACRIM-S14-014-2025) Orientation-dependent reinforcing mechanisms of SiC/carbon nanotube composites: A reactive molecular dynamics simulation study (Invited)

Y. Su^{*1}; Y. Wang²; Y. Ootani¹; N. Ozawa³; M. Kubo¹

1. Tohoku University, Institute for Materials Research, Japan
2. Research Institute of Frontier Science, Southwest Jiaotong University, China
3. Tohoku University, New Industry Creation Hatchery Center, Japan

Carbon nanotube (CNT) fibers are reported to enhance the toughness and strength of SiC ceramic matrices, but their reinforcement is limited by atomic-scale structural factors, particularly CNT orientation. The mechanisms by which orientation affects reinforcement remain unclear. This study employs bond-order-based reactive molecular dynamics simulations to investigate the mechanical properties and deformation mechanisms of SiC/CNT composites with varying CNT orientations. Results show that as the angle (θ) between CNTs and the tensile direction increases, CNT stretching magnifies while CNT bridging weakens. This leads to reduced composite strength due to reliance on CNT stretching, while toughness follows a volcano-type trend driven by competing both mechanisms. By considering the effects of SiC crystalline structure, CNT wall number, diameter, aspect ratio, and defects, this study introduces a modified and generalized rule of mixtures. It equates the CNT orientation correction factor to the cosine of θ , simplifying the theoretical prediction of tensile strength in fiber-reinforced ceramics matrix composites.

4:00 PM

(PACRIM-S14-015-2025) Synthesis pathways of (HfZrTiCe/La/Y) O_{2-x} nanoparticles via benzyl alcohol route at critical temperature (Invited)

F. Guo^{*1}

1. Shanghai Jiao Tong University, School of Materials Science and Engineering, China

High entropy oxides (RE-HfO₂) containing rare earth elements can provide excellent phase stability and oxidation resistance. However, the controllable synthesis of RE-HfO₂ at low temperature is a challenge due to poor understanding on nucleation. We synthesized the (HfZrTiLn)-HfO₂ nanoparticles with 15% ionic radius mismatch via benzyl alcohol route at 220 °C -5 min in presence of PtCl₄ and Fe(acac)₃. Nucleation pathways of the 5HfO₂ at the critical temperature were elucidated by using a comparison study of conventional heating and microwave irradiation heating. Consistency of XRD patterns and STEM-EDX observation indicate that the resultant Hf-OBN monomers acted as the nucleation center of the 5HfO₂, determined by diffusion kinetics. The nucleation rate depended on the metal monomers assembly and esterification reaction, which was accelerated by water vapor pressure produced in-situ by PtCl₄ catalyst. The Fe-metal organic cages served as the structure stabilizer of Zr/Ti monomers, and prevented early hydrothermal reaction route.

4:30 PM

(PACRIM-S14-016-2025) Creating anisotropic properties in conductive ceramics by incorporating hBN flakes

H. Liang^{*1}

1. Wuhan University of Technology, China

Tailoring physical properties in conductive ceramics is difficult, which is dominated by the continuous ceramic matrix. In this study, tunable anisotropic physical and mechanical properties in conductive ceramics were successfully realized by incorporating hBN flakes in their matrices. Two conductive TiB₂-AlN-hBN ceramics

(TAB) with different hBN amounts were fabricated by spark plasma sintering using powder mixtures containing TiN, Al, boron and hBN. Perpendicular to the load direction, flexural strength, fracture toughness, electrical conductivity and thermal conductivity of TiB₂-AlN-60 vol% hBN at room temperature were 151±6.34 MPa, 2.62±0.31 MPa•m^{1/2}, 5.3×10⁵ S/m and 77.87 W/m•K. Whilst electrical conductivity and thermal conductivity decreased to 2×10⁵ S/m and 32.25 W/m•K at the direction parallel to the load. These differences were created just by incorporating small amounts of extra aligned hBN flakes in conductive matrix, providing new opportunities to material selection and design.

PacRim S17 - Additive Manufacturing of Ceramics and Composites

PACRIM Symposium 17 - Additive Manufacturing of Ceramics and Composites III

Room: Prince of Wales

Session Chairs: Florian Bouville, ETH Zürich; Esther Valliant, Himed

1:15 PM

(PACRIM-S17-014-2025) Irradiative Ceramization of Chemically Bound Phosphate Ceramics (CBPCs) to Enable Direct Additive Manufacturing of Ceramic Composites (Invited)

M. D. Losego^{*1}

1. Georgia Institute of Technology, School of Materials Science and Engineering, USA

This talk will introduce a rapid, pressureless process to chemically bind ceramic parts via a combination of inorganic phosphate chemistries and electromagnetic irradiation. The ceramic components are synthesized from slurries of ceramic powders and Al(H₂PO₄)₃ binders. In initial studies, short-waved IR irradiation drives phosphate condensation reactions, however under these low irradiation powers (~0.2 W/cm²), condensation and ceramization requires minutes to tens of minutes to complete. Using a high-power flash lamp annealing (FLA) system (~10 kW/cm²) enables rapid ceramization in under 1 min and denser overall microstructures. Interestingly, though, the total irradiation energy required to drive complete ceramization is similar for both processes. The talk will also discuss the importance of light absorbers and the development of printed, high-temperature thermochromic ceramic sensors using this new additive manufacturing approach.

1:45 PM

(PACRIM-S17-015-2025) Inorganic/inorganic composites through emulsion templating (Invited)

T. Jiang¹; Y. Hong¹; E. Poloni¹; S. Zhou¹; E. Saiz¹; F. Bouville^{*1}

1. Imperial College London, Department of Materials, United Kingdom

Inorganic/inorganic composites are found in multiple applications crucial for the energy transition, from nuclear reactor to energy storage devices. Consequently, there has been a multitude of process developed to control them, from powder mixing and the use of short or long fibre, to tape casting for laminates up to recently 3D printing. Here, we combine emulsions and slip casting into a simpler, broadly available, inexpensive processing platform that allows for in situ control of composite's microstructure while also enabling complex 3D shaping. Our emulsions have particles loaded in both the oil and the water phase, enabling an independent control of both phase and a rich rheological behaviour. While these emulsions can be shaped by multiple processes, we show that slip casting triggers a two-steps solvent removal opening the possibility for the conformal coating of pores. We showcase this process by producing strong and light-weight alumina scaffolds reinforced by a conformal zirconia coating. In addition, by manipulating magnetically responsive droplets, we

can play with their distribution and, for example, form inorganic fibres inside an inorganic matrix in situ during slip casting. Using this approach, we have reinforced alumina with aligned metallic iron fibres to prepare composites with a work of fracture an order of magnitude higher than the pure ceramics.

2:15 PM

(PACRIM-S17-016-2025) Characterisation and Testing of 3D-printed ceramic and PM-parts with novel Thermo-Optical-Measuring application

A. Diegeler*¹

1. Fraunhofer ISC, Center of Device Development, Germany

Thermo-optical measurement devices have been developed at the Fraunhofer ISC during the last 20 years - recently also with atmospheric control (TOM-AC). This technique will be used to test and inspect additive manufactured ceramic and PM-parts during the whole temperature cycle inside the furnace to evaluate full functionality. This method allows to follow changes of sample shape (up to 50mm in diameter) with an accuracy of nearly 0.3 micron by contactless measurement. Due to the purely optical detection samples of any shape can be monitored inside the furnace. A sophisticated algorithm detects the contour of samples - and thus dimensional changes. Possible applications include simply measuring the shrinkage or shape distortions. By a computer-controlled program we realized full atmospheric control, i.e. changing the gas atmosphere inside the furnace (inert gas at different pressures, forming gas or vacuum) during the sintering process. Main focus according additive manufactured ceramic and PM-parts lies on quality and quality control during production process, and on characterization of behavior under thermal or other stress application. Thermo-Optical Measurement technique offers a wide range of contactless, optical detection of complex shaped ceramic and PM-parts with very high resolution.

2:35 PM

(PACRIM-S17-017-2025) Accelerating Discovery of Ultra-High-Temperature Ceramics via High-Throughput Methods and Additive Manufacturing (Invited)

K. Min¹; K. Wojtowicz¹; I. McCue²; C. Hansen*¹

1. University of Massachusetts Lowell, Mechanical & Industrial Engineering, USA
2. Northwestern University, Materials Science & Engineering, USA

The discovery of novel ceramic materials for extreme environments demands innovative approaches to accelerate the development process. In this work, we present the efforts of the High-throughput Materials Discovery for Extremes (HT-MAX) Center, a multi-university initiative leveraging high-throughput synthesis, characterization, modeling, and data science to speed material discovery. This presentation highlights our synthesis and processing strategies to fabricate Ultra-High-Temperature Ceramics (UHTCs). We use material extrusion additive manufacturing with a dual-reservoir system to print ceramic formulations, such as silicon carbide (SiC) and boron carbide (B₄C). This setup allows for on-the-fly compositional modifications, spanning from the extremes of individual reservoir compositions to any intermediate combination. Key formulation variables include particle composition, binder chemistry, particle size distribution, and volume fraction. Our combinatorial approach minimizes the preparation of unique formulations required to efficiently explore large parameter spaces. Machine learning further accelerates discovery by guiding experimental design and prioritizing data collection. High-throughput characterization links compositions to mechanical and thermal properties, creating a comprehensive framework that advances the discovery of UHTCs for extreme environments.

3:30 PM

(PACRIM-S17-018-2025) UV-assisted and rotational robocasting of ceramic composites for electrical insulation, catalysis and bone tissue engineering (Invited)

A. Gurlo*¹

1. Technische Universitaet Berlin, Chair of Advanced Ceramic Materials, Germany

An innovative strategy and our achievements in the additive manufacturing of advanced ceramic materials are presented. The first case study describes rotational robocasting combined with the sponge replication technique for the production of bone-mimetic scaffolds made of a composite bioceramic containing Cu-doped diopside and biphasic calcium phosphate. The customised nozzles with different geometries are applied to fabricate high-strength scaffolds with channel structures. The scaffolds have a high porosity while also demonstrating excellent compressive strength, comparable to that of human bone in both axial and lateral compression. The second case study presents the robocasting of curved electrical insulation composites made from a mica/photocurable silicone resin. To overcome the viscosity limitations of conventional robocasting, a two-stage curing process was used that combined UV curing with heat treatment. The results showed a significant improvement in print quality and provided an effective solution for the development of printable insulation in motors and generators. The third case study was concerned with the influence of the framework geometry (extruded, face-centred cubic and body-centred cubic) on the catalytic performance of the In₂O₃/ZrO₂ systems for CO₂ methanation.

4:00 PM

(PACRIM-S17-019-2025) Developing an Hydroxyapatite Ink for DLP 3D Printing: Lessons Learned by a Leading HA Manufacturer (Invited)

E. Valliant*¹

1. Himed, R+D, USA

Hydroxyapatite and other calcium phosphates have been used for decades in the medical device industry, specifically for orthopedic, spinal, and dental applications. These materials can form strong bonds to bone and encourage new bone growth. However, 3D printing of these materials for medical devices is still in its infancy, whereas additive manufacturing of metal implants has already been widely adopted. In this presentation, we will share insights from the manufacturing experience, highlighting the key obstacles that must be overcome to allow for the greater adoption of additive manufacturing of bioceramics for medical devices. One of these challenges is the suitability and availability of inks for use in a GMP production environment. To address this difficulty, we have leveraged our 30 years of experience in manufacturing various forms of calcium phosphates to develop new ink formulations. Our extensive understanding of powder properties allows us to fine-tune formulations effectively. We will discuss key factors to consider when selecting the best powders for ink formulation for use in DLP printing, including the importance of particle size, size distribution, surface area and morphology. Additionally, we will share some lessons learned from using these inks in a production setting, such as thermal processing, process control and quality control.

4:30 PM

(PACRIM-S17-020-2025) Defect Evaluation and Mitigation in the Material Extrusion of Highly-Loaded Alumina Paste

P. Brune*¹; M. Tammi¹; W. Parks¹; M. C. Patterson¹

1. Kratos Defense and Security Solutions, Kratos SRE R&D, USA

Mechanical properties of ceramics (e.g. strength, hardness, and fracture toughness) are largely defect driven due to the brittle nature of ceramics and propensity for catastrophic failure. For high performance therefore, great care should be taken during the formation of ceramic green bodies to reduce the size and number of defects. Significant

prior effort to classify and evaluate the defects that result from various ceramic additive manufacturing processes is available in the literature and has been studied to better understand how defect formation might be minimized during the formation of green ceramic bodies from different rheologies. Current work at Kratos SRE is focused on the characterization and mitigation of printing defects in the direct ink write process. To this end, two aqueous pastes were formulated with different rheology to investigate and classify the typical porosity defects that result. An attempt was made to mitigate defects in printed solid infilled structures by varying paste rheology, mixing parameters, and printing parameters. The resulting defect hierarchies were evaluated using micro-CT, scanning electron microscopy, and density measurements on green and sintered bodies produced from the direct ink writing of alumina paste using the material extrusion technique.

PacRim S20 - Advanced Functional Materials for Clean Energy Solutions

PACRIM Symposium 20 - Advanced characterization techniques I

Room: Georgia A

Session Chairs: Clemens Heske, University of Nevada Las Vegas; Marc Willinger, Technische Universität München

1:15 PM

(PACRIM-S20-021-2025) Emerging X-ray spectroscopy for energy materials (Invited)

C. Dong*¹

1. Tamkang University, Department of Physics, Taiwan

To pave the way for a zero-emission future, developing advanced energy materials holds significant importance, and thus we must tackle these challenges from multiple perspectives, with a specific emphasis on the materials that enhance energy conversion, storage, and conservation efficiencies. Improving the efficiency of existing energy materials is straightforward but presents technically challenges. The physical and chemical properties of materials are closely correlated with the atomic and electronic structures. Gaining a deep understanding of these fundamental characteristics, particularly their behavior at work, is essential for effective engineering and practical application. Synchrotron x-ray spectroscopies serve as powerful tools for investigating the atomic and electronic structures of energy materials. By employing in situ techniques, the dynamic changes in the atomic and electronic structures during operation can be monitored. The emerging scanning transmission x-ray microscopy offers spatially resolved x-ray spectroscopy, holding great potential for exploring energy science. This presentation aims to underscore the significance of x-ray spectroscopies in characterizing atomic and electronic structures of energy materials, such as photosynthesis materials, advanced nanocatalysts, and smart materials. Tamkang University end-stations at the Taiwan Photon Source TPS-45A & 27A will be also introduced.

1:45 PM

(PACRIM-S20-022-2025) X-ray spectroscopies for atomic-scale insights in energy materials for clean energy solutions (Invited)

S. Mukherjee*¹; S. Riva¹; K. Klementiev²; J. Scragg³; M. Wahlin³; H. Rensmo³

1. Uppsala Universitet, Department of Physics and Astronomy, Sweden
2. Lunds Universitet, Sweden
3. Uppsala Universitet, Sweden

Research on energy materials for clean energy solutions has reached a stage where future advancements require unlocking structure-function correlations at the atomic-level. This stems from the realization how local site-specific distortions within a lattice can remarkably alter the electronic landscape, i.e., band configuration, thereby modifying material properties. The key to construct the

future roadmap for functional materials, therefore, lies in the ability to identify and control such geometric-electronic structural links which allows for smart material designs for device fabrication, as well as finding novel phenomenon/materials. We are witnessing a recent surge in utilizing advanced x-ray techniques to explore such correlations in materials at different technological readiness levels, with increasing focus towards characterizations performed under real operating conditions. This seminar aims to highlight how and why such advanced x-ray characterization techniques can be effectively utilized to address critical challenges in the development of existing and emergent functional materials. Specifically I will look at case studies on wide range of photovoltaic materials, with some recent highlights from our battery research, and concluding with a perspective of that intergrates research goals in academia and industry landscapes combining both in-house and large facilities.

2:15 PM

(PACRIM-S20-023-2025) Discovery and Performance of New Electrocatalyst Materials for Energy and Sustainability (Invited)

B. E. Koel*¹

1. Princeton University, Chemical and Biological Engineering, USA

We discuss the synthesis, characterization, and performance of several new electrocatalyst materials that address energy and sustainability needs. An efficient acid-stable N₂-plasma treated Hf oxyhydroxide electrocatalyst showed unprecedented high catalytic activity and stability for earth-abundant materials for hydrogen evolution and oxidation reactions (HER and HOR) in strong acid. Reaction-driven restructuring of defective PtSe₂ created an ultrastable electrocatalyst for the oxygen reduction reaction (ORR) with 1.3 times the specific activity and 2.6 times the mass activity of a commercial Pt/C catalyst, and maintained this activity in accelerated durability tests. A highly active Hf-modified Ir oxide (IrHf_xO_y) electrocatalyst for the oxygen evolution reaction (OER) demonstrated activity 10 times higher in base (pH = 11) and 4 times higher in acid (pH = 1) than IrO_x. The highest intrinsic mass activity of the IrHf_xO_y catalyst in acid was 6950 A g_{IrOx}⁻¹ at an overpotential of 0.3 V. A phosphorus-doped Hf-Ru oxide (Hf_xRu_yPO) electrocatalyst exhibited highly efficient and stable OER activity over 40 h. XPS and Raman indicated that the durability of RuO₂ was improved by formation of a HfOOH phase with higher OER activity and lower impedance. Also, we report on studies of metal-organic frameworks (MOFs) and MOF-derived (MOF-d) materials as electrocatalysts.

2:45 PM

(PACRIM-S20-024-2025) Charge carrier dynamics of photo-functional semiconductor films in correlation with their device performance (Invited)

Y. Tachibana*¹

1. RMIT University, School of Engineering, Australia

Solar energy conversion is one of the most attractive processes to generate electricity (PV) or fuel (solar fuel). Their devices function by absorbing the sun light at a photo-functional semiconductor, followed by charge carrier generation and dissociation at or inside the semiconductor. PVs generate electricity by extracting the separated charge carriers at their respective electrode, while solar fuel such as hydrogen gas or alcohol is generated by reducing water or carbon dioxide with the generated and separated electrons. Highly efficient charge transfer reactions in addition to high charge separation efficiency and swift charge transport with minimum charge recombination are required to improve their device performance. Therefore, it is of immense importance to identify underlying key parameters controlling charge carrier dynamics in correlation with the device performance. In this presentation, we will demonstrate how charge carrier dynamics at typical photo-functional semiconductors such as halide perovskite films or TiO₂ photocatalysts influences their device performance. This work was partly supported by JSPS KAKENHI Grant (19H02813) and (22H02182), the Collaborative Research

*Denotes Presenter

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PACRIM Symposium 20 - Advanced characterization techniques II

Room: Georgia A

Session Chair: Lars Österlund, Uppsala Universitet

3:30 PM

(PACRIM-S20-025-2025) Material growth, self-organization, and pattern formation: Insights from multi-scale operando electron microscopy (Invited)

M. Willinger*¹

1. Technische Universität München, Chemistry, Germany

Multi-scale operando electron microscopy provides direct insights into processes that govern material growth and allows us to study functional materials in their “functional” state. Using the example of CVD growth of graphene, observed by in-situ scanning electron microscopy, it will be shown how the controlled balance between graphene growth and etching can be used for the fabrication of twisted layer graphene and formation of complex intertwined graphene spirals. Moving from material growth to the emergence of function, we will turn to catalysis. It will be shown how the dynamic interplay between reactive species and a metal catalyst can lead to the formation of dissipative structures and complex spiral patterns. The emergence of both is a direct consequence of and linked to the emergence of catalytic function. Self-organization in ongoing chemical reactions, or during material deposition and growth, involves feedback loops and coupling between dynamics that dominate at different scales. Both need to be considered for a better and more fundamental understanding. Using operando scanning and transmission electron microscopy, it is now possible to study processes and dynamics that occur at different time and length scales, and to move beyond the study of thermodynamically isolated static arrangements that has dominated electron microscopy for many years.

4:00 PM

(PACRIM-S20-026-2025) Symtheiss and investigation of Eu-doped ZnO nanosponges: Where are the Eu atoms? (Invited)

C. Tai*¹; S. Feng¹; S. Naim Katea²; M. Ek²; G. Westin²

1. Stockholms Universitet, Department of Chemistry, Sweden

2. Uppsala Universitet, Department of Chemistry - Ångström, Sweden

ZnO is a simple and low cost material. It has been applied to many applications from transparent electrodes, batteries, catalysts, photocatalysts, sensors, etc. By doping d- and f-block elements, add-on electrical, optical and magnetic properties can be obtained. Besides, the microstructural features can enhance the performance of a device. The larger the surface area is beneficial to, for example, catalysis and energy storage applications. A simple and low cost salt-based route was used to synthesize Eu-doped crystalline nano-sponges. After drying the mixture of dried zinc diacetate tetrahydrate, zinc dinitrate hexahydrate, europium nitrate pentahydrate, triethanolamine (TEA) and methanol, a two-step heating: 400 °C for 1 min, cooling to room temperature, and then to 600 °C for 3 mins, was applied. 5-33% Eu dopant can be implemented into ZnO. XRD and IR, combined electron microscopy techniques were employed to examine the samples from micron to atomic scale. STEM images and EDS shows the distribution of the Eu. In addition, pair distribution function (PDF) analysis was applied to examine the atom-atom. In addition, the co-existence of 4, 5 and 6 coordinations of Eu-O was revealed. The combined electron microscopy techniques reveals the structural variation of Eu-doped ZnO nanosponges, especially the short-range structural order or non-crystalline phases.

4:30 PM

(PACRIM-S20-027-2025) Chemical solution-based fabrication of piezoelectric materials for energy applications (Invited)

M. Einarsrud*¹

1. Norges teknisk-naturvitenskapelige universitet, Materials Science and Engineering, Norway

Aqueous chemical solution-based fabrication is a simple, environmentally friendly, and upscalable process to piezoelectric nanostructured and thin piezoelectric films for energy applications. The fabrication is based on a solution containing the precursors, followed by annealing, and finally crystallization. We have developed a unique set of in situ synchrotron X-ray-based characterization units to reveal nucleation and crystallization mechanisms of the as-fabricated materials. Using this information, we can tailor materials structure and orientation and thereby enhance the piezoelectric properties. Here we report on guidelines for how to design fabrication of nanostructured materials and thin films of several lead-free piezoelectric materials. We have investigated the formation of lead-free K_2NaNbO_3 and $Sr_xBa_{1-x}Nb_2O_6$ piezoelectrics from salt and oxide precursors by hydrothermal synthesis to tailor the properties. Control of the chemical solution deposition for piezoelectric thin films have been obtained during the solution deposition. In combination with in-situ IR spectroscopy and total scattering, understanding the evolution of the nucleation and crystallization of $BaTiO_3$, $K_{0.5}Na_{0.5}NbO_3$ and $Sr_xBa_{1-x}Nb_2O_6$ thin films is obtained. This understanding will guide us to design of the optimal procedure for fabrication and tuning the desired materials properties.

5:00 PM

(PACRIM-S20-028-2025) Multiscale modelling of molecules and materials (Invited)

P. Broqvist*¹

1. Uppsala University, Department of Chemistry- Ångström Laboratory, Sweden

The materials (and molecular) science community often deals with multiscale problems, i.e. problems that at the same time concern macroscale properties such as hardness, colour, and ductility, which in turn heavily rely on the microscale (electrons and atoms). In this community, multiscale modelling has evolved as a strategy to address scientific problems and to bridge many of the size- and time gaps existing between “first-principles” theoretical approaches and experiments. One strategy in multiscale materials modelling is to connect data from different distinguishable “levels” of models. A key obstacle in this work is to link and harmonize the different models. In some cases, the link can be obvious and made using empirical approaches. However, extending these simple empirical approaches to be used for more complex systems, where discrete and finite size effects are of importance, have been proven difficult. In these cases, machine learning has emerged as a promising tool to achieve efficient and accurate linking between levels. In this talk, I will present the development and use of multiscale materials modelling using three examples from my research. These are i) enhanced redox activity of ceria nanoparticles at small sizes, ii) the formation of molecular-like Eu_2O_3 clusters in ZnO, and iii) thermodynamic simulations and phase evolution of battery cathode materials.

PacRim S26 - Materials for Advanced Nuclear Energy Systems and Nuclear Waste Management

PACRIM Symposium 26 - Materials for Advanced Nuclear Energy Systems and Nuclear Waste Management I

Room: Plaza B

Session Chairs: Xiao-Ying Yu, Oak Ridge National Laboratory; John McCloy, Washington State University; Xiaonan Lu, Pacific Northwest National Lab; William Weber, University of Tennessee; Jim Neeway, Pacific Northwest National Lab

1:15 PM

(PACRIM-S26-001-2025) Use of Ion Beams to Simulate Alpha-Decay Damage in Nuclear Waste Forms (Invited)

W. J. Weber*¹

1. The University of Tennessee Knoxville Tickle College of Engineering, Materials Science & Engineering, USA

The principal source of radiation damage in ceramics for immobilization of actinide-containing nuclear waste is alpha-decay of the actinides, which occurs over geologic timescales. Alpha-decay produces energetic alpha particles (4.5 to 5.5 MeV) and recoil nuclei (70 to 100 keV) that result in radiation damage and the accumulation of helium. The evolution of radiation damage due to alpha-decay has been studied using short-lived actinides; however, ion beam irradiation has become the primary approach to study radiation damage in relevant materials due to decreased costs, shorter irradiation times, and the non-radioactive nature of the irradiated materials. Ion irradiations are conducted at relatively high dose rates compared to alpha-decay rates and often over a narrow range of conditions that limit predictive modeling of the kinetics of microstructure evolution, phase transformations, and swelling under alpha-decay damage rates in a repository. Several collaborative studies over the years have benchmarked MeV ion heavy-ion irradiation results on relevant materials with results from identical samples doped with short-lived actinides. Such benchmarking has demonstrated that bulk-like irradiation with MeV heavy ions, such as Au or Bi, provides the best simulation of damage accumulation from alpha decay, yielding swelling and phase transformation behavior that agree well with results from alpha-decay damage.

1:45 PM

(PACRIM-S26-002-2025) Machine Learning in Nuclear Waste Glass Formulation and Property Model Development (Invited)

X. Lu*¹; J. Vienna²

1. Pacific Northwest National Lab, Energy and Environment Directorate, USA
2. Pacific Northwest National Lab, USA

The US Department of Energy manages the Hanford Site's nuclear waste, planning to process it into low-activity waste (LAW) and high-level waste forms through vitrification. Waste vitrification has been practiced worldwide as the preferred method of treating highly radioactive nuclear wastes. Previously, algorithms for Hanford LAW glass formulation were developed using traditional methods such as partial quadratic mixture models. Since machine learning (ML) has been successfully used to model glass properties, this work reviews the integration of ML in nuclear waste immobilization, including efforts on database management, model development, uncertainty qualification, and glass formulation. Compared to the previous framework, ML-based optimization methods, as demonstrated in proof-of-principle studies, offer improved LAW glass designs and a streamlined approach to generation of data from optimally selected compositions and near real-time updates. Moreover, the review

highlights advancements in the glass optimization framework and available tools with examples. Lastly, we discuss prospects for glass property model development and formulation strategies.

2:15 PM

(PACRIM-S26-003-2025) Evolution of the physico-chemical behaviour of ceramic matrix composites in deep geological disposal

G. German*¹; E. Perret³; F. Rebillat¹; A. Debelle²; X. Bourbon²; J. Roger¹

1. Universite de Bordeaux, France
2. Agence nationale pour la gestion des dechets radioactifs, France
3. Institut de Recherche Technologique Antoine de Saint-Exupery, France

The Cigéo project, managed by Andra - French national radioactive waste management agency - aims to construct and monitor a deep geological disposal facility for high-level (HL) and long-lived intermediate-level radioactive waste. Low carbon steel is currently defined as the reference material for the liner of the micro-tunnels (or cells) in which the HL disposal packages should be placed. Due to the expected conditions in the cells, steel will experience corrosion. Although this phenomenon is fully considered in the safety case provided by Andra, the Agency is studying Ceramic Matrix Composite (CMC) as a potential alternative material. There is hence a crucial need to determine the behaviour of these materials in field conditions, i.e., in contact with pore water. To tackle this issue, an integrated approach aiming at identifying and quantifying potential material degradation processes has been implemented. This approach includes the development of both an accelerated ageing set-up and a methodology to characterize the materials and solutions, and the construction of a thermodynamical model to simulate the ageing experiments. This approach has been first tested by selecting alumina as a model material. Calculations and actual observations have proven to be consistent and allows a better understanding of the degradation mechanisms under hydrothermal conditions.

2:35 PM

(PACRIM-S26-004-2025) Advancements in Predictive Modeling of Refractory Corrosion for Enhanced Longevity of Nuclear Waste Glass Melters

D. P. Guillen*¹; J. Acierno¹; T. Jin²; J. Amoroso³; R. Pokorny⁴; A. A. Kruger⁵

1. Idaho National Laboratory, Materials Science and Manufacturing, USA
2. Pacific Northwest National Laboratory, USA
3. Savannah River National Laboratory, USA
4. University of Chemistry and Technology Prague, Czechia
5. US Department of Energy, Hanford Field Office, USA

This presentation highlights advancements in modeling refractory corrosion in nuclear waste glass melters, focusing on Monofrax® K-3 refractory. Refractory degradation significantly impacts the lifespan of melters used in nuclear waste vitrification. Our integrated computational-experimental approach uses data from static, bubbled, and rotating crucible experiments wherein K-3 coupons are exposed to seven surrogate waste glass compositions at 1100 to 1250°C for up to 12 days. Comprehensive data is obtained through optical microscopy, X-ray computed tomography, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and electron probe microanalysis. This data is vital for developing and validating computational fluid dynamics (CFD) models that predict refractory corrosion. Our CFD models use methodologies including volume of fluid, passive scalar diffusion, Marangoni convection, dynamic contact angle, and mesh morphing to simulate the complex multiphysics environment. This work aims to predict refractory material loss over time as a function of glass composition, with the ultimate goal of reducing melter downtime and extending the lifespan of nuclear waste glass melters. This presentation covers modeling methods, challenges, and initial findings that contribute to more reliable predictions and better mitigation strategies for refractory corrosion.

2:55 PM

(PACRIM-S26-005-2025) R&D for the Thermal Treatment of Nuclear Waste in the UK

M. T. Harrison*¹

1. United Kingdom National Nuclear Laboratory, Waste Management and Decommissioning, United Kingdom

In addition to the established vitrification process for high-level radioactive waste (HLW), thermal treatment is currently being considered for other radwastes in the UK. High temperature processing offers the advantages of volume reduction, destruction of organics, removal of reactivity and improvements in product quality compared to the baseline of cement encapsulation. Sellafield Ltd have recently completed a series of inactive trials under the HAW Thermal Treatment (HAWTT) project that focussed on two streams; (i) plutonium contaminated material (PCM) using plasma vitrification, and (ii) pumpable wastes by Joule-heated ceramic melters (JHCM). Following these, an interim R&D programme started in April 2024 focussed on de-risking thermal treatment and addressing the key knowledge gaps. In parallel, NNL is developing R&D capability to support thermal treatment as one of its internally funded 'Core Science Themes'. As well as funding several PhD projects, the theme also includes several tasks structured around the immobilisation of waste using thermal processes and product quality of the resulting wasteforms. The original focus on active analysis capability (Raman, XRF, etc.) has been expanded to include glass dissolution studies and advanced glass and ceramic wasteforms. This presentation will highlight some of the key recent activities, including GRAAL modelling, UF₄ vitrification, and microscopy of leached glasses.

3:30 PM

(PACRIM-S26-006-2025) Effect of Melt Conditions on Phosphate Glass Structure in Mixed Alkali Halide Waste Forms

L. Greiner*²; C. Lonergan¹

1. Missouri University of Science and Technology, USA
2. Missouri University of Science and Technology, Materials Science and Engineering, USA

The structural evolution and dechlorination of mixed alkali-containing iron phosphate glasses were systematically investigated to determine their viability for nuclear waste immobilization. A mixed alkali halide salt (NaCl, KCl, LiCl) was combined with phosphoric acid and iron oxide and then reacted in air and argon environments at varying temperatures. High-Performance Liquid Chromatography (HPLC) was employed to monitor changes in phosphate chain lengths and to determine the oxygen-to-phosphorus (O/P) ratios, providing insights into the polymerization of the glass network. Raman spectroscopy was utilized to examine the structural modifications within the phosphate framework throughout the dechlorination process. Argon atmosphere and lower-temperature melts exhibited higher retained Cl content, shorter chain lengths and higher O/P ratios than what is theoretically predicted for a mixed alkali iron phosphate. Mössbauer spectroscopy helped assess the iron redox states, elucidating the role of iron on the glass structure. These findings underscore the significance of melt conditions in tailoring the structural properties of phosphate glasses for immobilizing hazardous and nuclear wastes.

3:50 PM

(PACRIM-S26-007-2025) Processing Limits of Cermets for Nuclear Waste Form Applications

N. O. Marrero*¹; K. Matthies²; S. K. Sundaram¹

1. Alfred University, Inamori School of Engineering, USA
2. Alfred University, USA

Nuclear fuel cycles and processing produce widely different nuclear waste streams. Generally, nuclear waste streams are separated into high level and low-level waste, HLW and LLW respectively, based on radiation levels. Cermets or ceramic-metal composites can combine

different waste streams containing metals and ceramics, oxides and non-oxides. Cermet waste forms aims to incorporate all the positive aspects of each material class including ductility, chemical stability and overall strength of the final product. Model cermet systems of SS 316-ZrO₂ and SS 316-SiC cermets over ceramic-to-metal ratios of 20:80-50:50 vol%, were processed by spark plasma sintering (SPS) and hot uniaxial pressing (HUP). Temperatures and pressures of processing are 700-900°C and 32 or 50MPa for SPS and 900-1100°C and 85MPa for HUP. Density and porosity values of these cermets range from 70 to 100% and 20 to >1 vol%, respectively. We have used scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), and x-ray diffraction to image microstructure, map elements distribution, and identify phases. Additionally, using terahertz time-domain spectroscopy (THz-TDS) optical and dielectric constants were recorded. Several samples met the target density (>95% theoretical density) and porosity (< 5 %) values. Our results demonstrate that dense stable cermet waste forms can be a viable option to incorporate multiple waste streams.

4:10 PM

(PACRIM-S26-008-2025) Current status of treatment method for HWR resin waste and C-14 recovery technology in resin waste

K. Lee*¹; H. Park¹; G. Kim¹; H. Park²

1. Korea Atomic Energy Research Institute, Republic of Korea
2. SKTNS, Republic of Korea

The intermediate level spent resins waste generated from water purification for the the moderator and primary heat transport system during operation of heavy water reactor (HWR). Especially, moderator resins contain high level activity largely because of their C14 content. So spent resins are considered as a problematic solid waste and require special treatment to meet the waste acceptance criteria for a disposal site. Various methods have been studied for the treatment of spent resins which include thermal, destructive, and stripping methods. In the case of solidification methods, cement, bitument or organic polymers were suggested. In the 1990s, acid stripping using nitric acid and thermal treatment methods were actively investigated in Canada to remove C14 nuclide from waste resin. In Japan, thermal destructive method was studied in the 1990s. Since 2005, KAERI developed acid stripping method using phosphate salt. However, acid stripping method are not suitable due to large amounts of 2nd waste containing acid solution with various nuclides. To solve this problem, KAERI has been suggested the microwave treatment method for C-14 selective removal from waste resin in the 2010s. Commercial demonstration tests using radioactive waste resin generated from Wolsung unit 1 and unit 2 were successfully conducted and 95 % of C14 was selectively removed from the radioactive waste resin.

4:30 PM

(PACRIM-S26-009-2025) Geochemical Modeling of Quenched Blast Furnace Slag Alteration in Cementitious Waste Forms

J. Neeway*¹; S. Kerisit¹; C. L. Trivelpiece²; M. Asmussen¹

1. Pacific Northwest National Lab, USA
2. Savannah River National Lab, Environmental and Process Control Technology, USA

Unreacted reagents commonly found within cementitious waste forms undergo continued hydration that can drive mineral changes and impact contaminant release. Blast furnace slag (BFS) is a supplementary cementitious material involved in the hydration reactions forming the solidified matrix and, importantly for waste form applications, that provides reduction capacity to suppress the release of redox-sensitive contaminants (Cr, ⁹⁹Tc, etc.). Quenched BFS is a glassy material that is ground for use in cementitious waste forms but retains its amorphous structure. BFS particles that remain in the cured material can continually react over disposal time frames and replenish the species responsible for maintaining a reducing environment (e.g. Fe(II), sulfide) at a currently unknown rate. Here, we describe the development of a kinetic model aimed at predicting the long-term

alteration and thus reduction release rate of BFS within cementitious waste forms. The model combines a linear rate law for dissolution with a time-dependent hydration rate. Model parameterization was performed using literature data for a range of compositions altered at multiple temperatures and liquid-to-solid ratios. The model accounts for the observed initial rapid dissolution followed by long-term slow alteration and can serve as a source term for reduction capacity in large-scale models of cementitious waste form disposal.

4:50 PM

(PACRIM-S26-010-2025) Tritium and lithium transport along tritium breeding components

X. Yu^{*1}; J. Son¹; D. Senor²

1. Oak Ridge National Laboratory, Materials Science and Technology Division, USA
2. Pacific Northwest National Laboratory, USA

We investigated light isotope distributions of irradiated components in a tritium producing system consisting of cladding, getter, and pellet. Specimens were selected at different axial elevations along the Tritium-Producing Burnable Absorber Rod (TPBAR) and analyzed using powerful surface tools, namely time-of-flight secondary ion mass spectrometry (ToF-SIMS) and scanning electron microscopy (SEM) – focused ion beam (FIB). Specifically, SEM-FIB was used to prepare small specimens to reduce potential risk to the analytical platform and instrument analysts. The tritium (T or ³H) and lithium (Li) isotope distributions were characterized using ToF-SIMS primarily due to its superior surface sensitivity and selectivity. Post irradiation examination (PIE) results were used to infer transport mechanisms of light isotopes under neutron irradiation in light water fission reactors. This presentation will offer a summary of the key ToF-SIMS and SEM imaging and spectral results of the irradiated cladding, getter, and pellet analyses. Multimodal analyses using SIMS and SEM provide sensitive observations of the microstructural evolution of the cladding, getter, and pellet post neutron irradiation. The valuable data and understanding will be ultimately used to improve engineering design and contribute to tritium science and technology.

5:10 PM

(PACRIM-S26-011-2025) Bismuth-Induced Modifications in Iodine Solubility of Aluminoborosilicate Glasses Synthesized at High Pressure

S. Soudani^{*1}; J. Hamon³; M. Paris³; Y. Morizet²

1. Washington State University, Institute of Materials Research, USA
2. Nantes Université, Laboratoire de Planétologie et Géosciences, France
3. Institut des Matériaux de Nantes Jean Rouxel, France

Adding bismuth to borosilicate glass has gained interest for radiation shielding, optical properties, and as a solid sorbent for radio-iodine (¹²⁹I). Despite its low activity, ¹²⁹I is problematic due to its long half-life (15.7 Ma) and mobility. Bi-based sorbents could then be used as an iodine source for vitrification, but conventional methods cause iodine release. High-pressure synthesis prevents this, enabling higher I incorporation. Two aluminoborosilicate glass series (60-x) SiO₂-6B₂O₃-(5+x)Al₂O₃-20Na₂O-8CaO (x = 0 or 10 mol.%) were synthesized with 1, 2, 4, or 8 mol.% Bi₂O₃ under 1.0 GPa, adding iodine as I₂ or I₂O₅. SEM/EDS showed I content increases with Bi₂O₃, reaching 2.7 mol.% I. ¹¹B and ²⁷Al MAS-NMR revealed BO₄/BO₃ decreases with Bi in both “Al-rich” and “Al-poor” glasses, while Al coordination increases only in “Al-rich” glasses. XPS results show Bi “opens” the glass network, enhancing I incorporation. At high Bi content, depolymerization may reduce stability. Moderate Bi₂O₃ doping should then be optimal, balancing waste load and glass stability for nuclear waste applications.

PacRim S28 - Joining and Integration of Ceramics for Enabling Complex Components and Adv Apps

PACRIM Symposium 28 - Joining and Integration of Ceramics for Enabling Complex Components and Adv Apps II

Room: Seymour

Session Chair: Heloisa Ramlow, Swiss Federal Laboratories for Materials Science and Technology

1:15 PM

(PACRIM-S28-003-2025) Laser joining of ceramics and metals for manufacturing complex components in molten-salt batteries

H. Ramlow^{*1}; H. Ghasemi-Tabasi²; M. Harald³; A. Burn²; G. Blugan¹

1. Swiss Federal Laboratories for Materials Science and Technology, Laboratory for High Performance Ceramics, Switzerland
2. Switzerland Innovation Park Biel/Bienne AG, Switzerland
3. Battery Consult AG, Switzerland

The joining of ceramics to metals is crucial for enabling complex components in energy storage systems. This study explores the potential of laser joining as a faster and more scalable alternative to conventional furnace joining in molten-salt Na/NiCl₂ batteries. These batteries require durable, corrosion-resistant, and leak-tight α-Al₂O₃-metal joints to prevent short circuits between metal connectors and Na-doped β"-Al₂O₃ solid electrolytes. While furnace joining at 1000 °C is slow and costly, laser joining offers a more efficient solution. In this work, α-alumina, AgCuTi interlayer, and metal alloy components were joined using both laser and furnace techniques under an argon atmosphere. Laser joining reduced processing time significantly from 6 hours with furnace joining to just 3 minutes. Scanning electron microscopy and energy dispersive X-ray spectroscopy analyses showed a higher Ti concentration at the filler-metal alloy interface, likely due to reactions between Ti and Ni to form Ti_xNi_y intermetallic compounds. A few Ti_xO_y reaction layers formed at the alumina interface due to titanium scavenging, explained by the dissolution of nickel and iron from the alloy in the molten braze. These results demonstrate that laser joining not only shortens processing time but also enables the integration of ceramics into complex components, improving scalability and cost-effectiveness.

1:35 PM

(PACRIM-S28-004-2025) Microstructure of hot-pressed ZrC and ZrC-Ti-ZrC diffusion bonded interface

S. Karcher^{*1}; J. Tallan¹; J. McCloy¹

1. Washington State University, School of Mechanical and Materials Engineering, USA

Zirconium carbide ceramics offer high strength, corrosion and wear resistance at extreme temperatures, enabling their use for applications in areas such as hypersonic vehicles and jet engine components. ZrC ceramics were synthesized from nano-sized ZrC powders by hot uniaxial pressing at 1600° C and 40 MPa, resulting in <10 μm diameter, equiaxed ZrC grains. Polished sections of the ZrC pellet were diffusion bonded at temperatures up to 1600° C in a vacuum furnace, using a 10 to 50 μm thick Ti foil interlayer to facilitate diffusion while minimizing void formation. Various Ti layer thicknesses were used in order to achieve a homogenous microstructure at the interface and a continuous compositional gradient of Ti through the joint. The resulting microstructures were evaluated by SEM-EDS and electron backscatter diffraction (EBSD). XRD was used to characterize the initial ZrC powders and diffusion bonded joints. Raman spectroscopy was used to provide additional information on carbon and oxygen defects in non-stoichiometric ZrC and to evaluate minor phases present due to impurities in one of the starting ZrC powders.

1:55 PM

(PACRIM-S28-005-2025) Design Strategies for Joining Dissimilar Materials

M. C. Patterson*¹; P. Brune¹; R. Amaro¹; W. Parks¹; J. Tucker¹;
M. Kuttolamadom²; C. Mora Salcedo²; H. Nied³; A. Bujanda⁵; P. Allison⁴;
C. Ritter²; R. Swinney³; V. Yun⁶; G. Kim⁶; J. Benoit⁷

1. Kratos Defense and Security Solutions, Kratos SRE R&D, USA
2. Texas A&M University, USA
3. Lehigh University, USA
4. Baylor University, USA
5. US Army Combat Capabilities Development Command, USA
6. 3DFlexible, USA
7. Sciperio, USA

Traditionally, the manufacturing of different materials (metals, polymers and ceramics), has been performed separately with multi-material systems requiring additional strategies such as adhesives or brazes to combine materials and address the dissimilar interface properties. These interfaces can often perform in an inferior manner to the bulk materials due to residual stress and poor chemical bonding. The resulting interfaces can act as points of failure in multi-material systems particularly when exposed to environmental changes found in their use applications. The efficient generation of surface shapes afforded by additive manufacturing, provides a useful strategy to design interfaces for specific use environments while minimizing interfacial stress. Strategies for polymer/metal and metal/ceramic interfaces are discussed in the context of modeling and experimental validation. With flat designs, edge stresses are regions for increased scrutiny and require additional design strategies to minimize edge stress and provide more robust interfaces. Various strategies are considered in conjunction with the process necessary to fabricate the architecture interfaces, which as scale becomes smaller and more intricate, generate process related flaws that adversely affect the properties. Thus, a balance between design and process capabilities must be considered.

PacRim S29 - Progress in High-Entropy Materials

PACRIM Symposium 29 - Thermodynamic, kinetic, physical, and environmental properties II

Room: Plaza A

Session Chairs: Theresa Davey, Bangor University;
Shijun Zhao, City University of Hong Kong

1:15 PM

(PACRIM-S29-030-2025) On the role of chemical disorder on the irradiation and oxidation resistance of high-entropy carbide ceramics (Invited)

S. Zhao*¹

1. City University of Hong Kong, Hong Kong

High entropy carbide ceramics (HECCs) hold great potential as structural materials in advanced nuclear reactors that operate in harsh environments characterized by high temperatures and irradiation doses. Based on first-principles calculations, we explore the accumulation and evolution of irradiation-induced defects and anti-oxidation properties. Our results reveal that the high-entropy mixing of different transition metals within the cation sublattice only has a minor impact on the irradiation defect evolution. By examining the defect energetics and kinetics, we propose a parameter, that is, the recombination energy barrier of the Frenkel pair defects, to dictate the irradiation tolerance of rocksalt high-entropy ceramics. Leveraging first-principles data, we determine the heterogeneous oxygen adsorption ability of different constituent elements in HECs. Incorporating this fundamental-level understanding, multi-objective optimization (MOO) was performed to identify a compositional

region with potentially intrinsic oxidation immunity, achieving a balance between the compactness of the oxidation product and the thermodynamic stability of the HEC matrix. Based on our analysis, we propose a compositional design strategy involving the strategic reduction of elements with higher oxygen adsorption energies, to effectively improve the oxidation performance of HECs.

1:45 PM

(PACRIM-S29-031-2025) Transition Metal Distribution in Dual Phase High Entropy Boride-Carbide Ceramics (Invited)

W. Fahrenholtz*¹; S. M. Smith¹; G. Hilmans¹; S. Curtarolo²

1. Missouri University of Science & Technology, Materials Science and Engineering, USA
2. Duke University, Materials Science, Electrical Engineering and Physics, USA

Macroscopic thermodynamic was used to predict the distribution of transition metals between boride and carbide phases in dual phase high entropy ceramics. An ideal solution model was applied to predict the preference of metals for boride and carbide phases based on the Gibbs' free energies of formation. Individual metals were analyzed to determine the partitioning between the two phases along with the assumption that metals did not interact with each other. Predicted and actual metal contents showed a strong correlation. Subsequently, results from the model were compared to experimental results, which enabled estimation of the Gibbs' free energy of formation of phases for which no data were available. The model points to future needs for more detailed knowledge of solution thermodynamics in boride and carbide ceramics along with analysis of diffusion behavior in these systems.

2:15 PM

(PACRIM-S29-032-2025) Oxygen adsorption, absorption, and diffusion in FeCrNi medium entropy alloy: An ab initio study (Invited)

H. Zhang*¹

1. University of Alberta, Chemical and Materials Engineering, Canada

Despite significant advances in understanding interstitial diffusion in bulk medium entropy alloys (MEA) and high entropy alloys, the role of principal elements in governing surface interstitial diffusion remains unclear. In this work, we employ density functional theory to investigate oxygen adsorption, absorption, and diffusion in a model FeCrNi MEA. The adsorption energy for oxygen cohesion to all investigated surfaces was lowest for the sites containing Cr, suggesting a positive effect of Cr in producing a chromium oxide scale. The position of Cr at the surface or subsurface is the most important factor for adsorption energy and the permeation barrier, while the effect of Fe and Ni on the permeation barrier had less impact on diffusion. In addition, it was observed that diffusivity was highly sensitive to changes in Cr local concentration before and after the jump. This work provides insights into the formation of chromium scaling based on oxygen adsorption and permeation, with potential implications in the design of oxidation-resistant surfaces for high-temperature applications.

2:45 PM

(PACRIM-S29-033-2025) Structure and property relationship in high-entropy thermoelectric materials (Invited)

J. He*¹

1. Southern University of Science and Technology, China

In high-entropy materials, local chemical fluctuation from multiple elements inhabiting the same crystallographic site plays a crucial role in their unique properties. Using atomic-resolution chemical mapping, we identified the respective contributions of different element characteristics on the local chemical fluctuation of high-entropy structures in thermoelectric materials. Electronegativity and mass had a comparable influence on the fluctuations of constituent elements, while the radius made a slight contribution. The local chemical

fluctuation was further tailored by selecting specific elements to induce large lattice distortion and strong strain fluctuation to lower lattice thermal conductivity independent of increased entropy. The chemical bond fluctuation induced by the electronegativity difference had a noticeable contribution to the composition-dependent lattice thermal conductivity in addition to the known fluctuations of mass and strain field. Our findings provide a fundamental principle for tuning local chemical fluctuation and lattice thermal conductivity in high-entropy thermoelectric materials.

3:30 PM

(PACRIM-S29-034-2025) Phase stability, structure distortion, and local bonding in multi-principal component UHTC transition metal carbides (Invited)

T. Davey^{*1}; Y. Chen²

1. Bangor University, Nuclear Futures Institute, United Kingdom
2. Tohoku Daigaku, School of Engineering, Japan

High-entropy or multi-principal component ultra-high temperature ceramics (UHTCs), such as MC_{1-x} carbides (where the cation $M=Ti,Zr,Hf,Nb,Ta$), may have potential improved or tuneable properties such as melting point, hardness, ductility, and oxidation resistance. At high temperatures, the configurational entropy in these multi-principal component mixtures is thought to overcome any opposing enthalpic effects inhibiting mixing, resulting in single solid solution phases. However, despite the individual group IV and V transition metal carbides having similar properties and behaviour on an atomic or electronic scale, the elemental differences result in complex local behaviour, with significant distortion in the crystal structure and huge variations in bond strengths resulting from the local atomic environment. Although the thermodynamic stability can determine whether or not a mixture is a single phase at equilibrium, variations in the local structure may affect other features such as mechanical properties and oxidation rates. This work explores variation in local structural and bonding properties in MC_{1-x} ($M=Ti,Zr,Hf,Nb,Ta$) mixtures from binary to quinary systems and attempts to correlate them to phase stability.

4:00 PM

(PACRIM-S29-035-2025) Order to disorder transition due to entropy in layered MAX phases

B. C. Wyatt^{*1}; Y. Yang²; P. Michalowski³; D. Jiang²; B. Anasori¹

1. Purdue University, Materials Engineering, USA
2. Vanderbilt University, Department of Chemical and Biomolecular Engineering, USA
3. Siec Badawcza Lukaszewicz - Instytut Mikroelektroniki i Fotoniki, Poland

There is controversy in the high-entropy community regarding the relation of short-range ordering observed in compositionally complex materials to the competition between enthalpy and entropy effects. Due in part to this observation, the moniker “high-entropy” for many as-reported high-entropy material systems has become a point of contention within the general materials community. In this work, we use the unique structure of nanolayered MAX phases, with their many covalent-metallic-covalent interfaces, to address this controversy systematically. By experimentally synthesizing nearly 40 known and newly reported carbide MAX phases containing between 2 to 9 transition metals, we show that the enthalpy-related preference for short-range ordering of transition metals remains until the total number of transition metals causes the entropy-related effects to overcome this preference. Lastly, we also show that these MAX phases can be used to synthesize their corresponding MXenes by selectively removing the metallic layer in the MAX phase. Overall, this work represents a major step in understanding the competition of enthalpy and entropy on the short-range ordering in high-entropy materials.

PacRim S33 - Ceramics for Electrochemical Energy Storage

PACRIM Symposium 33 - Ceramics for Electrochemical Energy Storage I

Room: Plaza C

Session Chairs: Michael Naguib, Tulane University; Valerie Pralong, CNRS ENSICAEN

1:15 PM

(PACRIM-S33-001-2025) Advances in next generation sustainable energy storage systems (Invited)

S. Mathur^{*1}; D. Patrun¹

1. University of Cologne, Institute of Inorganic and Materials Chemistry, Germany

The present energy challenges require new concepts in battery design, beside the extensive studies being performed on optimization of established battery materials. The modification of electrode architectures is necessary to enhance performance, sustainability and adaptability to future energy needs. These include the ongoing integration of batteries in a variety of electronics from wearable electronic devices up to transportation and therefore improvements in energy density, faster charging rates and enhanced battery lifetime are required. Techniques like 3D printing of electrodes, anode-less batteries and dual integrated photo-battery systems are concepts for next generation battery devices, offering several advantages: (1) 3D printing is an adaptive technique, which provides high degree of freedom in designing the electrode structure, while being scalable and cost-efficient. (2) Anode-free lithium and sodium metal batteries are a safer and lighter alternative, because they eliminate the traditional host anode for the $Li^+/-Na^+$ -ions, resulting in enhanced energy density and reduced battery weight. (3) The photo-battery combines both electrode functions, energy harvesting and storage, thereby offering an innovative and promising solution for sustainable battery systems. All three concepts are suited for future integration in different alkali-ion batteries including compatibility with solid state electrolytes.

1:45 PM

(PACRIM-S33-002-2025) Design of new cathode material for Na and K-ion batteries (Invited)

V. Pralong^{*1}

1. CNRS ENSICAEN, France

One of the major challenges of the 21st century is the need to resolve problems linked to energy generated by constantly increasing consumption, demographics, and standards of living. It is therefore imperative to anticipate this energy demand in a context of sustainable development and security. Storage technologies are highly dependent on the materials used, so it is necessary to search for new materials with advanced properties that are also ecological and economical. Despite the high performance of lithium-based batteries, the production of lithium associated with environmental costs pushes scientists to develop alternative systems such as Na-ion or K-ion batteries. Indeed, sodium and potassium are abundant and uniformly distributed across the earth's crust. For these reasons, we decide to explore the inexpensive and non-toxic Na/K-Mn-O systems. We report for the first time the electrochemical behavior of a-(Na-K)₃MnO₄ phase. We will discuss the different systems and detail our strategy to offer new sustainable electrode materials.

2:15 PM

(PACRIM-S33-003-2025) Two-dimensional Molybdenum-Based MXene and MBene as Electrode Materials for Electrochemical Energy Storage

K. Eisawi^{*1}; E. Loni¹; A. Majed¹; M. Naguib¹

1. Tulane University, Physics and Engineering Physics, USA

MXenes are a large family of electrically conductive two-dimensional (2D) transition metal carbides and nitrides. Their ability to host ions, combined with low diffusion barriers for ion transport on their surfaces, makes them excellent candidates as electrode materials for ion batteries and capacitors. Mo-based MXenes are particularly notable as they can be synthesized both with and without ordered vacancies. Similarly, Mo-based borides (MBenes) can also be produced with ordered vacancies, similar to MXenes. This makes Mo-based MXene and MBene systems compelling for studying the effects of vacancies and the distinct roles of carbon and boron. Herein, we report the novel synthesis of Mo-based MXenes and MBenes, along with an evaluation of their electrochemical performance. These materials exhibit excellent performance at high specific currents; for example, $\text{Mo}_{4/3}\text{B}_2$ maintained a specific capacity of over 250 mAh/g after more than 500 cycles at currents up to 2 A/g. Our results highlight Mo-based MXenes and MBenes as promising candidates for energy storage applications, with potential use in both Li-ion batteries and Li-ion capacitors.

2:35 PM

(PACRIM-S33-004-2025) Experimental study of energy harvesting from mechanical load on cement-lead zirconate titanate composites

V. Kumar^{*1}

1. Birla Institute of Technology, MECHANICAL ENGINEERING, India

This paper presents the energy harvesting characteristics of a cement-lead zirconate titanate (PZT) composite through mechanical load. Four distinct composites were fabricated by incorporating 5%, 10%, 20%, and 40% PZT (weight%) into cement, utilizing PZT powder of approximately 1-micron size. The experiment involved 28-days water-cured unpoled composites. The study examines the waveform characteristics of the voltage generated by a unique energy harvesting circuit and the collected electromagnetic radiation (EMR) energy. The resultant peak EMR voltage and peak EMR energy are 1.47 V and 0.09 μW , respectively, with an applied mechanical energy of 500 mJ at 40% cement-PZT concentration. The sample with the highest cement-PZT proportion (i.e. 40% by weight) and maximum applied mechanical energy exhibits an increase in the generated EMR voltage and EMR energy waveform. Both DC voltage and the EMR energy acquired from the energy harvesting circuit exhibit an increasing pattern corresponding to an increase in applied mechanical energy. The wired and wireless sensor applications, such as structures and highway crack deformation, can benefit from the electromagnetic radiation energy harvesting response. This study improves our understanding of how to use impact-induced energy for efficient and sustainable structural purposes.

2:55 PM

(PACRIM-S33-005-2025) Metal-Organic Frameworks (MOFs) integrated separators for Li-ion Batteries

B. Saruhan-Brings^{*1}; N. Wood¹; A. Ray¹

1. Deutsches Zentrum für Luft- und Raumfahrt DLR, Institute of Materials Research, Germany

In recent years, many methods have been developed to extend the service life of LIBs and prevent effects that impact on service life and efficiency such as gas formation. Metal-organic frameworks (MOFs) could suitably absorb these gases. The development of MOF-integrated separators for absorption and storage of H_2 , O_2 , CO and RH are currently being carried out within the EU-funded project-PHOENIX. In this work, PVDF-HFS based polymer separators were functionalized with porous MOFs in order to increase the

porosity and surface area of the separators, thereby increasing the electrolyte absorption capacity and ionic conductivity to absorb gases. The selected MOFs (e.g. Zr-MOF, Ni-MOF) have been produced using solvothermal synthesis and characterized by XRD, SEM/EDX to ensure that the synthesis was successful. The synthesized MOFs have been embedded in a polymer matrix in order to produce MOF-polymer separators to fabricate LIB half-cells in form of coin cells. In addition, commercial polymer and glass fiber separators are coated with the synthesized MOFs to investigate the influence of MOFs on the electrochemical performance. GCD measurements were taken in a voltage window of 2.7-4.2 V and with C/10 for 5 cycles. The GCD measurements of the PVDF-HFP polymer separators showed a promising specific capacity of 80-100 (mAh/g).

3:30 PM

(PACRIM-S33-006-2025) Evaluation of low crystallinity in Li-rich layered oxide electrode by pair distribution function analysis (Invited)

M. Oishi^{*1}; K. Nakatsuka¹; Y. Otokura¹; S. Hiroi²; K. Ohara²

1. Tokushima Daigaku, Department of Science and Technology, Japan

2. Shimane Daigaku, Japan

Further improvements of lithium-ion secondary batteries are required. Conventional positive electrode materials exhibit excellent charge-discharge cycle characteristics because only Li-ions are extracted and inserted while maintaining the crystalline structure of the material. In contrast, Li-rich layered oxide (LLO) materials achieve high energy density. LLO materials change their crystal structure during the charge and discharge, and it shows a lower crystalline state at the charged state. In this study, X-ray total scattering measurements were performed. The crystal structure variations during the charging and discharging of LLO were evaluated. The structural parameters in the various states of charge/discharge of LLO material $0.3\text{Li}_x\text{MnO}_3-0.7\text{LiMeO}_2$ (Me=Ni, Co, Mn) were determined through a crystal pair distribution function (PDF) analysis. We clarified the existence of a low-crystal structure in LLO formed by the crystal structure change accompanying the migration of Me ions during the charge/discharge cycles.

4:00 PM

(PACRIM-S33-007-2025) Tailored NMC core/shell cathode powder for long cycle life LIB batteries

S. N. Krüger¹; B. N. Tasdemir¹; B. Saruhan-Brings^{*1}

1. Deutsches Zentrum für Luft- und Raumfahrt DLR, Institute of Materials Research, Germany

NMC ($\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$) cathode materials with high Ni content remain the most successful formulas, delivering strong overall performance and excellent specific energy. However, the increased reactivity of Ni with surface oxygen during charge-discharge cycles and larger Li/Ni cationic mixing can lead to chemical and structural degradation, resulting in poor cycling performance, rapid capacity fading and short cycle life. The present work deals in the frame of EU-funded PHOENIX project with the development of core/shell structured NMC-particles. This morphology provides surface stabilization of NMC90 core via Mn-rich (NMC 622) shell by keeping the energy storage capabilities at higher level and prevents cathode degradation. For its synthesis, an oxalate-assisted, two staged coprecipitation route and advanced in-situ Li-infiltration approach has been developed. Moreover, prior to application of Mn-rich shell, a thin WO_3 layer has been brought onto the surface of the Ni-rich core particles to prevent interdiffusion between the core and shell. Relying on a relatively high I(003)/I(104) ratio (1.59 at NMC90 and 2.18 at NMC622), it is shown that the formation of R3m structure via in-situ Li-infiltration can be achieved for both compositions already at 850 °C. Further electrochemical studies and long cycling tests have been carried with half-cell LiBs using core/shell NMC cathodes with and without WO_3 interlayer.

4:20 PM

(PACRIM-S33-008-2025) Optimizing TiNb₂O₇: Impact of Particle Size, Defects, and Crystallinity on Accelerated LithiationC. Sturgill²; I. Milisavljevic¹; S. Wechsler²; M. Muhić²; H. zur Loye²; S. T. Mixture^{*1}; M. Stefić²

1. Alfred University, USA
2. University of South Carolina, Department of Chemistry and Biochemistry, USA

Wadsley-Roth (WR) niobate phases have garnered significant attention as promising candidates for durable, fast-charging lithium-ion batteries. Among them, TiNb₂O₇ (TNO) stands out for its potential to enable rapid lithium diffusion while minimizing lithiation-induced strain during electrochemical cycling. This study aims to improve TNO battery performance by examining how crystallization, shaped by microstructure and defect-sensitive properties, affects key electrochemical behaviors. Spray-dried nanostructured TNO was heat treated in a temperature range of 600-1100°C. The sample annealed at 800°C showed the highest galvanostatic C-rate lithiation capacity retention at 5C of around 260 mAh/g. It also exhibited the lowest electrical resistivity as measured by the intermittent current interruption method. Detailed XANES and EXAFS analysis revealed progressive elimination of point/extended defects and increasing octahedral distortion with crystallization. The combination of changes resulted in TNO heat treated at 800°C having a remarkable 10C capacity of approximately 233 mAh/g, which compares favorably to other leading TNO examples. This research emphasizes the intricate atomic structure and architectural changes that take place during crystallization, potentially advancing our understanding of other WR battery materials.

4:40 PM

(PACRIM-S33-009-2025) Reducing Surface Energy Stress in Nano-LiCoO₂ with Lanthanum Doping (Invited)R. Castro^{*1}; S. Dahl²; K. Joshi¹

1. Lehigh University, Material Science & Engineering, USA
2. University of California Davis, USA

The dynamic environment within lithium-ion batteries causes significant changes in local thermodynamic functions, hindering accurate predictions of cathode stability during cycling. While delithiation primarily impacts the surface properties of the cathode structure, the evolution of interfacial energies with varying stoichiometry is not well understood. Here, we used microcalorimetry to quantify, for the first time, the thermodynamic changes between stoichiometric and partially delithiated nano-LiCoO₂ states. Mild delithiation from LiCoO₂ to Li_{0.71}CoO₂ reduced surface energy, weakening grain adhesion by ~0.4 J/m². The introduction of 1.0 atom % lanthanum lowered the surface energy of stoichiometric LiCoO₂ and stabilized surface energy during delithiation down to Li_{0.57}CoO₂, reducing thermodynamic stress between grains and mitigating degradation mechanisms. Lanthanum-induced surface stabilization also suppressed coarsening and dissolution of the cathode particles. Using electron microscopy, we proposed an atomistic mechanism by which lanthanum doping stabilizes surfaces, improving cathode durability.

PacRim S34 - Carbon based mtl's & smart struct for elec/phononics/elec-chemical/ MEMS & energy app**PACRIM Symposium 34 - Carbon based materials and smart structures for advanced engineering application I**

Room: Grouse

Session Chairs: Richard Fu, Northumbria University; Haitao Ye, University of Leicester

1:15 PM

(PACRIM-S34-001-2025) From diamond/ β -SiC composites to porous diamond networks (Invited)X. Jiang^{*1}

1. University of Siegen, Institute of Materials Engineering, Germany

Diamond composites are more attractive than diamond individually for some electronic, mechanic, physical, chemical and engineering applications since the components in such composites integrate the features of diamond with other materials. For years, my group has been working on the chemical vapour deposition of such diamond-based composites. In this presentation, recent processes and achievements with respect to the synthesis, characterization and applications of these diamond composite films will be presented. A briefly overview on all these composites will be given at the first part of my presentation, followed by the details about chemical vapor deposition of nanocrystalline diamond/ β -SiC composite films. The control of the crystal quality, grain size and phase distribution of both diamond and β -SiC phases in the composite films will be shown in detail. The application of these composite films for the fabrication of porous diamond network and porous SiC membranes will be highlighted. As case applications, the usage of these diamond composite film as cutting tool coating, as the substrates for sensing applications (e.g., for trace heavy metal detection) and as the bio-interfaces for selective protein adsorption and DNA immobilization, as the electrode for energy storage will be subsequently introduced. The future research directions and perspectives will be outlined at the end of my presentation.

1:45 PM

(PACRIM-S34-002-2025) Diamond High Power and Voltage MOSFETs: Inch-Sized Wafer Growth and Power, Dynamic, RF FET Characteristics (Invited)M. Kasu^{*1}; N. Saha¹; M. Eguchi¹

1. Saga University, Electrical and Electronic Engineering, Japan

Diamond possesses an ultrawide bandgap energy of 5.47 eV, a breakdown field of >10 MV/cm, higher thermal conductivity (22 W/cmK), and higher electron and hole mobilities (4500 and 3800 cm²/Vs, respectively) than GaN and SiC. Therefore, diamond is the most capable candidate for power semiconductor device applications. Diamond single-crystals have been limited to sizes of 4 mm. We have demonstrated a two-inch-diameter diamond wafer grown on an Ir/sapphire (a-Al₂O₃) (11-20) substrate. The heteroepitaxial diamond layer exhibited the highest crystal quality, with a dislocation density of 1.4x10⁷ cm⁻², and XRC FWHM of 98 arcsec. For diamond p-channel MOSFETs, we have established p-type doping on the H-terminated diamond using NO₂ gas, and the thermal stabilization and gate insulation with ALD Al₂O₃ layer. We have fabricated diamond MOSFET demonstrating a high drain current density of 0.68 A/mm, a low ON-state resistance of 50 Ω mm, and an extremely high OFF-state breakdown voltage of -2568 V. The specific on-state resistance was determined to be 7.54 m Ω cm², and the maximum available power, i.e., BFOM has been obtained to be 874.6 MW/cm², the highest ever in diamond. Diamond RF MOSFET

with a 157-nm long T-shaped gate has demonstrated a power-gain cut-off frequency (f_{MAX}) of 120 GHz, the highest ever. This indicates that diamond can be applied to millimeter-wave range amplifiers.

2:15 PM

(PACRIM-S34-003-2025) Carbon Nanotubes-Localized Surface Plasmon Fiber Optic Sensors for Gases Detection (Invited)

T. Allso²; M. Al Araimi³; R. Arif⁴; P. Davey⁵; D. Webb⁶; A. Rozhin^{*1}

1. Aston University College of Engineering and Physical Sciences, Nanoscience Research Group, Aston Institute of Photonic Technologies, United Kingdom
2. Grimsby Institute and University Centre Grimsby, Engineering, United Kingdom
3. University of Technology and Applied Sciences, Engineering, Oman
4. University of Sulaimani College of Science, Iraq
5. University of Plymouth, School of Engineering, Computing and Mathematics, United Kingdom
6. Aston University College of Engineering and Physical Sciences, Aston Institute of Photonic Technologies, United Kingdom

Single-Walled Carbon Nanotubes (SWNTs) have unique optical and surface properties, making them ideal for sensing applications. Traditional electronic gas sensors face limitations in explosive environments due to the risk of electrical sparks. To address this, we present a novel optical fibre sensor platform that combines Localized Surface Plasmon (LSP) technology with SWNTs for safe and selective gas detection. The platform is developed on a D-shaped optical fibre coated with a multi-layer structure of Ge, SiO₂, and platinum. Ultraviolet laser treatment creates an ordered array of nanowires capable of supporting LSPs. Functionalized SWNTs, adhered to the nanowire surface, enable selective gas detection. The sensor demonstrates excellent sensitivity and selectivity for both CO₂ and NO_x gases, achieving detection limits as low as 150 ppm for CO₂ and 109 ppm for nitrous oxide (N₂O), with rapid response times of under 20 seconds. This optical approach eliminates electrical hazards, making it particularly valuable for deployment in hazardous environments. The demonstrated platform can be extended for other gases detection by modifying the SWNT surface functionalization, offering a highly versatile solution for environmental monitoring and industrial applications.

2:45 PM

(PACRIM-S34-004-2025) Lithium electrolytes from sustainable mineral sources and their electrochemical performance

J. Rodrigues^{*1}; J. Restivo¹; J. P. Sousa¹

1. International Iberian Nanotechnology Laboratory, Portugal

The processing of lithium chloride to obtain lithium hydroxide using a sustainable efficient alternative in the form of membrane electrolysis opens pathways in the processing of lithium ores and brines. Ore processing through chlorine-based leaching and LiCl adsorption from brines are significantly more efficient processes. The viability of these pathways is highly dependent on the electrochemical performance of the obtained lithium salts. This work focuses on the assessment of the electrochemical performance of lithium salts. LiCl and LiOH electrolytes were doped with selected contaminants based on the composition of spodumene concentrates. The behaviour of the electrochemical cell was evaluated and compared with known references. The mechanisms involved are investigated and further validated through tests conducted with varying contamination levels, combinations of contaminants, and samples derived from the processing of natural lithium sources. The results reveal that the presence of aluminum and iron in the electrolyte enhances the oxygen evolution reaction. However, when carbon-based working electrodes are used, the carbon undergoes oxidation, resulting in the formation of insoluble lithium carbonate. These lithium carbonate salts accumulate on the electrode surface, obstructing access to the reaction medium and compromising the electrode's integrity.

3:30 PM

(PACRIM-S34-005-2025) Vertical 3D Field Effect Transistors With Nanoscale Gate-All-Around (Invited)

C. Gu^{*1}

1. Chinese Academy of Sciences Institute of Physics, China

Three-dimensional (3D) vertical gate-all-around (GAA) transistor has the strongest gate control ability and the capacity to effectively suppress the short channel effect. However, at present, there are still some problems, such as the difficulty of device processing and the complexity of electrodes interconnection, which greatly restrict and postpone the practical application of this device structure. In this work, we present a systematic investigation of 3D vertical GAA transistors. In order to simplify the fabrication processes and enhance the flexibility of electrode layout of 3D vertical GAA devices, a new method for fabricating 3D suspended electrodes is proposed. The electrodes prepared by this method can use air as an isolation layer to greatly reduce the parasitic effect between electrodes. Three vertical GAA devices with different channel materials such as Si, Diamond and ZnO are designed and fabricated by combining the fabrication method of suspended electrode. Focused ion beam (FIB) technology is used to realize the interconnection of devices' electrodes. By studying the fabrication processes and performance of these devices, the advantages of FIB technology and 3D suspended electrodes in 3D device processing are highlighted, such as high efficiency, high controllability and low cost.

4:00 PM

(PACRIM-S34-006-2025) Polyaniline/Ta₂C MXene nanocomposites for electromagnetic noise reduction

A. Arshad^{*1}; A. Elmarakbi¹; R. Y. Fu²

1. Northumbria University, Mechanical and Construction Engineering, United Kingdom
2. Northumbria University, United Kingdom

MXene-based nanocomposites are potential candidates to meet the escalating challenges posed by EMI and radiation. Despite the promising characteristics of MXene, the synthesis of flexible and long-term stable polymer-MXene nanocomposites with exceptional EMI shielding is considerably challenging. This study investigates novel PANI/Ta₂C MXene nanocomposites for EMI shielding. Chemically synthesised PANI/Ta₂C MXene nanocomposites are characterized, and their flexible free-standing films are prepared. PANI/Ta₂C MXene nanocomposites demonstrate synergistic behaviour to shield EMI superior to either component. A free-standing film of PANI/Ta₂C nanocomposite I exhibits an excellent shielding efficiency of 58 dB over a frequency range from 7 to 13 GHz, which corresponds to 99.999% shielding effectiveness and specific shielding performance (SSE) as high as 580 dB/mm. These ultra-thin, lightweight and flexible free-standing films may find application in next-generation EMI shielding solutions for flexible electronic packaging that demands both signal protection and portability.

4:20 PM

(PACRIM-S34-008-2025) Development of MOF-based composites as an efficient approach for CO₂ Capture and Storage

S. P. Fernandes^{*1}; J. P. Sousa¹

1. International Iberian Nanotechnology Laboratory, Portugal

Global greenhouse gas emissions have increased over the years. To overcome this problem, European Commission has adopted a set of proposals (European Green Deal) to tackle the current climate crisis, with the aim of achieving carbon neutrality by 2050. Thus, the development of carbon capture, utilization, and storage (CCUS) technologies has emerged as a promising alternative to conventional treatments, allowing CO₂ emissions to be reduced and CO₂ to be reused. The adsorption process, due to its low energy consumption, easy implementation and low operational cost, has been used as a

promising technique in CCUS. The choice of a suitable absorbent is a key factor. Metal-Organic Frameworks (MOFs), due to their high porosity, excellent crystallinity and tunability, have emerged as promising materials to be used as adsorbents for CO₂ capture. However, owing to their original form as a solid powder, the use and processing of MOFs under real conditions is difficult. Activated carbon (AC) are purely carbon-based materials with high surface area and thermal/chemical stability, which are inexpensive and easy to obtain in the form of pellets. However, the lack of selectivity of AC for the CO₂ molecule reduces its interest as adsorbent. Thus, the formation of hybrid materials composed of AC pellets and MOFs (AC@MOFs) will be addressed, and their performance for CO₂ capture will be evaluated.

4:40 PM

(PACRIM-S34-009-2025) Embedding Shape Memory Alloys into Carbon Fiber Reinforced Polymer via Embroidery for Improved Energy Absorption and Damping

E. Ghoniem^{*1}; H. Ong¹; J. Manrique²; S. Iwan³; A. Elmasry¹; R. Y. Fu¹; A. Elmarakbi¹

1. Northumbria University, Mechanical and Construction Engineering, United Kingdom
2. Fundacion para la Investigacion y Desarrollo en Transporte y Energia, Spain
3. thermoPre Engineering GmbH, Germany

Carbon Fiber Reinforced Polymers (CFRP) composites provide excellent strength-to-weight ratios, while Shape Memory Alloys (SMAs), such as Nitinol, offer unique shape-changing properties. However, combining these materials poses challenges, including mechanical compatibility, thermal stability, and manufacturing complexities. Existing methods for embedding SMAs, such as layering and adhesive bonding, face limitations regarding strength, performance, and structural integrity. Key factors like SMA wire dimensions, placement, actuation temperature, and interface adhesion must be optimized to prevent damage and enhance composite properties. This study explores embroidery as an innovative technique for embedding SMAs into CFRP composites. Embroidery enables precise SMA placement, improving mechanical integration and facilitating the development of advanced composite structures capable of responding to external stimuli. By carefully analyzing factors such as wire dimensions, actuation temperatures, and interface bonding, the research tests the performance of embroidered composites under various thermal conditions. Results demonstrate that this approach enhances energy absorption and damping capacity, confirming the potential of embroidered SMA-CFRP composites for high-performance engineering systems.

Friday, May 9, 2025

PacRim S2 - Frontier of modeling and Design of Ceramics and composites

PACRIM Symposium 2 - Modeling materials structure, stability, formation and degradation

Room: Balmoral

Session Chair: Laurent Karim Béland, Queen's University

8:00 AM

(PACRIM-S02-014-2025) High-Entropy Ceramics for Passive Radiative Cooling Applications: a Theoretical Standpoint (Invited)

C. Borghesi²; L. Latterini⁴; A. Pisello³; I. Castelli⁵; G. Giorgi^{*1}

1. The University of Perugia, Department of Civil & Environmental Engineering, Italy
2. Consiglio Nazionale delle Ricerche, Italy
3. The University of Perugia, Department of Engineering, Italy
4. The University of Perugia, Department of Chemistry, Biology, and Biotechnology, Italy
5. Danmarks Tekniske Universitet, Department of Energy Conversion and Storage, Denmark

The ever-increasing concentration of CO₂ is mainly associated with the fossil fuel consumption for energy production. Accordingly, while on one side the community had deeply focused since decades on renewables, the time has come to couple this field with that of a technology aimed at mitigating effects, i.e., able to reduce anthropogenic CO₂ production, particularly critical in those areas, the Urban Heat Islands, overheated contexts where ~68% of the global population lives. In this sense, Passive Radiative Cooling (PRC) represents an important mechanism. PRC is a natural nocturnal (exploitable also at daytime if proper conditions are fulfilled) phenomenon that can cool surfaces without energy consumption. Passive coolers directly emit heat through a transparent atmospheric spectral window ("atmospheric sky window", ATW, 8–13 μm) into the cold universe. Applied over buildings' envelopes, they have been shown to reach subambient surface temperature, improving comfort and saving energy in the built environment. In this scenario, High-Entropy Oxides (HEOs) seem to be compounds with relevant features as passive coolers. By means of a campaign of ab-initio calculations, in the present contribution we show that some of the discussed HEO combine the features of a wide bandgap and highly dispersive material with those of an excellent IR emitter, evenly spreading IR-active modes in ATW.

8:30 AM

(PACRIM-S02-015-2025) Phase stabilities of perovskite and non-perovskite lanthanide tungsten nitrides from first principles

C. Fisher^{*1}; T. Ogawa¹; H. Moriwake¹

1. Japan Fine Ceramics Center, Japan

A systematic comparison of crystal and electronic structures of perovskite nitrides LnWN₃ (Ln = La, Pr, Nd, Sm, Eu, Gd, Dy, Yb) calculated within the framework of density functional theory using various exchange-correlation functionals and pseudopotentials is reported. Lattice energies and phonon dispersion curves suggest that other lanthanides besides LaWN₃ may exhibit ferroelectricity, although the smallest lanthanide predicted to have a non-centrosymmetric perovskite structure as its ground state depends on the type of functional and pseudopotential used. The results highlight the importance of using sufficiently accurate and transferable functionals when small differences in energy are involved in comparing polymorphs.

8:50 AM

(PACRIM-S02-016-2025) Atomistic modelling of pyrolysis and material properties of polymer-derived silicon-oxycarbides using novel machine-learning methods (Invited)

J. Rohrer*¹; N. Leimeroth¹; L. Erhard¹; K. Albe¹

1. Technische Universität Darmstadt, Institut für Materialwissenschaft, Germany

Silicon-oxycarbides (SiOCs) are polymer-derived glass ceramics showing outstanding versatility in technological applications that range from protective coatings to energy storage and biomedical devices. This versatility originates from a tunable chemical composition and microstructure that can be tailored by the choice of precursor and pyrolysis temperature. Here we present a novel machine-learning potential (MLP) for quaternary Si-O-C-H systems, specifically designed for SiOCs. This MLP enables large-scale simulations of 100-thousands of atoms over several (10 - 100) nanoseconds on state-of-the-art compute clusters. We demonstrate its ability to simulate phase-formation under pyrolysis conditions and produce realistic model geometries with different compositions and morphologies of the turbostratic free carbon phase. We then study materials properties of these polymer-derived ceramics in relation to their structure and composition and investigate the role of hydrogen for their thermodynamic stability. A key finding is the delicate dependence of the stiffness on Si-C bonds that contradicts commonly assumed relations to the free carbon phase.

PacRim S10 - Ceramics of Tomorrow for Green Energy and Cleaner Environment

PACRIM Symposium 10 - Ceramics of Tomorrow for Green Energy and Cleaner Environment III

Room: Georgia B

Session Chairs: Marina Leite, UC Davis; Gurpreet Singh Selopal, Dalhousie University

8:00 AM

(PACRIM-S10-022-2025) Synthesis of hollow nanoparticles and their applications through composite with functional ceramics (Invited)

K. Ishii*¹; M. Fujii²

1. Nagoya Kogyo Daigaku, Advanced Ceramics Research Center, Japan
2. Nagoya Institute of Technology, Japan

Hollow silica nanoparticles consist of a void core and a silica shell. They exhibit unique properties due to the extremely small hollow spaces and the pore structure of the silica shell. In this presentation, we will discuss the technology for controlling the pore structure of hollow particles during the synthesis process and the functionality when titania is combined with the silica shell.

8:30 AM

(PACRIM-S10-019-2025) Investigating the Properties of TiO₂ with High-Concentration Nb Doping (Invited)

D. Hao*¹

1. Shanghai Institute of Ceramics Chinese Academy of Sciences, China

Titanium dioxide (TiO₂) is widely recognized as a practical and versatile photocatalyst due to its high chemical stability, low toxicity, and abundant availability. It has been extensively studied for applications including antiviral activity, deodorization, self-cleaning, organic contaminant degradation, and solar energy conversion. However, its wide band gap and reduced efficiency after immobilization—particularly following thermal treatment—have limited its broader application. In this study, high-concentration niobium-doped TiO₂ (25 at.%) nanoparticles were synthesized via solvothermal, sol-gel,

and plasma methods. The phase transformation, light absorption properties, and band gap evolution of the doped TiO₂ were systematically investigated at elevated temperatures. The visible light photocatalytic activity of the materials was evaluated after high-temperature heat treatment, revealing that the niobium-doped TiO₂ demonstrated superior thermal stability and visible light activity compared to commercial TiO₂. Furthermore, an interphase-dependent mechanism for enhancing photocatalytic performance under visible light was proposed, supported by electron spin resonance (ESR) measurements. This work provides a promising strategy for developing thermally stable TiO₂ with enhanced visible light photocatalytic activity.

9:00 AM

(PACRIM-S10-020-2025) Self-assembly of metal hydroxide salt monolayer nanoparticles toward efficient electrocatalysts (Invited)

N. Tarutani*¹

1. Hiroshima University, Graduate School of Advanced Science and Engineering, Japan

Transition metal-based layered hydroxides are known as potential catalysts for efficient oxygen evolution reaction. Since the discovery of the excellent electrochemical catalytic performance of exfoliated hydroxide nanosheets, many studies have focused on the synthesis and catalytic use of hydroxide nanosheets/nanoparticles. In general, conducting materials and binder materials are co-dispersed with hydroxide catalysts for electrochemical characterization. Drying the dispersion allows the formation of catalyst composites, which enables the evaluation of the electrochemical catalytic property with ease. However, influential factors such as aggregation structures and interface structures are difficult to control, which complicates the elucidation of materials design strategies. Here, we focus on the design of metal hydroxide electrocatalysts without conducting and binding materials through a self-assembly process. Metal hydroxide monolayer nanoparticles were prepared based on our previous report. Molecule-modified Au electrodes were dipped in the nanoparticle dispersions to trigger self-assembly and immobilization of nanoparticles. Assembled films of metal hydroxide nanoparticles showed >100 times higher weight-normalized catalytic performance compared with catalysts prepared by traditional methods using conducting and binder materials.

MOVED to Thursday, May 8 at 11:50 AM

(PACRIM-S10-021-2025) Hybrid multiscale ceramics: enhanced mechanical behavior and energy applications (Invited)

D. Giuntini*¹

1. Eindhoven University of Technology, Mechanical Engineering, Netherlands

The great potential of engineering materials at the nano- and microscale to foster emergent properties at the macroscale is particularly relevant for ceramics and ceramic-based composites. Nano/micro-structured ceramics combine the unique features of ultrasmall building blocks and their organization into tailored architectures to foster new functionalities. Many applications open up, e.g. in catalysis, energy and optoelectronics. The fabrication of such materials is however a tricky task. Control of the arrangement of nano- and micro building blocks requires finely tuned self-assembly procedures and careful compositional design, whilst interfaces between components largely control the macro scale material response. This talk will tackle these aspects for some promising examples of nano- and micro architected ceramic-based materials. A strategic combination of different material processing technologies will be shown, spanning colloidal assembly of hybrid building blocks and recent advancements in ultra-rapid material consolidation techniques.

10:20 AM

(PACRIM-S10-018-2025) Vertically Aligned MXene Nano-ceramics for High-Performance Lithium-Ion Battery Electrodes (Invited)H. Zarrin^{*1}; Y. Liu¹; D. Hwang¹

1. Toronto Metropolitan University Faculty of Engineering & Architectural Science, Chemical Engineering, Canada

Lithium-ion batteries are vital for sustainable energy solutions, particularly in electric vehicles and portable electronics. To meet increasing demands for higher capacity, faster rates, and greater stability, advanced ceramic materials like MXenes are key due to their excellent conductivity, stability, and tunable properties. This study introduces a novel method to fabricate vertically aligned MXene nano-ceramics with reduced graphene oxide, forming free-standing anodes for lithium-ion batteries. Using a modified microfluidic technique, we created 3D porous films with vertical alignment and macro-porosity, enhancing ion transport and conductivity. Optimization of fabrication parameters, including precursor concentration and flow rate, yielded reproducible high-performance structures. Electrochemical tests revealed specific capacities over 400% higher than commercial anodes, with improved cyclability and durability. This innovation highlights the potential of MXene-based nanocomposites and scalable fabrication techniques to revolutionize energy storage systems, aligning with sustainable energy goals.

10:50 AM

(PACRIM-S10-023-2025) Development of photocatalytic filters for the degradation of indoor air pollutantsI. M. Oliveira^{*1}; J. P. Sousa¹

1. International Iberian Nanotechnology Laboratory, Portugal

Most people spend 70–90% of their time indoors, where poor air quality can provoke serious health risks due to the release of volatile organic compounds (VOCs) from different sources. Unlike conventional air purifiers that mainly trap particulate matter, photocatalysis offers a promising solution by converting indoor air pollutants into harmless substances. Titanium dioxide (TiO₂) nanoparticles are widely used as highly effective photocatalysts due to their non-toxicity, low cost, and long-term stability. However, their photocatalytic activity is limited to UV radiation and presents a high recombination rate of electron–hole pairs, reducing efficiency. To overcome these limitations, TiO₂–C₃N₄ (carbon nitride) composites were developed to enhance visible light activity and decrease recombination rates. The composites were synthesized with different proportions of TiO₂ and C₃N₄ through a simple ball-milling method. Photocatalytic experiments under visible light, using a standard organic dye in water, identified 90% TiO₂–10% C₃N₄ as the most effective composite, achieving 70% degradation efficiency. The optimized material was further immobilized and tested for photocatalytic activity in a gaseous system, demonstrating its potential for indoor air purification under visible light. This study highlights TiO₂–C₃N₄ composites as a cost-effective and efficient solution for improving indoor air quality.

11:10 AM

(PACRIM-S10-024-2025) Role and functionality of nanocatalysis on hydrogen and energy research: Intermediate States through Synchrotron Based Spectroscopies (Invited)M. Huttula^{*1}

1. University of Oulu, Finland

Photocatalysis offers a prominent route for energy conversion e.g., water splitting, CO₂ reduction and pollutant degradation. Understanding the intermediate states formed during these reactions is crucial for optimizing photocatalytic efficiency and developing new materials with enhanced performance. Synchrotron radiation (SR), with its ability to provide detailed chemical and electronic structure information at the atomic and molecular level, serves

as a powerful tool in this analysis. By utilizing techniques such as X-ray absorption spectroscopy (XAS) and X-ray photoelectron spectroscopy (XPS), we can observe the formation, evolution, and disappearance of intermediate states in real-time. This allows us to construct a comprehensive picture of the photocatalytic process, from the initial light absorption to the final product formation. We have employed SR-based characterization to study a range of photocatalytic materials, including metals, metal oxides, sulphides, and hybrid nanomaterials. These studies have revealed critical insights into the role of surface states, charge carrier dynamics, and the impact of environmental factors on photocatalytic activity. Recently we have identified the role of transient species as key intermediates in the reaction pathway.

PacRim S17 - Additive Manufacturing of Ceramics and Composites**PACRIM Symposium 17 - Additive Manufacturing of Ceramics and Composites IV**

Room: Prince of Wales

Session Chairs: Zehui Du, Nanyang Technological University; Chang-Jun Bae, Korea Institute of Materials Science

8:00 AM

(PACRIM-S17-023-2025) Vat photopolymerization of SiC with submicron ceramic particles (Invited)Z. Du^{*1}; T. Y. HO¹; C. Gan²

1. Nanyang Technological University, Temasek lab, Singapore
2. Nanyang Technological University, School of Materials Science and Engineering, Singapore

Vat photopolymerisation (VP) 3D printing of SiC ceramics with dense or hierarchical porous microstructures makes it possible to fabricate various complex shapes for wide applications in energy management, aerospace and defence. However, SiC VP 3D printing remains challenging due to strong UV absorption and high refractive index of the SiC particles. Current approaches in realizing VP of SiC ceramics have been largely using large, micron-sized SiC particles to improve the cure depths of printed slurries, but at the detriment of sintering activity. In this work, we present a few strategies to enhance the cure depth of slurries prepared with sub-micron SiC particles, including particle surface modification, adding UV-transparent secondary phase and using longer-wavelength light for curing, etc. Simultaneous improvement on the cure depth of derived slurries (~40–60 μm) and the densification of the printed green bodies through sintering (up to ~90% relative density) have been obtained. The effects of the modification strategies on the cure depth and width of derived SiC slurries were studied systematically, and mechanistic insights were elucidated. Furthermore, the application of the 3D printed SiC ceramics as a heat sink and catalyst supports will be demonstrated.

8:30 AM

(PACRIM-S17-025-2025) Vat photopolymerization 3D printing and joining of large-scale and intricate Si₃N₄ structures with UV-thermal dual curable slurryZ. Koh^{*1}; C. Gan¹; Z. Du¹

1. Nanyang Technological University, Temasek lab, Singapore

Si₃N₄ ceramics have garnered significant attention as structural ceramic due to its exceptional mechanical and thermal properties. However, vat photopolymerization 3D printing of Si₃N₄ ceramics with large dimension and intricate structures remains challenging due to its strong UV light absorbance which limits cure thickness to be only ~30–50 μm, leading to high susceptibility to printing failure. In this work, Si₃N₄ slurry dual curable with UV light and/or

heat has been developed for vat photopolymerization 3D printing and joining of Si_3N_4 . The slurry exhibit high photo-cure thickness up to $\sim 72\mu\text{m}$ at UV energy density of $7.31\text{mJ}/\text{mm}^2$ and thermally curable at $\sim 150^\circ\text{C}$. The dual curing mechanism is discussed based on interaction between ceramic particle surface chemistry and resins. Complex Si_3N_4 structures with diameter/height up to $\sim 13\text{cm}$ have been successfully 3D printed with the slurry and sintered to $\sim 96\%$ density. The slurry were further used to bond two 3D printed Si_3N_4 green bodies, resulting in joined ceramics with flexural strength comparable to that of non-bonded counterpart. More complex Si_3N_4 structures that are difficult to one-step 3D print have been demonstrated with joining process using dual curable slurry. These results demonstrate potential of Si_3N_4 slurry for advancing scalability and application of Si_3N_4 ceramic additive manufacturing.

8:50 AM

(PACRIM-S17-026-2025) NiFe_2O_4 soft magnets obtained by Direct Ink Writing 3D printing

L. Wilk^{*1}; J. Marchewka¹; M. T. Sitarz¹

1. Akademia Gorniczko-Hutnicza im Stanislawia Staszica w Krakowie, Poland

In today's increasingly electrified and technologically advanced world, functional magnetic materials attract significant attention from academia and industry. The global market for magnetic materials, valued at USD 31 billion in 2021, is projected to reach USD 48 billion by 2030, driven by demand from the automotive, energy, and electronics sectors. Among these, spinel-structure ferrites stand out for their versatility, functioning as hard or soft magnets depending on chemical composition, while also offering high thermal and corrosion resistance and electrical resistivity. This study utilized the Direct Ink Writing (DIW) 3D printing method to fabricate nickel ferrite-based components. Additionally investigation of thermal treatment parameters on the structural, microstructural, and magnetic properties of the final products was carried on. Preliminary optimization of the initial material composition focused on selecting an appropriate liquid medium to ensure favorable rheological properties. The study also analyzed the spinel inversion parameter, which affects the magnetic properties of the materials. Structural characterization employed spectroscopic techniques such as Raman spectroscopy and Mössbauer spectroscopy. This research was supported by the "Excellence Initiative – Research University" program at AGH University of Krakow and the National Science Centre, Poland, under grant number 2024/53/N/ST11/02608

PacRim S18 - Nanostructured Metal Oxides and Metal Chalcogenides for Adv Functional Applications

PACRIM Symposium 18 - Nanostructured Metal Oxides and Metal Chalcogenides for Adv Functional Applications

Room: Seymour

Session Chairs: Theodosia Gougousi, University of Maryland, Baltimore County; Pelagia-Irene Gouma, The Ohio State University

8:00 AM

(PACRIM-S18-001-2025) Chalcogenide-based photonics integrated devices and applications (Invited)

J. Pan²; Z. Li^{*1}

1. Sun Yat sen University, China
2. South China Normal University, China

The sixth primary group of chalcogenide-based materials has attracted widespread attention due to its numerous advantages, including transmission from visible to mid-infrared wavelengths, ultra-low optical loss, high nonlinearity, and high elastic optical

coefficients. Here, we have conducted innovative research on chalcogenide-based materials, covering material systems based on chalcogenides, integrated photonics chip and device fabrication, and integrated chip demodulation systems and their applications. This manuscript discusses a novel chalcogenide-based material with excellent elastic optical coefficients and its manufacturing process, which can effectively detect highly sensitive ultrasound signals. A photonic micro-ring array device with a quality factor close to 10^6 and a noise equivalent pressure as low as $2.2\text{mPa}/\text{Hz}^{1/2}$ has been successfully fabricated, with an ultrasound signal bandwidth coverage of 175 MHz. Advanced parallel spectroscopic detection techniques have been employed to achieve wavefront array detection of ultrasound fields, enabling photoacoustic imaging in vivo zebrafish and demonstrating broad application prospects.

8:30 AM

(PACRIM-S18-002-2025) Optimization of Green Quantum Dots–Transforming the Landscape of Next-Generation Optoelectronic Technologies

G. Selopal^{*1}; K. Shanmugasundaram¹; U. Sohail¹; S. Madhu¹; M. Chinna¹

1. Dalhousie University, Department of Engineering/ Faculty of Agriculture, Canada

Colloidal quantum dots (QDs) hold great promise in optoelectronic technologies due to their remarkable and adjustable optoelectronic properties through the rationale involving size, atomic composition of core and shell, shapes, and surface states. However, most high-performing QDs in optoelectronic devices contain hazardous metal elements, including Cd and Pb, posing significant environmental risks and hindering commercialization development. In the past few years, green QDs, so-called eco-friendly, have attracted considerable attention due to their application in next-generation optoelectronics technologies. However, the performance of green QDs-based devices is still lower than conventional QDs due to unfavourable non-radiative recombination, insufficient separation and transfer of charge carriers, and limited stability. In the talk, the optimization of green QDs via core/shell and interface engineering will be discussed. A detailed discussion on the different synthesis approaches, the effect of different shell thicknesses, compositions, and interfacial layers of core/shell on the optoelectronic properties to develop structural-properties relationship will be discussed. Finally, the integration of optimized green QDs in different optoelectronic technologies, such as solar windows, green-hydrogen production and anti-counterfeiting, will be discussed.

8:50 AM

(PACRIM-S18-003-2025) A new route for synthesis of GeTe nanoparticles using organometallic precursors

M. Bouska¹; Y. Milasheuskaya¹; M. Slouf²; P. Knotek¹; S. Pechev³; L. Prokes⁴; L. Pecinka⁴; J. Havel⁴; M. Novak¹; R. Jambor¹; P. Neme^{*1}

1. University of Pardubice, Czechia
2. Institute of Macromolecular Chemistry, Czechia
3. Institut de Chimie de la Matière Condensée de Bordeaux – CNRS, France
4. Masarykova univerzita Přírodovědecká fakulta, Czechia

Nanoparticles can offer an alternative approach to fabricate phase-change materials such as GeTe. Up to now, the chemical synthesis of GeTe nanoparticles using organometallic precursors exploits high-boiling solvents and relatively high temperatures. The aim of this work is the preparation of GeTe nanoparticles by a low-temperature synthetic method exploiting specific organometallic precursors and common organic solvents. Indeed, different preparation methods and characterization of GeTe nanoparticles is presented. The characterization of the prepared nanomaterial was performed based on X-ray diffraction, transmission electron microscopy, scanning electron microscopy with energy dispersive X-ray spectroscopy, laser ablation time-of-flight mass spectrometry, Raman scattering spectroscopy, and dynamic light scattering. The results show that the low-temperature synthetic route leads to amorphous GeTe nanoparticles. Exploited

organometallic precursor is stabilised by neutral ligand which can be isolated after the reaction and repeatedly used for further reactions. Furthermore, GeTe nanoparticle size can be tuned by the conditions of the synthesis. The financial support of the Czech Science Foundation under the project No. 22-07635S is greatly acknowledged.

9:10 AM

(PACRIM-S18-004-2025) The effect of process temperature on the properties of ALD TiO₂ films (Invited)

T. Gougousi^{*1}

1. University of Maryland Baltimore County, Physics, USA

Temperature plays a critical role in determining the properties of thin films, particularly those deposited by Atomic Layer Deposition (ALD). In this study, we investigate the impact of deposition temperature on the properties of TiO₂ films grown using tetrakis dimethyl amino titanium (TDMAT) and water. Our focus is on the influence of temperature on phase formation and the incorporation of nitrogen into the films. Films deposited at 100°C crystallize in the anatase phase after inert annealing, while those deposited between 150–300°C transition to the rutile phase. At 350°C, films exhibit mixed phases that vary with thickness. In terms of composition, films deposited at temperatures above 200°C incorporate oxynitride bonding, significantly affecting both the linear and nonlinear optical properties, as well as electrical conductivity. These variations are most pronounced between 200 and 275°C, a temperature range commonly considered the “ALD window.” Our findings reveal previously unreported reaction pathways that significantly influence the optical and insulating properties of the films. This work provides new insights into the temperature-dependent behavior of ALD-grown TiO₂ films and offers critical guidance for optimizing film properties for optoelectronic applications.

9:40 AM

(PACRIM-S18-005-2025) The Ferrochromic Nature of ε-WO₃: A True Binary Ferroelectric

M. Rahaman^{*1}; J. Flores²; M. Noor³; M. Rahaman³; M. Rahaman¹;

M. Rahaman¹; M. C. Rahaman¹; M. Newburger²; P. Gouma¹

1. The Ohio State University, Materials Science and Engineering, USA

2. Air Force Research Laboratory, USA

3. The Ohio State University, USA

Developing ferroelectric polymorphs with rapid, energy-efficient dipole switching is vital for next-generation displays, memory devices, and neuromorphic systems. This study introduces ε-WO₃, a unique binary ferroelectric polymorph, and examines the electro-optical response of thin films made from nanopowders. Piezo-response Force Microscopy (PFM) revealed nano-domain switching at low electric fields (a few kV/cm). High harmonic generation analysis provided insights into nanodomain orientation, while their interaction with light caused a distinctive blue coloration under electro-optical stimuli. Visible light responses were confirmed through C-V measurements. The “ferro-chromic effect”—rapid, reversible coloration of ε-WO₃ thin films induced by voltage without electrolytes—was investigated using X-ray Photoelectron Spectroscopy and Linear Optical Measurements. These results highlight ε-WO₃'s potential for single-layer, solid-state devices, including ubiquitous displays, energy-efficient windows, and non-volatile memory systems, offering a promising solution for sustainable and advanced ferroelectric technologies.

10:20 AM

(PACRIM-S18-006-2025) Hybridizing Laser-Induced Graphene (LIG) and Molybdenum Oxide (MoO_x) Using Metal-Organic Decomposition for VOC Gas Sensing

A. Katsura^{*1}; O. Okanishi¹; Y. Hirose¹; T. Sugahara¹

1. Kyoto Kogei Sen'i Daigaku, Japan

Metal-Organic Decomposition (MOD) method has been widely utilized for the synthesis of metal oxides due to its broad adaptability, capability to produce high-purity metal oxides, and ease of processing. In recent years, researchers have employed MOD to synthesize molybdenum oxide (MoO_x) nanostructures for a variety of applications such as gas sensors, energy storage, and electrochromic devices. On the other hand, Laser-Induced Graphene (LIG), a carbon material fabricated by irradiating a polymer substrate with a laser, is a promising substrate material for gas sensors due to its high electrical conductivity, large surface area, and simple fabrication process. In this study, MoO_x nanostructures were deposited onto LIG using the MOD method. The resulting LIG/MoO_x samples were characterized by SEM, XRD, Raman spectroscopy, BET analysis, and electrical resistance measurements. Then, their sensing properties to volatile organic compounds (methanol, ethanol, acetone, and 2-propanol) were evaluated. The results showed that the LIG/MoO_x hybrid gas sensor displayed a pronounced n-type response at 300°C, achieving a sensitivity of 46.9% for 1098 ppm ethanol. These findings highlight the potential of LIG/MoO_x hybrids in high-performance flexible gas sensors.

10:40 AM

(PACRIM-S18-007-2025) Preparation of complex metal oxide ceramic nanofibers by electrospinning

I. Shepa^{*1}; K. Nemes¹; E. Mudra¹; P. Hviscova¹; R. Smolko²; F. Kromka¹;

M. Balaz³; M. Lisnichuk¹; K. Balazsi⁴

1. Institute of Materials Research Slovak Academy of Sciences, Ustav materialoveho vyskumu Slovenskej akademie vied, Košice, Košice Region, SK, academic/eng, Slovakia

2. Ustav experimentalnej fyziky Slovenskej akademie vied, Slovakia

3. Institute of Geotechnics, Slovak Academy of Sciences, Košice 040 01, Slovakia, Slovakia

4. Centre for Energy Research HAS, Thin Film Physics, Hungary

This work focuses on the preparation and detailed characterization of oxide ceramic nanofibers composed of group IV (Ti, Zr, Hf) and group V (Ta, Nb) transition metals, with the primary goal of achieving a single-phase material. The utilization of the reactive electrospinning allowed obtain in a single step, pre-ceramic composite PAN/MeO_x fibers, where Me = Ti, Zr, Hf, Nb, Ta, which were further transformed into porous ceramic MeO_x nanofibers via calcination at different temperatures. Thermogravimetric studies described the thermal properties of the precursor fibers and thus defined the necessary heat treatment profile. It was found that calcination at 600 °C results in pure ceramic fibers without carbon residues, while an increase in the heat treatment temperature resulted in the crystallization of the ceramic component and the gradual formation of distinct phases. The changes in fibrous morphology and mean diameter of the ceramic nanofibers obtained at different temperatures were analyzed via electron microscopy. A surface area was determined through nitrogen adsorption measurements, while X-ray diffraction was utilized to confirm the crystallinity and phase composition of the calcined fibers. Acknowledgment “Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00579.”

11:00 AM

(PACRIM-S18-008-2025) 3D Self Supported Nanofibrous Visible Light Photocatalysts based on Cu Doped TiO₂

F. Mikaeili^{*1}; M. Rahaman¹; P. Gouma¹

1. The Ohio State University, Materials Science and Engineering, USA

This study highlights the development of 3D, self-supported nanofibrous TiO₂ structures (nanogrids) synthesized via blend electrospinning. The incorporation of anatase and brookite phases in Cu-doped TiO₂ nanogrids significantly enhances their photocatalytic properties. Cu doping narrows the bandgap, shifting the absorption edge to the visible spectrum and enabling efficient separation of photogenerated charge carriers. The brookite phase further boosts performance by minimizing electron-hole recombination. Comprehensive characterization, including cyclic voltammetry and chronoamperometry, revealed that Cu-doped TiO₂ nanogrids generate a substantial photocurrent under visible light, demonstrating superior photocatalytic efficiency. These nanogrids outperform P25 Degussa, being activated by natural sunlight without requiring nanoparticle filtration. Their self-supported structure combines the advantages of nanomaterials without the associated challenges, making them highly effective for advanced photochemical applications in environmental remediation and energy production. This work offers valuable insights for designing efficient, sustainable photocatalysts.

PacRim S20 - Advanced Functional Materials for Clean Energy Solutions

PACRIM Symposium 20 - Synthesis and characterization of carbon and thermal management materials

Room: Georgia A

Session Chairs: David Patrun, University of Cologne;

Lars Österlund, Uppsala University

8:00 AM

(PACRIM-S20-029-2025) Improving Combustion Heating Energy and Emissions in Steel Manufacturing via Retrofit Ceramic Inserts (Invited)

K. Breder^{*1}; B. Nakanishi¹; D. Woolley¹; E. Buchovecky¹; F. Mirri¹; B. Yoon¹; T. Briselden²

1. Saint-Gobain Research North America, USA

2. Saint-Gobain, Performance Ceramics and Refractories, USA

Steel reheating in continuous annealing lines often relies on radiant tube combustion. By introducing ceramic retrofit heat exchangers and flame disruption inserts, the energy consumption and CO₂ emissions can be reduced by up to 30% while significantly lowering NO_x emissions. Advanced forming technologies for Siliconized Silicon Carbide (SiSiC) have enabled the use of this material to produce highly efficient and complex inserts that can be used in existing steel furnaces. This presentation will focus on the fundamental principles and opportunities for improving radiant tube heating efficiency with a focus on retrofit ceramic technologies. Through advanced, additive manufacturing complex shapes are manufactured on an industrial scale to significantly reduce manufacturing impact on the environment. The stresses in these complex shapes have been evaluated by thermal modeling, and strength testing and Weibull analysis have been performed to ensure the survival of the heat exchangers in the given application.

8:30 AM

(PACRIM-S20-030-2025) Multilayer Thin Films with Synergetic Catalytic, Self-Cleaning and Antipathogenic Properties (Invited)

L. Österlund^{*1}

1. Uppsala Universitet, Materials Science and Engineering, Sweden

Multilayer films have been made that synergistically improve their combined catalytic, self-cleaning and light collection properties. First, we show how multilayer structures exhibiting spectrally selective optical properties can be used to make self-cleaning and dynamic optical modulating films. Anatase TiO₂ films are deposited on thermochromic VO₂, which heats to the TiO₂ film as it absorbs near-infrared light absorption above the critical temperature for the semiconductor to metal phase transition, thus accelerating catalytic reactions. Second, we show how the same effect can be used to obtain an enhanced self-cleaning solar absorber TiAlN coating. Third, we show how super-acid titania can be made by means of a photo-fixation method of SO₂ and NO₂ gas molecules to produce sulfated and nitrate titania surfaces, respectively, with superacid properties. By doing so, the wetting properties and surface chemistry of the TiO₂ films are modified, resulting in sustainable organic catalysis and antimicrobial properties. Finally, we present results of a photochromic film structure that exhibits omnidirectional antireflection, dynamic solar control, and self-cleaning made by scalable colloidal lithography methods realizing Mie scattering nanopillars for wide angle light collection. We discuss how such materials could be implemented as energy efficient windows or cover glass coatings.

PACRIM Symposium 20 - Advanced synthesis and characterization of metal organic framework materials

Room: Georgia A

Session Chairs: Gunnar Westin, Uppsala University;

Peter Broquist, Uppsala University

9:00 AM

(PACRIM-S20-031-2025) Towards Broadband Photocatalysis (Invited)

D. Ma^{*1}

1. Institut national de la recherche scientifique Centre energie Materiaux Telecommunications, Canada

Forming nanomaterials junctions and using plasmons represent two important, promising strategies for realizing broadband photocatalysis in strategically important applications such as solar fuels and photocatalytic degradation of pollutants. In this talk, I will present some of our recent work on the rational design of nanohybrids and their applications in solar fuels and photocatalysis. One example is about the in situ synthesis of plasmonic Ag nanoparticles (AgNPs) and Ag-MOF. The intimate and stable interface between the AgNPs and Ag-MOF and hot electron transfer from the plasmonic AgNPs to MOF led to highly efficient visible-light photocatalytic H₂ generation in aqueous solution, which surpasses most of reported MOF-based photocatalytic systems. This work sheds light on effective electronic and energy bridging between plasmonic NPs and MOF.

9:30 AM

(PACRIM-S20-032-2025) Effect of Hydrophobicity on Porphyrin-Based Zr-MOFs for Photosynthesis of Hydrogen Peroxide

Y. Kondo^{*1}; S. Mizutani²; Y. Kuwahara²; K. Mori²; T. Sekino¹; H. Yamashita²

1. Osaka University, SANKEN, Japan

2. Osaka University, Graduate School of Engineering, Japan

Hydrogen peroxide (H₂O₂) has attracted much attention as not only an eco-friendly oxidant but also a liquid fuel. At present, H₂O₂ is produced by an anthraquinone oxidation process, but this process requires high energy due to the multistep reaction and produces

waste byproducts. Photosynthesis approach is a sustainable and facile method for H₂O₂ synthesis because it only needs earth abundant dioxygen (O₂), water (H₂O), and sunlight. Metal-organic frameworks (MOFs), which are a class of porous coordination compounds consisting of metal-oxo clusters and organic linkers, offer significant chemical diversity to develop highly efficient photocatalysts. In this work, we used Zr-MOFs (Zr-TCPP) containing a TCPP linker as a photocatalyst for H₂O₂ production. Zr-TCPP was modified with perfluoro-carboxylic acids with different alkyl chain lengths to hydrophobize it (Zr-TCPP-RFx). Hydrophobicity of Zr-TCPP-RFx increased as the alkyl chains of the modified perfluorocarboxylates became longer. Photocatalytic H₂O₂ production was performed using MOFs dispersed in an O₂-saturated aqueous solution under visible-light irradiation. The H₂O₂ production of hydrophobic Zr-TCPP-RFx was higher than that of the pristine Zr-TCPP. The photocatalytic activity was significantly improved by modifying perfluorocarboxylates with the optimal length of alkyl chains on Zr-TCPP.

10:10 AM

(PACRIM-S20-033-2025) Driving Sustainable and Clean Energy Solutions using Carbon Nanomaterials (Invited)

R. Naccache*¹

1. Concordia University, Chemistry and Biochemistry, Canada

Carbon dots have garnered significant interest with their compact size, versatile and tunable surface chemistry, simple and low-cost synthesis. While some of the reported works on these dots have focused on catalytic applications, their investigation as heterogeneous catalysts for the production of biofuels such as biodiesel remains unexplored. Biodiesel fuel production remains one of the most promising alternatives to non-renewable fossil fuels such as conventional oil and diesel. However, many challenges persist in its production particularly related to the tedious purification processes, high cost of production and unsustainable practices. Thus the need for the development of novel, sustainable and metal free heterogeneous catalysts is required. Here we show that these dots can trans/esterify the conversion of oils to biofuels with sustained catalytic efficiency for at least five reaction cycles. Our second and third-generation catalysts allow for a significant reduction of reaction temperature and operate at ambient pressure without a significant increase to the catalyst loading. Our work now tackles waste and inedible oils in order to reduce the overall cost of the process. This cost-efficient, sustainable and effective heterogeneous catalyst can have positive economic and environmental repercussions that can further drive academic and industrial research in this burgeoning area.

10:40 AM

(PACRIM-S20-034-2025) Photo-fenton degradation of carbon nanotubes in water: enhanced kinetics with pre-treated commercial materials

J. P. Sousa*¹

1. International Iberian Nanotechnology Laboratory, Portugal

With the rising interest in carbon nanotubes (CNTs), concerns about their impact on natural waters have grown. Identifying human exposure pathways beyond inhalation underscores the need for strategies to address water-based CNT contamination. The enzymatic degradation of CNTs has opened promising avenues for managing such contamination, with the Fenton reaction identified as the primary mechanism, driven by iron release from active centers. This mechanism has been replicated in the photo-Fenton degradation of multi-walled CNTs, but the lengthy degradation time (168 h) highlights the need for optimization. This study proposes pre-treatment of single-walled CNTs to enhance photo-Fenton degradation. Nitric acid oxidation introduces lattice defects and amorphous carbon, while ozone treatment adds oxygen-containing surface functionalities. Results show that increasing nitric acid strength (up to 7 M for 48 h) significantly accelerates degradation, achieving complete

breakdown within 48 h. However, extending oxidation beyond 24 h yielded only marginal improvements (90 to 92% degradation). Ozone pre-treatment was similarly effective, with comparable results to nitric acid. Combining both treatments further improved outcomes, achieving 95% degradation within 24 h.

PacRim S26 - Materials for Advanced Nuclear Energy Systems and Nuclear Waste Management

PACRIM Symposium 26 - Materials for Advanced Nuclear Energy Systems and Nuclear Waste Management II

Room: Plaza B

Session Chairs: Tyler Gerczak, ORNL; Xiao-Ying Yu, Oak Ridge National Laboratory; Tomas Grejtak, Oak Ridge National Laboratory

8:00 AM

(PACRIM-S26-012-2025) Insights into graphite-salt interactions via a multidisciplinary approach (Invited)

T. Grejtak*¹; J. Qu¹; J. Braatz²; W. Li³; J. D. Arregui-Mena¹; N. C. Gallego³

1. Oak Ridge National Laboratory, Materials Science and Technology Division, USA
2. Oak Ridge National Laboratory, Radioisotope Science and Technology Division, USA
3. Oak Ridge National Laboratory, Chemical Sciences Division, USA

Interest in molten salt reactors (MSRs) has surged in recent years as they represent a promising path towards clean and sustainable energy. In MSR, the graphite in-core components are in permanent contact with liquid salt which introduces new challenges in material compatibility. Although earlier experiments from the 1960s suggested that molten salts could be chemically inert to graphite, recent studies indicated that a continued exposure of graphite to molten salt can alter its local composition and microstructure and lead to changes in its mechanical, thermal and irradiation-resistant properties. This talk will outline a multidisciplinary approach to characterizing graphite-molten salt interactions to address key knowledge gaps in this area. Neutron imaging was used to investigate molten salt intrusion into the open pores of nuclear graphite with varying grades and microstructures, across a range of parameters, to visualize and quantify salt intrusion in graphite. Wetting behavior of molten salt on graphite was characterized using contact angle measurements to examine the compatibility and interaction between the salt and graphite. Lastly, tribological studies of graphite in lubricated molten salt conditions were conducted to evaluate the wear and friction properties of graphite pebbles. The outcomes of this work could provide guidance for evaluating the integrity and service life of MSRs.

8:30 AM

(PACRIM-S26-013-2025) Waste management considerations for advanced fission and fusion reactors (Invited)

J. McCloy*³; A. Goel²; J. Vienna¹; B. J. Riley¹; X. Guo³

1. Pacific Northwest National Laboratory, USA
2. Rutgers The State University of New Jersey, USA
3. Washington State University, USA

With the rapid evolution of new nuclear reactor technologies, both fission and fusion, the technical community is striving to address issues around the back end of the fuel cycle, given a large amount of uncertainty about what technologies will be deployed in the United States. Various designs for small modular reactors of light water reactor technology, as well as high temperature gas reactors, microreactors, metallic fuel reactors, and molten salt reactors all have very different considerations for waste streams that would

require reprocessing or immobilization. Additionally, while fusion reactors in principle will have lower amounts of radioactive waste than fission reactors, the management of tritium remains a significant challenge. In this talk we will summarize what is known and estimated about the radionuclide content of various waste streams, as well as some potential strategies for processing and waste form development. The pros and cons of various waste forms including glasses, ceramics, glass-ceramics, metals, and cermets for various advanced reactors will be summarized.

9:00 AM

(PACRIM-S26-014-2025) Sorbents for mercury and iodine capture

K. Carlson^{*1}; L. Sharpless¹

1. University of Nevada Reno, USA

The Hanford Site in Washington State is in the process of commissioning the Waste Treatment and Immobilization Plant to process a portion of the 54 million gallons of radioactive and chemical waste from Cold War weapon production. Technologies for the capture of volatile species of concern are still being assessed, and new methods and materials are developed as operational and flowsheet mission risks are identified. One such area still being assessed is the abatement efficacy of the Carbon Adsorber units to retain gaseous mercury and ¹²⁹I released during processing. It is challenging to predict the mercury chemistry due to the variability of the feed, and different methods/materials are required for the capture of gaseous Hg⁰ and Hg^{II} compounds. While pilot-scale studies can be used to produce prototypical off-gas streams, there are concerns regarding mercury quantification using common characterization methods due to interferences with other compounds present. Additionally, as the current sorbent is unable to chemically bind iodine, physical entrapment as an immobilization strategy must be assessed. This talk will focus on the fundamental challenges of gaseous mercury and iodine capture and characterization, as well as the new materials and robust evaluation methods that our group has developed to assist with abatement.

9:20 AM

(PACRIM-S26-015-2025) Structural Studies of Phosphate-based Electrorefiner Salt Waste Stream using X-ray Diffraction and Raman Analysis **WITHDRAWN**

I. C. Ajoku^{*1}; H. Werth²; K. Carlson²; P. Murray²; B. J. Riley³; C. Lonergan¹

1. Missouri University of Science and Technology, Materials Science and Engineering, USA
2. University of Nevada Reno, Chemical and Materials Engineering, USA
3. Pacific Northwest National Laboratory, Nuclear Science Division, Radiological Materials Group, USA

The immobilization of salt waste streams from chloride-based molten salt reactors through waste vitrification relies on the dechlorination efficacy and chemically durable structures that allow for long-term waste storage. This study investigated the impact of (Li, Na, K)₂O on the structural characteristics of (Li, Na, K)₂O-P₂O₅ waste glasses using H₃PO₄ precursor. The studied glasses were characterized utilizing x-ray diffraction (XRD) and Raman spectroscopy tools. Alkali salts appeared in samples at 300 and 400 °C in argon, while samples at 300, 400, and 600 °C in air were amorphous, utilizing XRD analysis. Strong POH bonds in phosphoric acid were revealed by Raman analysis of samples between 25 and 200 °C in Argon and air atmospheres at low-frequency bands. Strong P-O-P bonds in Q² and lithium species incorporated in the waste glasses under study were observed to dominate in samples at 300, 400, 500, and 600 °C in argon using a higher frequency band. For 50 mol% (Li, Na, K)₂O, samples in Argon at ≥ 300 °C revealed similar Q² structures in both the calculated O/P ratio and analyzed phosphate structure using Raman spectroscopy. XRD and Raman analysis revealed that samples at ≥ 300 °C in argon contained alkali cations.

9:40 AM

(PACRIM-S26-016-2025) Structural analysis of the thorite (ThTi₂O₆) and aeschynite (LaTiNbO₆) systems

M. C. Dixon Wilkins^{*1}; N. S. Yaw²; X. Guo²; N. C. Hyatt⁴; J. McCloy³

1. Washington State University, Institute of Materials Research, USA
2. Washington State University, Department of Chemistry, USA
3. Washington State University, School of Mechanical and Materials Engineering, USA
4. University of Bristol, School of Earth Sciences, United Kingdom

Brannerite (ATi₂O₆, A = Ce, Th, U) and aeschynite (REETiNbO₆, REE = La³⁺ to Dy³⁺) ceramics are of interest in a range of fields, including the immobilization of radioactive wastes and microwave dielectrics. Significant work exists examining Ce- and U-brannerites, with Th- and Pu-brannerites relatively less well studied. Of note is the existence of the low temperature α polymorph of ThTi₂O₆ alongside the high temperature brannerite structure; neither UTi₂O₆ nor CeTi₂O₆ have been reported to show such polymorphism. Similarly, La-aeschynites (LaTi(Nb/Ta)O₆) display polymorphism not observed for other aeschynites, with the aeschynite structure the low temperature polymorph, and a high temperature polymorph isostructural to α-ThTi₂O₆. In this work, the synthesis and characterization of the polymorphs of ThTi₂O₆ and LaTiNbO₆ will be reported, with a focus on structural analysis by Rietveld method refinements of diffraction data and Raman spectroscopy. Structural relations between the polymorphs and other related structures will be examined, particularly with respect to ionic size constraints and polyhedral connectivity. Given the applications of these materials, a deep understanding of the underlying structural chemistry is necessary to ensure stability of the desired phases over operational lifetimes.

10:20 AM

(PACRIM-S26-017-2025) The challenges facing adoption of coated particle fuel for the next generation of nuclear reactors (Invited)

T. J. Gerczak^{*1}; E. Lopez Honorato¹; G. Helmreich¹

1. Oak Ridge National Laboratory, USA

Tristructural isotropic (TRISO) coated particle fuel technology in the US was re-established under the US DOE Advanced Gas Reactor Fuel Development and Qualification (AGR) Program. The focus was on establishing a fuel qualification basis data package for uranium oxide/uranium carbide (UCO) kernel-TRISO fuel, under high temperature gas-cooled reactor (HTGR) concept operating envelopes. TRISO fuel particles consist of an all-refractory ceramic construction with a fissile kernel (UCO) coated with layers of low-density carbon buffer, dense inner pyrolytic carbon, silicon carbide, and dense outer pyrolytic carbon with each layer providing functionality. The success of the US AGR program has resulted in multiple advanced reactor concepts pursuing TRISO fuel, many with operational needs outside of the established envelope. A deeper understanding of the response of modern TRISO and other coated particle fuels to in-pile conditions and accident scenarios and the influence of property variations on performance is needed to extend the operational envelope. While consideration of new materials systems and particle architectures may be needed to adapt TRISO functionality to reactor concepts beyond HTGRs. The status of TRISO fuel research and development in the US and the challenges facing development of new coated particle fuel concepts for advanced reactor applications will be discussed.

10:50 AM

(PACRIM-S26-018-2025) Microwave-Assisted Recovery of Carbon-14 from Spent Ion Exchange ResinsG. Kim^{*1}; K. Lee¹; H. Park¹

1. Korea Atomic Energy Research Institute, Republic of Korea

Spent ion exchange resins (spent resins) play a critical role in liquid radioactive waste management at nuclear power plants (NPPs). The IRN-150 mixed-bed ion exchange resin, commonly used for purification processes, consist of cationic and anionic exchange resins. While the cation exchange resin removes radionuclides like Cs and Co, the anion exchange resin targets anions such as $\text{H}^{14}\text{CO}_3^-$. Spent resins containing carbon-14 (C-14) are categorized as low to intermediate level radioactive waste and require treatment to comply with disposal regulations in South Korea. In this study, we investigated microwave-assisted treatment for efficient recovery of C-14 while minimizing functional group degradation in the spent resins. Experiments were performed using simulated resins preloaded with HCO_3^- ions. Microwave treatments were applied with varying moisture contents in mock resins. To assess C-14 desorption efficiency, an acid stripping process with H_3PO_4 solution was employed. Additionally, the structural integrity of the resins was evaluated using ^{15}N NMR spectroscopy to analyze the functional group status post-treatment. The findings indicate that a controlled moisture content significantly enhances C-14 recovery while preserving the resin's functional groups. The optimized microwave treatment demonstrated potential for improving the safe and efficient management of intermediate level radioactive waste.

11:10 AM

(PACRIM-S26-019-2025) Sintering behavior of buffered UO_2 fuel doped with niobium oxidesS. Gobert²; F. Audubert²; J. Heintz^{*1}

1. ENSMAC-Bordeaux INP, ICMCB, France

2. CEA, DES, IRESNE, DEC, Cadarache, France

The nuclear fuel pellets (UO_2 or $\text{UO}_2\text{-PuO}_2$) used in pressurised water reactors are stacked in a metal cladding of zirconium alloy. During irradiation, particularly during power ramps, the fuel undergoes a reducing perturbation linked to the increase in temperature at the centre of the pellet. This results in a decrease in oxygen potential, which can increase the risk of cladding failure and therefore limit the fuel's lifespan. The objective of this study is to develop an innovative nuclear fuel containing a redox buffer to regulate the partial oxygen pressure ($p\text{O}_2$) within the reactor, thereby limiting stress corrosion cracking of the cladding. The selected redox buffer couple is $\text{Nb}_2\text{O}_5/\text{NbO}_2$. We will present the investigation of the densification behaviour of doped UO_2 fuel. The impact of dopant concentration and particle size has been evaluated through the monitoring of linear shrinkage and oxygen release from the pellet during the sintering process under a reducing atmosphere. This method has revealed a reduction of niobium oxides during sintering, leading to oxygen release, which appears to influence both the densification behaviour and the microstructure of the doped fuel.

PacRim S29 - Progress in High-Entropy Materials**PACRIM Symposium 29 - Manufacturing and characterization**

Room: Plaza A

Session Chairs: Yongho Sohn, University of Central Florida; William Weber, University of Tennessee

8:00 AM

(PACRIM-S29-036-2025) New Alloy Development Need for Additive Manufacturing (Invited)Y. Sohn^{*1}

1. University of Central Florida, Materials Science and Engineering, USA

Additive manufacturing (AM) of metallic alloys via powder fusion enables unprecedented geometrical complexity and customization in engineering components. However, its widespread adoption for critical applications is constrained by a key challenge: manufacturability, often referred to as printability. Many commercial alloys, originally designed for traditional manufacturing, are poorly suited to the extreme thermo-kinetic conditions of AM processes. This challenge presents a unique opportunity to develop novel alloys, including high-entropy alloys (HEAs), tailored to AM's specific conditions while ensuring manufacturability. By optimizing alloys to balance required properties, performance, and manufacturability, AM can unlock new possibilities in materials science. Our work focuses on alloy design and modification, driven by experimental studies in gas atomization, laser powder bed fusion, and detailed microstructural and mechanical characterization. We will document findings from newly designed, compositionally modified, and commercially available alloys, including Mg, Al, Ti, Fe, Ni, and HEAs. Advancing alloy development is crucial for addressing manufacturability challenges, enabling broader adoption of AM, and realizing its transformative potential in engineering and manufacturing.

8:30 AM

(PACRIM-S29-037-2025) Novel Refractory High-Entropy Metal-Ceramic Composites (Invited)B. Cui^{*1}; X. Chen¹; F. Wang¹; S. Hu²; X. Liu²; S. Humphry-Baker³; M. Gao⁴

1. University of Nebraska-Lincoln, USA

2. West Virginia University, USA

3. Imperial College London, United Kingdom

4. National Energy Technology Laboratory, USA

A new concept of refractory high-entropy metal-ceramic composites (HEMCC) has been proposed that combines the outstanding physical properties of both refractory high-entropy alloy (HEA) and high-entropy ceramic (HEC). As the first HEMCC system, $\text{TiTaNbZr-(TiTaNbZr)C}$, has been developed by a powder metallurgy process. Both the HEA and HEC phases with non-equimolar compositions exhibit body-centered cubic (BCC) and rock-salt B1 crystal structures, respectively, and both have non-equimolar compositions. With the increase of the HEC phase in HEMCC, the hardness is enhanced while the density and fracture toughness are decreased. HEA50C shows a favorable combination of flexural strength and fracture toughness at room temperature and a high compressive strength at 1300 C. The optimized mechanical performance of HEMCC might be attributed to the combination of the ductile HEA and strong HEC phases, smaller grain size, and crack trapping at HEC/HEA interfaces.

9:00 AM

(PACRIM-S29-038-2025) Synthesis and Characterization of High Entropy Nitrides (Invited)

Z. Cheng^{*1}; S. Das²; V. Drozd³; A. Durygin²; M. Sozal²; W. Li²; X. Bai³; Y. Ding⁴; Y. Guan⁵; Z. Mao⁵; M. Cinibulk⁶

1. Colorado State University, Mechanical Engineering, USA
2. Florida International University, Mechanical and Materials Engineering, USA
3. Virginia Tech, Materials Science and Engineering, USA
4. Georgia Institute of Technology, USA
5. The Pennsylvania State University - University Park Campus, USA
6. Air Force Research Laboratory, USA

Bulk near single-phase high-entropy nitride solid solutions, such as $(Al_{0.17}Nb_{0.17}Ta_{0.17}Ti_{0.32}Zr_{0.17})N$, have been prepared from binary nitride powder mixtures using a reactive flash sintering (RFS) technique. In situ synchrotron study carried out during RFS captured in real time the formation of HEN, which was preserved upon cooling, suggesting thermodynamic stability of the HEN phase, even up to extreme pressure (~35.6 GPa). SEM, STEM, and EDS reveal decent uniformity for the HENs, even down to submicron scale. Some properties of the obtained bulk HENs, e.g., hardness and bulk modulus, are close to rule-of-mixture (ROM) estimates from the constituent binary nitrides. Meanwhile, the fracture toughness for the HENs (e.g., $7.81 \pm 1.40 \text{ MPa}\cdot\text{m}^{0.5}$ or higher) turns out to be more than double of the expected ROM estimates, which is attributed to the observed nano-layered structure of the HENs. In addition, $(Al_{0.17}Nb_{0.17}Ta_{0.17}Ti_{0.32}Zr_{0.17})N$ HEN displays superconductivity. Future investigations are needed to confirm the observations, while detailed structural/chemical characterization as well as theoretical modeling at different length scales, are all needed to fully understand the inter-relationships between composition, processing, structure, and properties for these HENs and develop new, related materials for different applications.

9:30 AM

(PACRIM-S29-039-2025) Precursor-derived high-entropy carbides and oxides: from synthesis to additive manufacturing of customized parts (Invited)

H. Yang¹; A. Gurlo^{*1}

1. Technische Universitaet Berlin, Chair of Advanced Ceramic Materials, Germany

We describe a new precursor-based route for the synthesis of various types of high-entropy ceramics based a modified Pechini process. The polyesterification reaction causes steric immobilisation of the ions and subsequent homogeneous cation distribution in the pyrolyzed /calcined materials, shortening the diffusion distance of the atoms during calcination and significantly reducing the temperature required to form high-entropy ceramics. High-entropy carbides, high-entropy perovskite oxides and high-entropy spinel oxides were synthesised using this method. The process of forming high-entropy ceramics and their crystal structure were investigated using ex situ and in situ X-ray diffraction methods. The high-entropy carbides show an altered crack propagation mode, including crack deflection and higher fracture toughness compared to materials synthesised by a solid-state method. The high-entropy spinel oxides produced by this method have higher specific capacities and better cycle performance as anode materials. The additive manufacturing of high-entropy ceramics by digital light processing using the liquid ceramic precursor is demonstrated for the first time.

10:20 AM

(PACRIM-S29-040-2025) Properties and Ion Beam Modification of High-Entropy Oxides (Invited)

W. J. Weber^{*1}; R. Tanveer¹; V. Keppens¹

1. The University of Tennessee Knoxville Tickle College of Engineering, Materials Science & Engineering, USA

High-entropy oxides (HEOs) have recently gained recognition for their unique electrical, magnetic, thermal, and optical characteristics with diverse potential applications. The addition of compositional diversity in these oxides with five or more cations on a given lattice site offers the opportunity for property engineering by taking advantage of the high compositional disorder, lattice distortions, mass fluctuation, cation size variations, and integration of diverse cation species. High entropy oxides have the potential to revolutionize applications in areas such as energy storage, electronics, and photonics, as well as in high radiation environments. Ion beam modification provides another opportunity to further tune or pattern the functionalities of HEOs; however, little is known about their response to high energy ion beams. Some unique properties of these HEOs with different structure types will be reviewed, and the irradiation response to a range of ions and energies will be discussed. At high ion energies (several hundred MeV), amorphous ion tracks, microns in length, are formed along the ion trajectory, creating columnar-like defect structures. At intermediate energies (hundreds of keV to tens of MeV), irradiation-induced defects are introduced and amorphization often occurs.

PacRim S33 - Ceramics for Electrochemical Energy Storage

PACRIM Symposium 33 - Ceramics for Electrochemical Energy Storage II

Room: Plaza C

Session Chairs: Michael Naguib, Tulane University

8:00 AM

(PACRIM-S33-011-2025) Investigation of LiPON and LiSiPON amorphous electrolytes using high-throughput experiments

W. Berthou²; M. Legallais²; V. Motta-Ros³; S. Sorieul¹; G. Yildirim²; F. Le Cras^{*1}

1. CEA, LITEN, France
2. Commissariat à l'Énergie Atomique et aux Énergies Alternatives, CEA Tech Nouvelle Aquitaine, France
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LiPON is the solid electrolyte material of choice in thin-film lithium batteries (microbatteries), and is increasingly being considered as an interphase material to stabilize electrode/electrolyte interfaces in new battery designs (all-solid-state lithium batteries). In this work, we prepared 76-sample libraries of $\text{Li}(\text{P,Si})(\text{O,N})$ thin films by combinatorial synthesis (co-sputtering) that cover extended compositional ranges, to study correlations between chemical composition, local structure and ionic conductivity. They were characterized using automated spatially-resolved techniques to determine dimensions (profilometry), composition (LIBS, EDS, ICP-OES, RBS/NRA), local structure (Raman) and conduction properties (EIS) of each sample. This provided a unified picture of the conduction behavior of amorphous LiPOs and LiPONs for $0.8 < \text{Li/P} < 4.0$, that revealed similar trends in the evolution of the conductivity in two parts (gradual increase then saturation) and a constant beneficial effect of N introduction on the mobile charge carrier concentration over the whole Li/P range. This suggests that the improvement in conductivity is not specifically related to the presence of $[\text{O}_3\text{P-N}_d\text{-PO}_3]$ units, but more generally to the presence of bridging nitrogen. Subsequently, the study of the LiSiPON system revealed additional effects of the structure on ionic conductivity.

8:20 AM

(PACRIM-S33-012-2025) TEM observations of the SnB₂O₄ glass electrode in all-solid-state lithium-ion batteriesS. Mori*¹¹. Osaka Metropolitan University, Materials Science, Japan

As an environmentally friendly Pb-free material, SnO-B₂O₃ glass is considered a next-generation negative-electrode active material for all-solid-state lithium-ion batteries. Using SnB₂O₄ (50SnO50B₂O₃) as a negative-electrode active material, the all-solid-state cells exhibit a high initial discharge capacity of approximately 950 mAh g⁻¹. In this study, the microstructures of the SnB₂O₄ glassy electrode composites are investigated to clarify the charge-discharge behavior and charge-discharge mechanisms of the SnB₂O₄ glassy electrode composites using transmission electron microscopy (TEM). Here, ex situ TEM observations capture Sn and Li-Sn alloy nanocrystallites in the amorphous matrix. Li⁺ is incorporated into Sn, and Li-Sn alloy nanocrystallites are formed after initial lithiation. Further, Li⁺ is extracted from Li-Sn alloys to form Sn nanocrystallites after initial delithiation. In particular, Sn is lithiated and delithiated during the first cycle. However, as the cycle number increases, the capacity deteriorates. Ex situ TEM observations further reveal that Li-Sn alloys remain unchanged even after delithiation, and the crystallite size increases significantly. It is thus found that the capacity deterioration is attributed to the irreversible Li insertion/extraction between Sn and Li-Sn alloys.

8:40 AM

(PACRIM-S33-013-2025) Understanding grain boundary processes to improve the performance of oxide solid-state batteries (Invited)C. Roitzheim*¹; D. Fattakhova-Rohlfing¹¹. Forschungszentrum Jülich GmbH, Institute of Energy Materials and Devices IMD-2: Materials Synthesis and Processing, Germany

The garnet phase Li₇La₃Zr₂O₁₂ (LLZO) is attracting attention as a ceramic electrolyte for safe and robust solid-state batteries (SSBs) due to its relatively high ionic conductivity, non-flammability, processability in air and direct compatibility with lithium metal anodes, which enable cells with potentially high energy density. The technical challenges in the practical implementation of garnet SSBs lie in the need for high-temperature sintering, which often leads to phase separation at the grain boundaries and undesirable chemical reactions with the active cathode material, which has a negative impact on cell performance. Further challenges are associated with the protonation of the moisture-sensitive LLZO during processing and the irreversible loss of lithium during sintering. I will present our results on understanding the processes at the different LLZO interfaces during battery component processing and operation and explain the strategies to improve the battery performance.

9:10 AM

(PACRIM-S33-014-2025) Development of fluoride ion conductors based on LaF₃K. Kawahara*¹; R. Ishikawa¹; S. Sasano¹; N. Shibata¹; Y. Ikuhara¹¹. Tokyo Daigaku, Japan

All solid-state fluoride ion batteries are considered to be higher energy density and safer energy storages than current lithium ion batteries. Ba-doped LaF₃ (La_{0.9}Ba_{0.1}F_{2.9}; LBF) is mainly used as a solid-state electrolyte in fluoride ion batteries. However, room temperature conductivity of LBF is considerably low, on the order of 10⁻⁶ S cm⁻¹ and it is still unclear the optimal elements to be doped to LaF₃. In this study, we synthesized La_{0.9}Sr_xBa_{0.1-x}F_{2.9} (x = 0, 0.01, 0.025, 0.05, 0.1), in which Ba in LBF is substituted for Sr and investigated the composition dependence of F⁻ ion conductivity. We found that the higher concentration of Sr without Ba can improve the F⁻ ion conductivity. The maximum F⁻ ion conductivity of La_{0.9}Sr_{0.1}F_{2.9} is 1.5 × 10⁻⁵ S cm⁻¹ at room temperature, which is one order magnitude larger than that of

LBF (3.9 × 10⁻⁶ S cm⁻¹). The La_{0.9}Sr_{0.1}F_{2.9} total conductivity of 10⁻⁴ S cm⁻¹ can be achieved at 350 K, which lowers operating temperature of fluoride ion batteries down to 350 K. This presentation is based on results obtained from a project, JPNP21006, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

9:30 AM

(PACRIM-S33-015-2025) Electrochemical characteristics of oxyhalide glass-ceramic electrolytes according to crystallization for all-solid-state batteriesJ. Lee*¹; T. Kang¹; Y. Park¹; S. Kim¹¹. Korea Institute of Ceramic Engineering and Technology, Republic of Korea

All-solid-state batteries, that use solid electrolytes instead of liquid electrolytes, are promising energy storage systems due to their electrochemical stability, non-flammability, long cycle performance, high energy density, and potential for large-scale use in electronic devices. Key aspects of these batteries include the synthesis methods, stability, ionic conductivity, and interface properties of solid-state electrolytes. Glass-based solid electrolytes have attracted attention for their low sintering temperature and high resistance to dendrite formation. In this study, a Li₂O-LiX (X = Cl or Br)-B₂O₃-Al₂O₃-based glass composition system using an oxyhalide framework was developed by optimizing the B₂O₃ and Al₂O₃ ratios. The glass matrix was fabricated using the melt-quench method, and the halide-based glasses were sintered at their crystallization temperatures. The crystallization phases of the glass-ceramic electrolytes were analyzed using X-ray diffraction (XRD) patterns. Additionally, the variation in ionic conductivity and chemical stability as a function of crystallization conditions was studied, and the ionic conductivity mechanism was investigated. Finally, coin cells with the glass-ceramic electrolyte, LiCoO₂ as the cathode, and lithium metal as the anode were subjected to charge-discharge cycling analysis using a battery cyclers.

10:10 AM

(PACRIM-S33-016-2025) Development of LAGP-based glass/powder composite solid electrolyte sheet for all solid-state batteriesY. Park*¹; T. Kang²; S. Kim²¹. Korea Institute of Ceramic Engineering and Technology, Display Materials center, Republic of Korea². Korea Institute of Ceramic Engineering and Technology (KICET), Republic of Korea

The application of lithium-ion batteries (LIBs) is extending to electric vehicles and smart grid energy storage systems, due to their high energy density and long lifetime. Especially, all-solid-state rechargeable batteries using inorganic solid electrolytes offer enhanced safety, electrochemical stability, and performance. Among these, NASICON-type Li-based solid electrolytes, especially lithium aluminum germanium phosphate (LAGP), are promising due to their high ionic conductivity and moisture stability. In this study, LAGP-based solid electrolyte ceramic sheets were prepared composite of different ratio of glass frit and crystalline powder, and these ratios are 95:5 (5%), 90:10 (10%), 85:15 (15%), and 80:20 (20%) respectively. The resulting LAGP glass/powder composite ceramic sheet (GPCS) solid electrolytes exhibited no impurity phases and maintained the hexagonal NASICON structure. The 10% composite showed the highest ionic conductivity (4.93 × 10⁻⁴ S/cm), attributed to improved crystallinity and density from reduced porosity. This composite approach is a simple yet effective method to enhance ionic conductivity. Finally, a coin cell with the composite electrolyte, LCO cathode, and Li foil anode delivered a charge capacity of ~130 mAhg⁻¹, demonstrating the potential of LAGP GPCS solid electrolytes for advanced solid-state batteries.

10:30 AM

(PACRIM-S33-017-2025) Enhancing Lithium Ion Conduction in LLZO-Based Solid Electrolytes through Anion Doping for Advanced Energy Storage: Insights from MD Simulations

C. Lopez Puga^{*1}; J. Du¹

1. University of North Texas, Material Science and Engineering, USA

Solid-state electrolytes (SSEs) have emerged as promising alternatives to traditional liquid electrolytes due to their enhanced safety, higher stability and energy density in energy storage applications. Among SSEs, cubic $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) is considered particularly promising, offering high lithium ion conductivity, high chemical stability and a wide electrochemical stability window. Nevertheless, the cubic phase converts to a less conductive tetragonal phase during cooling in pure LLZO. We have investigated the effects of fluorine doping on the phase stability and ion conductivity of LLZO, exploring fluorine concentrations ranging from 1 to 10% across a wide temperature range of 300–1400 K using MD simulations. Doping at 1% was found to be insufficient to stabilize the cubic phase, while high fluorine concentrations (>4%) inhibited ion migration pathways due to stronger electrostatic interactions between point defects. Defect formation energies were also calculated to study their effect on lithium ion conduction. Lithium ion diffusion pathways and mechanisms are also explored by using trajectories from MD simulations. This study provides insights into the optimization of fluorine-doped LLZO, suggesting that moderate doping levels (around 3%) offer a balance between phase stability and ionic conductivity.

PacRim S34 - Carbon based mtl's & smart struct for elec/photonic/elec-chemical/ MEMS & energy app

PACRIM Symposium 34 - Carbon based materials and smart structures for advanced engineering application II

Room: Grouse

Session Chair: Changzhi Gu, Chinese Academy of Sciences Institute of Physics

8:00 AM

(PACRIM-S34-010-2025) Surface functionalised diamond for antimicrobial applications (Invited)

R. Zhang¹; N. Peng²; M. Sims³; H. Ye^{*1}

1. University of Leicester, School of Engineering, United Kingdom
2. University of Surrey, United Kingdom
3. University of Leicester Space Research Centre, United Kingdom

Microorganism-induced corrosion in marine engineering has resulted in significant losses. Antibacterial coatings, grown using chemical vapor deposition, such as ultrananocrystalline diamond (UNCD), nanocrystalline diamond (NCD), and microcrystalline diamond (MCD), have shown promise as a solution. These coatings exhibit varying hydrophobic/hydrophilic properties due to different sp³/sp² carbon bond ratios, influencing their anti-adhesion behavior against bacteria. This property is crucial for their antibacterial effectiveness. The results indicate that UNCD, NCD, and MCD coatings kill bacteria through a combination of mechanical effects and surface functional groups. These coatings are effective against both Gram-negative (*E. coli*) and Gram-positive (*B. subtilis*) bacteria within 1-6 hours of contact. Prolonged contact, especially with MCD coatings, significantly reduces bacterial colonies and enhances bacteriostatic rates for both *E. coli* and *B. subtilis*.

8:30 AM

(PACRIM-S34-011-2025) Diamond and diamond like carbon for ultrasonic and acoustic wave applications (Invited)

R. Y. Fu^{*1}

1. Northumbria University, United Kingdom

Diamond or diamond-like carbon (DLC) thin films show unique and attractive material properties, including high values of Young's modulus, hardness, tensile strength and high thermal conductivity, low thermal expansion coefficient. Along with their highest acoustic velocity of any known material, chemical inertness, low coefficients of friction and good wear resistance, they have been found wide applications in achieving high frequency resonators ultrasonic or acoustic wave MEMS. Using the multi-layer structures combing piezoelectric thin films and diamond or DLC films can greatly increase the acoustic wave velocity and electromechanical coupling coefficient. In this talk, various issues about using diamond coatings, nano-crystalline diamond films, DLC films, and also doped DLC films integrating with piezoelectric thin films have been discussed thoroughly for surface acoustic wave (SAW) and film bulk acoustic wave (FBAR) applications. Recent technologies development in this field have been introduced. Their applications and challenges into microfluidics, micro sensors and lab-on-chips in various mechanical, biological or chemical, energy applications have been discussed.

9:00 AM

(PACRIM-S34-012-2025) Plasma Jet Printing and in Situ oxidation of Mxene surfaces (Invited)

S. Krishnamurthy^{*1}

1. University of Surrey, Surrey Ion Beam Centre, United Kingdom

We developed an innovative approach to print TiO_2 - Ti_2C MXene heterostructures with promising applications in photocatalysis. Leveraging a low-powered atmospheric pressure plasma jet (APPJ) for in situ oxidation of Ti_2C MXene provides a controlled and energy-efficient route to forming TiO_2 layers with tailored electronic and structural properties. The in-situ oxidation method using APPJ promotes the formation of defect-rich TiO_2 on the Ti_2C substrate, which can enhance photocatalytic performance due to improved light absorption and charge separation. The creation of vacancies and mixed oxidation states of Ti and C likely contributes to a broadening of the absorption spectrum and facilitates electron mobility, crucial for efficient photocatalysis. The introduction of vacancies and the variation in valence states of titanium and carbon enhances the electronic density of states near the Fermi level. This modification may improve the MXenes catalytic efficiency by reducing electron-hole recombination rates and enabling more effective charge transfer.

Monday, May 5, 2025

GOMD S1 - Fundamentals of the glassy state**GOMD S1 S3 - Structural characterizations of glasses and melts I**

Room: Saltspring C

Session Chairs: Daniel Neuville, IPGP-CNRS-UPC; Dominique de Ligny, University Erlangen-Nürnberg; Ashutosh Goel, Rutgers University

1:15 PM

(GOMD-S1-S3-001-2025) Thin-Film Glassy Solid Electrolytes as a New Functionality for Glass Enabling High Energy Density Li and Na All Solid State Batteries (Invited)S. W. Martin*¹

1. Iowa State University, Materials Science & Engineering, USA

Fast ion conducting glasses have long been considered as alternatives to flammable liquid electrolytes in Li batteries. However, to date, there has never been before the unique combination of required electrochemical properties in any one such glass for its use as a solid electrolyte with the equally important requirements of viscoelastic behavior to form them into thin films suitable for high ion conductivity separators. In this first ever report of thin film fast ion conducting glasses, we will summarize our efforts to produce thin films of Li and Na ion conducting glasses and test in them in symmetric, asymmetric, and full cells.

1:45 PM

(GOMD-S1-S3-003-2025) NMR study of alkali segregation in the aluminophosphate-silicate systemP. Polette*¹; L. Montagne¹; F. Alousque²; F. O. Mear¹

1. University of Lille - UCCS, France

2. Safran Landing System, France

Several studies have investigated the influence of P₂O₅ in silicate glasses to enhance the understanding of nucleation and bioactivity in phosphosilicate glasses. Other studies have explored the aluminosilicophosphate structure, revealing that the phosphate network forms at the expense of the silicate network, which undergoes polymerization. The aim of this work is to elucidate the segregation mechanisms in this system, considering that alkali ions control the degree of network polymerization and, consequently, the material properties. We investigated the interaction between sodium silicate and aluminophosphate by mixing precursors and heating them at different temperatures. NMR spectroscopy was employed to characterize the evolution of the vitreous network after various thermal treatments. Our observations show that the silicate network fully polymerizes as a result of complete alkali migration to the phosphate network. This segregation phenomenon could have significant implications for nucleation driven by P₂O₅ in silicate glasses.

2:05 PM

(GOMD-S1-S3-004-2025) Influence of Strontium and Calcium Oxide Replacement on the Structure of Bioactive and biocompatible GlassesB. M. AlHasni*¹

1. University of Technology and Applied Sciences, Oman

In this context, extensive molecular dynamics (MD) simulations were performed to calculate various microscopic properties of the glass matrix. The present article demonstrates that the "Buckingham potential with long-ranged Coulomb interaction" can be effectively used to simulate glasses of varied compositions: 45SiO₂-28Na₂O-2P₂O₅-25SrO, 45SiO₂-12.5CaO-28Na₂O-2P₂O₅-12.5SrO, and 45SiO₂-25CaO-28Na₂O-2P₂O₅. The MD results show good agreement with experimental data. In this structure, Na, Ca, and Sr all act as

network modifiers, with mean coordination numbers of 5, 6, and 6, respectively. The MD results also reveal that Sr and Ca share the same octahedral environment, with the average Sr-O bond distance closely matching the RMC and experimental results at 2.60 Å. The agreement between the measured structure factors, bond distances, and coordination numbers from the experimental and MD results is quite good, reflecting the success of the models presented in this study.

2:25 PM

(GOMD-S1-S3-005-2025) Development and Testing of a Mercury-Free Drop Calorimeter to Measure Heat Capacity of Molten GlassH. Tokunaga*¹; T. Sugawara²; S. Yoshida¹

1. AGC Inc., Japan

2. Akita University, Japan

The heat capacity of molten glass is one of the physical properties required for studying the simulation of glass flow in a melting furnace and is also important for estimating the energy needed to melt the glass. In recent years, accurate measurement of the heat capacity of molten glass increases in importance, because it is now also used in phase equilibrium calculations and evaluations of glass-forming ability. While an abundance of data exists in geophysics for the specific heat capacity of high-temperature melts, there are very limited experimental data available for multi-component glass melts. It has long been known that a drop-type calorimeter is one solution to obtain highly accurate heat capacities of high-temperature melts. In this method, a crucible containing glass melt is dropped into the calorimeter, and the heat capacity of the melt is determined by measuring the volume change caused by the melting of ice inside the calorimeter. Mercury as an anti-freezing liquid has long been used in this type of calorimeter to increase the sensitivity of volume change detection, but mercury-free calorimeters have been desired due to environmental issues. We have constructed a mercury-free calorimeter using only water and implemented various measures to improve measurement accuracy. In this talk, the calorimeter configuration and some measurement results will be introduced.

GOMD S1 S3 - Structural characterizations of glasses and melts II

Room: Saltspring C

Session Chair: Laurent Cormier, Sorbonne University - CNRS

3:30 PM

(GOMD-S1-S3-006-2025) Formation of a zirconium oxide crystal nucleus in the initial nucleation stage in aluminosilicate glass investigated by X-ray multiscale analysis (Invited)Y. Onodera*²; Y. Takimoto¹; H. Hijiya¹; Q. Li¹; H. Tajiri³; T. Ina³; S. Kohara²

1. AGC Inc., Japan

2. National Institute for Materials Science, Center for Basic Research on Materials, Japan

3. Japan Synchrotron Radiation Research Institute, Japan

Glass-ceramics are composed of precipitated crystals and a glass matrix and are utilized in many industrial products. To understand the structure of a commercially important glass-ceramic ZrO₂-doped lithium aluminosilicate system during its initial nucleation stage, we conducted an X-ray multiscale analysis by combining diffraction, small-angle scattering, absorption, and anomalous scattering techniques. Element-specific pair distribution function analysis using anomalous X-ray scattering (AXS) data showed the formation of edge-sharing structure between ZrO_x polyhedra and (Si/Al)O₄ tetrahedra during the initial nucleation stage. The edge-sharing polyhedral connection was not a typical structural feature of glass-forming materials; a corner-sharing polyhedral network is formed in typical glass-forming materials, e.g., silica glass. Furthermore, AXS data indicated that the local structure of the Zr⁴⁺ ions, which resembled a cubic or tetragonal ZrO₂ crystalline phase, formed after

2 h of annealing the pristine glass. Therefore, the Zr-centric periodic structure surrounded by the (Si/Al)O₄ tetrahedral network was potentially the initial crystal nucleus for the ZrO₂-doped lithium aluminosilicate glass-ceramic.

4:00 PM

(GOMD-S1-S3-007-2025) Impact of Fe₂O₃ and P₂O₅ on Structure, Rheology, and Crystallization in Na₂O–Al₂O₃–B₂O₃–SiO₂ Glasses (Invited)

A. Goel^{*1}; Y. Zhang²; N. Balasubramanya²; N. Stone-Weiss³; S. Kamali⁴; R. Youngman⁵; P. Florian⁶

1. Rutgers University, USA
2. Rutgers-The State University of New Jersey, Materials Science and Engineering, USA
3. Corning Incorporated, Science and Technology, USA
4. University of Tennessee Space Institute, Department of Mechanical, Aerospace and Biomedical Engineering, USA
5. Corning Incorporated, Science & Technology Division, USA
6. CEMHTI-CNRS, France

The study investigates the structural changes in Na₂O–Al₂O₃–B₂O₃–SiO₂ glasses induced by Fe₂O₃ and P₂O₅ using advanced characterization techniques, including MAS NMR, Raman, and Mössbauer spectroscopies. The research examines how varying Fe₂O₃/Al₂O₃ and P₂O₅ content affect glass structure across diverse compositions. Results reveal that P₂O₅ repolymerizes Fe₂O₃-free glasses but minimally impacts iron-rich glasses' network connectivity. A significant tetrahedral avoidance is observed between AlO₄ and FeO₄ units. In P₂O₅-free glasses, iron primarily bonds with borate and silicate units, whereas P₂O₅ promotes iron-phosphate associations over borate or silicate. Additionally, the study links structural characteristics to the rheological and crystallization behaviors, aiming to establish composition–structure–property relationships in this glass system.

4:30 PM

(GOMD-S1-S3-008-2025) Atomic Structures of Ti-Bearing Multi-Component Silicate Glasses Using High-Resolution NMR

E. El Ghazaoui^{*1}; S. Lee²

1. Seoul National University, Earth and Environmental Science, Republic of Korea
2. Seoul National University, Republic of Korea

Titanium is known for enhancing mechanical properties of silicate glasses, but its structural role remains underexplored. Our study investigates the short- and medium-range structural characteristics of Ti-rich glasses. Specifically, we examine the structural order in Ti-bearing multi-component silicate glasses using ²⁹Si, ¹⁷O, and ²⁷Al NMR. Our findings show that TiO₂ substitution for Na₂O in sodium trisilicate and metasilicate glasses increases network polymerization. Conversely, in aluminosilicate glasses, replacing Al₂O₃ with TiO₂ reduces network connectivity and promotes the formation of non-bridging oxygen (NBO) as Na–O–Si. ¹⁷O 3QMAS spectra suggest the presence of highly coordinated Ti (^{5,6}Ti), based on a broad signal attributed to Ti–O–Si bonds. This observation enables semi-quantitative calculations of the oxygen species fraction within the glass. There is no evidence of Ti–O–Al species, confirming titanium-aluminum avoidance in silicate glasses. For the first time, ²⁷Al 3QMAS data provide clear evidence of an increase in Al-coordination state due to changes in the NBO configuration or the TiO₂/SiO₂ ratio in Ti-rich multi-component glasses. Our results validate titanium's role as a network-modifying cation, establish a non-linear correlation between the fraction of Ti–O–Si species and mechanical properties, and demonstrate a dependence of Al coordination states on Ti content.

4:50 PM

(GOMD-S1-S3-010-2025) Evaluation of the cooling rate during aerodynamic levitation glass processing using glass memory effect

D. de Ligny^{*1}; M. Cicconi¹; H. Reinfelder¹; B. Moulton²; S. K. Wilke⁴; R. Weber³

1. FAU - Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Glas und Keramik (WW3), Germany
2. Alfred University, Glass Science and Engineering, USA
3. MDI, USA
4. Materials Development, Inc., USA

The dependence of the glass structure on its cooling rate gives it a memory. Indeed, if this dependence is known, using glasses subjected to controlled cooling rates, it is then possible to trace back by measuring the structural data the speed at which it crossed the glass transition region. This effect has already been successfully applied to glasses formed under extreme conditions, such as fibers. When studying laser impacts, it has also been possible to identify a residual stress signature by coupling complementary spectroscopic information. It is proposed here to extend this approach to glasses prepared using the aerodynamic levitation technique. Under these conditions, gas flow and laser heating can lead to extreme cooling conditions. Temperature differences between the center and surface of a sphere is known to induce residual stresses similar to Prince Rupert's drop. Among the glasses whose calibration curves are known, four were used. A common soda-lime glass, a borosilicate for which the Bore coordination change can be used as a reliable calibrator, and two alkaline or alkaline-earth aluminosilicates. For each of these four glasses, a series of spheroids with diameters ranging from 1 to 3 mm was synthesized. By coupling Raman, Brillouin and Nd³⁺ luminescence spectroscopy profiles, it is possible to trace back both cooling rates and residual stresses.

GOMD S1 S5 - Data-driven modeling and machine learning for glass science I

Room: Moresby

Session Chairs: N M Anoop Krishnan, Indian Institute of Technology Delhi; Xiaonan Lu, Pacific Northwest National Lab

1:15 PM

(GOMD-S1-S5-001-2025) Vitrification Modeling and Machine Learning for Nuclear Waste Glass Design (Invited)

K. D. Miller^{*1}; J. E. Saal¹

1. Citrine Informatics Inc, External Research, USA

The design and testing of nuclear waste glass typically costs hundreds of millions of dollars, comprising a massive barrier to innovation in waste form development. We developed a flexible machine learning framework to optimize key properties of nuclear waste glasses, including glass formability. Using a large language model (LLM)-assisted extraction process, we generated a glass formability training data set with >70k entries, including select synthesis conditions. This data set provided the foundation for a machine learning model that predicts vitrification as a function of chemistry and synthesis conditions. In concert with predictive models for melting temperature, mechanical stability, thermal stability, and chemical durability, we leveraged this model to perform iterative design of phosphate waste forms for next-generation nuclear molten salt reactor applications.

1:45 PM

(GOMD-S1-S5-002-2025) Machine Learning with Gradient-Based Optimization of Nuclear Waste Vitrification with Uncertainties and ConstraintsL. Gunnell*¹; K. Manwaring¹; X. Lu²; J. Reynolds³; J. Vienna⁴; J. Hedengren¹

1. Brigham Young University, Chemical Engineering, USA
2. Pacific Northwest National Lab, Energy and Environment Directorate, USA
3. Washington River Protection Solutions LLC, USA
4. Pacific Northwest National Lab, USA

Gekko is an optimization suite in Python that solves optimization problems involving mixed-integer, nonlinear, and differential equations. The purpose of this study is to integrate common Machine Learning (ML) algorithms such as Gaussian process regression, support vector regression, and artificial neural network models into Gekko to solve data-based optimization problems. Uncertainty quantification (UQ) is used alongside ML for better decision making. An optimization problem involving nuclear waste glass optimization is presented to demonstrate the benefit of ML in the glass formulation field. ML models are compared against the current partial quadratic mixture model in an optimization problem in Gekko. This effort is an example of bringing modern computational tools like ML and UQ and applying them in industries in need of higher precision and accuracy with their modeling tools.

2:05 PM

(GOMD-S1-S5-003-2025) Leveraging machine learning to predict nepheline crystallization in high level waste glassesN. D. Joseph*¹; S. Mannan³; V. Badoni²; N. Krishnan³; A. Goel¹

1. Rutgers University, Materials Science and Engineering, USA
2. Princeton University, USA
3. Indian Institute of Technology Delhi, Civil Engineering, India

The devitrification of nepheline ($\text{Na}_2\text{O}\cdot\text{Al}_2\text{O}_3\cdot 2\text{SiO}_2$) – like phases is a well-known problem during the vitrification of sodium- and alumina-rich high-level waste. This problem, particularly pronounced during canister-centerline cooling (CCC) conditions, poses a risk to the chemical durability of the final waste form. Existing literature highlights the development of conservative empirical/semi-empirical models using the nepheline discriminator (ND) and optical basicity (OB), with a combined misclassification rate of approximately 30%. Addressing these limitations, we employ the support vector classification (SVC) model, significantly enhancing the performance in predicting nepheline crystallization. Moreover, we integrate the SVC model with chemo-structural descriptors, thereby strengthening the prediction of glass composition beyond the confines of the training dataset. Results obtained from this study will form the baseline for future, more complex nepheline crystallization models and nuclear waste studies.

2:25 PM

(GOMD-S1-S5-004-2025) Leveraging Textual and Numerical Features for Advanced Glass Dissolution Rate PredictionS. Mannan*¹; I. Mandal²; N. Gosvami³; N. Krishnan¹

1. Indian Institute of Technology Delhi, Department of Civil Engineering, India
2. Indian Institute of Technology Delhi, School of Interdisciplinary Research, India
3. Indian Institute of Technology Delhi, Department of Materials Science and Engineering, India

The long-term chemical resistance of glass plays a crucial role in the immobilization of radioactive waste. The chemical resistance is governed by both intrinsic factors as well as extrinsic factors, including the surrounding environment and thermodynamic conditions. No universal data-driven method or analytical model currently exists for accurately predicting dissolution rates of highly multicomponent glass compositions. To address this, we curated a dataset ~2000 glasses, including parameters such as chemical composition,

pH, and temperature. The descriptor-based machine learning (DML) model was developed to predict glass dissolution rates by combining ML techniques with physical and chemical descriptors. However, this model demonstrated insufficient accuracy when applied to unseen glass compositions. We improved our predictive DML model by incorporating additional features like testing conditions and processing conditions. By converting textual information into numerical features using Natural Language Processing (NLP), we developed a more robust predictive model called NLP-DML. Results shows that the NLP-DML model significantly outperforms the DML model. Overall, this framework provides accurate predictive model for predicting the dissolution rate of any glass compositions that can potentially be used to design and discover novel glass compositions for radioactive waste applications.

2:45 PM

(GOMD-S1-S5-009-2025) Discovering Symbolic Laws Directly from Trajectories with Hamiltonian Graph Neural NetworksS. Bishnoi*¹; R. Bhattoo¹; J. Jayadeva²; S. Ranu³; N. Krishnan¹

1. Indian Institute of Technology, India
2. Department of Electrical Engineering, Indian Institute of Technology Delhi, India
3. Indian Institute of Technology Delhi Department of Computer Science and Engineering, India

We present a new type of graph neural network (GNN), called a Hamiltonian GNN (HGNN), which is designed to model the dynamics of physical systems described by Hamiltonian equations of motion. Our approach extends the standard GNN framework by incorporating physical conservation laws and strong inductive bias into the model architecture and training procedure to learn the Hamiltonian of a particle-based system directly from the trajectory. We demonstrate the effectiveness of our method on several benchmark tasks, including the simulation of n-springs, n-pendulums, gravitational systems, and binary Lennard Jones systems. Our results show that HGNN learns the dynamics in excellent agreement with the ground truth from small amounts of data. We also evaluate the ability of HGNN to generalize to larger system sizes. Finally, employing symbolic regression on the learned HGNN model, we infer the underlying equations relating to the energy functionals, even for complex systems such as the binary Lennard-Jones liquid. Our framework facilitates the interpretable discovery of interaction laws directly from physical system trajectories. Furthermore, this approach can be extended to other systems with topology-dependent dynamics, such as cells, polydisperse gels, or deformable bodies.

GOMD S1 S5 - Data-driven modeling and machine learning for glass science II

Room: Moresby

Session Chairs: N M Anoop Krishnan, Indian Institute of Technology Delhi; Xiaonan Lu, Pacific Northwest National Lab

3:30 PM

(GOMD-S1-S5-005-2025) Harnessing Machine Learning Potentials for Glass Science: From Oxide Glasses to Sodium-based Solid Electrolytes (Invited)A. Pedone*¹

1. University of Modena and Reggio Emilia, Italy

The rise of artificial intelligence has revolutionized materials modeling, offering new pathways to accelerate discoveries in glass science. Machine learning potentials (MLPs) have emerged as transformative tools, bridging the computational efficiency of classical molecular dynamics and the accuracy of density functional theory. In this lecture, I will discuss the application of state-of-the-art MLP frameworks, specifically DeePMD and MACE, to model oxide glasses and sodium-based solid electrolytes. Our analysis highlights the strengths and limitations of each approach in capturing structure and

*Denotes Presenter

properties. The role of dispersion interactions and their critical impact on reproducing glass density will be discussed. This work demonstrates the capability of data-driven models to advance glass science and support materials development for industrial applications.

4:00 PM

(GOMD-S1-S5-006-2025) Enhancing Sodium Ion Diffusion in NaPSO Glassy Solid-State Electrolytes via Oxygen Doping: A Molecular Dynamics Study (Invited)

K. Luo¹; R. Zhou¹; S. W. Martin¹; Q. An^{*1}

1. Iowa State University, Materials Science and Engineering, USA

All-solid-state sodium batteries (ASSSBs) with nonflammable solid-state electrolytes (SEs) and abundant sodium anodes are promising for grid-scale energy storage. Oxygen doping in Na-P-S-O (NaPSO) glassy solid-state electrolytes (GSEs) enhances ionic conductivity, mechanical strength, and formability. A maximum Na ion conductivity occurs at the composition with O doping of 0.15, with further oxygen additions reducing conductivity. However, the mechanisms behind Na ion motion and diffusion in these GSEs are not fully understood. Here, we employ machine learning force field molecular dynamics simulations to study Na diffusion in NaPSO GSEs. Our results show that oxygen doping reduces free volume, which would typically hinder Na diffusion. Paradoxically, it also increases the flexibility of the amorphous framework, facilitating Na movement. This dual effect leads to an initial increase in diffusion coefficients at lower oxygen levels, followed by a decline as oxygen content rises, aligning with experimental observations. Our findings provide atomic-level insights into how oxygen doping affects Na diffusion in NaPSO GSEs. Enhancing the flexibility of the amorphous framework emerges as a viable strategy to improve ionic conductivity in solid-state electrolytes, potentially leading to more durable and cost-effective ASSSBs for grid-scale energy storage.

4:30 PM

(GOMD-S1-S5-007-2025) Machine Learning-Based Boron Coordination Prediction in Glass System: Unveiling Structural Insights

A. Jose^{*1}; S. Mannan²; N. Krishnan²; A. Goel³

1. Rutgers University, Material Science and Engineering, USA
2. Indian Institute of Technology Delhi, Department of Civil Engineering, India
3. Rutgers University, USA

Boron is present in glass structures in either a 3-coordination or 4-coordination configuration. The exploration of how boron coordination evolves with changes in glass composition originates in the twentieth century. Despite early efforts to comprehend the relationship between boron coordination and glass composition, existing prediction algorithms have predominantly focused on simple systems, often proving inadequate for accurate calculations in multicomponent scenarios. To address this limitation, we deploy diverse machine learning models on a large dataset comprising 912 experimental data points curated from different existing literature. Our approach aims to unravel the nuanced interplay between boron coordination and the complicated compositions present in multicomponent systems. Further, feature importance analyses shed light on the critical structural descriptors influencing boron coordination, offering valuable insights into the factors governing boron's coordination chemistry. Furthermore, the developed ML models provide a predictive tool for estimating boron coordination numbers in novel and yet-to-be-synthesized compounds, facilitating the exploration of boron-based materials with tailored

4:50 PM

(GOMD-S1-S5-008-2025) Uncertainty Propagation Methods for Nuclear Waste Vitrification and Constrained Optimization

L. Gunnell^{*1}; X. Lu²; J. Vienna³; D. Kim³; B. J. Riley³; J. Hedengren⁴

1. Brigham Young University, Chemical Engineering, USA
2. Pacific Northwest National Lab, Energy and Environment Directorate, USA
3. Pacific Northwest National Lab, USA
4. Brigham Young University, Chemical Engineering, USA

An ongoing effort to immobilize non-solid nuclear waste is to mix and melt the waste with glass-forming chemicals (GFCs) to form a waste glass. Algorithms to determine the ideal mixing recipes are formalized as constrained optimization problems to maximize waste loading in the glass product, with constraints on several properties of the glass melt and final product. An important aspect of these algorithms is how uncertainty is used to inform optimization. Assumed input distributions are typically propagated through a system with Monte Carlo sampling resulting in output distributions, which can be used for intervals used as buffers from constraints. Analytical methods of input uncertainty propagation, such as first order error propagation and surrogate modeling with machine learning, can produce uncertainty intervals equivalent to standard sampling approaches in a fraction of the time. These advanced numerical methods are implemented within a gradient-based optimization problem to yield faster waste glass formulation with trustworthy uncertainty intervals.

GOMD S1 S6 - Mechanical properties of glasses I - Indentation responses

Room: Pender

Session Chair: Yueh-Ting Shih, National Taipei University of Technology

1:15 PM

(GOMD-S1-S6-001-2025) Deformation and Cracking Behavior of Glass under Sharp Contact Loading: Role of Densification (Invited)

L. Huang^{*1}; H. Liu²; Y. Shi²

1. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA
2. Rensselaer Polytechnic Institute, USA

Despite extensive studies, what controls crack initiation in glass under sharp contact loading remains elusive. The difficulty arises from experimental complexity associated with in-situ investigations at a local scale (tens of microns) under complex and non-uniform stresses. In this context, classical molecular dynamics (MD) simulations were carried out to reveal how the stress field and the glass structure evolve underneath an indenter. To generate stress/strain fields and deformation patterns in glass that can be directly compared with instrumented experimental studies, we developed a 3-D nanoindentation protocol to mimic real-life loading conditions, and applied it in a model metallic glass favoring shear flow to understand the shear band activation/interaction mechanism. After validating our results with multiple experimental studies, we conducted a systematic 3-D nanoindentation study in metallic and silica glasses with different densification capabilities. The comparisons between silica and metallic glasses suggest that balancing shear deformation with a combination of instantaneous and permanent densification can provide multiple pathways to dissipate energy under indentation, thus increasing the load to initiate cracks and improving the damage resistance of glass.

1:45 PM

(GOMD-S1-S6-003-2025) Size Dependence of Indentation Modulus in Silicate glassesP. Shrestha²; M. Kazembeyki³; M. Bauchy¹; C. G. Hoover^{*2}

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA
2. Arizona State University, School of Sustainable Engineering and the Built Environment, USA
3. Keysight Technologies Inc, USA

The indentation size effect (ISE) in glasses is often characterized by a decrease in Hardness (H) with increasing applied force. Since the indentation modulus (M) is also calculated from indentation force vs displacement curves, this motivated us to see if the modulus also displayed an ISE. In this study, we investigate the ISE in M, determined using the Oliver and Pharr method, for commercially available fused silica and soda-lime silica (SLS) glasses, using micro-indentation with a Vickers probe. We found that M decreases by ~8% for fused silica and ~11% for SLS as the applied peak force increases from 12.5 to 200 grf in fused silica and from 12.5 to 100 grf in SLS. AFM measurements using Yoshida's annealing method show that the fraction of the total inelastically deformed volume that densifies decreases at higher forces. Since M and densification are, in general, positively correlated, we hypothesize that the observed ISE in M arises from the reduced percentage of densification volume at higher forces, leading to a lower modulus, compared to M at lower forces.

2:05 PM

(GOMD-S1-S6-004-2025) Strain Rate Sensitivity in Indentation Size Effect of a Glassy ZIF-62, a Zeolitic Imidazolate FrameworkP. Shrestha^{*3}; F. Cao¹; M. M. Smedskjaer¹; M. Bauchy²; C. G. Hoover³

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. University of California, Los Angeles, Civil and Environmental Engineering Department, USA
3. Arizona State University, School of Sustainable Engineering and the Built Environment, USA

It was previously shown through thermal annealing that uncracked ZIF-62 dissipates inelastic energy primarily through densification. The extent of the indentation size effect (ISE), the change in indentation hardness (H) due to increasing maximum applied force, is controlled by the relative proportion of densification and μ -ductility. The volume of μ -ductility, and the ISE, was previously shown to be strain rate sensitive for soda-lime silica glass. This motivated us to investigate if the ISE in a melt quenched ZIF-62 glassy metallic organic framework (gMOF) was also strain rate sensitive. We performed microindentation on the ZIF-62 gMOF, using a constant loading rate protocol, with six different average strain rates (0.002, 0.005, 0.01, 0.025, 0.5 and 1 s⁻¹) for each of eight maximum indentation forces. We found that, compared to oxide glasses in the same force range, the ZIF-62 gMOF exhibits low H due to its high porosity. The overall shape of the ISE was essentially strain rate independent. However, faster strain rates have higher hardnesses, compared to slower strain rates, for the same force range. This is opposite to what was seen in a soda-lime glass, where slower strain rates yielded higher H for the same force.

2:25 PM

(GOMD-S1-S6-005-2025) Enhancing Mechanical and Tribological Properties of Sodium Alumino-Phosphosilicate Glass Through Ion-Exchange TreatmentsK. S^{*2}; S. Mannan¹; A. Amarnath Reddy³; N. Gosvami²; N. Krishnan¹

1. Indian Institute of Technology Delhi, Department of Civil Engineering, India
2. Indian Institute of Technology Delhi, Department of Materials Science and Engineering, India
3. CSIR-Central Glass and Ceramic Research Institute, Energy Materials and Devices Division, India

Oxide glasses, valued for their optical transparency and chemical durability, are extensively used in lenses, display panels, coatings, biomedical devices, solar cells, and energy storage. However, their inherent brittleness restricts their use in load-bearing and structural applications. To address this limitation, we investigated the mechanical and scratch behavior of sodium alumino-phosphosilicate glasses subjected to ion-exchange treatments of varying durations. The ion-exchange process significantly improves crack resistance, increasing it nearly 15-fold (from 11.2 N for base glass to 150 N for ion-exchanged) within just 30 minutes. Nanoindentation technique reveals the mechanical response under normal and lateral contact conditions as a function of ion-exchange duration. Furthermore, the tribological performance of ion-exchanged glasses, evaluated using a tribometer, shows frictional behavior influenced by ion-exchange duration. Overall, the findings indicate that these ion-exchanged glasses hold significant promise for advanced engineering applications that demand enhanced durability, including load-bearing components and scratch-resistant surfaces.

GOMD S1 S6 - Mechanical properties of glasses II - Characterization techniques

Room: Pender

Session Chair: Liping Huang, Rensselaer Polytechnic Institute

3:30 PM

(GOMD-S1-S6-006-2025) In situ characterization of glasses during sharp contact loading by X-ray nano diffraction (Invited)M. M. Smedskjaer^{*1}; J. Christensen¹; M. Jalaludeen¹; X. Ge¹; S. S. Sørensen¹; A. K. Christensen¹; A. Davydok²; S. Kalbfleisch³

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. Helmholtz-Zentrum Hereon, Institute of Materials Physics, Germany
3. MAX IV-laboratoriet, Sweden

Stronger oxide glasses are critically needed to enable new applications and reduce their carbon footprint by making them thinner. In turn, this requires an in-depth understanding of how strength-reducing surface damages form under sharp contact loading. This is typically tested using instrumented indentation and it has been found that the structural deformation mechanism varies among different glass families. However, structural probing is typically performed after indentation although it is known that certain stress-induced structural changes are reversible upon unloading. To this end, we here use state-of-the-art synchrotron techniques to perform indentation of different oxide glasses while simultaneously observing their local structural response using an indenter coupled to a nanofocus X-ray scattering setup. These experiments provide spatially resolved information at different stages of the indentation process, showing the formation and evolution of the induced densification zone and different types of cracking with resolution on the nanoscale.

4:00 PM

(GOMD-S1-S6-007-2025) Visualizing invisible subsurface defects in glass made by physical contact

S. H. Kim*¹

1. Pennsylvania State University, Chemical Engineering & Materials Science, USA

Because glass is a non-equilibrium solid material, its structure is not a state function, but a path function. In other words, its properties cannot be fully described or predicted with its composition, temperature, and pressure; they vary depending on the history such as cooling rate from the melt or annealing temperature. This adds a great deal of complexity in structure-property relationships of bulk glass. When it comes to surface properties, it is even more complicated because glass surface is exposed to humid air and often touched by other physical objects. This talk presents spectroscopic evidence showing invisible structural changes in the region that is physically touched with a load that is low enough not to leave topographically visible damage to the surface.

4:20 PM

(GOMD-S1-S6-008-2025) Crack initiation load of silica glass surfaces formed during sub-critical crack growth

J. Endo*¹; T. Sekine²; S. Shimizu²; S. Yoshida¹

1. AGC Inc., Materials Integration Laboratories, Japan
2. AGC Inc., Innovative Technology Laboratories, Japan

Crack initiation load of the freshly fractured surface of silica glass was evaluated to investigate the controlling factors which reduce the intrinsic strength of undamaged silica glass. The fracture surfaces were formed during sub-critical crack growth in the regions I, II and III of the stress intensity factor (K_I) - crack velocity (V) curve. The ring/(cone) crack forming probability during ball indentation was the lowest for the fracture surface formed in the region III. Surface conditions which are topography, relative non-bridging oxygens (NBO), hydrogen concentrations, and Si-O three- or four-membered ring structures, were measured by atomic force microscopy, X-ray photoelectron spectroscopy, dynamic secondary ion mass spectrometry, and Raman spectroscopy, respectively. No distinct difference in NBO and hydrogen concentrations nor in the ring structures was found among the fracture surfaces formed in different regions of the K_I - V curve. The peak to valley height of the fracture surface formed in the region III was lower than that of the fracture surface formed in the regions I and II. Therefore, it is deduced that the roughness or topography of the freshly fractured surface is one of the controlling factors which alter the strength of silica glass.

4:40 PM

(GOMD-S1-S6-009-2025) Local brittle-ductile-transition and activation of viscous flow via electron irradiation in oxide glasses

S. Bruns*¹; D. de Ligny²; K. Durst¹

1. Technische Universität Darmstadt, Physical Metallurgy, Germany
2. Friedrich-Alexander-Universität Erlangen-Nürnberg, Materials Sciences and Engineering, Germany

The increasing use of oxide glasses in high-tech applications illustrates the demand of novel engineering techniques on nano- and microscale. Conventional shaping operations of glass require temperatures close the point of glass transition T_g in order to lower the viscosity and prevent brittle failure. Recent studies have shown that electron irradiation is able to reduce the glass viscosity as well, facilitating viscous flow at room temperature on nano- and microscale. The present contribution aims to demonstrate the potential of electron irradiation for local microengineering via in-SEM nanoindentation. The experiments were performed with cube corner indenter under various electron irradiation conditions on a selection of silica glasses with increasing network complexity: fused silica, soda lime silica glass and Boroplate. The results show a significantly reduced deformation resistance as well as a suppression

of crack nucleation under active electron irradiation. The significant increase in strain rate sensitivity under active irradiation indicates changes in the deformation processes. The irradiation induced state of low glass viscosity has a short lifetime and vanishes once the beam is turned off. Raman spectroscopy and discolorations visible for high irradiation doses, however, demonstrate remaining modifications of the network structure after irradiation.

GOMD S2 - Glass and interactions with its environment - Fundamentals and applications

GOMD S2 S3 - Materials for waste immobilization I

Room: Cortes

Session Chairs: Jessica Rigby, PNNL; Richard Pokorny, University of Chemistry and Technology Prague

1:15 PM

(GOMD-S2-S3-001-2025) Investigation into the processing parameters of phosphate-based dehalogenation for chloride-based waste salt (Invited)

K. Carlson*¹

1. University of Nevada Reno, USA

The increasing need for energy independence and security may lead the U.S. to recycle used nuclear fuel. Electrochemical processing is a demonstrated recycling technology that is being advanced through recent U.S. DOE programs. The chloride-based waste salt generated during this reprocessing can be dechlorinated before disposal to reduce waste volume while simultaneously making it easier to immobilize radioactive cations in a durable waste form. This talk will cover different processing conditions used to investigate dechlorination, including phosphate-based precursors and processing atmosphere, as well as material interactions during processing and recycling of the off-gas material.

1:45 PM

(GOMD-S2-S3-002-2025) Lessons in Iodine Capture from Offgas of Nuclear Waste Vitrification

D. Dixon*¹; J. Lang¹; M. Hall¹; J. C. Rigby²; J. Marcial²; R. K. Brown¹; W. C. Eaton¹

1. Pacific Northwest National Lab, USA
2. PNNL, Radiological Materials Group, USA

The Waste Treatment and Immobilization Plant (WTP) will process and stabilize nuclear waste stored in tanks located on the Hanford Site. At the WTP, the tank waste will be combined with glass-forming additives to make a slurry called melter feed, which will then be vitrified in joule-heated melters. The continuous laboratory-scale melter (CLSM) system at Pacific Northwest National Laboratory integrates a small, externally heated melter with an offgas treatment system. The CLSM is used to process melter feeds containing either simulated or actual (radioactive) tank wastes. The experiments performed with the CLSM enable collection of information related to melter feed processability, validation of simulant formulations, and partitioning of components of interest within the glass and offgas system. Semi-volatile components that can be captured in the CLSM offgas treatment system include iodine, a radioactive component that may be present in certain wastes. Melter feeds using simulant wastes were spiked with iodine salts and processed in the CLSM and behavior of iodine was observed through analysis of the offgas treatment system samples. Minor quantities of iodine were captured on filters while most was captured in the liquids poured from collection units, such as a condenser and submerged bed scrubbers.

2:05 PM

(GOMD-S2-S3-004-2025) Effect of Solids Loading on Simulated Melter Feed Rheology

J. Zaengle*¹; J. C. Rigby¹; J. Marcial¹; J. Chun¹; N. Bohrmann¹; S. K. Sundaram²; M. Hall¹; W. C. Eaton¹; A. A. Kruger³

1. Pacific Northwest National Laboratory, USA
2. Alfred University, Inamori School of Engineering, USA
3. US Department of Energy, Office of River Protection, USA

The study of the rheological properties of slurries has been a key area of research across multiple industries for decades due to its significance in optimizing processing efficiency. Various physical and chemical factors such as particle size, solids loading, water content, pH, and ionic strength can influence rheology. This is relevant to nuclear waste processing efforts, such as those at the Hanford Site in eastern Washington, to ensure safe and efficient waste transfer in a liquid form and slurry feed to the vitrification melter. A typical Hanford low-activity waste (LAW) is combined with glass-forming chemicals (GFCs) to form an aqueous solution containing high concentrations of dissolved salts, metal hydroxides, oxides, and GFCs. This is referred to as a LAW melter feed. This results in a diverse, highly flocculated structure with complex rheological behavior. The addition of glass-forming chemicals significantly influences the rheological properties of an already complex LAW supernatant. The current glass formulation models can be improved by incorporating additional melter feed rheological characteristics. In this study, we examine the effects of water content and solids loading on the rheological properties of a melter feed, providing insights into the interactions that influence its flow behavior.

2:25 PM

(GOMD-S2-S3-005-2025) Aggregation and Settling of Solids in Continuous Melters Processing Radioactive Waste Glass

P. Hrma*¹

1. Hanford Field Office, USA

The settling of crystalline materials and their accumulation on the melter bottom is one of the major factors that limits high-level waste glass formulation. The thermodynamic equilibria constraints, such as the minimum liquidus temperature or the maximum fraction of equilibrium crystallinity at a given temperature, are unduly limiting the waste loading and are unable to prevent large crystals and aggregates of small crystals from settling. The main factor that determines the rate of settling of individual crystals is their size. The tiny crystals of RuO₂, too small to settle, readily form aggregates, the settling rate of which depends on their apparent density and size. The aggregates originate early in the melting process and then grow by shear-flocculation mechanism. Melt convection, whether driven by gravity or pneumatic stirring, affects sludge formation by both flocculation and breakage depending on the shear rate.

2:45 PM

(GOMD-S2-S3-007-2025) Alternative Reductants for Vitrifying Radioactive Waste: Fundamental Structural Evolution to Scaled Melter Tests

J. C. Rigby*¹; J. Marcial²; J. Lang³; D. Dixon³; R. K. Brown³; M. Hall²; A. A. Kruger⁴

1. PNNL, Radiological Materials Group, USA
2. University of Chemistry and Technology, Prague, Laboratory of Inorganic Materials, USA
3. Pacific Northwest National Lab, USA
4. US Department of Energy, Office of River Protection, USA

The vitrification of radioactive waste is vital for environmental remediation efforts at the Hanford Site, transforming hazardous waste into stable glass. Sucrose, the baseline additive for redox and foam control produces toxic acetonitrile as a byproduct and poses handling and

environmental risks. This research explores both organic and inorganic alternatives. Bench-top studies showed that BN (boron nitride) and coke dust (a petroleum byproduct), effectively reduce acetonitrile by over 90%, while also controlling foaming and redox state. Scaled-up testing evaluated the viability of both BN and coke dust as alternatives to sucrose using Continuous Laboratory Scale Melter tests with both inactive simulant waste and actual radioactive tank waste from the Hanford site's first Low-Activity Waste (LAW) melter. These alternatives could provide operational flexibility for processing of LAW at the Hanford Waste Treatment and Immobilization Plant (WTP), while further testing may also provide this option for high-level waste. The study also displays the broader potential of alternate raw materials in reducing CO₂ emissions and utilizing industrial byproducts, offering a promising path for the future of the glass industry, if not these compounds, then the mechanisms of foam and redox control presented that obviate introduction of excess organics.

3:30 PM

(GOMD-S2-S3-006-2025) Structural origins of high MoO₃ solubility in peraluminous alkali aluminoborosilicate glasses

N. D. Joseph*¹; H. Kamat²; R. Saini³; G. Tricot⁴; K. Wang⁵; R. Youngman⁶; A. Goel¹

1. Rutgers University, Materials Science and Engineering, USA
2. James R. Glidewell Dental Ceramics, Glass & Glass-ceramics, USA
3. Rutgers University, USA
4. Universite de Lille, France
5. Alfred University, USA
6. Corning Incorporated, Science & Technology Division, USA

Owing to its high ionic field strength, molybdate oxyanion [MoO₄]²⁻ is known to induce phase separation in peralkaline (e.g. Na/Al > 1) borosilicate glasses, leading to the crystallization of alkali/alkaline-earth molybdate phases (e.g. Na₂MoO₄, CaMoO₄) that have low-to-moderate chemical durability in aqueous environments. This presents a significant challenge in the vitrification of MoO₃ containing high-level waste, as the low solubility of MoO₃ (~1 mol%) limits the overall waste loading capacity, thereby increasing vitrification costs. Hence, there is continuing interest in developing new glass formulations which can accommodate higher MoO₃ concentrations. Our recent studies have demonstrated a multi-fold increase in MoO₃ solubility in peraluminous (Na/Al < 1) sodium aluminoborosilicate glasses compared to their peralkaline counterparts. This increase in MoO₃ solubility is attributed to structural changes in the glass network, where Mo⁶⁺ (1) shifts its coordination from tetrahedral [MoO₄]²⁻ units to octahedral MoO₆⁶⁻ moieties and (2) partially reduces to Mo⁵⁺ to facilitate its integration within the glass matrix. The possible mechanisms governing the incorporation of MoO₃ in these glasses and the impact of its addition on the glass network will be discussed as deduced by a suite of characterization techniques, including XRD, EPR, TEM/EDS, NMR, and Raman Spectroscopy.

3:50 PM

(GOMD-S2-S3-008-2025) Effect of Alternative Reductants BN and Coke on Redox Chemistry in Hanford Low Activity Waste Feeds

J. George*¹; J. C. Rigby¹

1. Pacific Northwest National Lab, USA

Conventional formulations of Hanford low-activity waste melter feed include the addition of sucrose to reduce the amount of foaming during melting and to improve processing rates. Alternative reductants to sucrose have been explored in an attempt to limit acetonitrile production in the off-gas condensate as acetonitrile may exceed bounding limits and increase the cost of effluent management. A variety of alternative reductants to sucrose were previously evaluated with boron nitride (BN) and carbon coke both showing success at reducing foaming while decreasing acetonitrile production. This study further explores the effects of these alternative reductants on

feed chemistry, particularly redox of multivalent ions in the glass such as Re (a surrogate for Tc) and Fe. Feeds produced with BN show more reduced Re and Fe than those made with sucrose or coke. The redox results will be discussed alongside evolved gas analysis and foaming behavior properties.

4:10 PM

(GOMD-S2-S3-009-2025) Increasing Tc/Re retention during nuclear waste vitrification by selection of alumina source and silica particle size

R. Pokorny*¹; J. Klouzek¹; P. Cincibusova¹; L. Lowy¹; M. Eret¹; J. George²; P. Hrma³; A. A. Kruger⁴

1. University of Chemistry and Technology Prague, Czechia
2. Pacific Northwest National Lab, USA
3. AttainX, USA
4. DOE Hanford Field Office, USA

Volatilization of Tc-99 is of concern during the conversion of low-activity waste (LAW) feed to glass. Thus, the development of feed formulations ensuring high single-pass retention of Tc (or Re, its non-radioactive surrogate) is crucial for improving vitrification process efficiency. Previously, we demonstrated that using gibbsite or boehmite as the alumina source in LAW feeds increased the Re retention in the produced glasses by up to 20 and 25 %, respectively, compared to the nominal LAW feed containing kyanite. In this work, we performed leaching tests, XRD, and ²⁷Al NMR to show that the enhanced Re retention is caused by faster incorporation of Re into the transient glass-forming melt between 500 and 900 °C, and that the earlier formation of nanocrystalline alumina in the boehmite-containing feed is the likely key factor behind its superior performance. In addition, we show that Re retention in produced waste glasses increases with decreasing silica particle size, despite the increase in primary foaming. Since smaller silica particles dissolve faster in the borosilicate glass-forming melt, increasing its volume fraction in melter feed, we hypothesize that this enhances the rate at which Re is being incorporated.

GOMD S5 - Glass manufacturing

GOMD S5 S1 - Manufacturing I

Room: Saturna Island Ballroom

Session Chairs: Lisa Lamberson, Corning Incorporated;

Katelyn Kirchner, Celsian Glass USA

1:15 PM

(GOMD-S5-S1-001-2025) Our efforts to recycling of waste glass from end-of-life vehicles (Invited)

T. Kuzuya*¹; T. Naganuma²; H. Matsushima²; K. Sawada¹; N. Sawaguchi¹; A. Sato³; K. Deguchi⁴; H. Inano⁵

1. Muroran Kogyo Daigaku, Japan
2. Hokkaido Daigaku, Japan
3. MATEC Inc., Japan
4. Fukagawaglass, Japan
5. Chiho Dokuritsu Gyosei Hojin Hokkaidoritsu Sogo Kenkyu Kiko, Japan

Because end-of-life vehicle (ELV) waste glass has a low economic and environmental impact, most of it ends up in landfills. However, ELV waste glass is a carbon dioxide-free and energetically efficient glass-making material. Recently, recycled products have become popular as people are more environmentally conscious. Therefore, we started to produce and sell handicraft products using ELV waste glass. In this study, we tried to tune the thermal and mechanical properties of ELV waste glass by adding biomass, which abounds in alkaline metals. These serve as network modifiers to improve the processability of waste glass. Adding coconut ash increased the coefficient of thermal expansion and reduced the glass transition temperature. Conversely, the hardness tended to increase with an increase in the amount of coconut ash. It is considered to be an

effective tuning agent for the thermal and mechanical properties of ELV waste glass. To expand the use of ELV waste glass, we need to create products that make the most of waste glass's unique properties and composition. We focused on the additives of ELV waste glass and tried to create functional materials. In this study, the selective corrosion of glass condensed these additives on the surface to form an alternation layer. We examined the metal absorption and catalysis ability of this layer. It was found to exhibit good absorption ability for Ag and a strong basicity.

1:45 PM

(GOMD-S5-S1-002-2025) Reducing Energy Consumption and Carbon Dioxide Emissions from Glass Manufacture

E. Ahizi*¹; D. Deng²; D. Kabir¹; P. A. Bingham²

1. Sheffield Hallam University, Engineering and Maths, United Kingdom
2. Sheffield Hallam University, Materials and Engineering Research Institute, United Kingdom

There is a global effort to reduce the energy demand and carbon dioxide emissions from glass manufacture to meet the current net zero targets for a sustainable environment. Alternative raw materials are being sourced which have the capacity to reduce energy usage and limit CO₂ emissions from glass manufacture. Among these is wollastonite (CaSiO₃), which has been identified as a rich source of calcium oxide potentially capable of partially or completely replacing limestone in glass batches whilst also delivering faster melting kinetics, leading to energy saving during glass manufacture. Different lab-scale experimental analyses have been carried out to ascertain the viability of wollastonite as a limestone substitute in soda-lime-silica (SLS) glass manufacture. Among the analyses carried out were glass melting including a stages-of-melting study, with XRF, XRD, DSC/TGA and Micro-XRCT. Following the findings so far, when a batch containing wollastonite as the only calcium oxide source in SLS glass is compared to a benchmark glass composition containing limestone (CaCO₃) as the calcium oxide source, wollastonite maintained faster reaction kinetics which points to lower energy demand during the batch reaction processes and consequently, lower melting energies. Further analyses are underway to quantify melting behavior and potential energy savings.

2:05 PM

(GOMD-S5-S1-003-2025) Development of a sustainable, high-quality Ba-, Sb- and B-free art glass

C. H. Roos*¹

1. Rheinisch-Westfälische Technische Hochschule Aachen, Glass and Glass Ceramic, Germany

Many glass products are still based on older glass chemistries that can no longer be considered environmentally friendly and sustainable under today's conditions. The presentation will show the optimization of the glass composition for a leading manufacturer of high-quality tableware and art glass, which is used for both manual and automated production. The glass is colored using a feeder coloring process if required. The specifications for the new glass composition were correspondingly strict on the part of the client and presented a variety of challenges. The requirements were decisive: - Sb₂O₃ completely removed and BaO at least significantly reduced, also ideally B₂O₃ removed - Color of the flint glass unchanged - Improvement of the thermal shock resistance - Improvement in mechanical resistance with regard to both scratches and edge chipping - Improved dishwasher resistance to class 2 - Reduction of emissions (particulate emissions from the composition and gaseous emissions) - All current colors reproducible - Centrifuge and pressed products produced from the same glass mass - No setbacks in production speed and manual production - All current processes applicable almost unchanged The presentation shows the work and the procedure for such a demanding development from cradle to successful production.

2:25 PM

(GOMD-S5-S1-004-2025) New Pathways to Reduce the Carbon Footprint of Glass?D. R. Neuville^{*1}; T. Arnal¹; L. Cormier²; N. Schibille³

1. IPGP, Geomat, France
2. Sorbonne University - CNRS, IMPMC, France
3. Institut de Recherche sur les Archeomatériaux, France

Glass is a versatile material, essential for daily life and future carbon-neutral technologies. However, current glass production generates significant CO₂ emissions. Achieving a carbon-neutral supply chain by mid-21st century requires developing sustainable raw materials and melting processes. Several strategies to reduce CO₂ and energy consumption have been explored, such as increasing hydrogen use in gas mixtures, adopting electric furnaces, and incorporating cullet in production. While recycled materials are widely used, innovation potential remains. An alternative approach is to replace CO₂-bearing raw materials with volcanic lava, up to 50% by weight, mixed with glass cullet. This could eliminate carbonates—key CO₂ emission sources—and significantly reduce energy consumption in melting processes. A challenge lies in ensuring the glass's thermal working range remains compatible with its physical and chemical properties. Our research focuses on developing new glass compositions by mixing cullet with volcanic lava. Preliminary results are promising, suggesting the potential for producing bottles and other containers while aligning with carbon-neutral goals.

2:45 PM

(GOMD-S5-S1-005-2025) ZeroCO₂ Glass: Advancing the Path to Carbon-Neutral Container ManufacturingD. K. Orzol^{*1}; S. Thiele¹; S. Pietsch¹

1. IPGR - International Partners in Glass Research e.V., Germany

Achieving carbon neutrality in the container glass sector is a critical step toward sustainable manufacturing. To address this challenge, the ZeroCO₂ Glass project has established a state-of-the-art pilot facility capable of replicating industrial-scale glass production at 2.4 tons per day. This facility enables the systematic investigation of innovative strategies to decarbonize glass melting processes while maintaining industrial relevance. Key advancements include the integration of electric boosting as a primary energy source and the substitution of natural gas combustion with hydrogen. Additionally, traditional glass compositions have been re-engineered to incorporate alternative raw materials that minimize or eliminate CO₂ emissions during melting. This presentation will provide an overview of the pilot facility, operational since October 2024, and its initial findings. Topics will include energy efficiency, melting behavior, and the industrial applicability of the modified glass formulations. By sharing these insights, the project contributes to advancing carbon-neutral technologies and supporting the broader transition toward environmentally sustainable practices in glass manufacturing.

GOMD S5 S1 - Manufacturing II

Room: Saturna Island Ballroom

Session Chairs: Irene Peterson, Corning Incorporated; Lisa Lamberson, Corning Incorporated

3:30 PM

(GOMD-S5-S1-006-2025) Sustainable Manufacturing: Ideas to Overcome Technical Barriers to Wider Adoption of Electric MeltingS. Cooper^{*1}; K. Kirchner¹; E. Muskovin¹; J. Lang³; J. Blevins⁴; E. Nausken⁴; S. Rutkowski²

1. Corning, USA
2. RoMan Manufacturing, USA
3. Pacific Northwest National Laboratory, USA
4. Toledo Engineering Co., USA

The adoption of fully electric melting for large-scale glass manufacturing offers significant opportunities to reduce CO₂ emissions but also presents technical challenges that limit its widespread implementation. Key issues include foaming, refractory degradation, achieving higher pull rates, and meeting quality standards. To address these, CelSian, Pacific Northwest National Laboratory (PNNL), TECO, and RoMan Manufacturing have partnered under the Glass Manufacturing Industry Council (GMIC) to investigate the underlying physics and chemistry of electric melting and develop practical solutions. This presentation explores hypotheses for causes of foaming, limited heat transfer in dark-colored glasses, and corrosion. Methods include cold top melting experiments, raw material pellet testing, and computational fluid dynamics (CFD) modeling. The goal is to demonstrate the potential for an 85% reduction in CO₂ emissions in industrial glass melting processes while maintaining market performance and economic viability. We aim to spark discussion on cold top melting's chemistry and physics to accelerate adoption of sustainable glass melting.

3:50 PM

(GOMD-S5-S1-007-2025) Shaping the Future of Glass: Advances in Modeling and Measurements for Sodium-Reduced GlassesM. Bay^{*1}; S. Thiele²; C. H. Roos¹

1. Rheinisch-Westfälische Technische Hochschule Aachen, Institute of Mineral Engineering - Chair of Glass and Glass-ceramic, Germany
2. International Partners in Glass Research (IPGR) e.V., Germany

The Zero-CO₂-Glass project is focused on advancing the sustainability of glass production by reducing CO₂ emissions. Central to this effort is the investigation of sodium-reduced glasses, with SLS glass used as a reference under natural gas firing conditions. By capturing detailed measurements of wall thickness, glass temperatures, and mold temperatures, a comprehensive dataset is being established to inform simulation models. These models are refined through an iterative process to reflect real-world conditions, providing insights into the interplay of forming parameters such as timing and temperature. The goal is to optimize wall thickness distribution systematically while maintaining process efficiency. This work addresses global sustainability challenges while responding to a growing shortage of skilled workers. By fostering a deep understanding of the forming process, predictive models can support operators with varying levels of expertise, enabling efficient production with reduced reliance on experience-based knowledge.

4:10 PM

(GOMD-S5-S1-008-2025) From differential equations to melting furnace design (Invited)

W. Kuhn*¹

1. Fives Stein, Glass division, France

The glass melting process is of considerable complexity as it involves fluid dynamics, heat transfer, chemical thermodynamics/kinetics, and complex material properties. Glassmakers always tried to better understand the glass melting process and improve the melting tanks by empirical approaches. Scientific methods helped to deepen the knowledge on the different items of the melting process. Numerical modelling allows today tackling the coupled non-linear partial differential equations of the melt convection, integrodifferential equation of the radiation, multi-phase processes and complex glass chemistry. On this basis, glass technologists search for improvements of the melting process and tank design beyond a purely empirical approach. However, the complexity of the process and the huge number of adjustable parameters renders any optimization even with numerical tank models quite laborious. In the talk, the basic equations that govern the melting process are revisited. Appropriate reductions of the differential equations allow to better understand the impact of parameters such as tank dimensions and melt properties. Some of the key parameters are reviewed on their consequences for the tank design.

4:40 PM

(GOMD-S5-S1-009-2025) The effects of high water vapor atmosphere on float glass and its production process (Invited)

T. Maehara*¹; H. Tokunaga²; T. Miura¹

1. AGC Inc., Innovative Technology Laboratories, Japan
2. AGC Inc., Materials Integration Laboratories, Japan

CO₂ emissions for each ton of flat glass produced in a regenerative float furnace is approximately 0.5 ton. This includes 0.34 tons from fossil fuel combustion and 0.16 tons from carbonate raw materials. Methods for reducing CO₂ from burning fossil fuels can be categorized into energy saving and switching from fossil fuels to low-carbon energy sources. Energy saving measures, such as oxy-fuel combustion, various types of waste heat recovery system are already viable technologies, but they alone will not produce sufficient CO₂ reduction effects. To achieve dramatic CO₂ reduction effects, we must switch from fossil fuels to low-carbon energy sources. Alternative combustion gases are hydrogen, ammonia, and biogas. Electricity can also be used as a heat source other than combustion. When hydrogen or ammonia is burned in a furnace instead of fossil fuels, the water vapor partial pressure in the glass melting atmosphere increases significantly. Glass melting in a high water vapor atmosphere results in glass with a high water (-OH) concentration. In this study, glass samples with a wide range of water concentrations were prepared and various physical properties that affect the forming characteristics of the glass were evaluated. This presentation is based on results obtained from a project, JPNP21012, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

5:10 PM

(GOMD-S5-S1-010-2025) Thermodynamic analysis of the chemical reactions in the float bath: Development of the SnO-SnO₂-SiO₂-Al₂O₃ thermodynamic database and its applications

J. Lee*¹; I. Jung¹

1. Seoul National University, Material Science and Engineering, Republic of Korea

The float glass process is designed to produce flat glass with high homogeneity and controlled thickness. In the float bath, chemical reactions induced by Sn bath and evaporation of glass component pose significant challenges. For example, due to the evaporation of volatile species (Sn, SnO, ...) at the entering temperature, Sn can condense at the exit temperature and create surface defects.

In addition, Na evaporated from the glass can react with SiC heater on the roof of the chamber to form Na₂O-SiO₂ liquid. This liquid glass can drip onto the glass causing local inhomogeneity of glass composition, which may induce breakage. Furthermore, the reactions between sodium from the molten glass can degrade fireclay bottom block refractories by forming nepheline phase. In order to address these challenges, the thermodynamic database of the SnO-SnO₂-SiO₂-Al₂O₃ was developed based on the phase diagram experiments and critical evaluation of the literature data. After integrating new Sn oxide database with the existing Na₂O containing database, complex thermodynamic calculations on the oxygen/sulfur cycle, SiC degradation, and refractory degradation in the float bath were performed to understand the chemical reactions. All the calculations in this study were conducted using the FactSageTM thermochemical software.

GOMD S6 - Jonathan Stebbins Honorary Symposium

GOMD S6 - Jonathan Stebbins Honorary Symposium I

Room: SaltSpring AB

Session Chair: Jingshi Wu, Corning Incorporated

1:15 PM

(GOMD-S6-001-2025) Oxide Glasses and Liquids: Intriguing Journeys Past, Present and Future (Invited)

J. Stebbins*¹

1. Stanford University, USA

Oxide glasses and glass-forming liquids remain of central interest in advanced technologies, Earth and planetary sciences, and condensed matter physics. Several themes can illustrate the wide potential relevance of connections between the local and intermediate-range structure and the chemical behavior and physical properties of silicate glasses and melts, as well as key questions that remain unresolved. Here, important clues that have been viewed through the window of NMR spectroscopy will be highlighted, but there remain many future research challenges where new experimental and theoretical tools could lead to major breakthroughs. Examples include the molecular-scale dynamical processes that control critical properties such as diffusion and viscous flow, the temperature and pressure effects on structure beyond the most obvious changes in short-range coordination, and their connections to free energy, entropy and density, and the network connectivity from anionic (e.g. oxide ion) viewpoint. Such issues will be considered with a view both to historical development and future prospects.

2:05 PM

(GOMD-S6-002-2025) Aluminium Local Environment and Dynamics in Aluminosilicate Melts: in-situ High-Temperature Nuclear Magnetic Resonance Approach

P. Florian*²; D. R. Neuville¹; D. Massiot²

1. Institut de Physique du Globe de Paris, France
2. Conditions Extremes et Matériaux Haute Temperature et Irradiation, France

Despite real technological challenges, we have developed in our laboratory capabilities to perform Nuclear Magnetic Resonance (NMR) experiments from room-temperature up to 2400°C. This allowed us to observe the local structure (coordination state) and dynamics of aluminum controlling the macroscopic properties of aluminum-rich refractory melts. Heating sodium aluminosilicates across the glass transition temperature (~800°C) show a clear increase of the ²⁷Al concentration, a transient unit increasing the T_g of the glasses. Rare-earth aluminosilicate melts (>1700°C) also show an important presence of "minor" ²⁷Al species. For Ca-based compositions viscosity, electrical conductivity and ²⁷Al NMR relaxation processes in the melt are the same, pointing to a coupling between

the rate of Al-O bond exchange, the viscous flow and the motion of Ca ions. For Sr-based compositions the structure of the depolymerized melts is controlled by the Al/Si distribution, while the depolymerized melts show smaller rings with the presence of non-bridging oxygens on AlO_4 lost during cooling. The NMR correlation times provide a measure of the oxygen self-diffusion coefficient and its compositional dependence. The dominant parameter controlling the temperature dependence of the melts is the distribution of $\text{Al}-(\text{OSi})_p(\text{OAl})_{(4-p)}$ units.

2:25 PM

(GOMD-S6-003-2025) Application of High-resolution ^{95}Mo Solid State NMR in structural studies of alkali molybdate crystals and glasses

S. Sen^{*1}; I. Hung²; Z. Gan²

1. University of California, Davis, Department of Material Science and Engineering, USA
2. National High Magnetic Field Laboratory, USA

The Mo-O coordination environment is probed in a series of simple and complex crystalline alkali molybdates as well as in mixed-alkali molybdate glasses using high-field (20.0 T) ^{95}Mo MAS and MQMAS NMR spectroscopy. When taken together, the ^{95}Mo NMR spectroscopic results indicate that somewhat contrary to the conventional wisdom the corner- and edge- shared MoO_6 octahedral sites in these alkali molybdates are characterized by higher values of the isotropic shift and quadrupolar coupling constant (C_Q) compared to the MoO_4 tetrahedral sites. These anomalous trends are hypothesized to be related to the unusually strong distortion of MoO_6 octahedra in corner- and edge- shared configurations and strong relativistic effects on the chemical shift. While the ^{95}Mo C_Q of the MoO_4 sites displays an approximately linear positive correlation with the degree of tetrahedral distortion, no such correlation is observed for the MoO_6 sites. ^{95}Mo NMR results show the coexistence of tetrahedral and octahedral Mo-O environments in the structure of alkali molybdate glasses, with the relative fraction of the latter environment increasing with the Mo content. The results indicate that high-resolution ^{95}Mo NMR spectroscopy at high magnetic fields (~20 T or higher) may prove to be a promising tool for investigating the Mo-O coordination environments in nuclear waste glasses.

2:45 PM

(GOMD-S6-004-2025) An advanced NMR protocol for the structural characterization of transition metals in oxide glasses (Invited)

H. Eckert^{*1}; H. Bradtmüller¹; L. Hernandez¹; M. de Oliveira¹; R. B. Pena¹

1. University of Sao Paulo, Sao Carlos Institute of Physics, Brazil

Despite the great current interest in transition metal (TM) oxide containing glasses owing to their unique linear and non-linear optical properties, the short- and medium range order of the TM intermediate oxide species (such as TiO_2 , La_2O_3 , and Nb_2O_5) and their role in transforming the glass structure is poorly understood. Although solid state NMR techniques have, in principle, the potential of providing such information, the full potential of this method has, to date, been underutilized for glassy materials. The present contribution introduces an advanced multinuclear solid state NMR protocol involving spinning speed dependent magic-angle spinning at variable magnetic field strengths and numerous dipolar recoupling NMR methods, complemented by modelling studies and Raman spectroscopy, which shed light on the network-former role of Nb_2O_5 in niobium-containing silicate, borate and phosphate glasses. Funded by FAPESP, process no 2013/07793-6 (Center of Research, Technology and Education in Vitreous Materials), and processes 2023/17069-5, 2022/14232-0, and 2022/01937-5.

GOMD S6 - Jonathan Stebbins Honorary Symposium II

Room: SaltSpring AB

Session Chair: Sabyasachi Sen, University of California, Davis

3:30 PM

(GOMD-S6-005-2025) Stebbins and Silicate Melts (Invited)

A. Navrotsky^{*1}

1. Arizona State University, USA

I have known Jonathan Stebbins since he was a graduate student and I was a young faculty member. We have been friends and collaborators and have grown old together. Looking back on our careers, the “microscopic to macroscopic” aspects of crystalline, glassy, and molten silicates are constant common ground. Together and separately, we continue to link structure, properties, and thermodynamics. Complex multicomponent molten silicates are indeed “high entropy alloys”, with their enthalpy enhanced and their entropy significantly reduced by short range order. In this talk honoring Jonathan, I review the progress of experimental techniques in spectroscopy, diffraction, and calorimetry applied to silicate melts and glasses, with emphasis on what’s new, how we got there. And where we go next.

4:00 PM

(GOMD-S6-006-2025) Composition and pressure effects on the structure, elastic properties and hardness of calcium-aluminoborosilicate glass

J. Wu^{*1}

1. Corning Incorporated, Science & Technology, USA

In oxide glass, aluminum and boron can exist with multiple coordination numbers, which can be influenced by aspects like composition and pressure. We synthesized a series of calcium-aluminoborosilicate glasses with varying $\text{B}_2\text{O}_3/\text{SiO}_2$ ratios. These were then isostatically compressed at temperatures exceeding their glass transition temperatures at 1 and 2 GPa. We quantified the coordination numbers of boron and aluminum in recovered samples using ^{11}B magic angle spinning (MAS) nuclear magnetic resonance (NMR) and ^{27}Al MAS NMR spectroscopy at room temperature and pressure. We observed an increase in average coordination numbers as pressure on the glass was increased. Glasses with a higher boron concentration showed greater recoverable densification. The densification of the glass significantly impacts Young’s modulus and Vickers hardness number. Both show strong correlations with oxygen packing density in this series of glass. However, for accurate predictions of these properties, individual bond energy (or bond strength) must also be considered. Generally, Poisson’s ratio decreases as the average coordination number of network formers increases. However, the changes in Poisson’s ratio with pressure for each glass composition are complex and do not show a straightforward trend with compaction.

4:20 PM

(GOMD-S6-007-2025) Structure, composition, and reactivity of less ordered phases in cementitious systems from solid-state NMR

J. Skibsted^{*1}

1. Aarhus Universitet, Denmark

Less-ordered phases are crucial components in Portland cement-based materials, impacting their pozzolanic reactivity, and strength. For example, the principal binding phase in hydrated cements is a less-order Al-substituted calcium-silicate-hydrate (C-S-H) phase with variable composition and structure. Also, blast furnace slags and calcined clays, with CAS glass-like compositions and structures, are often used in cement blends as latent hydraulic components. A highly reactive pozzolanic material can also be formed by aqueous carbonation of end-of-life concrete, where an amorphous alumina-silica gel and is the reactive component. Solid-state NMR has played a vital role as a microstructural characterization tool for elucidation of structure, composition, and reactivity of these phases in cement

blends. ^{29}Si and ^{27}Al have been the most studied nuclei but information has also been derived from ^1H , ^{13}C , and ^{23}Na NMR. The most crucial challenge of the cement industry is to reduce its CO_2 footprint which accounts for 6 – 8 % of the anthropogenic CO_2 emissions. This presentation will focus on recent progress in the development of low- CO_2 supplementary cementitious materials from structural characterization and compositional modifications of the less-ordered/amorphous phases in CAS glasses, calcined clays, and carbonated recycled concrete fines from solid-state NMR experiments.

4:40 PM

(GOMD-S6-008-2025) Structures of Glasses at High Pressure: Our Journey to the Megabars

S. Lee*¹

1. Seoul National University, Republic of Korea

In this presentation, we highlight the recent experimental efforts to reveal the structures of densified glasses via solid-state nuclear magnetic resonance spectroscopy, the field that has been pioneered by Professor Stebbins. Our homonuclear- and heteronuclear correlation NMR results involving quadrupolar nuclides under pressure revealed previous unknown structural details of oxide glasses at high pressure up to ~90 GPa. We also present ab initio calculations of structure and NMR properties of prototypical oxide glasses under multi-megabar pressures, yielding a quantitative window to establish the relations between topological arrangement within glass network and the nature of nuclear spin interactions. We also provide an overview of our recent experimental progress via synchrotron inelastic x-ray scattering spectroscopy of multi-component oxide glasses under megabar pressure conditions, which reveals the electronic structures of non-network formers including iron, along with oxygen and framework cations, in amorphous networks under extreme deformation.

5:00 PM

(GOMD-S6-009-2025) The glass transition: adding a material parameter to geosciences & emergent technologies (Invited)

D. B. Dingwell*¹

1. Ludwig-Maximilians-Universität München, Earth and Environment, Germany

The central role of relaxation as a defining feature of volcanic processes has been a discovery of the first order in earth sciences. The defining power of the liquid to solid transition in glassforming systems in nature has led to a host of petrological and volcanological insights and tools. Glassy geomaterials, either initially present in the earth system, or molten materials generated during the interaction of environmental materials with extant technologies is also a rapidly expanding area of investigation usually requiring scaling to the glass transition. As we stand on the threshold of expanding our experience to planetary missions and goals we are faced with a further plethora of engineering challenges regarding the near ubiquitous presence of glassy materials, volcanic and impact, on planetary surfaces. The parameterisation of their thermal behavior is fully wrapped around the glass transition. Finally, as an essential element of grasping the fundamentals of planetary degassing, atmosphere development and its implications for exoplanets and the signals we receive from them, the modelling of volcanic (glassy) rock-forming processes on extraterrestrial bodies stands in the center of a mechanistic understanding of the fate of worlds. Some recent examples of novel glass transition determinations will be used to illustrate where these considerations have led us.

Tuesday, May 6, 2025

GOMD Award Lectures

GOMD - George W. Morey Award

Room: Saturna Island Ballroom

Session Chairs: Collin Wilkinson, Alfred University;

Madoka Ono, Hokkaido University

8:00 AM

(GOMD-Awards-001-2025) The Properties of Glass and Melt

D. R. Neuville*¹

1. IPGP-CNRS-UPC, Geomat Lab, France

Between 1938 and 2025, our understanding of glass has evolved dramatically. Once thought to be limited to silicate-based systems, we now know that glass can be formed with nearly every element in the periodic table and across all types of chemical bonds. Today, glass is best defined as a state of matter characterized by structural disorder and the glass transition phenomenon. Yet, fundamental questions remain: What exactly governs the glass transition? How do different chemical elements influence the properties of both glass and melts? And most importantly, how can we bridge the gap between atomic-scale structure and macroscopic behavior? In my talk, I will explore the structural roles of chemical elements—as network formers, charge compensators, or network modifiers—and their direct impact on material properties like viscosity. Beyond that, I will examine how these roles influence nucleation mechanisms and redox reactions. Understanding these processes is not just a matter of academic curiosity; it has real-world implications, from deciphering mass transfer in magmatic chambers to engineering low-carbon glass compositions that are essential for the energy transition.

GOMD S1 - Fundamentals of the glassy state

GOMD S1 S3 - Structural characterizations of glasses and melts III

Room: Saltspring C

Session Chair: Dominique de Ligny, University Erlangen-Nürnberg

9:20 AM

(GOMD-S1-S3-011-2025) Structure of rare earth aluminum garnet melts, $\text{RE}_3\text{Al}_5\text{O}_{12}$, and influence of ionic radii

S. K. Wilke*¹; A. Al-Rubkhi¹; C. J. Benmore²; J. Neuefeind⁴; R. Youngman³; C. Koyama⁵; T. Ishikawa⁵; R. Shimonishi⁵; R. Weber¹

1. Materials Development, Inc., USA
2. Argonne National Lab, X-ray Science Division, USA
3. Corning Incorporated, Science & Technology Division, USA
4. Oak Ridge National Laboratory, USA
5. Japanese Aerospace Exploration Agency, Japan

Rare earth aluminum garnets are important materials as lasing media, phosphors, Faraday isolators, and thermal environmental barrier coatings. Conventionally employed in crystalline form, these compositions can be vitrified by levitation melt quenching for rare earths with sufficiently large ionic radii. We have measured the structure of $\text{Yb}_3\text{Al}_5\text{O}_{12}$ melts, using X-ray and neutron diffraction with three Yb isotope substitutions, and the melt density, via imaging of electrostatically levitated drops. Models from empirical potential structure refinement (EPSR) of the diffraction data indicate that Al-O environments are mostly 4- and 5-coordinate, and Yb-O ranges 5- to 8-coordinate. Cation-oxygen polyhedra are connected predominantly by corner-sharing, with up to ~1/3 edge-sharing connections between polyhedra containing Yb or higher-coordinated Al. The -Al-O- network seems conducive to glass formation in terms

of mean oxygen coordination, polyhedra connectivity, and ring statistics, yet $\text{Yb}_3\text{Al}_5\text{O}_{12}$ cannot be cooled to form crystal-free glass. Structural comparison is made to a series of glass-forming $(\text{La},\text{Y})_3\text{Al}_5\text{O}_{12}$ to elucidate the effect of rare earth ionic radius on network structure and glass forming ability. Coordination distributions for Al-O from nuclear magnetic resonance spectroscopy (NMR) of the glasses are consistent with temperature extrapolations of the X-ray diffraction and EPSR models.

9:40 AM

(GOMD-S1-S3-012-2025) Achieving structural determination in glasses via first-principles molecular dynamics

C. Massobrio*¹

1. Laboratoire des Sciences de l'Ingenieur de l'Informatique et de l'Imagerie, France

One of the major issues of glass science is the precise determination of atomic structures devoid of topological order and mostly unattainable for experimental probes when it comes to describing the overall arrangement in terms of structural units variously connected. Invaluable help in this context can be provided by atomic-scale modelling, in particular by first-principles molecular dynamics (FPMD) ensuring a reliable treatment of chemical bonding and of its changes as a function of temperature. This talk will entirely focus on FPMD results obtained within our team on glassy systems, mostly (but not exclusively) chalcogenides. Concepts and crucial features inherent in the FPMD approach will be briefly recalled, as a prerequisite to capture the importance of the theoretical framework to complement and enrich realistically experimental structural determinations. Examples will be provided for a set of systems like SiN, GeTe_4 , $\text{Ge}_2\text{Sb}_2\text{Te}_5$ and those belonging to the $\text{Ge}_x\text{Se}_{(1-x)}$ family.

10:00 AM

(GOMD-S1-S3-013-2025) Crystal-Like Atomic Arrangement and Optical Properties of R_2O_3 - MoO_3 Binary Glasses Composed of Isolated MoO_4^{2-}

A. Masuno*¹; S. Munakata²

1. Kyoto University, Graduate School of Engineering, Japan
2. Hiroasaki University, Graduate School of Science and Technology, Japan

Transparent R_2O_3 - MoO_3 (R = rare earth element) binary glasses were prepared in bulk form using a levitation technique. The glass-forming range was limited, with the primary composition centered around 25 mol% R_2O_3 . X-ray absorption fine structure and Raman scattering analyses revealed that the $25\text{La}_2\text{O}_3$ - 75MoO_3 glass structure closely resembles the $\text{La}_2\text{Mo}_3\text{O}_{12}$ due to the presence of isolated MoO_4^{2-} units, whereas disordered atomic arrangement around La atoms was confirmed. The glass demonstrated broad optical transparency from 378 nm to 5500 nm and from 6.5 to 8.0 μm . This extended infrared transparency is attributed to the reduced diversity of MoO_n units and limited Mo-O-Mo connectivity, resulting in decreased multi-phonon absorption. Additionally, the glass transition temperature of $25\text{R}_2\text{O}_3$ - 75MoO_3 glasses increased monotonically with decreasing ionic radius of R^{3+} , while the local structure around Mo atoms remained largely unchanged. The glass formation of R_2O_3 - MoO_3 , deviating from conventional glass-forming rules, produced unique glasses with crystal-like atomic arrangements.

10:20 AM

(GOMD-S1-S3-014-2025) Oxide melt density measurements in an aero-acoustic levitation instrument

S. K. Wilke*¹; J. Rafferty¹; A. Al-Rubkhi¹; R. Weber¹

1. Materials Development, Inc., USA

Melt density is an important property in fundamental structure studies and for the design of melt processes in glassmaking. Yet, experimental measurements on refractory oxides are challenging due to crucible-induced reactions and crystal nucleation. One solution to

these challenges is to use containerless processes such as levitation, combined with silhouette imaging of molten droplets. We apply this technique in a novel instrument, the aero-acoustic levitator (AAL), which employs a heated gas jet and an actively controlled acoustic positioning system to levitate and laser beam heat oxide samples ca. 2-4 mm in diameter. The combination of aerodynamic and acoustic forces opens up unobstructed optical access to the full sample cross-section. Upon melting, the molten droplets are imaged with a monochromatic light source and narrowband-filtered camera. Melt volume is then calculated from the silhouette cross-sections and used to determine density as a function of temperature. As examples, we report densities for CaAl_2O_4 , $\text{Ca}_{12}\text{Al}_{14}\text{O}_{33}$, CaSiO_3 , their Fe_2O_3 -bearing analogues, and 83TiO_2 - $17\text{RE}_2\text{O}_3$ (RE = La or Nd) over 1530-1920 K, including up to 350 K of supercooling. This study aims to benchmark the capabilities, estimate the uncertainties, and explore the outlook for this technique.

10:40 AM

(GOMD-S1-S3-015-2025) Structures of mixed (Li,Na) silicates from MD simulations

A. Cormack*¹; D. Neuville²

1. Alfred University, USA
2. CNRS - Institut de physique du globe de Paris, France

The mixed alkali effect, first described 140 years ago, still lacks a universally accepted explanation. In this presentation, we add to the discussion the results of a structural investigation of mixed (Li,Na) silicate glasses, using molecular dynamics simulations. Four compositions were modelled: $\text{R}_2\text{O} \cdot 2\text{SiO}_2$; $\text{R}_2\text{O} \cdot 3\text{SiO}_2$; $\text{R}_2\text{O} \cdot 4\text{SiO}_2$ and $\text{R}_2\text{O} \cdot 10\text{SiO}_2$. Simulation boxes containing ~6000 atoms were created by randomly populating the boxes with atoms in the appropriate stoichiometry. The system was then heated at 2500 K for 1,000,000 timesteps (2 ns) and cooled to 300 K in steps of 100 K, with trajectories of 10 ns at each temperature. Pair distribution functions of the resulting structures were obtained and will be discussed. The detailed atomic scale structural environment of the alkali ions will also be described.

11:00 AM

(GOMD-S1-S3-016-2025) Structure of vanadium-containing sodium aluminoborosilicate glasses

P. Malviya*¹; R. Youngman²; J. Kaewkhao³; C. Sarumaha³; W. Busayaporn⁵; A. Yaremchenko⁶; A. Pedone⁴; M. Bertani⁴; A. Goel¹

1. Rutgers The State University of New Jersey, material science and engineering, USA
2. Corning Incorporated, USA
3. Nakhon Ratchasima Rajabhat University, Thailand
4. Universita degli Studi di Modena e Reggio Emilia, Italy
5. Synchrotron Light Research Institute, Thailand
6. Universidade de Aveiro CICECO, Portugal

Vanadium, as a transition element, exhibits varying oxidation states that are intricately influenced by the bulk chemistry of glass. This variation in oxidation states significantly alters the physical and chemical properties of glasses. For instance, when incorporated into borosilicate glasses, vanadium is known to increase sulfur solubility. What makes vanadium particularly compelling is the ambiguous underlying mechanism behind its ability to do so. Although numerous hypotheses exist within the literature, there remains a notable gap in understanding the precise mechanisms involved. This ambiguity prompts further investigation, as elucidating the underlying mechanisms could unearth potential to tailor practical applications in various areas of interest. Therefore, the present study aims at elucidating the structure of vanadium containing sodium aluminoborosilicate glasses, where the V_2O_5 concentration varies between 0 to 5 mol.% in the peralkaline, metaluminous, and peraluminous glass systems. The redox behavior of V as a function of Na/Al ratio and V_2O_5 concentration has been unearthed using V K-edge XANES, while the consequential impact on the glass

structure has been followed using Raman spectroscopy, electrical conductivity, combined with ^{11}B , ^{23}Na , ^{27}Al , and ^{51}V MAS NMR spectroscopy and molecular dynamics simulations. The results will be discussed in the presentation.

11:20 AM

(GOMD-S1-S3-017-2025) Nature of Mixing of Modifier Cations in Phosphate Glasses: Results from ^{17}O Solid-State NMR Spectroscopy

S. Chuang^{*1}; S. Sen¹

1. University of California, Davis, Department of Material Science and Engineering, USA

The degree of ordering in the distribution of modifier alkali and alkaline-earth cations in single- and mixed- modifier phosphate glasses is investigated using ^{17}O nuclear magnetic resonance (NMR) spectroscopy. ^{17}O isotope-enriched metaphosphate glasses are synthesized via a gas-to-solid isotope exchange method. The phosphate speciation in the resulting samples is characterized using ^{31}P magic angle spinning (MAS) NMR. ^{17}O NMR experiments, including MAS and triple-quantum MAS (3QMAS) NMR reveal the bridging (BO) and non-bridging (NBO) oxygen sites, while the compositional evolution of the NMR line shape of the NBO sites enables the identification and quantitation of distinct NBO environments associated with the various constituent modifier cations. The NBO speciation in mixed-modifier glasses is compared with that expected from a random distribution of the two constituent modifier cations, which sheds light on the role of field strength of these cations and the thermal history of the glass on their spatial distribution. The results, when taken together, contribute to a broader understanding of the mixed-modifier effect on various physical properties of these glasses and their parent supercooled liquids.

11:40 AM

(GOMD-S1-S3-018-2025) Enhancing Nb Solubility in Aluminosilicate Glasses via Phosphorus Addition

V. Kerling^{*1}; D. de Ligny¹; M. Cicconi¹

1. Friedrich-Alexander-Universität Erlangen-Nürnberg, Institute of Glass and Ceramics, Germany

$\text{Na}_{0.5}\text{K}_{0.5}\text{NbO}_3$ (KNN) crystallizes in a perovskite structure, exhibiting properties useful for energy storage and conversion applications. This study focuses on the development of transparent glass-ceramics containing KNN within an aluminosilicate matrix. In this talk, we will discuss the impact of P incorporation on the solubility of niobates in polymerized aluminosilicate glasses and on the crystallization behavior of the glasses. 6 and 9 mol% P_2O_5 were added to NAS glass having Al/Na molar ratio = 1. Subsequently, KNN was added up to its solubility limit, and the resulting homogeneous glasses were characterized. Polarized Raman spectroscopy revealed the disappearance of the $\text{Q}_p^4\text{-O-Al}$ fingerprint in the VV spectra with KNN addition, suggesting relevant variations in the glass topology. In particular, an interaction between P and KNN is proposed, likely forming P-O-Nb bonds or NbO_6 clusters in alkali-rich regions near phosphorus. Thermal events were identified by DSC, and heat treatments of glasses containing 10 and 20 mol% KNN resulted in transparent glass-ceramics. XRD confirmed the crystallized phase as a perovskite-like alkali niobate, with a secondary phase. Overall, the addition of phosphorus effectively increased the solubility of KNN in the polymerized NAS glass, enabling the formation of transparent glass-ceramics with higher KNN content and perovskite-like crystals.

GOMD S1 S6 - Mechanical properties of glasses III - Designing high-strength glass

Room: Pender

Session Chair: Jun Endo, AGC Inc.

9:20 AM

(GOMD-S1-S6-010-2025) Structural design of a hard and crack-resistant glass (Invited)

A. Goel^{*1}; A. Yadav¹; A. Rebecca¹; S. Kapoor⁴; Y. Shih³; L. Huang²

1. Rutgers University, USA
2. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA
3. National Taipei University of Technology, Department of Materials and Mineral Resources Engineering, Taiwan
4. Sterlite Technologies Limited, India

The industry has long sought to develop glass that is “hard” and “crack-resistant.” However, achieving these properties simultaneously in oxide glasses has proven exceptionally challenging. While Al_2O_3 -rich oxide glasses with both hardness and crack resistance have been reported in recent years, their industrial application faces two major obstacles: (1) high processing temperatures exceeding 2000 °C and (2) limited glass-forming regions near the eutectic point. Our study introduces a structurally engineered high-modulus, hard, and crack-resistant glass designed within the peraluminous region of the $\text{MgO-Al}_2\text{O}_3\text{-B}_2\text{O}_3\text{-SiO}_2$ system containing rare earth oxides. This glass can be processed at temperatures ≤ 1650 °C and demonstrates a Vickers hardness (Hv) greater than 7 GPa (under a 1.96 N load), crack resistance (CR) of 26.5 N, and optical transmittance of $90 \pm 2\%$. This presentation will explore the development process behind this glass and ongoing efforts to address challenges related to its scale-up and commercialization.

9:50 AM

(GOMD-S1-S6-011-2025) Effects of Ion Exchange on Lithium Disilicate Glass-Ceramics

Y. Shih^{*1}; C. Chang¹; H. Yeh¹

1. National Taipei University of Technology, Department of Materials and Mineral Resources Engineering, Taiwan

The hardness of lithium disilicate (LS2) glass is significantly enhanced through rapid surface crystallization followed by an ion exchange (IOX) process. This study fabricated lithium disilicate glass-ceramics (LS2-GCs) with varying crystallinities via nucleation and growth within two hours, preserving transparency and minimizing dimensional changes. The LS2-GCs demonstrated greater hardness than their parent LS2 glass, with hardness further enhancing as crystallinity rose. The IOX process further improved the hardness of LS2-GCs using different molten salt baths: NaNO_3 , KNO_3 , and a sequential bath ($\text{NaNO}_3 \rightarrow \text{KNO}_3$). X-ray diffraction (XRD) patterns revealed that the IOX primarily occurred in the glassy phase. Crystallization in LS2 glass effectively mitigated flaw formation during ion exchange; meanwhile, the hardness of LS2-GCs increased with both higher crystallinity and extended IOX duration. Among the IOX baths, the sequential bath yielded the highest hardness, followed by KNO_3 and NaNO_3 . Moreover, prolonged soaking in KNO_3 during the sequential bath further enhanced hardness. The transmittance of LS2-GCs in the visible light range decreased with increasing crystallinity and IOX duration. Of the three IOX baths, the KNO_3 bath maintained the highest transmittance, followed by NaNO_3 and the sequential bath. Additionally, transmittance further diminished with longer soaking times in NaNO_3 during the sequential bath.

10:10 AM**(GOMD-S1-S6-012-2025) Effect of Al₂O₃/SiO₂ and MgO/CaO ratio on the mechanical properties and chemical strengthening of sodium aluminosilicate glasses**J. Cho^{*1}; J. Chung¹; J. Kim¹

1. Korea Institute of Ceramic Engineering and Technology, Republic of Korea

This study aims to investigate the effect of Al₂O₃/SiO₂ and MgO/CaO ratio on the mechanical properties and chemical strengthening of sodium aluminosilicate glasses. The density increased with increasing Al₂O₃/SiO₂ and MgO/CaO ratio. The structure of glasses was analyzed by ²⁷Al and ²⁹Si MAS-NMR. It was confirmed that the amount of non-bridging oxygen decreased with increasing Al₂O₃ and MgO contents. Mechanical properties such as hardness and elastic modulus increased with increasing Al₂O₃ and MgO contents due to the reduction of the amount of non-bridging oxygens. In addition, the hardness of all samples increased after chemical strengthening and the increase in hardness after chemical strengthening increases with increasing Al₂O₃ and MgO content. The surface compressive stress (CS) and depth of layer (DoL) increased with Al₂O₃ and MgO content since the glass structure became more dense and the fraction of bridging oxygen increased. These results indicate that the chemical strengthening effect improved with increasing Al₂O₃ and MgO contents. We hope our results to be widely used in commercialization of chemical strengthened display glasses.

10:30 AM**(GOMD-S1-S6-014-2025) Biaxial strength testing of special glass samples**R. Bermejo^{*1}; F. Maurer²; R. Danzer¹; P. Supancic¹1. Montanuniversitat Leoben, Materials Science, Austria
2. Schott AG, Germany

Sheet-like glassy components are increasingly used in technical applications. Examples are window glasses in buildings, flexible cover sheets in smartphones or parabolic mirrors. The strength of these products is a key property for its design and therefore accessing reliable strength data via adequate strength tests is necessary. For testing flat plates the ring on ring (RoR) test is standardized and well established. The (circular or rectangular) plate is positioned on a support ring and bent via a second smaller loading ring, which is concentrically positioned on the opposite side of the plate. However, certain restrictions have to be fulfilled by the specimens (e.g. the aspect ratio of thickness to support diameter) to obtain valid data. For example, high strength materials with low elastic modulus can hardly fulfil the required limits. In this work the strength of special glass specimens, which cannot be measured by the conventional RoR-test, will be investigated by variants of the Ball-on-Three-Balls test (B3B): (i) bent glass plates, whose non-flat geometry is not compatible with the RoR-test, and (ii) thin glass sheets, which show a too large flexibility. A main feature of the B3B-test is that three support balls make a stable specimen support, which can also be used for strength testing of non-planar specimens. Miniaturization of the B3B-test allows also the accurate strength testing of thin and small specimens.

10:50 AM**(GOMD-S1-S6-015-2025) Evaluation of brittle properties in silicate glasses through a combination of phase-field method and single-notch microbeam test**G. A. Rosales-Sosa^{*1}; Y. Kato¹; G. Molnár³; T. Ohmura⁴; T. Nakashima¹; E. Barthel²; G. Kerrouche⁵; S. Nakane¹; H. Yamazaki¹1. Nippon Electric Glass, Fundamental Technology Division, Japan
2. CNRS/ESPCI, SIMM, France
3. University of Lyon, INSA-Lyon, LaMCoS, France
4. Busshitsu Zairyo Kenkyu Kiko, Research Center for Structural Materials, Japan
5. Ecole des Mines de Saint-Etienne, Physique et Mécanique des Matériaux (PMM), France

The critical energy release rate (G_c) is one of the fundamental properties of brittle materials related to the material's ability to absorb energy before failure. The phase-field method has recently proven effective in simulating static and dynamic failure in brittle materials by considering G_c and elastic moduli as basic properties in the model. This work proposes evaluating G_c in oxide glasses by combining single-notched microbeam tests and phase-field calculations. Single-notched silica (SiO₂) and soda-lime-silicate (SLS) glass microbeams were fabricated using the Focused Ion Beam (FIB) technique and tested with a nanoindenter in atmospheric conditions. The experimental load-displacement curves showed that the force required for fracture decreased with increasing depth of the notch in both glass compositions and that the fracture was brittle as expected. High reproducibility was observed in the experiments. The phase-field calculations allowed for direct evaluation of G_c for silica and SLS glasses. The approach proposed in this work proved promising for evaluating the brittle properties of materials, including the material's fracture toughness and fracture surface energy. The advantages and disadvantages of this new approach will be discussed.

11:10 AM**(GOMD-S1-S6-016-2025) Modeling the effects of thermal residual stresses on fracture of microstructured glasses**E. Barros de Moraes^{*1}; X. Xu¹; J. Harris¹; C. Smith¹

1. Corning Incorporated, USA

Microstructured materials such as composites, phase-separated glasses, and glass-ceramics, potentially have higher fracture toughness than single-phase homogeneous amorphous glasses. Due to elastic and thermal properties mismatch between phases, residual tensile or compressive stresses can be present and either enhance or deteriorate the fracture properties of the material. Experimental exploration of mechanisms and effects of thermal residual stresses is a challenge due to small scales of microstructural features and tri-dimensional nature of stress fields. In this talk, we present a computational framework to simulate and analyze the effect of thermal residual stresses in two-phase materials. The approach combines a phase-field model to generate complex 3D microstructures followed by mechanical simulations using peridynamics. We discuss how the mismatch in coefficient of thermal expansion interacts with other mechanical properties from each phase.

GOMD S2 - Glass and interactions with its environment - Fundamentals and applications

GOMD S2 S3 - Materials for waste immobilization II

Room: Cortes

Session Chairs: Jaime George, Pacific Northwest National Lab;
John Zaengle, Pacific Northwest National Laboratory

9:20 AM

(GOMD-S2-S3-010-2025) A Kinetic Model of the Long-Term Corrosion of Multiphase Waste Forms

S. Kerisit^{*1}; B. Parruzot¹; J. Neeway¹; J. T. Reiser¹; J. M. Westman¹;
P. D. Sutton²; D. Gregg²; M. Asmussen¹; G. L. Smith¹

1. Pacific Northwest National Lab, USA
2. Australian Nuclear Science and Technology Organisation, Australia

Multiphase waste forms show promise for increased waste loading and for the ability to dispose of contaminated solid and particulate wastes through direct densification. However, achieving predictive capability for long-term durability of multiphase waste forms, and thus assessing their possible deployment, requires expanding the current, limited knowledge base. Here, we describe the development of a corrosion model of a two-phase waste form consisting of crystals of known volume fraction embedded in a glass matrix. This model accounts for the dissolution of both the crystalline and glass phases as well as the hydration of the glass phase through an ion exchange reaction. Because of the large difference in solubility between the two phases, the reactive surface of the crystalline phase is a function of the extent of dissolution of the glass phase in this model. Model parameterization was performed using corrosion data, such as from single-pass flow-through tests, for the individual phases. The parameterized corrosion model was evaluated against static dissolution test data for a glass-ceramic multiphase waste form. This evaluation demonstrated the model's ability to reproduce the time-dependent release of key tracers of glass and crystalline phase dissolution. Hence, the development of a kinetic model provides a pathway for long-term durability predictions and thus the use of multiphase waste forms.

9:40 AM

(GOMD-S2-S3-011-2025) Glass Dissolution at Different Surface-Area-to-Volume (S/V) Ratios: An Approach to More Realistic Disposal Conditions

J. Neeway^{*1}; S. Kerisit¹; J. V. Crum¹; I. Burch¹; J. M. Westman¹; J. Ferrer¹;
S. Choi¹; J. T. Reiser¹; B. Parruzot¹; M. Asmussen¹; G. L. Smith¹;
D. Swanberg²; R. Skeen²

1. Pacific Northwest National Lab, USA
2. Washington River Protection Solutions LLC, USA

A performance assessment (PA) is used to estimate the impact of the disposal of immobilized low-activity waste (ILAW) glass and other wastes at the Integrated Disposal Facility (IDF) located at the Hanford Site, Washington State, USA. In the IDF PA, the release of contaminants from the ILAW glass is predicted with the ILAW glass corrosion model (IGCM). The IGCM has been developed, parameterized, and validated with data from static corrosion tests conducted with a large number of glass compositions at different temperatures. However, these tests were only conducted at one glass surface-area-to-volume (S/V) ratio, namely 2,000 m⁻¹. Because it is known that static tests performed at different S/V ratios will result in solutions of varying degrees of saturation with respect to solid phases, which will, in turn, affect the extent and rate of glass dissolution, it is important to verify that the IGCM is capable of predicting glass corrosion rates at various S/V ratios. For this reason, we have conducted a series

of tests at different S/V ratios and the data have been compared to IGCM predictions. This approach will help in assessing the general robustness of the IGCM and aid in the validation of the use of the model in the much higher S/V ratios expected in a disposal scenario.

10:00 AM

(GOMD-S2-S3-012-2025) Effect of in-situ γ dose rate on the alteration of nuclear glass

M. Taron^{*1}; H. Arena²; F. Chupin²; K. Ressayre²; R. Podor¹; M. Tribet²; S. Peugot²

1. Institut de Chimie Separative de Marcoule, France
2. CEA, France

In France, long-lived radioactive wastes are vitrified in a borosilicate glass matrix for disposal in a deep geological repository. After several thousand years, groundwater will interact with the glass, causing its degradation. Additionally, the self-irradiation of the glass due to the radionuclides affects its properties. To verify the safety of the repository, it is necessary to study the long-term behavior of nuclear glasses, considering alteration, self-irradiation, and their synergy. The effects of self-irradiation can be partly simulated using external irradiation beams on inactive samples, before alteration. However, it is also important to study the effects of irradiation on the alteration solution and the possible impact of its radiolysis on alteration kinetics. To this end, experiments were carried out at the Gammatec facility (STERIS, Marcoule), combining underwater alteration and γ dose rate. Glass samples were first submitted to several external irradiations scenarios using electrons and/or Au³⁺ ions, and then altered under a gamma dose rate of about 1,200 Gy/hr generated by a ⁶⁰Co source. The alteration kinetics were analyzed and the solids were characterized by ToF-SIMS and cryo-TEM. This study has therefore made possible to assess the impact of γ dose rate on glass alteration, and to identify a possible synergy with pre-irradiation, which simulates the effect of $\alpha\beta\gamma$ cumulative doses.

10:20 AM

(GOMD-S2-S3-013-2025) Self-irradiation of nuclear glasses simulated by external beams: recovery effect induced by electronic interactions

M. Taron¹; H. Arena^{*1}; S. Miro¹; C. Gillet¹; R. Podor²; S. Peugot¹

1. CEA, France
2. ICSM, Microscopy, France

Nuclear glasses containing radionuclides are submitted to their self-irradiation, which has an impact on the glass structure, properties and long-term behavior. Alteration experiments conducted on radioactive glass are cumbersome to carry out, as they have to take place in hot environments (glove boxes or shielded cells). Complex sequences of external irradiations were therefore used on inactive surrogate glasses, to simulate the electronic and nuclear interactions induced by self-irradiation. Nuclear interactions were generated by a 7 MeV Au³⁺ ions beam and the electronic interactions were induced by two particles with different stopping powers: 2.5 MeV electrons and/or 1.7 MeV He⁺ ions. In addition, complex sequential irradiation scenarios were carried out to study nuclear-electronic coupling. The irradiated glasses were then characterized by several techniques to assess changes in composition, structure, hardness and density. The effects of Au irradiation were much higher than that of He, and electron irradiation had very little impact on pristine glass. However, a recovery effect was observed when electronic irradiation was performed on samples previously damaged by nuclear interactions.

10:40 AM**(GOMD-S2-S3-014-2025) Elemental releases from enhanced low-activity waste glasses tested by 48-hour room temperature methods**

J. Marcial*¹; S. Choi²; N. Bohrmann²; A. Kennedy²; J. Hager²; L. Brown³; J. Neeway³; C. L. Thorpe³; R. J. Hand³; C. Pearce³; D. Kosson³; A. A. Kruger⁴

1. Pacific Northwest National Laboratory, Materials Testing and Development team, USA
2. Pacific Northwest National Lab, USA
3. University of Sheffield, Materials Science and Engineering, United Kingdom
4. US Department of Energy, Office of River Protection, USA
5. Vanderbilt University, USA

The Glass Leaching Assessment for Durability (GLAD) program seeks to develop new strategies to understand the elemental releases from nuclear waste glasses in near-surface conditions. Previously our team endeavored to develop linear compositional property models of enhanced Hanford low-activity waste (LAW) glasses tested using the United States Environmental Protection Agency (EPA) Leaching Environmental Assessment Framework (LEAF) EPA method 1313. The EPA method 1313 is a 48-hour, tumbled test where glass powders are immersed in different pH solutions at room temperature. Previous modeling demonstrated that the solution pH exhibited a dominant effect on elemental release as exhibited by the large change in initial pH and final pH during the conventional EPA method 1313. We explored the evolution of the solution pH during the test and investigated alternative methods to control the solution conditions during the entire 48 hours of testing, including the use of an autotitrator and buffered solutions with a statistically designed matrix. Compositional modeling was performed on the resulting normalized elemental release into solution.

11:00 AM**(GOMD-S2-S3-015-2025) Accounting for Alteration Layer Formation in Simulation of the Long-Term Corrosion of Nuclear Waste Glass**

S. Kerisit*¹; J. V. Crum¹; B. Parruzot¹; J. Neeway¹; G. L. Smith¹; M. Asmussen¹

1. Pacific Northwest National Lab, USA

Low-activity waste at the Hanford Site will be vitrified and disposed of on site at the Integrated Disposal Facility (IDF). The IDF performance assessment analyzes the long-term performance of the planned disposal system, including contaminant release from immobilized low-activity waste (ILAW) glass as predicted by the ILAW glass corrosion model (IGCM). The IGCM is composed of four coupled processes: glass dissolution, ion exchange (IEX), secondary phase formation, and aqueous speciation. Here, we describe an improvement to the IGCM, which involves the use of retention factors (RF) for key glass components to simulate the formation of a glass alteration layer. The RFs are parameterized simultaneously with the dissolution and IEX IGCM components using static test data for a matrix of 24 ILAW glasses that provides statistical coverage of major components in the ILAW composition space expected to be produced at the Hanford Waste Treatment and Immobilization Plant. The use of Al and Si RFs significantly improved agreement with static test data (B, Na, and Si concentrations) for all 24 glasses. For select cases, the predicted alteration layer composition was compared to energy-dispersive X-ray spectroscopic measurements of reacted glass cross sections. This work indicates the use of RFs is an effective way to improve the accuracy of long-term glass corrosion predictions.

11:20 AM**(GOMD-S2-S3-016-2025) Investigation of alkali and alkaline-earth phases in crystallized LAW glasses**

A. J. Lere-Adams*¹; J. McCloy¹

1. Washington State University, Mechanical and Materials Engineering, USA

Simplified Hanford low-activity waste (LAW) glasses were formulated to assess the effects of non-framework cations on crystallization and chemical durability. Glasses with different amounts of Na and Ca were heat treated using different schedules to induce crystalline phase formation via different paths. This will model the slow cooling of the melts at the canister centerline. The glassy structure was determined by Raman spectroscopy while the resultant phase assemblages were quantified by X-ray diffraction and confirmed by Electron Probe Micro-Analysis (EPMA) and Energy-Dispersive X-ray Spectroscopy (EDS). Chemical distribution of phases and alkali and alkali-earth elements in heated glasses were obtained. A Product Consistency Test (PCT) was conducted to determine the concentrations of chemical species released. To track the nucleation and growth of identified phases, diffraction data was collected while simultaneously heat-treating glasses. Overall, characterization helped to provide some understanding of the roles of non-framework cations.

11:40 AM**(GOMD-S2-S3-017-2025) Solubility of uranium oxide in aluminosilicate glass melts**

O. Podda¹; L. Tissandier²; M. Hunault³; E. Deloule²; A. F. Laplace*¹

1. CEA, University of Montpellier, Marcoule, France
2. CNRS, CRPG, University of Lorraine, France
3. Synchrotron SOLEIL, France

The immobilization of highly radioactive waste using vitrification process has been in application since many decades. Indeed, the incorporation of waste into the structure of a glass matrix can reduce the potential for radionuclides migration or dispersion. This process is under investigation for conditioning Intermediate Level and Long Life Waste (ILW-LL) using aluminosilicate glasses as host matrices. The vitrification must be able to maintain, within a certain range of compositions and redox potential, the actinides solubility. It is known that uranium chemistry is complex in glass-forming systems due to the presence of many oxidation states (VI, V, IV). This paper presents a study of the uranium solubility in aluminosilicate glass melts as a function of melt composition and redox potential. Ternary SiO₂-Al₂O₃-CaO (CAS) and SiO₂-Al₂O₃-MgO (MAS) systems are considered. In this study, the glass Al content is increased while keeping the Si/Ca and Si/Mg ratios constant. Further HERFD-XANES at the U M₄-edge analyses performed on MARS beamline at SOLEIL synchrotron (France) on selected samples enabled precise quantification of uranium oxidation states. The specific experimental methodology to cover a wide redox range is detailed and solubility results combined with uranium oxidation state data are discussed.

GOMD S3 - Optical and electronic materials and devices - Fundamentals and applications

GOMD S3 S4 - Rare-earth and transition metal-doped glasses and ceramics for photonic applications I

Room: Moresby

Session Chair: Brian Topper, Clemson University

9:20 AM

(GOMD-S3-S4-001-2025) Pushing the Limits: Stabilizing Unusual High Oxidation States of Transition Metals in Glasses (Invited)

D. Möncke^{*2}; B. Topper¹; A. Ashjari²; L. H. Hess³

1. Clemson University, USA
2. New York State College of Ceramics at Alfred University, USA
3. Northvolt AB, Sweden

Transition metal (TM) ions have been used early on as colorants in glasses. Especially 3d ions used in such fashion, or as fluorescing phosphors, are most often found in the di- or trivalent state. Developing glasses with high oxidation states of TM ions, such as Mn⁵⁺ for temperature sensing or imaging, presents a challenge for future photonic glassy materials. We were able to stabilize unusually high oxidation states of TM ions in cesium barium silicate and borate glasses of exceptionally higher optical basicity ($\Lambda = 0.72\text{--}0.81$). Stabilized species include blue Mn⁵⁺ (3d²), green Mn⁶⁺ (3d¹), yellow Co³⁺ (3d⁶), blue Ni³⁺ (3d⁷) or brown iron in tetravalent or higher oxidation states. Variations in composition resulting from synthesis including crucible dissolution to cesium oxide evaporation affects the redox ratio, but reproducible glasses can be made for a given melting protocol. High valence states were confirmed by UV-Vis, photoluminescence, and Raman spectroscopy. Notably, Raman spectroscopy detects vibrational modes for some transition metal anions present in very low quantities, for example, MnO₄ species can be identified with resonance Raman at concentrations well < 0.01%.

9:50 AM

(GOMD-S3-S4-002-2025) Characteristic luminescence properties of Eu³⁺ ions in mixed-anion coordination environment (Invited)

Y. Kitagawa^{*1}

1. Sangyo Gijutsu Sogo Kenkyujo Kansai Center, Japan

Eu³⁺ ions exhibit orange-red luminescence with sharp spectral lines owing to the interconfigurational 4f-4f transitions, making them valuable as red phosphors in various lighting and display applications. Regardless of shielding by the outer 5s and 5p orbitals, the optical properties of Eu³⁺ 4f-4f transitions are influenced by the local coordination environment, including the geometry of coordination polyhedra, site symmetry, nephelauxetic effects induced by coordinating anions, crystal field effects, and bonding characteristics. Mixed-anion coordination around a single Eu³⁺ ion directly modulates its luminescence properties. In this study, we investigated the luminescence properties of Eu³⁺-doped oxynitride YSiO₂N:Eu³⁺ and oxyhalide YOX:Eu³⁺ (X = Cl or Br). Partial substitution by nitride or halide anions within the coordination sphere introduced an asymmetric local field, significantly enhancing red luminescence peaking in the range of 610–630 nm. The elevation of the valence band maximum, attributed to the p orbitals of covalent anions, lowered the charge transfer transition energies and reduced the thermal quenching temperature of Eu³⁺ luminescence. These findings are compared with previously reported Eu³⁺-doped oxysulfides and oxyhydrides. Furthermore, material design guidelines for achieving efficient red luminescence under near-UV excitation are discussed.

10:20 AM

(GOMD-S3-S4-003-2025) Rare Earth Doped Titanate Glass Disks and Fibers for Optical Device Applications

R. Weber^{*1}; J. Tolliver⁴; A. Neumann⁴; S. K. Wille³; A. Al-Rubkhi¹; B. Topper²

1. MDI, USA
2. Clemson University, USA
3. Materials Development, Inc., USA
4. University of New Mexico, USA

Recent development of titanate network glasses has led to a new host for rare earth ions. The glasses contain ~80 mole% titanium oxide with the balance rare earth oxide. The network is composed mainly of corner and edge shared octahedra. The glasses have relatively low phonon energy combined with a high solubility for rare earth ions. Glasses have been formed into spheres and fibers directly from the liquid phase, with spheres post-processed to make disks. Results of optical property measurements including fluorescence lifetime and bandwidth for erbium and neodymium doped glasses, measurements of gain in Yb-doped fibers and laser demonstration in Nd-doped disks will be presented. The results will be discussed in the context of developing new optical devices enabled by the materials.

10:40 AM

(GOMD-S3-S4-004-2025) Magneto-optical effect of rare-earth-rich borate glasses prepared using a levitation technique

S. Sasaki^{*1}; K. Tanaka¹; A. Masuno¹

1. Kyoto University, Department of Material Chemistry, Japan

Borate glasses containing a large amount of R³⁺ ions (R = rare-earth element) have been prepared by using an aerodynamic levitation furnace. Optical and magneto-optical properties of R₂O₃-B₂O₃ glasses were investigated. The glasses were transparent in visible region except for coloration caused by the absorption due to the electronic transition of R³⁺ ion. Among the series of rare-earth borate glasses, R = Tb and Dy glasses displayed remarkably large Faraday effect in the visible region. R₂O₃ content dependence of Faraday effect of Tb₂O₃-B₂O₃ binary and Dy₂O₃-B₂O₃ binary glasses showed that the Verdet constants increased with increasing Tb₂O₃ and Dy₂O₃ content. The Verdet constant of 58Tb₂O₃-42B₂O₃ reached 229 rad/T m at 633 nm, surpassing the value of commercially available single-crystalline Tb₃Ga₅O₁₂, Tb₂O₃-Dy₂O₃-B₂O₃ ternary glasses were also fabricated by a levitation technique. The Verdet constant of the glasses was gradually increased with an increase of Tb³⁺ concentration. This suggests that the effect of rare-earth ion mixing on Verdet constant can be simply explained in terms of additivity. R₂O₃-B₂O₃ glasses have wide glass forming region when the levitation technique is applied, which means that the magneto-optical properties can be tuned greatly by changing the composition ratio of rare earth ions.

11:00 AM

(GOMD-S3-S4-005-2025) Development of new radiophotoluminescence materials and applications of real-time radiation measurements

G. Okada^{*1}; M. Koshimizu²; M. Sakai⁶; K. Shinsho³; H. Tanaka⁷; W. Kada⁴; K. Watanabe⁵; G. Wakabayashi⁸; H. Nanto¹

1. Kanazawa Institute of Technology, Japan
2. Shizuoka University, Japan
3. Tokyo Metropolitan University, Japan
4. Tohoku University, Japan
5. Kyushu University, Japan
6. Gunma University, Japan
7. Kyoto University, Japan
8. Kindai University, Japan

Radiophotoluminescence (RPL) is a phenomenon where luminescence centres are formed upon interaction with ionizing radiation. These centres, or so-called RPL centres, can be detected using conventional photoluminescence (PL) techniques. The PL intensity is proportional

to the concentration of RPL centres, which correlates with the accumulated radiation dose. As a result, RPL serves as an indirect probe for measuring accumulated radiation exposure dose and has been used in commercial dosimeter badges by Chiyoda Technol since 2000. A distinct advantage of RPL is that the signal can be read multiple times, reducing statistical deviations and enabling precise, reliable dose estimation. However, a major drawback of conventional RPL detectors, such as Ag-doped sodium aluminophosphate glass, is signal instability immediately after exposure, with intensity gradually increasing over time at a rate strongly influenced by temperature. This behaviour limits their use in real-time radiation monitoring. In this study, we conducted an intensive search for new RPL materials and identified candidates exhibiting stable signals. Additionally, we demonstrated their capability to detect photon, neutron, and heavy ion radiation.

11:20 AM

(GOMD-S3-S4-006-2025) Effect of the reduction of water and thulium doping concentration on the lifetime of thulium and other properties of the thulium - TZN system

L. J. Henry^{*1}; M. Klopfer²

1. Air Force Research Laboratory, Directed Energy Directorate, USA
2. Leidos, USA

There is an interest in finding a robust, alternate host aside from silica for heavily thulium doped optical fiber. This is the result of power scaling limitations brought about by the pedestal workaround necessary to offset the impact of the need to co-dope the silica fiber core with aluminum on the beam quality. Silica is also a non-ideal host for thulium because of a high maximum phonon energy of 1100 cm^{-1} which results in some non-radiative de-excitation of the $^3\text{H}_4$ pump level to the next lower $^3\text{H}_5$ level lowering the efficiency of the system. Heavy metal oxide glasses are good candidates to investigate as alternate matrices since they have been shown to accept high doping levels of thulium in addition to generally having lower maximum phonon energies. One such matrix is based on tellurium, zinc and sodium (TZN) which has a maximum phonon energy of $\sim 730\text{ cm}^{-1}$. For a range of thulium concentrations, the work presented here will show the impact of both the dry glove box environment as well the substitution of a fluoride for an oxide component on the lifetime of thulium and other properties of the thulium / TZN glass matrix system.

11:40 AM

(GOMD-S3-S4-007-2025) Broad NIR luminescence of Cr³⁺/Cr⁴⁺ doped silicate and germanate garnets

Y. Shigemura¹; J. Xu²; T. Nakanishi³; J. Ueda^{*1}

1. Hokuriku Sentan Kagaku Gijutsu Daigakuin Daigaku, Japan
2. Kyoto University, Graduate School of Human and Environmental Studies, Japan
3. Busshitsu Zairyo Kenkyu Kiko, Japan

Near-infrared spectroscopy (NIR spectroscopy) is widely used in the medical and agricultural fields for non-destructive qualitative and quantitative analysis of organic substances, due to the presence of absorption peaks specific to organic substances. However, conventional near-infrared light sources like halogen lamps have drawbacks, such as large size, low electro-optical conversion efficiency, and poor emission intensity stability. Phosphor-converted broadband near-infrared LEDs (pc-NIR-LEDs) are anticipated to overcome these challenges, necessitating the development of near-infrared phosphors with high emission efficiency, broad emission spectra, and various peak wavelengths. For near-infrared phosphors, the $4\text{T}_2 \rightarrow 4\text{A}_2$ transition of Cr³⁺ in the octahedral site and the $3\text{T}_2 \rightarrow 3\text{A}_2$ transition of Cr⁴⁺ in the tetrahedral site are promising near-infrared emission transitions and are actively being studied. Silicate and germanate garnets have trivalent octahedral sites and tetravalent

tetrahedral sites. Thus, these host materials can be good candidates as host materials for Cr³⁺ and Cr⁴⁺. In this study, we investigated the temperature dependence and pressure dependence of luminescent properties of Cr³⁺/Cr⁴⁺-doped Ca₃Sc₂Si₃O₁₂ and Ca₃Ga₂Ge₃O₁₂ garnet.

GOMD S5 - Glass manufacturing

GOMD S5 S1 - Manufacturing III

Room: Saturna Island Ballroom

Session Chairs: Terutaka Maehara, AGC Inc.; Madeleine Schmidlin, Corning Incorporated

9:20 AM

(GOMD-S5-S1-011-2025) Environmental conditions affecting the solidification behavior of natural basaltic melts (Invited)

S. Kolzenburg^{*1}

1. University at Buffalo, Geology, USA

Natural basaltic melts exist between liquidus and solidus conditions during storage, transport, eruption, and emplacement on Earth and other Planets. In these environments, where melts crystallize, they encounter a range of non-equilibrium thermal and environmental conditions, such as lower oxygen fugacities ($f\text{O}_2$) than in the atmosphere. Both the thermal environment and the melt's oxygen fugacity are known to influence the onset, phase-dynamics, and kinetics of crystallization. Thus, they have profound effects on glass forming ability. Yet, their influence on both glass formation and rheology remains largely uncharted, and most data derive from measurements at atmospheric conditions. Here I present an overview of the available data that constrain both rheology and solidification behavior of crystallizing basaltic melts at subliquidus temperatures, and reduced conditions. Available data show that at reduced conditions 1) the onset of crystallization can be significantly delayed 2) the crystallization kinetics are much slower. 3) the volume fraction of crystals decreases, and with that, the effective suspension viscosity is reduced. 4) the composition of the crystallized phases changes. 5) small variations in composition can extend / narrow the solidification window by several tens of degrees, causing challenges for the production of glasses and glass-ceramics from natural starting materials.

9:50 AM

(GOMD-S5-S1-012-2025) Development of the Na₂O-Al₂O₃-ZrO₂-SiO₂ thermodynamic database and its application to the glass melting furnace

J. Lee^{*1}; I. Jung¹

1. Seoul National University, Material Science and Engineering, Republic of Korea

The glass melting furnace operates at high temperatures to produce glass melt, often relying on alumina-zirconia-silica (AZS) refractories for their thermal stability. However, prolonged exposure to high temperatures can lead to the degradation of AZS refractories, potentially causing various defects to form in glass. In order to address these challenges, the thermodynamic database for the Na₂O-Al₂O₃-ZrO₂-SiO₂ system was developed based on the phase diagram experiments for the Na₂O-ZrO₂, Na₂O-Al₂O₃-ZrO₂, and Na₂O-ZrO₂-SiO₂ systems and the critical evaluation of the existing literature data. After integrating this ZrO₂-containing database with the existing oxide thermodynamic database, complex thermodynamic calculations to analyze the refractory degradation and defect formation in the melting furnace were performed to understand and mitigate the chemical reactions involved in the industrial problems. All the calculations in this study were conducted using the FactSageTM thermochemical software.

10:10 AM

(GOMD-S5-S1-013-2025) Redox in glass production: impact, challenge, measurement (Invited)

P. Georges*¹

1. Corning SAS, Characterization Science, France

The glasses usually incorporate multivalent elements, present in low concentration (typically lower than 1 mol%) but having a key role for various purposes (fining, color). The product properties as well as the ability to process glasses are strongly dependent of the relative proportions of the different valences of these elements. The redox ratio for an element is dependent of several factors (temperature, glass composition, atmosphere) but it is also dependent of the presence of other multivalent elements. By adjusting these conditions, manufacturers can manipulate the interactions between these elements, thereby customizing the properties of the glass to suit specific applications. Therefore, a meticulous control of redox conditions during glass production is needed but also very challenging, due to the high-temperature, corrosive environment. Existing methods for redox determination often necessitate sampling and offline analysis, which fail to provide real-time control and raise the question of the representativity of measurements on cooled samples vs state of melt at high temperature. In this discussion, we will present some examples showcasing the impact of redox on glass properties and the corresponding measurements we've done with their limitations and the essential breakthroughs or advancements needed in the field to enhance our understanding and control of redox in glass production.

10:40 AM

(GOMD-S5-S1-014-2025) Redox and gas release control for waste vitrification process (Invited)

A. F. Laplace*²; L. Pereira¹; O. Pinet²; F. Pigeonneau³; C. Laurin²; J. Agullo²

1. Université de Munich (LMU), Germany

2. CEA, France

3. MINES Paris, CEMEF, France

Vitrification is a method of immobilizing nuclear waste currently used on an industrial scale, particularly for highly radioactive waste. In France, the waste, which often contains several multivalent species, is incorporated into a borosilicate glass melted over 1000°C. The incorporation of such waste, into a glass-forming liquid can lead to gas releases, including those of oxygen resulting from redox reactions between dissolved species in the melt. It can have an impact on both the process and the final properties of the glass. Controlling redox properties and off-gassing is of major interest. Thermodynamic data were acquired for various redox couples. A model was developed, mainly based on the assessment of multivalent species (in waste and vitrification additive) and on thermodynamic redox equilibrium equations. Specific vitrification additives containing relevant multivalent species have been developed in order to better control the melt redox. Besides, work has also been carried out to understand the mechanisms of oxygen bubble formation and growth, and how they are linked to redox reactions. An approach combining experiments and numerical modeling was adopted. This talk reviews the studies we have conducted on these two subjects. Recent experimental developments enabling in situ monitoring of exchanges between gas and multivalent species in the melt will be presented.

11:10 AM

(GOMD-S5-S1-015-2025) Oxygen-related Bubbles and Pt Inclusions in Glass Melt (Invited)

J. Lee*¹

1. KCC Glass Corporation, R & D Center, Republic of Korea

Bubbles and Pt inclusions are the most concerning defects when molten glass passes through Pt structures at high temperatures, and a new phenomenon has been found in which bubbles occur when

water-cooled structures are used in feeders. Both these bubbles and Pt inclusions are related to oxygen, and solutions are proposed based on the results obtained in the production of LCD substrate glass. Even if β -OH is decomposed into O_2 and H_2 in the glass melt and H_2 permeation occurs through the Pt wall, no bubbles occur if the pO_2 balance between the O_2 donor group and the O_2 acceptor group remains within the safe range. Pt is oxidized by physically dissolved O_2 in the glass melt and incorporated into the glass melt, and as pO_2 decreases, the Pt ions are reduced to Pt metals, resulting in Pt inclusions. When the temperature of the Pt connection tube connected to the furnace was raised, Pt inclusions were greatly reduced, which is interpreted as inhibiting the oxidation of Pt by lowering the physically dissolved O_2 concentration on the Pt surface in contact with glass. And, bubble generation due to reheating after molten glass cooling is described with respect to the O_2 shift with changes in oxygen solubility and pO_2 with temperature change. This oxygen migration is interpreted as thermophoresis of oxygen by applying the Soret effect, and bubble generation by thermophoretic oxygen shifts is described as a new type of reboil.

11:40 AM

(GOMD-S5-S1-016-2025) The effect of iron redox state on viscosity of phonolitic magmas

L. Pereira*¹; K. Hess¹; D. B. Dingwell¹

1. Ludwig-Maximilians-Universität München, Germany

On Earth and other rocky bodies, iron occurs in at least two valence states (i.e., Fe^{+2} and Fe^{+3}) within silicate structures, significantly influencing viscosity and therefore high-temperature processes. We measured the viscosity of microlite- and nanolite-free phonolites with varying iron redox ratios using concentric cylinder coupled with gas-mixing device and micro-penetration techniques. Complementary analyses included differential scanning calorimetry, iron speciation, and viscosity modeling were executed. Our results show that viscosity decreases with iron reduction and the effect is amplified at lower temperatures. Current viscosity models and neural network tools overestimate viscosity, prompting us to propose an empirical model for iron-bearing phonolites. Additionally, the glass transition temperature depends on iron speciation, while the shift factor (K) remains unaffected by redox state of this family of melts. These findings provide insights into the viscosity of iron-bearing silicate melts and form a foundation for future viscosity models incorporating iron speciation.

GOMD S6 - Jonathan Stebbins Honorary Symposium

GOMD S6 - Jonathan Stebbins Honorary Symposium III

Room: SaltSpring AB

Session Chair: Scott Kroeker, University of Manitoba

9:20 AM

(GOMD-S6-010-2025) Investigating the Role of Phosphorus in the Structure of Aluminosilicate Glasses Using Inverse Methods for Two-Dimensional NMR Spectra (Invited)

Z. Boothe¹; R. Cowen¹; L. McCarthy-Carney¹; D. Srivastava¹; J. Wu²;

P. J. Grandinetti*¹

1. Ohio State University, Chemistry, USA

2. Corning Incorporated, Glass Research, USA

Ion exchange is a powerful tool for strengthening glasses, offering advantages over other methods. Minor modifications in the composition of aluminosilicate glasses can significantly impact the ion exchange process. Specifically, adding low concentrations of phosphorus pentoxide enhances the diffusion rate during processing, resulting in stronger glasses produced in less time. Phosphorus in aluminosilicate glasses forms tetrahedral sites, but its 5+ charge

necessitates maintaining charge neutrality by forming a double bond with oxygen or bridging to an aluminum tetrahedron. Consequently, adding phosphorus is expected to reduce network connectivity, which can favor ion exchange processes. However, experimental evidence on the depolymerization of the network by phosphorus addition is still lacking. Recently, we developed statistical learning methods for the model-free linear inversion of 2D NMR spectra of glasses into NMR parameter distributions. Building on the success of our 2D Si-29 NMR spectrum inversion methods in providing detailed information about the local structure of glasses, we demonstrate that applying these methods to P-31 2D NMR spectra presents an exciting opportunity to investigate the role of phosphorus in the aluminosilicate glass network structure and its influence on the modifier cation diffusion mechanism.

9:50 AM

(GOMD-S6-011-2025) Lone electron pairs on lead in glass: their effect on a atomic and electronic structure, and optical response

J. Zwanziger*¹

1. Dalhousie University, Chemistry, Canada

Lead confers extraordinary optical properties in glass, but why? Here we study this problem from the perspective of the structure directing lone pair that the lead ions may carry. We use a combination of structural probes, primarily NMR and XPS, to determine the local lead bonding geometry and the geometries around surrogates such as barium and tin, and correlate the results with bulk measurements, including mechanical, optical, and opto-mechanical studies. In addition, we use first-principles modeling studies to help interpret primarily the NMR and optical observables, including chemical shielding and index of refraction. Our previous results in this area provided an empirical model correlating lone pairs with stress-optic response, but correlations are not explanations. We hope here to provide more mechanistic detail into how the lone pairs determine both the optical and elasto-optic response.

10:10 AM

(GOMD-S6-012-2025) Understanding the dissolution behaviour of borophosphate glasses through their network connectivity: an NMR approach

M. Abbasi*¹; A. Krishnamurthy¹; H. Eckert²; S. Kroeker¹

1. University of Manitoba, Department of Chemistry, Canada
2. Instituto Federal de Educacao Ciencia e Tecnologia de Santa Catarina, Brazil

While silicate-based glasses have been successfully commercialized for treating bone and dental injuries, borate and borophosphate glasses are emerging as leading candidates for soft-tissue regeneration due to their desirable dissolution behaviour. To understand the relationship between the structure of borophosphate glasses and their dissolution behaviour, we have investigated a series of sodium borophosphate glasses before and after partial dissolution using ³¹P and ¹¹B magic-angle spinning nuclear magnetic resonance (MAS NMR) spectroscopy to obtain information on short-range structure. The network connectivity between boron and phosphorus was explored using rotational echo double resonance (REDOR) NMR spectroscopy. By interpreting the NMR data with the aid of Pauling bond strengths and charge-compensation principles, the phosphate and borate units were quantified to estimate the number of X – O – Y linkages and relate them to the dissolution behaviour of the glasses. Solution-state ³¹P NMR spectroscopy provides real-time insight into the phosphate species released during dissolution. These findings reveal that the balance between B–O–B and P–O–B linkages is a key factor influencing the degradation rate of borophosphate glasses.

10:30 AM

(GOMD-S6-013-2025) Water in nominally anhydrous mantle minerals: Insights from comprehensive spectroscopic measurements and first-principles calculations (Invited)

X. Xue*¹; M. Kanzaki¹

1. Okayama University, Institute for Planetary Materials, Japan

Water may be present in all major mantle mineral structures as hydroxyl (OH) defects and significantly alter various thermodynamic and physical properties of the mantle. Despite extensive studies, often using IR spectroscopy, how water is incorporated in the crystal structures of minerals is still not well understood. Recently, we were able to clarify the incorporation mechanisms of water in a number of major mantle minerals, including MgSiO₃ orthoenstatite and clinoenstatite, and aluminous orthoenstatite, via a comprehensive approach of IR/Raman and NMR measurements and first-principles calculations. In this presentation, we review our recent findings. Both MgSiO₃ orthoenstatite and clinoenstatite were found to contain OH defects in both Mg vacancies and Si vacancies, with the latter increasing in proportion with pressure. Their hydrogen bonding and NMR and vibrational spectroscopic features are, however, distinct from those of olivine and hydrogarnet, and strongly hydrogen-bonded OH are also present, but have been overlooked by previous IR studies. Our study also revealed that the generally believed paired substitutions of Al+H for 1Si or 2Mg, although present, are not the dominant mechanisms for the enhancement of water incorporation by Al. These findings call for examination of other major mantle minerals as well.

11:00 AM

(GOMD-S6-014-2025) NMR spectroscopy of strontium immobilization in vitrified zeolites

T. R. Elumalai*¹; S. Kroeker¹

1. University of Manitoba, Chemistry, Canada

⁹⁰Sr is generated during the operation of nuclear reactor and is a potentially dangerous component in high-level radioactive waste. Strontium behaves similarly to calcium and can accumulate on bone surfaces, making it a hazardous fission product with a radioactive half-life of 30 years. Clinoptilolite has been used as an ion exchanger for immobilizing strontium. This study investigates the potential of vitrifying Sr-loaded clinoptilolite with B₂O₃ for long-term immobilization, combining the favorable zeolitic adsorption properties with the high chemical durability of borosilicate glass to form geoglass. Solid-state ¹¹B MAS NMR spectroscopy is used to measure the proportions of three- and four-coordinated boron within the glass structure, while ²⁹Si MAS NMR provides insight into the degree of network polymerization, both of which can be related to chemical durability. The specialized pulse sequences will be employed to characterize the strontium sites in geoglasses. The observation of ⁸⁷Sr MAS NMR before and after aqueous dissolution provides valuable information about the partitioning of strontium between crystalline and glassy phases. Such structural knowledge will support the optimization of compositions to maximize both waste-loading and chemical durability, leading to high-volume, high-performance waste forms for radioactive ions.

11:20 AM

(GOMD-S6-015-2025) Dose rates, ordering and amorphisation in highly radioactive oxides observed by high-resolution NMR (Invited)

I. Farnan*¹

1. University of Cambridge, Earth Sciences, United Kingdom

Obtaining NMR spectra of nuclear materials requires a range of safety protocols because radioactive and, on occasion, fissile materials are spun very rapidly. The quantitative nature of NMR and the ability to apply it equally to amorphous or crystalline materials makes it a unique probe of materials used as nuclear fuels, and

Abstracts

waste forms. Examples will be given where NMR spin-counting has been used to obtain very precise absorbed neutron doses of zircon and xenotime material placed in nuclear reactors and the structure of the radiation damaged fractions produced. Very high resolution ^{17}O MASNMR spectra of actinide containing oxides have demonstrated the efficacy of new nuclear fuel fabrication techniques by providing unique details of the ordering of the fissile component and its uniform distribution in mixed oxide nuclear fuels.

GOMD Award Lectures

GOMD Norbert J. Kreidl Award

Room: Saturna Island Ballroom

Session Chairs: Collin Wilkinson, Alfred University;

Madoka Ono, Hokkaido University

12:00 PM

(GOMD-Award-002-2025) The Structure-Property Relationships of Iron Phosphate Nuclear Waste Glasses: A Combined MD Simulation and QSPR Approach

J. Kalaha*¹; T. S. Mahadevan¹; X. Lu²; J. Vienna³; B. J. Riley³; J. Du¹

1. University of North Texas, Materials Science and Engineering, USA
2. Pacific Northwest National Lab, Energy and Environment Directorate, USA
3. Pacific Northwest National Lab, USA

Iron phosphate glasses are highly durable and versatile, ideal for immobilizing nuclear wastes. Understanding their composition and properties is crucial for optimization in nuclear waste management and other applications. Molecular dynamics (MD) simulations have been invaluable in elucidating their structures, revealing how Fe_2O_3 content, alkali concentrations, and iron redox ratios affect network connectivity and glass properties. Structural analyses highlight the roles of P^{5+} and Fe^{3+} , with P-O and Fe-O bond distances aligning well with experimental values. Higher Fe_2O_3 levels enhance connectivity through more P-O-Fe linkages, reduce non-bridging oxygens, and shift from Q_1 and Q_2 to polymerized Q_4 units. Alkali modifiers associate with Fe^{3+} , while Fe^{2+} disrupts P-O-P bonds, depolymerizing the network. Mechanical properties and glass transition temperatures show monotonic trends with increasing Fe_2O_3 . QSPR analyses correlate MD structural features with glass properties. Data from over 30 glasses identify descriptors like Fe-O-P linkage density and modified F_{net} parameters as effective predictors of density, elastic moduli, and dissolution rates. These insights underline the critical roles of glass formers, modifiers, and redox conditions in shaping iron phosphate glasses, advancing their design for nuclear waste management and other applications.

GOMD S1 - Fundamentals of the glassy state

GOMD S1 S2 Glass Crystallization and Glass-Ceramics I

Room: Pender

Session Chair: Kenji Shinozaki, AIST

3:30 PM

(GOMD-S1-S2-001-2025) Vitrification of sodium ion conductive $\text{Na}_3\text{Zr}_2\text{Si}_2\text{PO}_{12}$ via laser-induced powder bed fusion technology (Invited)

T. Honma*¹; C. Fujii¹; E. Tamura¹; M. Affatigato²

1. Nagaoka University of Technology, Department of Materials Science and Bioengineering, Japan
2. Coe College, Physics, USA

$\text{Na}_3\text{Zr}_2\text{Si}_2\text{PO}_{12}$ (NZSP) is well known as a sodium superionic conductor (NASICON) structure crystal. By tuning the sintering process, NZSP exhibits superior sodium ion conductivity of 1 mScm⁻¹ at room temperature. However, improving the ionic conductivity of NZSP by

the usual solid-state reaction process requires long heat treatment, and the grain boundary resistance governs its ionic conductivity. Therefore, it is important to synthesize solid electrolytes that combine densification and ionic conductivity. In this study, we propose the fabrication of NZSP films by laser melting without conventional sintering. Morphology, crystallinity, and ionic conduction in the laser-induced layer were investigated. NZSP was prepared using the sol-gel process and conventional heat treatment. Acetylene black was added to NZSP as a laser light absorbent. A nano-second pulse laser with a 1064nm wavelength was irradiated on the surface of compact powder. Melt pool has formed in the 20 μm depth from the surface. Powder X-ray diffraction and differential thermal analysis showed that the melt-solidified region was amorphous. Nanocrystals of ZrO_2 could be observed, but they were found to be crystallized from high-temperature melts. When the amorphous NZSP was heat-treated again at 1000°C for 10h, the NZSP recrystallized while retaining its high-density morphology.

4:00 PM

(GOMD-S1-S2-002-2025) Precipitate Chiral LiGa_5O_8 Crystals from Glass under CO_2 Laser Irradiation

J. Zhao*¹; K. Kizaki¹; T. Omatsu²; M. Ono¹

1. Tohoku Daigaku, Department of Applied Physics, Japan
2. Chiba Daigaku, Graduate School of Science and Engineering, Japan

Circularly polarized luminescence (CPL) provides different emission intensities of right or left circularly polarized light, and can be used in telecommunication, photoelectric devices, enantioselective synthesis, etc. Glass is known for its reliability in harsh environments and capability in hosting luminescence centers. When using glass-based chiral material to generate CPL directly, energy loss can be reduced compared to the commercial method, and the product is compatible with most of optics systems. To fabricate glass-based chiral material, a vortex CO_2 laser beam is utilized to precipitate chiral crystals from glass. In my research, LiGa_5O_8 ($\text{P}_{43}32$ or $\text{P}_{41}32$) is chosen to precipitate from glass, because their enantiomeric feature is essential for achieving chirality, and the cubic structure makes optical chirality distinguished from birefringence. However, Ga-containing silicate-based glass also suffers from phase separation, where $\gamma\text{-Ga}_2\text{O}_3$ (Fd-3m) could precipitate from the Ga-enriched separated phase. In this talk, I will present current results in glass composition design to achieve LiGa_5O_8 precipitation, and crystallization behavior under CO_2 laser irradiation.

4:20 PM

(GOMD-S1-S2-004-2025) Thermal Expansion of Gillespite Glass-Ceramics

L. Moore*²; M. Wallen²; E. Stapleton¹; B. Wheaton¹; G. H. Beall²

1. Corning Incorporated, Characterization Sciences, USA
2. Corning Incorporated, Glass Research, USA

The thermal expansion of recently discovered gillespite ($\text{BaFeSi}_4\text{O}_{10}$) glass-ceramics has been studied. Crystallization studies of reduced $x(\text{BaO})_x(\text{FeO})_y4\text{SiO}_2$ (where $x+y=2$ and $y/x=0.125$ to 3.1) glasses showed gillespite formation in compositions with $y/x \geq 0.35$ heat treated at 800°C for 4h. Gillespite glass-ceramics were made by crystallizing glasses with $y/x=0.4$ to 1.35. The coefficient of the thermal expansion (CTE, 25-300°C) of the glass-ceramics decreased from 8.4 ppm/°C to 3.4 ppm/°C from $y/x=0.4$ to 1, then increased to 4.3 ppm/°C at $y/x=1.35$. XRD analysis of the glass-ceramics showed phase assemblages comprising gillespite, sanbornite (BaSi_2O_5), and a small amount of cristobalite. The initial decrease in CTE correlated with an increase in the amount of gillespite and a decrease in sanbornite (BaSi_2O_5). No sanbornite formed at the highest Fe/Ba ratio of 1.35, but a higher amount of cristobalite was detected. The thermal expansion coefficients of sanbornite and cristobalite are known to be high (> 10 ppm/°C), but no data on the thermal expansion of gillespite could be found in the literature. Using high temperature XRD data collected on a gillespite glass-ceramic, an average linear

CTE of around 2 ppm/°C was calculated for gillespite. Therefore, glass-ceramics with CTE < 3.4 ppm/°C should be attainable if the composition and process are controlled to eliminate sanbornite and cristobalite while maximizing gillespite.

4:40 PM

(GOMD-S1-S2-005-2025) Unraveling origin of crystal rotation during crystal growth: a simulation approach

R. Thapa^{*1}; M. E. McKenzie²; E. J. Musterman¹; V. Dierolf³; H. Jain⁴

1. Lehigh University, Material Science and Engineering, USA
2. Corning Incorporated, Science & Technology, USA
3. Lehigh University, Physics, USA
4. Lehigh University, International Materials Institute for New Functionality in Glass, USA

A rotation of crystals during the early stages of growth has been experimentally observed in laser-induced crystallization of glasses. Considering that glass is generally considered isotropic, the underlying cause of this rotation and its eventual cessation remain unclear. In this project, we propose to apply seeded crystal growth simulations to study the rotations of seeds inside the glass and explore the origins of such rotations. This will be extended to study torques in different regions of the seeded glass and compare how torque differs between the glass and the crystal. With insights from these molecular dynamics simulations, we hope to better understand the experimentally observed crystal rotation during early stages of laser induced crystallization.

GOMD S1 S3 - Structural characterizations of glasses and melts IV

Room: SaltSpring C

Session Chair: Yohei Onodera, Busshitsu Zairyo Kenkyu Kiko

1:15 PM

(GOMD-S1-S3-019-2025) What is the Role of Zinc in Silicate Glasses and Melts?

D. R. Neuville^{*1}; D. S. Brauer²

1. IPGP-CNRS-UPC, Geomat Lab, France
2. Friedrich-Schiller-Universität, Otto-Schott-Institut, Germany

Zinc oxide is a critical component in industrial glass formulations, yet its influence on physical properties remains poorly understood. To address this, we investigated the viscosity of Zn-bearing silicate glasses across a wide temperature range, including above the liquidus and near the glass transition. Our findings reveal that replacing alkaline earth metals with zinc significantly reduces viscosity and glass transition temperatures, despite zinc's low coordination number (~4). This behavior suggests that ZnO acts as a network modifier, disrupting the glass structure more effectively than other network modifiers. These results shed new light on the thermodynamic and structural role of ZnO in glasses and melts, with implications for optimizing industrial glass processes.

1:35 PM

(GOMD-S1-S3-020-2025) Influence of redox equilibria and multivalent element interactions on coloration and properties of silicate glasses

L. Cormier^{*1}

1. Sorbonne University - CNRS, IMPMC, France

The redox equilibrium not only governs coloration but also plays a critical role in glass fabrication, affecting viscosity, homogeneity, and fining. Multivalent elements interact dynamically depending on composition, concentration, and synthesis conditions such as melting temperature and furnace atmosphere, highlighting the complexity of redox processes. This study investigates the complex relationships between redox state and color in silicate glasses, focusing on the influence of transition metals, especially copper, and its interactions with other multivalent elements. Optical and

electron paramagnetic resonance (EPR) spectroscopies reveal that the redox state of copper significantly impacts color, with Cu⁺ ions contributing to blue and green hues through distinct UV absorption characteristics. Variations in glass composition and copper oxidation states, as quantified by EPR and XANES spectroscopies, demonstrate a shift from blue to green coloration due to increasing Cu²⁺-Cu⁺ intervalence charge transfer (IVCT). Additionally, site distortions and clustering phenomena further modulate these effects.

1:55 PM

(GOMD-S1-S3-022-2025) Structure-Property Correlations in the Bi₂O₃-ZnO-B₂O₃ Pyroborate Glass System and the Effects of Crucible Dissolution

L. Haight-Stott^{*1}; N. Tagiara³; R. Youngman²; E. I. Kamitsos³; D. Möncke⁴

1. New York State College of Ceramics at Alfred University, Glass Science, USA
2. Corning Incorporated, Science & Technology Division, USA
3. National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute (TPCI), Greece
4. Alfred University, Hall of Glass Science, Rm 100, USA

Glasses of the compositional series xZnO-(1-x)Bi₂O₃-(1.5-x)B₂O₃ (0 ≤ x ≤ 1) were prepared by the conventional melt-quench technique using either alumina or platinum-gold crucibles. Despite keeping the oxygen to boron ratio at a constant value of 2.5 - nominally expecting pyroborate units only as borate species - significant structural variations were observed by infrared (IR), Raman and ¹¹B and ²⁷Al NMR spectroscopy. Structural changes were correlated with thermal and optical properties including density, calculated refractive index, and glass transition temperature (T_g). Varying the conditional modifiers (Zn²⁺ versus Bi³⁺) influences speciation of borate units as the borate network under-modified in bismuth-rich glasses while zinc-rich glasses are characterized by disproportionation of pyroborate into orthoborate and metaborate units. Alumina crucible dissolution resulted in the presence of [AlO₄]⁻ tetrahedra and consequently changes in borate speciation.

GOMD S1 S4 - Vibration properties

Room: Pender

Session Chairs: Shingo Urata, AGC Inc.; Alfonso Pedone, University of Modena and Reggio Emilia

1:15 PM

(GOMD-S1-S4-001-2025) Understanding Phonon Modes in Glasses Through Hybrid Models

L. McClanahan²; E. Akirmak-Yamac¹; R. Welch¹; C. Wilkinson^{*1}

1. Alfred University, Inamori School of Engineering, USA
2. Coe College, USA

Phonons in solid state systems encode information about the structure and the properties, as they arise due to normal directions encoded in the 3N dimensional energy landscapes. Vibrational spectroscopic studies, as a result, have become the most common way of measuring and understand glass structure. The interpretation of the resultant spectra often relies on selection rules, small cluster models, or crystalline analogues. These analogues can be a challenge for quantitative interpretation as the long-range interactions that affect the intensity of the peak are geometry dependent, leading to most studies being qualitative. Here we present a unified machine learning/atomistic modeling approach to quantify the IR spectra of any oxide structure with an emphasis on understanding the phonon modes. A quantitative comparison of the phonon modes derived from glasses and from the corresponding crystals are compared and the ramifications for vibrational spectroscopy are discussed.

1:35 PM

(GOMD-S1-S4-002-2025) Semi-phenomenological Model of Glass Dynamics: Effect of Spatial Heterogeneity in Glass and Supercooled Liquid

W. Takeda^{*}; P. Lucas¹

1. The University of Arizona, Department of Materials Science and Engineering, USA

Dynamic and spatial heterogeneities are fundamental characteristics of glasses and supercooled liquids. They cause some of the key features of systems' dynamics such as temperature dependence of nonexponentiality and spatial enthalpy fluctuations. Commonly used phenomenological models such as Tool–Narayanaswamy–Moynihan (TNM) model fail to fully capture this phenomenon. In this presentation, I will describe a new model that computes the temperature dependence of spatial heterogeneity in the supercooled liquid to capture its frozen distribution at the glass transition and its evolution during relaxation. It requires only four adjustable parameters and one parameter estimated from the high-temperature limit of nonexponentiality in equilibrium liquids, which is generally equal to one for most oxide and chalcogenide glasses. The effects of spatial and dynamic heterogeneities on glass relaxation and enthalpy fluctuations are explored in this work. Notably, the model successfully reproduces Kovacs' expansion gap paradox. Furthermore, it describes the measured relaxation dynamics of glasses across a broad range of temperatures using a set of parameters, whereas the TNM model requires multiple parameter sets to achieve comparable results.

1:55 PM

(GOMD-S1-S4-003-2025) Effect of three-body interaction on structural features of phosphate glasses from molecular dynamics simulations

J. Du^{*}; N. Marchin¹; S. Urata²

1. University of North Texas, Materials Science and Engineering, USA
2. AGC Inc., Japan

Phosphate glasses find important technological applications from biomedicine, photonic devices to nuclear waste disposal, yet there are still challenges in understanding their atomic structural features. In this talk, we report the effect of addition of three-body potential (TBP) to the widely adopted partial charge pairwise potentials on the short and medium range structures of phosphate glasses by using Molecular dynamics (MD) simulations, a powerful approach to study glass and amorphous materials. Our results show that addition of TBP improves the structural descriptions, including reproducing the P-O-P bond angle and P Qⁿ distributions across compositions. It also improves agreement with experimental neutron structure factors, particularly for sodium-rich glasses, and captures the structural evolution induced by modifier addition, from depolymerization to network reorganization. These findings underscore the critical role of multi-body interactions in accurately simulating the structural features of phosphate and potentially other network glasses.

2:15 PM

(GOMD-S1-S4-004-2025) Comparing the Vibrational Properties of Common Glass Interatomic Potentials

E. Akirmak-Yamac^{*}; S. S. Sørensen²; R. Welch¹; M. M. Smedskjaer²; C. Wilkinson¹

1. Alfred University, Inamori School of Engineering, USA
2. Aalborg University, Department of Chemistry and Bioscience, Denmark

The vibrational and configurational properties of glasses are controlled by the emergent potential energy landscape (PEL). Practically, the PEL topography is determined by the choice of an interatomic potentials in classical systems, here we evaluate 5 such interatomic potentials (Matsui, PMMCS, BMP, Du, and SHIK) for the silica and calcium aluminosilicate systems, comparing structural, vibrational, and

thermal properties with experimental data. The properties compared include the vibrational density of state, the heat capacity, structure, diffusion, and ultimately the thermal conductivity. Insights into the validity of each potential are derived with a special emphasis on understanding the underlying energy landscape. The discussion is framed based on a Taylor series expansion of the energy of a basin.

2:35 PM

(GOMD-S1-S4-005-2025) Impact of Long-Range Coulombic Interactions and Dynamical Heterogeneities on Ionic Conductivity within Metaphosphate Glass Systems

W. L. Kiff^{*}; C. Wilkinson¹

1. Alfred University, Glass Science, USA

Emerging glasses have been proposed as prospective candidates for all solid state battery electrolytes due to our ability to systematically manipulate the structure and properties of these materials. Despite recent progress, fundamental structure/property relationships for ionic mobility remain elusive. Here, to further our understanding of ion mobility, we carry out a broad study of structural and thermodynamic effects on modifier sites using molecular dynamics. From the study it was found that the ionic packing of the charge carriers determined the structural arrangement of the glass system, in turn creating a net long-range interaction which electrostatically contributed to mobile charge carrier sites within the glass. The site energies were strongly correlated with the activation barrier of charge carrier mobility. However, when attempting to understand more local interactions and the propensity at these charge carrier sites, there are unknown nuanced mechanisms driving individual charge carrier mobility. Our research is placed within the context of other common models for ion mobility.

2:55 PM

(GOMD-S1-S4-006-2025) Atomistic Simulation of Subcritical Crack Growth in Glass in Vacuum

S. Gupta^{*}; M. Wilson²; S. Grutzik³; D. Warner⁴

1. Cornell University, USA
2. Sandia National Laboratories, Computational Materials and Data Science, USA
3. Sandia National Laboratories, Materials and Failure Modeling, USA
4. University of Canterbury, New Zealand

Atomistic simulations have become vital for studying crack propagation, revealing mechanisms of crack growth with nanometer-scale precision and picosecond-scale resolution. While these simulations enhance our understanding of material failure, a significant challenge remains in connecting atomistic models with experimental observations, particularly in brittle materials where crack propagation is localized at the tip. Here, we investigate crack growth rates in silica glass, under various loads below the dynamic limit using large-scale simulations and advanced parallel computing. With a system size of approximately 400,000 atoms, our simulations are large enough to minimize finite size effects compared to previous studies. Our findings demonstrate crack growth rates that correlate closely with experimental measurements, supporting the use of atomistic modeling in subcritical regimes for brittle materials. Notably, we identify a thermally activated stick-slip behavior that persists up to crack growth velocities nearing 1 km/sec, a significant finding that supports existing theoretical models and highlights the complex dynamics of fracture processes. This work paves the way for future investigations into the interplay between glass structure, chemistry, and mechanical integrity, with implications for understanding how environmental factors influence crack propagation.

GOMD S1 S4 - Dynamics/Mechanical

Room: SaltSpring AB

Session Chairs: Jincheng Du, University of North Texas;

Shingo Urata, AGC Inc.

3:30 PM**(GOMD-S1-S4-007-2025) Thermal conductivity of disordered nanomaterials by first-principles molecular dynamics (Invited)**E. Martin*¹

1. Laboratoire des Sciences de l'Ingenieur de l'Informatique et de l'Imagerie, France

The mechanism of thermal conduction in disordered materials is much less understood than in crystals. To date, measurements have only demonstrated a reduction of thermal conductivity in thin films for the case of amorphous Si. While this is due to the limited resolution of thermal measurements (50 nm) one can conjecture that disorder could potentially cause the size effects to manifest themselves at smaller thicknesses. As a contribution toward a more precise understanding of these phenomena, first-principles molecular dynamics (FPMD) can be employed. This approach provides a quantitative atomic scale description of materials including anharmonicity effects largely impacting thermal conduction. In this presentation, I will show how the thermal conductivity of disordered materials described by FPMD can be obtained using thermal transients (via the approach-to-equilibrium AEMD method) for a range of amorphous materials. The physical origins of the size dependence of thermal conductivity for different systems will be discussed, by pointing out the quantitative agreement with the experimental data for bulk sizes. Changes in thermal conductivity obtained at short lengths will be rationalized by invoking current theories of thermal transport in disordered materials. Finally, the impact of these effects on applications based on amorphous materials, such as phase-change devices, will be considered.

4:00 PM**(GOMD-S1-S4-008-2025) Exploring Structural and Mechanical Properties of Glass-Crystal Interfaces via Molecular Dynamics**F. Lodesani*¹; S. Urata¹; Y. Takato¹

1. AGC, Innovative Technology Laboratories, Japan

Glass-ceramic materials are renowned for their superior mechanical properties compared to homogeneous glass materials. A significant challenge in this field is the development of new materials with even more advanced properties. The ability to predict the mechanical response of these materials could represent a substantial breakthrough. While the properties of glass and crystal can be estimated experimentally or theoretically, determining the behavior of the interface between these two phases remains challenging due to its reduced size. To investigate how the interface affects the macroscopic response of glass-ceramic materials, we applied molecular dynamics simulations of the glass-crystal interface. In this work, we investigated the glass/crystal interface of $x\text{Li}_2\text{O}-(1-x)\text{SiO}_2$ systems incorporating $\text{Li}_2\text{Si}_2\text{O}_5$ crystal, as a prototypical glass-ceramics material. To generate the glass/crystal interface model at the nanoscale, various methods were examined, and the biaxial loading method was employed to assess the mechanical properties of the interface. The profiles of Young's modulus and Poisson's ratio were calculated in the model, extending from the crystal to the glass through the interface. Different profiles were obtained by varying the crystalline plane, highlighting some interesting features of the interface.

4:20 PM**(GOMD-S1-S4-009-2025) Prediction of Nepheline crystallization in aluminoborosilicates combining molecular dynamics and machine learning**M. Benassi*¹; M. Bertani¹; L. Gottardi¹; A. Pedone²; A. Goel³

1. University of Modena and Reggio Emilia, Departement of Chemical and Geological Sciences, Italy
2. University of Modena and Reggio Emilia, Italy
3. Rutgers University, USA

Crystallization in glasses is widely studied to find compositions with low devitrification tendencies, as glass producers often want their products to be stable against crystallization. Crystallization must be avoided in nuclear waste confinement as it reduces chemical durability. However, controlled crystallization is important in applications like glass-ceramics for kitchens, dentistry and phone screens due to their great mechanical properties. Empirical models linking composition and crystallization often require big experimental datasets. Conversely, we applied computational methods: first, Molecular Dynamics simulations were done on aluminosilicate glasses containing B, P, Ca, Na, Fe, and Li, using a core-shell potential, known for structural accuracy. The simulated data were validated against experimental results. We then applied Cluster, a homemade code that quantifies the similarity between atomic environments in the glass and the nepheline crystal. The hypothesis, confirmed by our experiments, is that a high similarity, particularly in oxygen environments, increases crystallization tendency. Using these results, a Machine Learning Classification model is used to predict whether a glass composition will crystallize nepheline as the primary phase. This method reduces the need for experimental synthesis, offering significant economic and environmental benefits.

4:40 PM**(GOMD-S1-S4-010-2025) Structure and Fracture Behavior of Hydrated Sodium Aluminosilicate Glasses**E. J. Pedersen*¹; J. Christensen¹; T. Du¹; S. S. Sørensen¹; R. Christensen¹; M. M. Smedskjaer¹

1. Aalborg University, Department of Chemistry and Bioscience, Denmark

Water has for decades been considered harmful for oxide glasses, as water penetration into the glass network can cause glass corrosion and enhance crack growth when stress is applied. However, recent studies found that hydrothermal treatment can induce compressive stress and improve, e.g., the crack initiation resistance of certain oxide glasses. As such, additional studies are needed to understand glass-water reactions and how they impact the mechanical properties of oxide glasses. Here, using reactive molecular dynamics simulations, we explore the structural response during fracture of $x\text{H}_2\text{O}-(30-x)\text{Na}_2\text{O}-10\text{Al}_2\text{O}_3-60\text{SiO}_2$ glasses. We study the fracture behavior of precracked structures with varying Na/H ratio, finding that the fracture mechanism becomes less brittle upon substituting Na with H. This is caused by an increasing adaptability of the glass network, as revealed by bond switching analysis, where coordination number changes during fracture are studied. Overall, our findings reveal that water can increase the nanoscale ductility of certain glass compositions, but at the same time make the glass networks less stiff.

5:00 PM**(GOMD-S1-S4-011-2025) Decoding Hardness: Nano-Indentation Insights into the Albite-Anorthite Glass Series**A. Pallini*¹; A. Pedone²; L. Talirz³; W. Mannstadt³

1. University of Modena and Reggio Emilia, Chemical and Geological Sciences (DSCG), Italy
2. University of Modena and Reggio Emilia, Italy
3. SCHOTT, Germany

Hardness is a key property that determines how solid materials respond mechanically to applied stress. In this work, we use MD simulations to perform nano-scale indentation tests, offering new

insights into the fundamental processes influencing hardness. The study focuses on examining how the structure of oxide glasses is altered during their interaction with a diamond cone-shaped indenter. To investigate the role of aluminium and the effect of different cations within the glass network, we focus on the albite-anorthite series, spanning from sodium (albite, NaAlSi₃O₈) to calcium (anorthite, CaAl₂Si₂O₈) aluminosilicate. This allows us to analyze how replacing sodium with calcium impacts the charge compensation of AlO₄-tetrahedra and its role in modifying the glass network. We analyze the structural changes occurring during and after the indentation, linking these alterations to the mechanical properties of the glasses. The effects of densification are also examined, with attention to changes in bulk and surface structure, elastic properties, and hardness across the series. This investigation offers a deeper understanding of the nano-scale mechanical behavior of aluminosilicate glasses. By exploring the interplay between composition, structure, and mechanical performance, the study provides valuable knowledge to guide the design and optimization of glassy materials for advanced applications.

GOMD S3 - Optical and electronic materials and devices - Fundamentals and applications

GOMD S3 S3 - Optical fibers and waveguides, optoelectronic glass-based devices I

Room: Cortes

Session Chair: Xianghua Zhang, University of Rennes/CNRS

1:15 PM

(GOMD-S3-S3-001-2025) Pixelated Electrically Tunable Phase-Change Metasurface Array for Multifunctional Applications (Invited)

Y. Li^{*1}, Z. Li¹

1. Sun Yat-Sen University, China

Antimony selenide (SbSe), a lead chalcogenide, stands out among phase-change materials for its exceptional NIR transmission properties, which render SbSe-based phase-change metasurfaces highly potent for diverse optical field manipulation. Our research integrates metal microheater arrays with multifunctional SbSe phase-change metasurfaces, marking the first demonstration of pixelated, independently controllable phase transitions in two-dimensional SbSe metasurface arrays. This array exhibits over 2000 stable phase-change cycles with crystallization speed below 50 μ s. Capitalizing on its low-loss and quasi-continuous phase transition, we achieve multi-level amplitude-dominated modulation of over 10 dB and phase-dominated modulation covering over 120°. Building upon pixelated phase-change transition, we construct a high-dimensional, low-correlation spectral transmission matrix using a 6x6 metasurface array, enabling the first demonstration of broadband, integrated spectral detection in the NIR range (1100-1700 nm), showcasing the array's potential for multifunctional photonic applications.

1:45 PM

(GOMD-S3-S3-002-2025) The Subtle and Functional Role of Glass Substrates and Surfaces in Modern Electronics (Invited)

R. G. Manley^{*1}

1. Corning Incorporated, Thin Films and Coatings, USA

As electronics and technology advance, their properties and functions increasingly depend on their surfaces. High-tech glass, initially used for flat panel displays, is now key to RF applications, sensors, antenna/phase shifters, MEMS, IC packaging, and large-area electronics. Even if not in the final product, glass may serve as a production substrate. Various glass types are selected for different applications, each posing unique integration challenges linked to the glass surface. During fabrication, glass substrates undergo chemical, thermal, and mechanical changes. Simple water exposure can affect film growth,

resistance, and etching. Electrostatic properties can also be modified, impacting reliability. Altering the glass surface's electronic structure may change performance, potentially enhancing it. Understanding these surfaces and their evolution will improve glass integration and electronic design. This talk aims to inform on glass substrates and surfaces, highlighting their practical impact in electronics and fabrication beyond mechanics, adhesion, and cleanliness.

2:15 PM

(GOMD-S3-S3-003-2025) Characterization of potassium niobium germanate core - borosilicate clad glass optical fiber fabricated via the molten core method

B. Topper^{*1}, B. Baldus¹, K. Chapman¹, M. Walton¹, L. Dong¹, T. Hawkins¹, J. Ballato¹

1. Clemson University, USA

Novel optical fibers have been fabricated using the molten core method employing a low-alkali borosilicate cladding (Duran) with a potassium niobium germanate core glass. Compositions with upwards of 20 mol% niobium oxide have been successfully drawn. This talk will discuss fabrication and optical characterization of the bulk precursor glasses and the optical fibers. Active rare-earth ions were introduced for spectroscopic study, including Yb, Tm, Ho, and Eu. Notably, a Yb-doped fiber was used as a gain fiber to amplify a 1030 nm input signal under 976 nm core pumping.

2:35 PM

(GOMD-S3-S3-004-2025) Who put the β in photodarkening?

B. Poletto Rodrigues^{*1}, S. Kuhn¹, N. Haarlammer¹, T. Schreiber¹

1. Fraunhofer-Institut für Angewandte Optik und Feinmechanik IOF, Germany

Photodarkening — the increase in optical absorption over time in light-irradiated materials — is a critical challenge for the development of high-power laser systems. Despite its importance, a fundamental understanding of its time-dependent behavior remains elusive. This work seeks to elucidate the origin of the stretched exponential time dependency observed in photodarkening by linking it to the well-established “diffusion to traps” model, commonly used to describe relaxation processes in glassy materials. Combining this model with an analysis of glass network topology, provides a physical interpretation of the dimensionless stretching parameter β . Our approach not only explains the time-dependent dynamics of photodarkening but also offers predictive insights that could guide the design of more robust laser materials.

2:55 PM

(GOMD-S3-S3-005-2025) Elaboration of tapered chalcogenide glass fibers for in operando monitoring of chemical reactions in Li-ion batteries

S. Coudray^{*1}, C. Boussard-Pledel¹, C. Leau², A. Gautier¹, T. Jouan¹, Y. Wang², T. Safarik², J. Tarascon², X. Zhang¹

1. Université de Rennes, France
2. Collège de France, France

Infrared fiber optic evanescent wave spectroscopy (IR-FEWS) is an innovative technology that captures chemical phenomena and reactions occurring in lithium-ion batteries throughout charge and discharge cycles. Understanding these complex phenomena paves the way for more durable and high-performing batteries. The optical fiber selected for this study, made from Te₂₀As₃₀Se₅₀ (TAS) glass and characterized by low optical losses, provides access to the vibrational modes of chemical bonds in molecules involved in electrolyte reactions. We present the production of tapered fiber using a tapering machine designed specifically for soft glasses. The study aims to compare detection results using a 125-micron optical fiber and fibers with varying input diameters, with a 125 μ m tapered region. These tapered fibers are employed to analyze an electrolyte composed of ethylene carbonate (EC), dimethyl carbonate (DMC), and lithium salt (LiPF₆), and to evaluate improvements in the sensor's sensitivity.

Finally, the tapered sensor was integrated into different half-cells, enabling the monitoring of electrolyte decomposition mechanisms, ion solvation dynamics and the structural evolution of electrode materials during cycling. In addition, it permits the following of the formation of the solid-electrolyte interface (SEI).

3:30 PM

(GOMD-S3-S3-006-2025) Exploring and extending the limit of vapor deposition fabrication for silicate optical fibers (Invited)

Y. Messaddeq¹; T. Meyneng^{*2}; K. Sanggon¹; R. Kashyap³

1. Université Laval, Optic-Photonic Pavillion, Canada
2. Université Laval, COPL, Canada
3. Chemin de Polytechnique, Canada

Silica, one of the gold standards in photonics, is among the most widely used glass materials in an ever-expanding range of applications. Its exceptional properties are a key factor, with attenuation losses approaching its theoretical limit. Equally important is its design flexibility, which extends from simple single-mode fibers to advanced multi-core photonic crystal fibers. At the foundation of silica's outstanding performance are vapor deposition fabrication methods, which enable these remarkable features. In recent years, our research has focused on exploring the limits of these processes to address specific application-driven design challenges. To further enhance or unlock new applications, we are also developing novel accessory methods, to enlarge the capacity of such processes. The presented work aims to first review the current technological state of vapor deposition technologies, highlighting some of their limitations. We will demonstrate how innovative designs can mitigate these challenges, with applications in biophotonics, telecommunications and fiber lasers. We also intend to provide insights into the future of these technologies and how they will contribute to further expanding the already extensive capabilities of silica optical fibers.

4:00 PM

(GOMD-S3-S3-007-2025) Optical and Structural Characterization of Reactively Sputtered SnO_x-SiO_x Binary Thin Films

M. S. Dailey^{*1}; B. G. Potter¹; K. Simmons-Potter²; P. Thelen³

1. The University of Arizona, Dept. of Materials Science and Engineering, USA
2. The University of Arizona, Dept. of Electrical and Computer Engineering, USA
3. Sandia National Laboratories, USA

The control of optically active structural point defects in glass via deposition conditions and compositional variation remains central to the development of thin film optical behavior. We have used reactive RF-magnetron sputter deposition from composite Sn/Si targets to produce a suite of glass thin films with Sn contents of 6.6±1.9 and 18.5±1.6 at% and deposited under varied oxygen partial pressures to influence oxygen deficiency in the structure. Optical absorption studies coupled with x-ray photoelectron spectroscopy (XPS) and valence-band-XPS (VB-XPS) have provided insight into the constituent bonding environments and their correlation with as-deposited, UV-vis absorption behavior. In the context of the anticipated application of these materials, we have found different classifications of UV-induced absorption change spectral response with variation in film metal stoichiometry and oxygen content. This suggests the potential to tune the resulting photomediated refractive index change to produce optical device structures with tailored performance in these materials.

4:20 PM

(GOMD-S3-S3-008-2025) In-situ photodegradation monitoring from ultra-sensitive SERS fiber probes based on Ag nanoparticle and Ag₃PO₄ nanocube composite

T. Hu^{*1}; X. Han¹; J. Zhang¹; J. Xie¹

1. Wuhan University of Technology, China

Ag nanoparticles and silver phosphate (cubes and tetrapods) composites based glass fiber probes fabricated, and applied for ultra-sensitive SERS detection and in-situ photocatalytic degradation monitoring based on surface-enhanced Raman spectroscopy (SERS). The combination of localized surface plasmon resonance (LSPR) from Ag nanoparticles and the photocatalytic performance of Ag₃PO₄ can realize SERS in-situ detection and develop recyclable SERS substrates. The formation of Ag/Ag₃PO₄ nanoparticles was verified by UV-Vis-NIR, XRD, FE-SEM, TEM, EDS and XPS. The lowest detection limit of CV for both composite particle based fiber probes is 10-14 M. The detection substance was catalyzed and degraded under irradiation. The decrease of the absorption peak detected by the LSPR effect of Ag confirmed the decrease of the corresponding content of the detected substance. For the prepared fiber probes, the degradation rate of CV and PATP reached more than 90% under SERS in-situ monitoring after one hour of illumination. The high electromagnetic field intensities generated by two kinds of Ag/Ag₃PO₄ nanoparticles were analyzed using the finite element method. This research indicates that the Ag/Ag₃PO₄ fiber probes fabricated by Ag₃PO₄ cubes and tetrapods have great application potential in the trace detection and SERS in-situ monitoring.

4:40 PM

(GOMD-S3-S3-009-2025) Characterization of Calcium Germano-Aluminate Glasses for Mid-Infrared Applications

A. Shearer^{*1}; J. C. Mauro¹

1. Pennsylvania State University, Materials Science and Engineering, USA

Calcium aluminate glasses have emerged as promising candidates for optical applications, particularly due to their potential for infrared transparency. However, their practical use has been hindered by challenges in glass-forming ability and inherent fragility, which complicate their manufacturing processes. Recent studies suggest that the incorporation of SiO₂ into the calcium aluminate matrix could enhance the polymerization of the glass network, thereby reducing crystallization tendencies and mitigating fragility. This study investigates the effects of increasing GeO₂ content on the structure and properties of calcium aluminate glasses through evaluating thermal, mechanical, and optical characterization methods. The results indicate that the addition of GeO₂ significantly stabilizes the glass structure, reduces fragility, and lowers the thermal expansion coefficient. However, mechanical property analysis reveals a decrease in both modulus and hardness with increasing GeO₂ concentration. Optical property measurements further suggest that these modified glasses possess favorable attributes for optical applications, with improved transparency in the infrared spectrum. This study provides valuable insights into the role of GeO₂ in enhancing the performance and manufacturability of calcium aluminate glasses for potential use in advanced optical devices.

5:00 PM

(GOMD-S3-S3-010-2025) Quantitative Assessment of Hinge Creases in Folding Devices

J. Banerjee^{*1}; K. Lindberg¹; D. Pikula¹

1. Corning Incorporated, USA

We present a novel method for assessing cosmetic defects in folding devices, with a primary focus on hinge region creases which induce tactile and optical distortions. The technique applies to a range of devices, including foldable phones and IT devices showcasing diverse hinge designs from elliptical to tear drop. The analytical approach leverages deflectometry, an existing characterization technique capable of measuring surface topography across a large field of

view. This enables swift data acquisition (< 30 sec) of surface shape across the entire device or component. With this algorithm, crucial metrics like crease depth, peak gradient, and extrema curvature magnitude, which are significant for light reflection distortion, are reported. The analysis algorithm and extrema (not mean) curvature metric are designed to capture critical points of the crease profile to ensure consistent reporting for both standard and non-standard shape profiles. This method shows high agreement with optical distortion through visual observations and zebra board imaging, allowing for high confidence in relative ranking and trend analysis of devices. The approach successfully tracks crease formation post-bending events and monitors its relaxation over time when the device is open. Therefore, it presents valuable insights for R&D efforts aiming to mitigate crease distortion.

GOMD S3 S4 - Rare-earth and transition metal-doped glasses and ceramics for photonic applications II

Room: Moresby

Session Chair: Jumpei Ueda, Hokuriku Sentan Kagaku Gijutsu Daigakuin Daigaku

1:15 PM

(GOMD-S3-S4-008-2025) Optical and geometrical functionality of active glass-based materials: 3D display chamber and tissue mimicking phantom (Invited)

Y. Wei^{*1}; H. Ebendorff-Heidepriem¹

1. The University of Adelaide, Australia

The geometry of optically active glass-based materials is as critical as their optical functionality for real-life applications such as stained glass windows and fiber lasers. This talk highlights glass-based materials with tailored optical properties and geometries for two applications: Glass cube as imaging chamber for 3D volumetric display: We evaluated the two-step, two-frequency upconversion (TSTF) performance of Er³⁺-doped tellurite and germanate glasses, benchmarking them against Er³⁺-doped fluoride glass. Combining experiments with simulations, we identified Er³⁺-doped tellurite glass as a scalable imaging chamber material with high TSTF upconversion performance – surpassing fluoride glass when both exciting lasers have pulsed output with optimized laser modulation parameters. Glass phantoms as calibration standards for fluorescence imaging systems: We developed a range of Sm³⁺ and Ag nanoparticles doped glass ceramic samples to mimic the absorption, scattering and fluorescence of healthy and malignant tissues. These glass ceramic samples were processed into small chip phantoms and assembled to form a calibration standard – which demonstrated excellent photostability, homogeneity, and long-term shelf-life. The calibration standard was further validated via a commercial surgical fluorescence imaging system.

1:45 PM

(GOMD-S3-S4-009-2025) CsPbBr₃ Perovskite Nanocrystal Embedded Borosilicate Glasses as a Robust Green Color Converter

W. Chung^{*1}; D. Gelija¹; T. T. Pham¹

1. Kongju National University, Division of Advanced Materials Engineering, Republic of Korea

Cesium lead halide (CsPbX₃) perovskite nano-crystals (PNCs) have been extensively studied as color converters in display applications due to their high photoluminescence quantum yield (PL-QY) and narrow emission bandwidth, enabling a wide color gamut suitable for ultra-high definition (UHD) TV. However, their ionic characteristics and organic passivation layers result in weak chemical, thermal, and photonic stabilities, which can be mitigated by introducing inorganic glass matrices. PNC-embedded glasses (PNEGs) have thus demonstrated practical feasibility as color-converting materials by composing white LEDs with a wide color gamut. In order to

extend their practical applications, a more chemically stable matrix is required. In this study, we fabricated CsPbBr₃ PNEGs based on a borosilicate glass system to obtain a green color converter with high PL-QY. We carried out a compositional study on the glass matrix and PNC elements, optimizing heat treatment conditions to improve PL-QY up to 70%. The formation of CsPbBr₃ nano-crystals was examined using XRD and HR-TEM, while Raman and XPS analyses were used to investigate the compositional role in the PNEG. The thermal, photonic, and chemical stabilities of the PNEG were compared with those of germanate PNEG. A white LED composed of the obtained PNEG demonstrated a wide color gamut up to 131% of the NTSC-defined area.

2:05 PM

(GOMD-S3-S4-010-2025) Effect of soda alumino germanate glass composition and bismuth source valence on the optical properties of the bismuth dopant and matrix

L. J. Henry^{*1}; M. Klopfer¹; K. Richardson²

1. Air Force Research Laboratory, Directed Energy Directorate, USA

2. University of Central Florida, CREOL, USA

Alteration of the alkali / aluminum ratio in a germanate glass is known to affect not only non-bridging oxygens and glass structure but also the environment dopants see in the glass matrix. Bismuth (Bi) is a dopant known to exist in multiple valence states which display unique optical properties. When Bi₂O₃ is melted with raw materials of a glass matrix, the glass network impacts the equilibrium valence state of Bi, driving the species via reduction towards metal (Bi⁰) and metal ion clusters when melted at higher temperatures or for longer melt times. The multi-valent nature of Bi can serve to stabilize charged defects in the glass matrix and the matrix itself can also work to stabilize Bi emission sites. The work presented here will show how the optical excitation and emission properties of Bi change for glass matrices having an atomic excess and deficit of Na relative to Al, across the 1:1 Na/Al ratio. It will also show that the reduction equilibrium of Bi established when melting Bi₂O₃ (Bi³⁺) or Bi metal (Bi⁰) with components of a soda alumino germanate glass matrix in air, does not largely impact the glass' resulting structure or optical properties. Finally, we will show how the presence of Bi in a doped glass affects the balance of charge and formation of matrix defects relative to what is seen in the analogous undoped, Bi-free glass.

2:25 PM

(GOMD-S3-S4-011-2025) Evolution of Pore Structure During Annealing of Fine-Grained Yttrium Based Transparent Ceramics

J. M. Tallan^{*1}; J. Bussey³; S. Karcher²; J. McCloy²

1. Washington State University, Materials Science & Engineering, USA

2. Washington State University, School of Mechanical and Materials Engineering, USA

3. Washington State University, USA

Transparent Y₂O₃ was first prepared in the 1960s, and has remained one of the most prevalent and promising materials in the field of transparent ceramics, particularly in areas such as IR windows and laser hosts. Achieving high transparency in Y₂O₃ ceramics requires high density, homogenous pore structures, a homogeneous microstructure and low impurity concentration. During the sintering process of Y₂O₃ based transparent ceramics the material is commonly reduced from Y₂O₃ to Y₂O_(3-x) and returning Y₂O₃ to its original stoichiometry requires an additional annealing process under oxidic conditions. During annealing, migration and consolidation of pores at grain boundaries and junctions can lead to changes in the density and optical properties. In this work the impact of annealing conditions on the pore structures and optical properties of Y₂O₃ based ceramics is investigated. Y₂O₃ pellets were prepared via hot uniaxial pressing using commercially available nano powders. FTIR was used to assess the IR transparency of as-sintered and post-annealing Y₂O₃ ceramics. Nano-CT was used to study the migration and growth of

pores as a function of annealing conditions. IR microscopy and electron backscatter diffraction were used to monitor changes in the grain structure after annealing. Hydrostatic weighing and pycnometry were used to assess changes in open and closed porosity after annealing.

2:45 PM

(GOMD-S3-S4-012-2025) Spectroscopic properties of Cr²⁺/Fe²⁺ doped ZnS hot-pressed transparent ceramics

M. Poitou^{*1}; K. Ereemeev²; S. Mauree¹; G. R. Durand¹; P. Loiko²; A. Le Coz¹; F. Starecki²; V. Nazabal¹; P. Camy²; A. Braud²; O. Merdrignac¹

1. Universite de Rennes, France
2. Universite de Caen Normandie, France

Zinc chalcogenide crystals (ZnS, ZnSe) doped with transition metal ions (e.g., Cr²⁺, Fe²⁺) have garnered significant interest as broadband gain media and efficient saturable absorbers for lasers operating in the infrared regions. These wide bandgap II-VI semiconductors offer broad transparency, tetrahedral coordination for dopant ions and low phonon energies. The low phonon energies contribute to a weak non-radiative decay pathway, enhancing the quantum yield of luminescence at room temperature. Cr²⁺-doped ZnS is well-known for its application in broadly tunable and femtosecond mode-locked lasers that emit in the 2.1–2.5 μm range. Fe²⁺-doped ZnS emits in the mid-IR range (3–5 μm). High-quality (Cr²⁺, Fe²⁺):ZnS is typically produced via chemical vapor deposition, followed by hot isostatic pressing, with chromium or iron doping introduced through thermal diffusion. However, this process is complex, costly and the resulting materials exhibit moderate laser-induced damage threshold and non-uniform distribution of (Cr²⁺, Fe²⁺) ions. Hot pressing offers a promising alternative to this conventional method. Recently, we fabricated transparent ZnS ceramics from high-purity nanopowders, which were synthesized by using a combustion method and subsequently densified by hot pressing. In this study, we apply this method to produce (Cr²⁺, Fe²⁺)-doped ZnS transparent ceramics and assess their emission properties.

GOMD S5 - Glass manufacturing

GOMD S5 S1 - Manufacturing IV

Room: Saturna Island Ballroom

Session Chairs: Luiz Pereira, Université de Munich (LMU);

Irene Peterson, Corning Incorporated

1:15 PM

(GOMD-S5-S1-017-2025) Advances in Studying Silicate and Carbonate Melts through Flash DSC (Invited)

K. Hess^{*1}

1. Ludwig-Maximilians-Universität München, Earth Sciences, Germany

Flash Differential Scanning Calorimetry (Flash DSC) has transformed the investigation of high-temperature melts, providing unparalleled insights into the thermal and kinetic properties of structural glasses. This review synthesizes recent experimental findings that leverage Flash DSC to study rapid phase transitions, crystallization kinetics, glass formation and structural relaxation in these complex materials. Flash DSC's ultra-fast heating and cooling rates, exceeding 10,000 K/s, enable detailed exploration of metastable states, rapid crystallization, and glass formation processes. For example, investigations into ultramafic compositions have highlighted the intricate interplay between viscosity and undercooling, deepening our understanding of volcanic glass formation and magma or lava flow dynamics. Recent advancements in the study of amorphous carbonates have further expanded the scope of Flash DSC. These materials have been shown to exhibit a calorimetric glass transition, confirming their classification as structural glasses. This

discovery situates amorphous carbonates within the broader family of glasses produced through diverse mechanisms, such as evaporation and electrodeposition. This review also addresses experimental challenges, including sample preparation and the interpretation of data.

1:45 PM

(GOMD-S5-S1-018-2025) Radiative properties of waste glasses and their implications on glass production rate

P. Ferkl^{*1}; J. Marcial¹; J. C. Rigby¹; P. Hrma²; A. A. Kruger³; R. Pokorny⁴

1. Pacific Northwest National Lab, USA
2. AttainX, USA
3. U.S. DOE, Hanford Field Office, USA
4. University of Chemistry and Technology Prague, Czechia

Defense nuclear waste currently stored at the Hanford site in the US will be mixed with glass-forming and modifying chemicals and immobilized in durable glass forms. The large diversity in the chemical composition of the waste and the optimization of the waste content in glass will result in a broad range of melter feed and glass compositions produced at the Waste Treatment and Immobilization Plant. The processing rate is affected by the melter feed makeup, melter operating conditions, and the properties of the melt such as melt viscosity and thermal conductivity. In this work, we present experimental characterization of radiative properties of multiple low-activity and high-level waste glasses at several temperatures and redox conditions. Additionally, we show how these properties can be estimated by modeling speciation of transition metal ions given the oxygen partial pressure. Finally, we discuss the effect of small bubbles and undissolved particles on radiative properties, thermal conductivity, and glass production rate for a wide compositional range of waste glasses.

2:05 PM

(GOMD-S5-S1-019-2025) Evolved gas analysis studies of melter feeds for Hanford nuclear waste vitrification

J. Marcial^{*1}; W. Choi²; J. Seo³; J. C. Rigby²; M. Hall²

1. Pacific Northwest National Laboratory, Materials Testing and Development team, USA
2. PNNL, Radiological Materials Group, USA
3. Pacific Northwest National Laboratory, USA

High-temperature evolved gas analysis during glass melting has been used for decades to understand processes that occur during glass production and to improve the overall process efficiency. For both commercial glassmaking and nuclear waste vitrification, this method is used to study the influence of composition and makeup of commercial glass batches and waste glass melter feeds on the conversion process and the phenomena that influence the rate of glass production, especially foaming. We present an overview of experimental configurations used to elucidate aspects of batch-to-glass conversion with specific focus on batch reactions and foaming. This includes evolved gas analysis (EGA), a method that provides insight into the modes of gas production. Gases produced can either escape the samples through open porosity or become trapped in the glass-forming melt resulting in foam growth and collapse in heated glass batch samples. We are in the process of developing an observation setup in which gas evolution during batch melting can be monitored. Obtained results will be presented as a function of varying melter feed chemistry to determine effect of melter feed chemistry on the makeup of evolved gases.

2:25 PM

(GOMD-S5-S1-020-2025) Investigations on the Wetting and Spreading Behavior of Silicate Glass Melts on Metals and their Oxides

P. Engelmann^{*1}; C. H. Roos¹

1. Rheinisch-Westfälische Technische Hochschule Aachen, Institute of Mineral Engineering - Chair of Glass and Glass-ceramic, Germany

The interaction between a cooling glass melt and metallic molds plays a crucial role in the hollow glass forming process. Mold wear-out and oxidation eventually lead to gob sticking, causing surface defects in the final product. For the development of mold materials and coatings enabling an improved forming process, it is important to better understand the glass melt's behavior on metallic and ceramic surfaces and to revise the existing theories on sticking. Therefore, the wetting and spreading behavior of different glass melts is investigated by means of different thermo-optical methods. Previous investigations in a heating microscope showed a high influence of the substrate material on the wetting and sticking behavior. The time- and temperature-dependent contact radii and angles obtained from the experimental data were successfully used to describe the dynamic wetting and spreading behavior by means of a molecular kinetic model. Current work focuses on understanding the influence of different atmospheres and interface reactions and the relation of molecular kinetic parameters to glass structure and substrate properties. A lab scaled setup where a glass droplet is generated at industrial gob temperature and poured onto an individually heated substrate, held at mold temperature was constructed to enable non-isothermal trials and a better depiction of the industrial process.

2:45 PM

(GOMD-S5-S1-021-2025) Modelling Refractory Corrosion During Industrial and Waste Glass Melting

J. Klouzek^{*1}; R. Pezl¹; P. Cincibusova¹; D. P. Guillen²; P. Hрма³; A. A. Kruger⁴; R. Pokorny⁵

1. University of Chemistry and Technology, Prague, Laboratory of Inorganic Materials, Czechia
2. Idaho National Laboratory, Materials Science and Engineering, USA
3. AttainX, USA
4. US Department of Energy, Office of River Protection, USA
5. University of Chemistry and Technology Prague, Czechia

Understanding and managing refractory corrosion is critical to ensure the longevity and efficiency of glass-melting furnaces while maintaining glass product quality. The presented experimental work focuses on developing a corrosion rate model for refractory material as a function of temperature, melt flow rate, and glass composition. Corrosion tests were conducted under both static and dynamic conditions, simulating the effect of forced convection of the melt on the corrosion rate. The rate of subsurface corrosion increases with the melt flow rate. The melt line corrosion rate is independent of the melt flow. The influence of glass composition, specifically the content of chromium, alumina, iron oxides, and alkali metal oxides, is identical for both linear and subsurface corrosion. The experimental setup allows to estimate the diffusion coefficients of the dissolving refractory components, an important property that will be used for the development of detailed K-3 corrosion models based on diffusion-controlled dissolution. The measured data will be used directly in the CFD melter model to evaluate the effect of melter processing conditions, such as temperature, bubbling rate, or the chemical composition of glass melt, on the corrosion rate, and help optimize the melter long-term performance.

GOMD S5 S1 - Manufacturing V

Room: Saturna Island Ballroom

Session Chairs: Terutaka Maehara, AGC Inc.; Irene Peterson, Corning Incorporated

3:30 PM

(GOMD-S5-S1-022-2025) Measurement of the dispersion of the stress-optic coefficient in ion-exchanged sodium aluminosilicate glass

J. Hunt^{*1}

1. Corning Incorporated, Optical Physics and Materials, USA

Non-destructive optical stress measurements through analysis of the optical birefringence are essential for product development and quality control in the technology of chemically strengthened glass. These measurements rely on accurate knowledge of the stress-optic coefficient (SOC) to convert measured birefringence to stress. However, the SOC is not constant, and the wavelength dependence of the SOC becomes important when the measurement wavelength is different from the wavelength at which a nominal value of the SOC is provided. Furthermore, the stress values are usually reported based on the assumption that the SOC of the ion-exchanged material is the same as the SOC of the base glass. This work reports on a measurement of the dispersion of SOC in sodium-aluminosilicate glass that has been ion exchanged with potassium, by analyzing the birefringence profiles extracted using the inverse-IWKB method. The SOC-dispersion obtained for the ion-exchanged material did not distinguish from the SOC-dispersion of the bulk material beyond the uncertainty limited by the deviations of the bulk data from their trend.

3:50 PM

(GOMD-S5-S1-023-2025) Silica viscosity measurement via the elongation method

C. Nie^{*1}; G. Calkins¹; J. McCarthy¹; A. Sarafian¹

1. Corning Incorporated, USA

Viscosity is a critical material property for understanding forming processes. This work focuses on viscosity measurements of high temperature silica glasses using an elongation methodology that was developed in 1929. These measurements are challenging due to the high temperature requirements involved. The results obtained from this study are compared with existing literature and highlight differences between the elongation method and other techniques such as MCVD collapse, draw tension, and penetration methods.

4:10 PM

(GOMD-S5-S1-024-2025) The Impact of Glass Waste Filler on Density and Flame Retardancy in Sawdust-Reinforced Composite Ceiling Boards

K. J. Jomboh^{*1}; A. O. Adejo²; A. D. Garkida³

1. University of Maiduguri, University of Maiduguri, Nigeria
2. Federal University Lafia, Nigeria
3. Ahmadu Bello University, Nigeria

The development of composite ceiling boards involved the formulation of sawdust/saturated polyester resin (UPR), glass waste/UPR, sawdust/glass waste/UPR and a control group (100% UPR). Density was used as a factor to evaluate flame resistivity, with the horizontal burning method performed in accordance with ASTM D635 standards, utilizing specimens sized at 125mm x 13mm x 5mm. The resulting data included the extent of burning (mm) and ignition time (s). Results indicated that sawdust/glass waste/UPR hybrid composites demonstrated high resistivity to the flame test, with glass acting as a flame retardant. The hybrid sample containing 13/27/60 % sawdust, glass waste and UPR had the highest flame resistance of 3.34 mm with a density of 1.41 g/cm³. In contrast, the control sample (100% resin) had the poorest flame resistance of 16.15 mm extent of burning with a density of 1.11 g/cm³. Density increased in accordance

with the filler loading, with the control group having the lowest density of 1.11 g/cm³, and the sample containing 0/40/60 % glass waste/UPR having the highest density of 1.91 g/cm³, which is typical of bulk materials.

GOMD S5 S2 - Additive manufacturing of glass

Room: Saltspring C

Session Chair: Beck Walton, Lawrence Livermore National Lab

3:30 PM

(GOMD-S5-S2-001-2025) Additive Manufacturing of Lattices Using Digital Glass Forming (Invited)

M. Azad¹; N. Khadka¹; R. Landers¹; E. Kinzel¹

1. University of Notre Dame, USA

Digital Glass Forming is a process for printing glass. A glass filament is fed relative to a moving workpiece. A laser locally heats the glass above the transition temperature. The forces from the workpiece (positioned by 4-axis stages) and feeder deform the glass locally so that it can be fused to create fully dense freeform objects or bent in the air to print freestanding structures. In this talk, we discuss new work printing lattices. The laser is used to fuse the filament to the substrate and the substrate moved in the same direction that the filament is fed from. This creates a freestanding, straight piece of glass. After a specified length the laser is used to locally heat the glass while the substrate and filament are moved in opposite directions to break the glass. The substrate is rotated 120 deg. and repeated. After a 3rd piece is added the tops are fused with laser heating. Repeating this process allows the fabrication of complete primitive cubic unit cells. The advantage of this approach is that no laser heating is required during most of the structure which speeds fabrication and preserves the initial tempering of the glass filaments. The procedure is described and initial results using 2 mm borosilicate cane will be presented along with a general overview of ongoing Digital Glass Forming Work.

4:00 PM

(GOMD-S5-S2-002-2025) Novel Colloidal Materials for Additively Manufacturing Optical Glasses (Invited)

J. F. Destino¹; M. Murthi¹; N. Tobin¹; J. Chou¹; A. R. Carr¹; R. M. Wayne¹; A. Fernandes¹; L. O'Keefe¹; S. Garapati¹; A. Kayton¹; F. Lopez¹; J. Varguez¹

1. Creighton University, Chemistry & Biochemistry, USA

The advancement of additive manufacturing (AM) or 3D printing has shown extraordinary potential to revolutionize many fields, including glass science. We present the development and characterization of sol-gel-derived hybrid colloidal feedstocks designed for fabricating glass by direct ink write (DIW) AM. Our research mainly focuses on binary silica-based feedstocks targeting specific optical properties, including improved optical transmission, tunable refractive indices, and color filtering. We report multiple sol-gel approaches for synthesizing hybrid colloids of various morphologies and compositions and confirm their physical and chemical structural properties by electron and atomic force microscopies and Raman and FTIR spectroscopies, respectively. We also investigate how colloidal feedstock structure influences glass network formation upon thermal processing and densification using those same techniques. Ongoing research seeks to compare the resulting glass structures fabricated from sintered sol-gel colloidal feedstocks with melt-quench glasses of the same composition.

4:30 PM

(GOMD-S5-S2-003-2025) A New Method to Guide the Processing of Additively Manufactured Glass

R. J. Pao^{*1}

1. Alfred University, Inamori School of Engineering, USA

Additive manufacturing of glasses requires inefficient and lengthy guess and check methods to find optimal sintering parameters. Titanosilicates glasses have been additively manufactured and sintered to full density using these guess and check methods, however this often results in crystallization. To bypass the traditional Edison-ian methods we developed a new model based on recent insights into crystallization, sintering, and slumping to streamline the development of a sintering procedure. It was found that the model can accurately predict at what time and temperature to sinter titanium silicate glass up to 97% densification. The method proposed here is based on rational design and offers a route to additively manufacturing future glasses of interest.

4:50 PM

(GOMD-S5-S2-004-2025) 3D printing glass via UV-DIW

T. Yee¹; B. Walton²; A. Browar²; V. Vuppuluri²; D. Nguyen²; R. J. Dylla-Spears³; N. Dudukovic²

1. Lawrence Livermore National Laboratory, Materials Science Division, USA
2. Lawrence Livermore National Laboratory, USA
3. Lawrence Livermore National Laboratory, Optics and Materials Science & Technology, USA

Direct ink writing (DIW) has shown promise to fabricate glass structures with geometries and spatial compositions not possible with conventional manufacturing techniques. With this method, a glass slurry or ink is extruded from a nozzle to build a part layer by layer. Previous work has relied purely on viscoelastic properties for shape retention, although parts were sensitive to handling and achievable aspect ratios were limited. Alternatively, utilizing a UV curable glass ink, which can be exposed to light immediately after extrusion, can provide increased print robustness for greater yields as well as for structures such as thin walls. Fully dense glass is then achieved through heat treatment, which requires more stringent processing than non-UV techniques. We also evaluate the properties of AM glass such as mechanical strength and chemical compatibility. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. LLNL-ABS-2002054. Abstract for consideration for an oral presentation at the Glass and Optical Materials Division meeting, Vancouver, BC, Canada May 4 – 9, 2025.

GOMD S6 - Jonathan Stebbins Honorary Symposium

GOMD S6 - Jonathan Stebbins Honorary Symposium IV

Room: Saltspring AB

Session Chair: Sung Keun Lee, Seoul National University

1:15 PM

(GOMD-S6-016-2025) Exploring the Surface Structure and Chemistry of Oxide Catalysts with ¹⁷O Solid-State NMR Spectroscopy (Invited)

L. Peng^{*1}

1. Nanjing University, Chemistry, China

The surface structure of catalysts, in particular, the local structure at the molecular and atomic scale, determines their performances. This information is a prerequisite for catalyst studies, but it is challenging to obtain. In the past ten years, we developed an approach

based on ^{17}O solid-state NMR spectroscopy to extract the detailed structural information of oxide catalysts, which is able to distinguish oxygen sites at different surface layers, facets, and chemical environments, providing rich opportunities for further exploring chemistry on oxides. Recently, we demonstrated that species oxygen species responsible for gas adsorption and activation can be identified with ^{17}O solid-state NMR spectroscopy, by using MgO adsorbing CO_2 and ZnO activating H_2 as examples. The reasons behind the different adsorption capacities of the MgO nanosheets treated at different conditions and the detailed mechanisms of H_2 activation on ZnO nanorods at different temperatures were elucidated. In addition, the surface structure and catalytic properties of the emerging metal-oxide single atom catalysts (SACs) can also be determined. These methods provide key information for understanding the structure-properties relationship of oxygen catalysts, as well as the rational design of better adsorbents and catalysts.

1:45 PM

(GOMD-S6-017-2025) NMR studies of borosilicate glass alteration in aqueous environments: Implications for nuclear waste immobilization

S. Kroeker¹; M. Brytskiy¹; K. Penner¹; A. Krishnamurthy³; A. Farrant²

1. University of Manitoba, Chemistry, Canada
2. Dalhousie University, Chemistry, Canada
3. Purity-IQ Inc, Canada

The dissolution behaviour of silicate glasses in aqueous environments is key to evaluating the suitability of materials for radioactive waste disposal, as the formation of an alteration layer limits ionic transport and improves radionuclide retention. In borosilicates, layer thickness is estimated by measuring B release into solution, assuming that B is not incorporated into the layer. Recent work has shown that this assumption is unreliable, but little is known about how B is incorporated into borosilicate alteration layers. Alteration layers formed on alkali boroaluminosilicate glasses are analyzed by NMR to obtain a clearer picture of B incorporation and network connectivity. Boron retention differs for different alkali glasses but shows a concentration gradient across the altered region. ^{11}B NMR of altered glass reveals elevated BO_3 fractions relative to the bulk Na-based glass, whereas B speciation in the analogous Li glass layer differs only slightly from that of the unaltered bulk. $^{11}\text{B}\{^1\text{H}\}$ D-HMQC spectra reveal insight into the local bonding environments of the BO_3 and BO_4 . $^{29}\text{Si}\{^1\text{H}\}$ cross-polarization NMR of isolated layers shows a high fraction of silanol groups, consistent with some models of silicate glass alteration. SEM of the layer thickness confirms that using B as an alteration tracer leads to underestimation of the true alteration layer thickness.

2:05 PM

(GOMD-S6-018-2025) Chemical strengthening of float glasses: effect of composition and structure

V. M. Sglavo¹; S. Dire¹; E. Callone¹

1. University of Trento, Italy

Two silicate float glasses were considered in the present work: a typical clear soda lime silicate glass and a soda magnesia silicate glass. The two materials were subjected to chemical strengthening in KNO_3 and a different behavior was pointed out in terms of potassium penetration and corresponding surface compression; soda magnesia silicate glass is revealed to be much proner to be reinforced by the exchange of sodium with potassium owing to a much higher inter-diffusion coefficient, although the activation energy for the process was substantially identical for the two materials. The difference performance in terms of Na/K exchange can be only partially correlated to the slightly larger amount of sodium in the soda magnesia silicate glass which is instead characterized by a more open structure, characterized by a large amount of 5-6 or more members rings, as revealed by NMR and FT-IR/micro-Raman spectroscopy.

The structure appears dictated by the chemical composition of the glasses, soda magnesia silicate material being richer in formers (like silica and alumina, and, very likely, magnesia), which cause the presence of more abundant Q^3 units and more limited Q^2 and Q^4 ones for a faster movement of the alkaline atoms.

2:25 PM

(GOMD-S6-019-2025) A study of sub-Tg relaxation in aluminosilicate glasses and its link to total pitch variation in high performance display manufacturing (Invited)

T. Kiczanski¹; O. Gulbitten²; S. Koseba¹; G. G. Moore³; M. E. DeRosa²; B. M. Guy²; L. Moore⁴; A. Sarafian⁵; A. J. Ellison²

1. Corning Incorporated, Inorganic Materials, USA
2. Corning Incorporated, Science & Technology Division, USA
3. Corning Incorporated, Characterization Sciences, USA
4. Corning Incorporated, Glass Research, USA
5. Corning Incorporated, USA

To enable perfect registration of the various layers of a TFT in the manufacture of a display, the dimensional change of the glass substrate must be very small and very repeatable. The metric currently used by the display industry to capture this behavior is “total pitch variability”, where total pitch is defined as the distance a feature moves during a given step in the TFT process. We will discuss the various glass attributes contributing to total pitch variability such as viscous relaxation, stress relaxation, elastic distortion, and sub-Tg relaxation. We will then focus on quantification of the sub-Tg relaxation and our attempts to link it back to structural changes in the glass.

GOMD S7 - Emerging frontiers - Glasses in new technology

GOMD S7 - Emerging frontiers - Glasses in new technology I

Room: Moresby

Session Chairs: Madoka Ono, Hokkaido University;
Collin Wilkinson, Alfred University

3:30 PM

(GOMD-S7-001-2025) Virtual Center for Nuclear Waste Glass Science (Invited)

M. Singh¹; X. Lu⁴; E. M. Tsekrekas²; C. Wilkinson³; C. L. Trivelpiece²; D. Aidhy¹

1. Clemson University, Materials Science and Engineering, USA
2. Savannah River National Lab, Environmental and Process Control Technology, USA
3. Alfred University, Glass Science, USA
4. Pacific Northwest National Lab, Energy and Environment Directorate, USA

In 1982, borosilicate glass was deemed the “best demonstrated available technology” for the disposal of high-level nuclear waste (HLW) and since that decision, glass has also been demonstrated as an effective waste form for low-activity waste (LAW). Since then, enormous amount of data has been generated by relating to the properties of nuclear waste glasses. Until recently, most of this data could only be accessed from isolated reports or institutional databases. This non-centralized data prevents current and future generations of glass researchers from using state-of-the-art computational tools to design, test, and produce next generation waste glass formulations. Our team has created the first online, open-access repository of nuclear waste glass data called the Virtual Center for Nuclear Waste Glass Science. The website consolidates the data into a single source that can be used from around the world to study radioactive waste forms. The database includes a forward-facing “landing page” for the front and filtering methods that allow researchers to target specific glass properties such as composition, viscosity, and durability. With these

developments, the Center provides centralized access to decades of data, facilitate evaluation of existing models for predictive insights—including those using machine learning methods—and support data management and maintenance for newly generated data.

4:00 PM

(GOMD-S7-002-2025) Digitalization of Glass Development (Invited)

U. G. Fotheringham^{*1}; F. Teepe¹¹; L. Pfeifer¹⁰; M. to Baben²; A. de Camargo⁹; T. Hickel³; L. Wondraczek⁵; M. Sierka⁵; K. Thurow⁶; A. Vu⁸; R. Müller⁷; J. Janssen³; P. Dolabella Portella⁴

- Schott AG, Germany
- GTT-Technologies, Germany
- Max-Planck-Institut für Nachhaltige Materialien GmbH, Germany
- Fraunhofer-Institut für Werkstoffmechanik IWM, Germany
- Friedrich-Schiller-Universität Jena, Germany
- Universität Rostock Fakultät für Informatik und Elektrotechnik, Germany
- Technische Universität Clausthal, Germany
- Fraunhofer-Institut für Produktionstechnologie IPT, Germany
- Bundesanstalt für Materialforschung und -prüfung, Germany
- LTB Lasertechnik Berlin GmbH, Germany
- PRALL-TEC GmbH, Germany

Funded by the German Federal Ministry for Education and Research, the Innovation Platform MaterialDigital has been launched in 2019 with the goal to pioneer in the digital standardization of materials data and materials information. Carefully balancing out necessarily public issues like standardization and ontologies on one side and guaranteeing the rights of authors, data sovereignty, and data protection on the other, an attractive forum for the material science community has been developed. Material Digital is fed by funded projects. Glass has been part of these activities from the very beginning. The first was “GlasDigital”, an academic project with associated industrial partners, that laid the groundwork for the development of data-driven workflows for an accelerated glass development. This work is currently carried on by the industry-led project “GlasAgent” (from “glass” and “software agent”), which targets both the speed and the flexibility of glass development, the latter with the goal of allowing recycled glass as raw material for a broad variety of glasses.

4:30 PM

(GOMD-S7-003-2025) Process Digital Twin for Optimizing High-Precision Laser Glass Machining (Invited)

S. Tani^{*1}

- Rikagaku Kenkyujo, RIKEN Center for Advanced Photonics, Japan

Ultrashort pulsed lasers have become indispensable tools for glass modification and processing, offering unparalleled precision and deep penetration into glass materials. However, optimizing processing conditions remains challenging due to the vast parameter space and the incomplete understanding of multiscale physical mechanisms. Key processes, including multi-photon ionization, electron-phonon coupling, and bond dissociation, span diverse temporal and spatial scales—from angstroms and femtoseconds to millimeters and seconds—complicating modeling and control efforts. To overcome these challenges, we developed a deep neural network-based simulator trained on an extensive experimental dataset for laser-driven glass processing. This innovative simulator enables the optimization of laser processing parameters beyond the training dataset, providing a powerful platform for virtual parameter exploration and optimization in cyberspace. By bridging the gap between experimental data and predictive modeling, our approach advances control and efficiency in ultrashort laser-based glass processing.

Wednesday, May 7, 2025

GOMD Award Lectures

GOMD Stookey Lecture of Discovery

Room: Saturna Island Ballroom

Session Chairs: Collin Wilkinson, Alfred University;
Madoka Ono, Hokkaido University

8:00 AM

(GOMD-Awards-003-2025) Discovery of strong and damage-resistant glasses through indentation studies

T. M. Gross^{*1}

- Corning Incorporated, Physical Properties, USA

The response of glass to indentation provides considerable information regarding modes of deformation and propensity towards cracking. Learning to tailor the observed glass response through composition design has resulted in several key discoveries. In between normal glasses that deform with a considerable volume displacing shear component and anomalous glasses that deform primarily by densification, a third type of glass, defined as intermediate, was shown to display enhanced indentation crack resistance. By designing ion-exchangeable compositions with intermediate indentation deformation behavior, Vickers cracking threshold values exceeding 30 kilograms force were observed for the first time. This discovery paved the way for multiple generations of Corning® Gorilla® Glass. The discovery of a composition space that exhibited large ring cracks on the anomalous end of the deformation spectrum resulted in highly break-resistant Corning® Fusion5® windshield glass. The large ring crack provides a barrier to the extension of radial cracks that result in windshield failure. Lastly, indentation studies on glasses designed specifically to enable high water diffusion resulted in a surprising observation of high stored strain energy at failure. Subsequent analyses revealed a significant stress profile induced by hydration and damage resistance comparable to ion-exchanged glass.

GOMD S1 - Fundamentals of the glassy state

GOMD S1 S2 Glass Crystallization and Glass-Ceramics II

Room: Pender

Session Chairs: Laurent Cormier, Sorbonne University - CNRS;
Tsuyoshi Honma, Nagaoka University of Technology

9:20 AM

(GOMD-S1-S2-006-2025) Controlling crystallization in perovskite glass-ceramics (Invited)

M. Cicconi^{*1}

- Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science and Engineering, Germany

Perovskite-bearing glasses and glass-ceramics (GCs) play an important role in several technological applications. In particular, the niobate and titanate families are known for their enhanced optical and dielectric properties, and energy storage applications. Combining key glass qualities such as optical properties, manufacturability, and thermal/chemical-resistance with the symmetry-dependent properties of perovskite crystals (e.g., piezo-/pyro-electricity, SHG) creates significant opportunities for advanced multifunctional GCs. These materials are especially promising for photorefractive and electro-optical applications. First, selecting an adequate glass composition is crucial, followed by investigating the correct nucleation and growth parameters. However, the wide range of applications demands different microstructures, such as fine-grained structures (nano-sized) for enhanced optical transparency, oriented crystals for improved piezoelectric performance, and porous frameworks for catalytic applications.

Therefore, this talk will provide an overview of the different crystallization paths used to develop transparent or texturized GCs. Both ex-situ and in-situ methods were employed to understand the development of the crystal phases and their arrangement. Another aspect of particular interest to many fields is the study of stress in the residual glass, and a few examples will be provided.

9:50 AM

(GOMD-S1-S2-008-2025) Vanado-tellurite glass-ceramics containing copper oxide: effect of chemical composition on microstructural-electrical properties

C. Sgarlata^{*1}; A. Iannuzzi¹; M. Affatigato²; C. Siligardi¹

1. Università degli Studi di Modena e Reggio Emilia, Engineering "Enzo Ferrari", Italy
2. Coe College, Physics Department, USA

This study extends previous research concerning the study of the electrical conductivity of a glass system containing transition metal oxides. Starting from a reference glass $20\text{CuO}-48\text{V}_2\text{O}_5-32\text{TeO}_2$ previously studied, two glass systems $14.07\text{CuO}-53.93\text{V}_2\text{O}_5-32\text{TeO}_2$ and $20\text{CuO}-48\text{V}_2\text{O}_5-25\text{TeO}_2-7\text{TiO}_2$ were examined by varying some stoichiometric ratios in the first system, and introducing a percentage of TiO_2 in the second. Glassy samples synthesized under static air, were then subject to different time of heat treatments to obtain glass-ceramics and then investigated using different techniques such as electrical conductivity, X-ray diffraction (XRD), electron microscopy FEG-SEM, and thermal analysis DTA. Furthermore, all glass ceramic samples were etched with HCl to study the role of the glassy and crystalline phases, and the microstructural influence on the analyzed properties. The results confirmed a significant increase of conductivity in the two systems, due to the thermal treatment of the glasses and the crystallization of the samples, depending on the time of treatment. Some results seem to confirm an improvement in conductivity with the presence of TiO_2 . Finally, the correlation of the presence of the copper vanadium bronze crystalline phase in the samples with conductivity was deepened.

10:10 AM

(GOMD-S1-S2-009-2025) Lithium Alumino-silicate glass-ceramic: Salient properties and thermal characteristics

P. Barick^{*1}; P. Biswas¹; M. Suresh¹; D. C. Jana¹; B. P. Saha¹; P. Jain¹; R. Vijay¹

1. International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI) Hyderabad India, Centre for Advanced Ceramic Materials, India

Lithium Alumino-Silicate (LAS) glass-ceramic is an indispensable material for many applications namely telescope mirror, fast ion conductor, and cooktop panel because of its unique combination of ultra-low thermal expansion, high thermal shock resistance, high visible-light transparency, and low birefringence. The LAS glass is produced through melt-quench technique using a mixture of several chemical compounds like Li_2CO_3 , NaNO_3 , KNO_3 , SiO_2 and others. Thereafter, the glass is annealed and crystallized under an appropriate heat treatment cycles. Upon analysis, XRD pattern revealed the signature peak of $(\text{Li,Mg,Zn})_{1.7}\text{Al}_2\text{O}_4\text{Si}_6\text{O}_{12}$ which is isostructural to β -quartz solid solution (βQSS) - a stuffed derivative of β -quartz. The TEM results demonstrates that nanometer sized βQSS -like crystals ($\approx 20\text{nm}$) uniformly grown in the glassy matrix, favorable for higher optical transparency ($\approx 85\%$) and achieving low thermal expansion (≈ 0.12 ppm). In addition, a state-of-the-art heating stage microscope (HSM) is employed to understand the thermal behavior of glass as a function of temperature and record the real-time images and corresponding temperatures pertaining to: crystallization regime, softening, sphere formation, half-sphere formation, and melting. The crystallization temperature regime is also compared with DSC result.

10:30 AM

(GOMD-S1-S2-010-2025) Crystallization enables suppressing thermal conduction in oxide glasses

M. B. Østergaard^{*1}; L. Thomsen¹; H. Johra²; Y. Yue¹

1. Aalborg University, Chemistry and Bioscience, Denmark
2. SINTEF Community, Architectural Engineering, Norway

Oxide glasses are important materials to overcome great societal challenges within energy and environment. The thermal conduction in oxide glasses is a key controlling factor for developing new materials used for fast heat transport or thermal insulation. Unfortunately, the thermal conductivity of oxide glasses is scarcely studied. It is well known that the thermal conductivity of glasses is usually lower than that of their crystalline counterparts due to the lack of long-range order in glasses, limiting the phonon mean free path. Thus, glasses are better thermal insulators than crystals. But how can we reduce the thermal conductivity of glasses even further? Here, we demonstrate a new way to suppress the thermal conduction in glasses. Specifically, the new way is based on our recent new finding, i.e., the thermal conductivity of glass-ceramics exhibits an abnormal trend with varying crystallinity. Upon initial crystallization, the thermal conductivity of a silicate glass system decreases by approx. 20 % compared to that of the pure glass phase. Upon further crystallization, as expected, it increases again due to the enhanced degree of long-range order. The initial reduction in thermal conductivity could be ascribed to an enhanced scattering effect caused by crystallites. This scattering effect exceeds that of the pure glass phase.

10:50 AM

(GOMD-S1-S2-011-2025) Chiral crystallization of glass using optical vortex laser

K. Kizaki^{*1}; J. Zhao¹; T. Omatsu²; M. Ono¹

1. Tohoku Daigaku, Department of Applied Physics, Japan
2. Chiba Daigaku, Graduate School of Engineering, Japan

Chiral materials are vital in biotechnology and pharmaceuticals for their optical and pharmacological properties. Recently, circularly polarized luminescence (CPL) materials have gained attention for optical communication applications. CPL refers to the unequal emission of left- and right-circularly polarized light from chiral substances. Organic and metal-complex CPL materials are limited by low stability, but inorganic phosphors offer greater durability. We investigated $\text{LaBSi}_x\text{Ge}_{1-x}\text{O}_5$ (LBSGO), which have chiral crystal structures and a glass forming ability. Applying thermal process for LBSGO solution yields non-selective crystallization of left- and right-handed crystals. X-ray diffraction is performed to determine the handedness of the precipitated crystals. CPL measurements are done to examine the relationship between the crystal structure and optical property. We also develop crystallization with selective handedness using an optical vortex laser with orbital angular momentum.

GOMD S1 S4 - AIMD/ML potentials

Room: SaltSpring AB

Session Chairs: Alfonso Pedone, University of Modena and Reggio Emilia; Jincheng Du, University of North Texas

9:30 AM

(GOMD-S1-S4-012-2025) Ab Initio Molecular Dynamics Study of Trivalent Rare Earth Rich Borate Glasses (Invited)

T. Ohkubo^{*1}

1. Chiba University, Faculty of Engineering, Japan

Trivalent rare earth (RE)-rich borate glasses, such as $30\text{La}_2\text{O}_3-70\text{B}_2\text{O}_3$, $50\text{La}_2\text{O}_3-50\text{B}_2\text{O}_3$, $60\text{La}_2\text{O}_3-40\text{B}_2\text{O}_3$, and $50\text{Y}_2\text{O}_3-50\text{B}_2\text{O}_3$, were modeled using ab initio molecular dynamics (AIMD) simulations through the melt-quenching process. The resulting structures contained isolated borate units (monomers, dimers, trimers) terminated with non-bridging oxygen atoms. Polymeric units with four

or more boron atoms were also identified, some containing three-membered boron rings (Brings). Increasing La_2O_3 content led to more isolated units, indicating La_{3+} ions act as network modifiers. These units form through polymer reactions without Brings. The RE coordination environment was analyzed and compared to LaBO_3 and YBO_3 crystal structures. Notably, Y_{3+} in YBO_3 exhibited unique coordination with Brings, absent in RE borate glasses. This study provides insights into RE-rich borate glasses and coordination environments of heavy elements in glass matrices.

10:00 AM

(GOMD-S1-S4-013-2025) Structural features of glasses through first-principles molecular dynamics: meeting the million-atom challenge

C. Massobrio*¹

1. Laboratoire des Sciences de l'Ingenieur de l'Informatique et de l'Imagerie, France

In the area of disordered systems, first-principles molecular dynamics (FPMD) has proved to be an essential theoretical tool to predict and describe structural properties by accounting (in most cases within density functional theory) for the subtleties of chemical bonding. However, the predictive power of FPMD is somehow criticized and even refuted on the grounds that affordable system sizes are too small and time trajectories are too short. While these statements cannot be totally dismissed, it remains true that the advantages of using FPMD to obtain quantitative information directly comparable with experiments largely compensate its intrinsic limits. This talk will focus on recent FPMD results on glassy systems (mostly ionic-covalent) by pointing out both the most relevant successes in terms of agreement with measurable properties and some significant shortcomings. The use of FPMD as a database for building up well performing machine-learning interatomic potentials will be highlighted, thereby allowing to make predictions on million-atom disordered systems.

10:20 AM

(GOMD-S1-S4-014-2025) Million-atom models of amorphous silicon simulated using machine-learned interatomic potentials

S. Elliott*¹

1. University of Oxford, United Kingdom

Amorphous silicon (a-Si) is one of the simplest and most studied of non-crystalline materials and has many applications, e.g. solar cells, thin-film transistors etc. Its atomic structure has been studied using many experimental techniques (diffraction, NMR etc), and by computer simulation, including bond-switching and reverse-Monte Carlo fitting of experimental data. Perhaps the best method to simulate glass models is to use 'cook-and-querch' molecular-dynamics (MD) simulations, e.g. using empirical interatomic potentials or density-functional theory (DFT) calculations. However, the former are inaccurate; and, although the latter are reasonably quantum-accurate, they are cubic-scaling with system size ($O(N^3)$), limiting model sizes to <1000 atoms. Recently, machine-learned (ML) interatomic potentials have been developed, fitted to a training set of DFT potential-energy surfaces for a large number of different structural configurations; they are both DFT-accurate and also linear-scaling ($O(N)$). In this talk, I will describe results of structural analyses of ML MD simulations of models of a-Si, extending up to a million atoms. In particular, because the model sizes are so large, one can study, for the first time, rare events, such as the occurrence of three distinct types of low-concentration five-fold coordinated ('floating-bond') defects, as well as their clustering behaviour.

10:40 AM

(GOMD-S1-S4-015-2025) Li diffusion in oxygen-chlorine mixed anion borosilicate glasses using a machine-learning simulation

S. Urata*¹

1. AGC Inc., Innovative Technology Laboratories, Japan

Lithium-ion conducting borate glasses are suitable for solid-state batteries as an interfacial material between a crystalline electrolyte and an electrode, thanks to their superior formability. Chlorine has been known to improve the electron conductivity of borate glasses as a secondary anion. To examine the impact of chlorine on lithium dynamics, molecular dynamics (MD) simulations were performed with a machine-learning interatomic potential (MLIP). The accuracy of the MLIP in modeling chlorine-doped lithium borate (LBCL) and borosilicate (LBSCI) glasses was verified by comparing with available experimental data on density, neutron diffraction, and glass transition temperatures. The LBCL and LBSCI glass models exhibited increased lithium ion diffusion, and the ions were found to travel longer distance with an increase in chlorine content. According to the structural analyses, it was observed that chlorine ions primarily interacted with lithium ions rather than the network formers. Consequently, lithium ions that interacted with a higher amount of chlorine showed a moderate increase in mobility.

11:00 AM

(GOMD-S1-S4-016-2025) Computational study of oxy-thiophosphate glassy solid electrolytes for sodium-based batteries in the framework of the Ecosister project

M. Bertani*¹; A. Pedone¹

1. University of Modena and Reggio Emilia, Italy

The growing demand for energy storage is driving research for battery materials with high performance, safe and ecological synthesis, usage, and disposal. All-Solid-State-Batteries (ASSB) are gaining increasing attention as promising alternatives. Still, they require highly conductive, yet electrochemically stable Solid-State Electrolytes (SSE). Among them, Glassy Solid Electrolytes (GSE) are receiving growing interest because of their low-cost manufacturing and chemical stability. The lithium extraction from mines comes with ethical issues and the supply chain could face a shortage soon. Sodium-based batteries are possible alternatives, but a huge effort is needed in the study of suitable SSE. Most of the GSEs are based on sulfide glasses whose usage is hampered by the reactivity of these materials with atmospheric compounds. An alternative is the mixed oxy-sulfide (MOS) glasses that can maintain the conductivity of the pure sulfide GSE with higher stability. In this study, we trained Machine Learning interatomic potentials from ab-initio calculations to study the structure of a series of MOS glasses. We correlated the presence of structural units to the conduction mechanisms to help develop new MOS compositions. This project is funded under the PNRR Miss. 4, Comp. 2, Inv. 1.5, NextGenerationEU-Avviso 3277/2021 – ECS_00000033-ECOSISTER-spk06.

11:20 AM

(GOMD-S1-S4-017-2025) Developing Machine Learning Potentials for Local Structure Analysis of Multicomponent Glasses

T. Nishiyama*¹; A. Tanaka¹; A. Saito¹; T. Murata¹

1. Nippon Electric Glass, Research Division, Japan

Predicting the properties of industrial multicomponent glasses from their local structures is challenging. Accurate understanding requires both experimental and computational methods, but no well-established method exists. This study aims to overcome these limitations by understanding local structures from an atomistic computational perspective. We are working on establishing a method to generate machine learning potentials for arbitrary compositions, using calcium aluminosilicate as a benchmark. The training dataset is computed by density functional theory. Atomic environments are

encoded using polynomial structural features, built from group-theoretical rotational invariants. The potential energy surface is inferred with linear ridge regression, which is effective due to its low computational cost, allowing hyperparameter optimization. A major challenge is data generation, as molecular dynamics calculations often result in biased atomic structure distributions. In this study, we generate diverse datasets from different crystal prototype structures and validate the applicability of the machine learning potential through detailed property evaluations.

11:40 PM

(GOMD-S1-S4-019-2025) New generalized classical force-field for superionic chalcogenide-like materials

L. Poitras^{*1}; M. Micoulaut¹

1. Sorbonne Universite, Physics, France

A Buckingham-type empirical force field has been formulated for both glassy and crystalline chalcogenides. This model incorporates fractional charges, short-range repulsive interactions, long-range attractive dispersion, and harmonic interactions. The parametrization process relies on a least-squares minimization of numerical data against crystallographic benchmarks from crystalline phases, further refined by optimizing numerical scattering functions to align with experimental counterparts for glassy systems. The resulting force field exhibits remarkable consistency with experimental observations. Additionally, detailed analyses uncover structural characteristics commonly associated with silicates, such as the progressive depolymerization of the base network, enhanced ionic conductivity with ionic addition, the distribution of Qn species, and the disintegration of ring structures.

GOMD S1 S8 - Chalcogenide glasses and amorphous materials

Room: Cortes

Session Chairs: Pierre Lucas, University of Arizona;

Changgui Lin, Laboratory of Infrared Materials and Devices

9:20 AM

(GOMD-S1-S8-001-2025) Advanced Chalcogenide Glasses and Their Applications in Multifunctional Sensing (Invited)

S. Kang^{*1}; C. Lin²

1. Ningbo University, Laboratory of Infrared Materials and Devices, China
2. Laboratory of Infrared Materials and Devices, Research Institute of Advanced Technology, Ningbo University, China

Chalcogenide glasses are receiving increasing attention in infrared sensing because of their wide transmission range, low transmission loss, and excellent shaping ability. Besides the superior optical properties, chalcogenide glass also possesses good thermoelectric properties, including high Seebeck coefficient and low thermal conductivity, which is promising for temperature sensing application. Here I would like to present a brief report concerning the recent advances of novel chalcogenide glasses and their applications in multifunctional sensing.

9:50 AM

(GOMD-S1-S8-002-2025) Chalcogenide exposed core fiber made by additive manufacturing - Application to Mid-IR spectroscopy (Invited)

J. Troles^{*1}; R. Cheneviere¹; S. Coudray¹; L. Szymczyk²; A. Gautier¹; T. Jouan¹; C. Boussard-Pledel¹; F. Charpentier²; Y. Guimond²; G. Renversez²; F. Cheviré¹

1. University of Rennes, France
2. UMICORE IR Glass, France
3. Aix-Marseille Universite, France

Chemical bonds of most of the molecules vibrate at a frequency corresponding to the near or mid infrared field. It is thus of a great interest to develop sensitive and portable devices for the detection of specific chemicals and biomolecules for various applications in health, the

environment, national security and so on. Chalcogenide glasses are known for their transparency in the infrared optical range and their ability to be drawn as fibers. Such optical fibers can transmit light from 2 to 12 μm depending on the composition of the glass constituting the fiber. They are consequently good candidates to be used in biological/chemical sensing. In this context, an exposed core chalcogenide fiber has been elaborated. This design consists of an optical fiber with a suspended micron-scale core that is partially exposed to the external environment. In this work the preform used for drawing the fiber has been fabricated an original 3D printing way. Indeed, the preform was realized by fused filament deposition. The optical quality of the fibers and the different designs obtained during the drawing will be presented and discussed. Preliminary studies of fiber evanescent wave spectroscopy measurements will be also presented.

10:20 AM

(GOMD-S1-S8-003-2025) Atomistic simulations of the crystallization kinetics of $\text{Ge}_2\text{Sb}_2\text{Te}_5$ in confined geometries

D. Acharya¹; O. Abou El Kheir¹; S. Marcorini¹; M. Bernasconi^{*1}

1. Universita degli Studi di Milano-Bicocca, Materials Science, Italy

Phase change alloys are among the most promising materials for the realization of artificial neurons and synapses for neuromorphic computing. In a recent experimental work, it was proposed that a superlattice (SL) geometry made of alternating layers of the phase change material Sb_2Te_3 and thermally stable confining layers of TiTe_2 would exhibit superior properties for neuromorphic computing. However, Sb_2Te_3 suffers from insufficient data retention due to its low crystallization temperature T_x . Substituting Sb_2Te_3 with a phase change compound with a higher T_x , such as $\text{Ge}_2\text{Sb}_2\text{Te}_5$ (GST), seems an interesting option in this respect. Nanoconfinement might, however, alters the crystallization kinetics with respect to the bulk. In this contribution, we will discuss the results of molecular dynamics simulations of the crystallization process of GST nanoconfined in geometries mimicking GST/ TiTe_2 SLs by exploiting a machine-learned interatomic potentials that we recently devised. The simulations reveal that nanoconfinement induces a mild reduction in the crystal growth velocities which would not hinder the application of SL in neuromorphic devices. The fragility of the supercooled liquid in the bulk and in confined geometry will also be discussed.

10:40 AM

(GOMD-S1-S8-004-2025) Sensing devices based on chalcogenide glasses / silicon platform

W. Zhang^{*1}

1. Ningbo University, China

Chalcogenide glasses (ChGs) are widely recognized as the material of choice for integrated photonics due to their broad transparency window, large linear and nonlinear refractive indices, low two-photon absorption and negligible free carrier absorption. Here we introduce high-quality waveguide and microring resonator sensing devices, based on $\text{Ge}_{28}\text{Sb}_{12}\text{Se}_{60}$ ChGs. Slot Bragg grating and slot waveguide microring resonator sensors, manufactured by electron beam lithography and inductively coupled plasma etching, which confine the effective mode in the low index slot region, could increase the interaction between the effective mode and the analyte, and improve the sensitivity of the sensor. The obtained chalcogenide SBG has a minimum feature size of 150 nm, which makes it easier to manufacture than silicon Bragg grating devices. Measurement results show a high sensitivity of 325 nm/RIU, compared to the conventional evanescent field waveguide sensor in the sensing experiment. Meanwhile, the chalcogenide slot waveguide microring resonator has achieved a quality factor of 1×10^4 , one of the highest quality factors reported for chalcogenide slot microring resonators. The sensitivity of the sensor is measured to be 471 nm/RIU, which leads to an intrinsic limit of detection of 3.3×10^{-4} RIU. This work illustrates the feasibility of Ge-Sb-Se glasses as materials for integrated photonics especially for sensing applications.

11:00 AM

(GOMD-S1-S8-005-2025) Glasses in the $\text{Ga}_2\text{S}_3 - \text{La}_2\text{S}_3$ Pseudo-Binary Prepared by Mechano-Chemical MillingD. P. Bayko^{*1}; P. Lucas¹

1. University of Arizona, USA

Lanthanide-based chalcogenide glasses has been investigated over several decades for their various optical properties and high rare-earth solubility. In particular, the Ga-La-S system permits to achieve high rare-earth content while also maintaining high chemical durability as well as exceptionally high glass transition temperatures. However, difficulties in synthesis arise due to the strong reactivity of La_2S_3 , which readily reacts with silica and other oxides. Therefore, a means of synthesizing glasses in the $\text{Ga}_2\text{S}_3 - \text{La}_2\text{S}_3$ via mechano-chemical milling has been explored. Glasses in the composition range between $x = 55-80 \times \text{Ga}_2\text{S}_3 - (1-x) \text{La}_2\text{S}_3$ were produced and characterized. Furthermore, considerations of mechano-chemical synthesis such as milling time and speed are investigated, as careful parameterization is needed to ensure chemical synthesis without overmilling. Additionally, analysis of crystalline compounds in the region was performed to evaluate reported phase compositions in the pseudo-binary as well as crystalline content of the milled materials. The results provide an alternative synthesis pathway to produce high-temperature infrared transparent glasses.

11:20 AM

(GOMD-S1-S8-006-2025) Chalcogenide glass solid state electrolyte and interface modificationC. Gao^{*1}; C. Lin²

1. Ningbo University, China

2. Laboratory of Infrared Materials and Devices, Research Institute of Advanced Technology, Ningbo University, China

Compared with commercial lithium-ion battery, the chalcogenide glass solid-state electrolytes are not only compatible with high-capacity lithium metal anode to improve the energy density of the battery, but also non-toxic, harmless and non-combustible itself. However, the stability of chalcogenide glass solid-state electrolytes is poor, which not only releases highly toxic H_2S gas when contacting air, but also causes interfacial side reactions when contacting electrode materials, which greatly affects the assembly cost and cycling life of solid-state batteries. In this study, the chemical and electrochemical stability of the electrolyte is regulated by the mixed glass network effect and component doping optimization. At the same time, for the interface between the electrolyte and electrodes, which is difficult to be directly detected, it is proposed to use dynamic in-situ electrochemical impedance method combined with non-in-situ testing techniques (XPS, Raman, etc.) to carefully monitor the evolution of the components and the structure of the interface, which provides an important foundation for the design and preparation of highly stable chalcogenide glass solid state electrolytes, and is conducive to promoting the development of long-cycle-life, high-security, low-cost solid state batteries.

11:40 AM

(GOMD-S1-S8-007-2025) Solution-Processed Chalcogenide Glass towards Functional Flexibility and IntegrationL. Tan^{*1}; C. Lin¹

1. Ningbo University, China

Rare-earth doped chalcogenide films are major components in flexible and integrated photonic and optoelectronic devices for modern communication systems, technology, and optical sensing. However, it is still challenging to develop a high concentration of rare-earth doping chalcogenide film with a smooth surface to realize efficient photoluminescence (PL). Here, we demonstrate that Er^{3+} -doped GeS_2 films are prepared by spin-coating based on a two-step dissolution process. Such a two-step process provides the high solubility of Er^{3+} in GeS_2 films and exhibits efficient emission at $\sim 1.5 \mu\text{m}$

crossing the telecommunication C-band. The highest PL emission intensity is obtained in GeS_2 films doped with 1.4 mol% of Er^{3+} , and this PL in GeS_2 films is reported for the first time. We propose adjustments of annealing parameters for improving the PL characteristics in such materials. Through the control precision of the heating rate and annealing temperature, the smooth surface of GeS_2 films enables efficient photo-luminescence. This two-step dissolution-based strategy would pave a new path to design luminescent chalcogenide films for application in flexible and integrated optoelectronics and photonics.

GOMD S2 - Glass and interactions with its environment - Fundamentals and applications**GOMD S2 S2 - Glass Surfaces and Functional Coatings**

Room: SaltSpring C

Session Chairs: Joy Banerjee, Corning Incorporated; Nicholas Smith, Corning Incorporated

9:20 AM

(GOMD-S2-S2-001-2025) Functional Glass Surface (Invited)P. Mazumder^{*1}; W. Senaratne¹; A. Mezzadrelli²; J. Chillon²; I. Karadzhov²; C. Graham²; V. Pruneri²

1. Corning Research and Development Corporation, USA

2. ICFO-Institut de Ciències Fotòniques, Spain

We live in the Glass Age, thanks to the pace of glass innovation and its role in our daily lives spanning a range of industries such as consumer electronics, telecommunications, architecture, and transportation, to name a few. While we are inundated with news related to advances in cutting-edge technologies involving technical glass including displays, smart windows, wearables, and many others, such advancements owe a great deal to the progress of surface and interfacial technologies. Glass surface thus offers an exciting playground for functional chemistry as well as micro-nanoengineering. In Corning, for many years, our team has explored various technologies, broadly along two routes - surface chemistry and nano-engineering - to achieve special functional properties (wetting, adhesion, optics, chemical reactivity, tribology, biocidal, etc.). In this talk, we will give a broad overview of our work and highlight a few select cases, for example, durable, broadband, omnidirectional, anti-reflection and self-cleaning glass nanostructures; ultrathin metal films (UTMF) as tunable infrared reflectors and plasmonic resonant structures; scalable dewetted nanometallic particles as antimicrobial agents; surface chemistry and coating for tuning adhesion with polymers and metals; and mechanical deactivation of bacteria on nanostructured surfaces with optimal hydrophobicity/oleophilicity.

9:50 AM

(GOMD-S2-S2-002-2025) Surface chemistry, water adsorption, and electrostatic charging of display glass panelS. H. Kim^{*1}

1. Pennsylvania State University, Chemical Engineering & Materials Science, USA

Surface chemistry of glass is a complex function of not only the elemental composition but also the treatment history. This talk epitomizes such complexities by analyzing subtle changes in surface chemistry and their impacts on water adsorption/desorption properties as well as electrostatic charging/discharging behaviors of a display glass panel. The study employed aqueous solutions with different pHs to immerse the glass samples for 1 min and then characterized them immediately after quick drying using various spectroscopic techniques. The results show that the surface-free

energy and overall elemental composition of the glass surfaces were insensitive to the exposure to different pH values. However, the oxygen speciation at the topmost surface was altered, and the water structure and desorption rate also varied among the samples rinsed with different pH solutions. Interestingly, it was found that the DI water treated surface appeared to discharge more slowly than the pH 1 or pH 13 solution treated surfaces, which correlated with the temporal change of water structure. Overall, this study provides important insights into the fundamental questions regarding the impact of surface preparation methods on various surface properties and what characterization techniques are sensitive to the chemistry change in the topmost layer.

10:10 AM

(GOMD-S2-S2-003-2025) Electrical characterization of glass surfaces via Kelvin Probe Force Microscopy (KPFM) analysis

G. Agnello*¹; D. Thelen¹; A. Antony¹; A. Nayyar²; J. Liu²

1. Corning Incorporated, USA
2. University at Buffalo, USA

Tribocharging of insulating surfaces and its characterization have historically been very challenging to quantify and understand. The Kelvin Probe Force Microscopy (KPFM) technique has been successfully utilized to investigate contact charge accumulation and dissipation in metallic and semiconducting materials, but it has not yet been adapted for the study of glasses. Here, we report results from new (KPFM) studies on the electrostatic charging behavior of glass surfaces by sliding a nanosized silicon-based atomic force microscopy (AFM) tip on sample surfaces and mapping the surface potential distribution. Using the developed methodology, our results show that the surface potential difference of the alkali-containing glass samples does not have a strong sample thickness dependence. Here, the observed trends of surface potential difference have been studied to determine whether the behavior can be explained by glass material properties such as relative permittivity.

10:30 AM

(GOMD-S2-S2-004-2025) Positron annihilation spectroscopy to probe surfaces of glassy materials

J. Bussey*¹; M. Weber¹; N. J. Smith²; C. V. Cushman²; J. McCloy¹

1. Washington State University, USA
2. Corning Incorporated, USA

Positron annihilation spectroscopy (PAS; Doppler broadening, DBPAS, or lifetime spectroscopy, PALS) relies on photon generation from positron-electron annihilations to study defects and free-volume. A variable energy beam enables the identification and assessment of vacancies as a function of depth. Doppler broadening of the annihilation line carries information about the annihilation site. A discussion is presented regarding the benefits of using PAS to probe near surface layers in glasses. Results are presented using PAS to probe aqueous alteration layers on the second International Simple Glass from vapor hydration. The presence of ortho-positronium indicate a gel layer of increasing depth with longer alteration time. These depths are compared with x-ray imaging. In addition, the use of PAS to interrogate layers formed by thermal poling and to detect changes in free volume during physical aging will be discussed.

10:50 AM

(GOMD-S2-S2-005-2025) Probing Surface Reactions on Multicomponent Glass using Reflection-Absorption Infrared Spectroscopy

M. Link*¹; Y. Lin¹; J. Banerjee²; N. J. Smith²; A. L. Ogrinc¹; Y. Guo¹; Y. Li¹; S. Yoo³; K. Oh³; J. Choi³; S. H. Kim⁴

1. The Pennsylvania State University, Chemical Engineering, USA
2. Corning Incorporated, USA
3. Korea Institute of Science and Technology, Republic of Korea
4. Pennsylvania State University, Chemical Engineering & Materials Science, USA

The chemical stability of silicate glasses is one of the key attributes of thin cover glass found in electronic devices. During the manufacturing, transportation, storage, and usage of such panels, their surfaces are exposed to various chemicals and environmental conditions and thus, the glass surface inevitably forms chemical defects that diminish this key attribute. Studies investigating these chemical interactions primarily used elemental analysis techniques, and—although such characterization methods provide insight on compositional changes—molecule-specific chemical reactions are not determined unambiguously. Thus, this study demonstrates the use of reflection-absorption infrared spectroscopy (RAIRS) as a technique to detect molecular species on monolithic silicate glass surfaces where acetic acid vapor was used as a model reactant to probe the reaction sites at the surface with or without aqueous pre-treatments of varied pH. With the assistance of theoretical calculations of spectral changes based on bulk complex refractive indices, it was possible to identify the molecular species removed from and produced at the glass surface. Although the reactivity of the glass surfaces with acetic acid was found to be insensitive to the pH of pre-treatment, the results of this study demonstrate the capability of RAIRS to deepen the current understanding of glass surface science.

11:10 AM

(GOMD-S2-S2-006-2025) Oxynitride Thin Films for Glass Surface Modification (Invited)

S. Ali*¹

1. Linnaeus University, Department of Built Environment and Energy Technology, Sweden

Oxynitride thin films in the M-Si-O-N systems (where M = alkaline-earth or rare-earth elements) are gaining attention due to their exceptional optical, mechanical, and chemical properties, which can be tailored by adjusting their composition. These films were deposited using RF magnetron co-sputtering from M and Si targets in an Ar/N₂/O₂ gas mixture on substrates such as soda-lime silicate float glass, silica wafers, and sapphire. The films were characterized using X-ray photoelectron spectroscopy, scanning electron microscopy, nanoindentation, and spectroscopic ellipsometry to investigate their properties. The composition was primarily controlled by the power applied to the M target and the reactive gas flow, which influenced N and M cation incorporation. Some films achieved nitrogen and cation concentrations exceeding 60%, a composition rarely observed in bulk M-Si-(Al)-O-N glasses. The films were homogeneous, transparent in the visible region, and showed refractive indices from 1.5 to 2.01 at 633 nm. Hardness values (up to 22 GPa) and reduced elastic modulus (120–210 GPa) were strongly correlated with nitrogen content and cation concentration. These films show potential for advanced applications in optical coatings, protective layers, and glass surface modifications. This presentation compares M-Si-O-N thin films with conventional bulk M-Si-(Al)-O-N glasses, highlighting their advantages for industrial applications.

GOMD S3 - Optical and electronic materials and devices - Fundamentals and applications

GOMD S3 S1 - Optical and electronic materials and devices - Fundamentals and applications

Room: Saturna Island Ballroom

Session Chairs: Casey Schwarz, Ursinus College; Rashi Sharma, University of Central Florida

9:20 AM

(GOMD-S3-S1-001-2025) Laser Ionization Time of Flight Mass Spectrometry Studies of Oxide Glasses (Invited)

M. Affatigato*¹

1. Coe College, Physics, USA

We report on our work on determining the short- and intermediate-range structure of glasses using laser ionization time-of-flight mass spectrometry. Gentle removal of structural units is possible using low-power ultraviolet (266 nm) light pulses, leading to desorption (and not higher-power ablation). Through the use of the isotopic resolution of the instrument, the precise mass of all molecular units—positive- and negatively charged—can be measured. This process allows for the identification of all molecular species present, and the relative abundance of each group can be determined. This report will cover our insights on traditional glassformers like lead silicates, lead borates, bismuth borates, and sodium-doped lead borosilicates. Less traditional families like the vanadates show similarities with the silicate structure. Significant differences also exist between families, such as the borates and the silicates. Other insights can also be derived from glasses containing rare-earth dopants, non-traditional networks like the aluminate family, and glasses containing mixed glassformers. Other characterization techniques—like Raman spectroscopy—were used to contrast their results with those of the LITOF-MS spectrometer. Work supported by the United States National Science Foundation under DMR-PECASE 9733724, DMR 05020518, DMR-0904615, DMR-1262315, DMR 1407404, and DMR-1746230.

9:50 AM

(GOMD-S3-S1-002-2025) Spatial Fidelity of Laser-Written Three-Dimensional Glass Structures and their Optical Functionalization (Invited)

M. Kang*¹; B. Triplett²; M. Shalaginov³; M. Truman⁴; E. Shirshneva-Vashchenko⁵; T. Karnik³; C. Schwarz⁴; M. C. Richardson⁵; A. M. Agarwal¹; C. R. Baleine²; J. Hu³; T. Gu³; K. Richardson⁵

1. Alfred University, USA
2. Lockheed Martin Corporation, USA
3. Massachusetts Institute of Technology, USA
4. Ursinus College, USA
5. University of Central Florida, USA

This talk introduces the first ever combined optical design - material processing - test methodology approach for realizing conformally patterned programmable large area infrared diffractive layers. Details of this first-time effort presented in this presentation will be of broad interest to the optics and optical materials community as the results expose new opportunities that will enhance and extend optical design paradigms with new flexibility for hybrid diffractive-refractive aberration-corrected imaging platforms. We present a versatile and scalable laser-based photo-chemical process to spatially tailor the geometry of micro-gratings within As_2S_3 films and employed a combined computational-experimental approach to functionalize resulting structures for broadband infrared diffraction optical elements (DOEs). The flexibility of the novel photo-chemical process and resulting optical functionality of the created DOEs provides a glimpse into our vision for thin surface-written grating-based

optical components that rival the performance of traditional bulky optics. Furthermore, our spatially programmable photo-chemical process is expected to enable a wide variety of surface structures to be conformally realized on arbitrarily shaped platforms, thereby making our approach an ideal candidate for many broadband optical applications.

10:20 AM

(GOMD-S3-S1-003-2025) The nature of the interface between fs laser formed single crystal and surrounding glass

R. W. Antonio*¹; C. O'Shaughnessy²; V. Dierolf³; H. Jain⁴

1. Lehigh University, Materials Science & Engineering, USA
2. Corning Incorporated, USA
3. Lehigh University, Physics, USA
4. Lehigh University, International Materials Institute for New Functionality in Glass, USA

Femtosecond laser heating allows for controlled single crystal growth deep inside a glass. Such laser-fabricated architectures provide model interfaces towards understanding the interactions between the crystal and glass phases. This is beneficial in the development of glass-ceramics where the crystal and glass interfaces play a key role in the mechanical and optical properties. We have investigated the structure and chemical distribution on either side of this interface using X-ray diffraction and X-ray absorption spectroscopy at National Synchrotron Light Source II, as well as transmission electron microscopy and electron energy loss spectroscopy on lanthanum borogermanate. This is a congruently crystallizing system with stoichiometry maintained between the glass-crystal transition, and will give insights towards more complicated systems. For example, lithium niobosilicate, which is crystallized to form lithium niobate, and does not contain the added silica. The effects of stoichiometry and crystallization mechanism on the interface will be discussed in the presentation.

10:50 AM

(GOMD-S3-S1-004-2025) Development of solution processing protocols for optical phase change materials (Invited)

R. Sharma*¹; D. Wiedeman²; E. Bissell²; G. Mullapudi²; P. Banerjee²; C. Schwarz²; B. Mills⁴; J. Hu³; K. Richardson⁵

1. University of Central Florida, College of Optics and Photonics, USA
2. University of Central Florida, Material Science and Engineering, USA
3. Ursinus College, Physics & Astronomy, USA
4. Massachusetts Institute of Technology, Materials Science and Engineering, USA
5. Massachusetts Institute of Technology, USA
6. University of Central Florida, CREOL, USA

Chalcogenide-based optical phase change materials play a crucial role in the development of optical and photonic devices for future technologies. Solution processing methods, such as drop-casting, offer a cost-effective and high-throughput approach for depositing thin films, enabling greater diversity in material compositions. In this study, we systematically investigated chalcogenide alloys in a solution mixture containing amine, thiol, and thioglycolic acid. The focus of this work is to identify key factors for selecting an optimal solution mixture to create a stable chalcogenide ink suitable for drop-casting into films. We analyzed the composition, morphology, and structural properties of the films using scanning electron microscopy, energy dispersive X-ray spectroscopy, Raman spectroscopy, and X-ray diffraction. Additionally, we present initial evidence supporting the viability of this solution processing approach for synthesizing and depositing O-PCM films.

11:20 AM

(GOMD-S3-S1-005-2025) Probing the Mechanisms of Ge Nanoparticle Formation in Glass Induced by Femtosecond Laser Irradiation

A. Tsekrekas^{*}; H. Jain¹; V. Dierolf²; S. Garner²

1. Lehigh University, Institute for Functional Materials and Devices, USA
2. Corning Research and Development Corporation, USA

Femtosecond laser irradiation enables precise, spatially resolved modifications within the bulk of oxide glasses, providing a versatile platform for developing 3D photonic integrated circuits (PICs). In the $\text{La}_2\text{O}_3\text{-B}_2\text{O}_3\text{-GeO}_2$ (LBG) glass system, these modifications can yield either single crystal LaBGeO_5 or Ge nanoparticles (NPs), depending on the laser and processing conditions. While the mechanisms underlying the crystallization of LaBGeO_5 are well established, the pathways leading to Ge NP formation remain poorly understood. The high intensity of femtosecond laser irradiation can cause numerous processes, potentially including oxygen bubble formation, color center generation, structural defects, and glass network rearrangement, all of which may drive the reduction of Ge ions for nanoparticle formation. To elucidate these mechanisms, characterization techniques such as Raman spectroscopy, electron energy loss spectroscopy (EELS), and UV-Vis spectroscopy have been conducted. These techniques can unravel the specific interactions responsible for Ge NP formation, establishing a direct correlation between femtosecond laser parameters and nanoparticle synthesis. Understanding these processes will contribute to the fabrication of nanoparticles in LBG glass and other glass systems.

GOMD S7 - Emerging frontiers - Glasses in new technology

GOMD S7 - Emerging frontiers - Glasses in new technology II

Room: Moresby

Session Chairs: Madoka Ono, Hokkaido University; Collin Wilkinson, Alfred University

9:20 AM

(GOMD-S7-004-2025) Advancements in Long-Haul Communication Fibers: A Detailed Discussion on Silica Core and its Comparisons with HCF and MCF (Invited)

S. Goyal^{*1}

1. Corning Incorporated, USA

The presentation will primarily focus on Silica Core fibers, their importance in the historical and current context of telecommunication systems, and their evolving role in the face of emerging technologies. While Silica Core fibers have been the bedrock of long-distance data transmission for years, the advent of Multicore(MCF) and Hollow Core Fibers (HCF) has added new contenders to the field. Despite this, the pervasiveness and existing ecosystem of Silica Core fibers continue to hold significant relevance. This talk will provide an in-depth analysis of Silica Core fibers, their inherent strengths, and challenges, while also briefly comparing these features with those of Multicore and HCF technologies

9:50 AM

(GOMD-S7-005-2025) Nanocrystal-doped Silica Optical Fibers: a Step Towards a New Generation of Optical Fibers (Invited)

V. Fuertes de la Llave^{*1}; J. Fernandez Lozano¹; S. LaRochelle²; Y. Messaddeq²

1. Consejo Superior de Investigaciones Científicas, The institute of ceramics and glass, Spain
2. Université Laval, Centre for Optics, Photonics and Lasers (COPL), Canada

Silica optical fibers are a well-established technology for a wide range of applications, such as fiber lasers or distributed optical fiber sensors (DOFS). Although silica glasses present excellent properties, they

have also certain limitations that restrict their use. One of the most promising approaches to solve this problem is their engineering by nanoparticle doping, which simultaneously incorporate new functionalities that are determined by the nanoparticle features. Despite the promising future of this technology, it is still in an early stage and has been limited to few suitable spherical nanoparticle compositions. This is partly due to the high temperatures of manufacture, >2000 °C, which modify the initial nanoparticle features or directly cause their dissolution. In this talk, we demonstrate by different advanced material characterization techniques the possibility of doping silica optical fibers fabricated by MCVD with nanostructures that remain stable after the optical fiber drawing process, apart from spherical nanoparticles, such as rod-shaped and cubic-shaped nanocrystals. Their application for DOFS based on Rayleigh scattering enhancement is also shown. In this presentation, we discuss the challenges and future prospects of nanoparticle-doped optical fibers towards the incorporation of unprecedented shape-dependent functionalities for DOFS and fiber laser applications.

10:20 AM

(GOMD-S7-006-2025) Optical nanofibers for cavity quantum electrodynamics (Invited)

T. Aoki^{*1}

1. Waseda Daigaku, Japan

A cavity quantum electrodynamics (QED) system, where atoms are coupled to light confined in an optical cavity, provides an ideal platform for studying the dynamics of atom-light interactions. In the strong coupling regime of cavity QED, where the rate of coherent energy exchange between the atom and the cavity exceeds the dissipation rates (such as spontaneous emission from the atom and leakage of light from the cavity), the system's coherent nature can be preserved throughout its dynamics. Conventionally, experimental studies in cavity QED have been conducted using free-space cavities with bulk mirrors. In this talk, we will present our approach to using optical nanofibers for cavity QED experiments and their potential applications in quantum computing and quantum networks.

Thursday, May 8, 2025

GOMD Award Lectures

Darshana and Arun Varshneya Frontiers of Glass Lectures - Glass Technology Award

Room: Saturna Island Ballroom

Session Chairs: Collin Wilkinson, Alfred University;

Madoka Ono, Hokkaido University

8:05 AM

(GOMD-Awards-004-2025) Glass for a Sustainable Future

J. C. Mauro^{*1}

1. Pennsylvania State University, Materials Science & Engineering, USA

Glass has proven to be a critically important material for the development of contemporary human civilization. Its influence continues to grow as new glass products and processes are developed to address global challenges in energy, the environment, healthcare, information technology, and more. Despite recent advances in glass science and technology, major challenges remain with respect to the sustainability of the glass industry, which generates more than 86 million tons of carbon dioxide annually. In this presentation, I will describe my own personal journey in glass from Alfred, New York to Happy Valley, Pennsylvania. After reviewing some recent advances in glass physics and chemistry, we'll peer into our glass (not "crystal") ball to discuss future glass technologies for a more sustainable future. The latter part of the presentation will introduce LionGlass, Penn State's

patent-pending glass compositional family that offers, for the first time, an alternative to standard soda lime silicate glass for reducing the carbon footprint of the glass industry by ~50%. LionGlass achieves this goal by lowering the melting temperature of everyday glass products by 400°C and eliminating the use of carbonate batch materials. LionGlass also offers 10× improvement in damage resistance compared to soda lime silicate, enabling the lightweighting of everyday glass products.

Darshana and Arun Varshneya Frontiers of Glass

Lectures - Glass Science Award

Room: Saturna Island Ballroom

Session Chairs: Collin Wilkinson, Alfred University;

Madoka Ono, Hokkaido University

9:05 AM

(GOMD-Awards-005-2025) What use is a really bad glass?

S. Elliott*¹

1. University of Cambridge, Chemistry, United Kingdom

In conventional glass science and technology, the thermal stability of a glass is often of primary importance. What then, rather counter-intuitively, might be the technological applications, if any, of glasses exhibiting extremely bad thermal-stability characteristics, i.e. with exceedingly fast crystallization kinetics? In this lecture, I will discuss such glassy materials, principally tellurides alloyed with metalloid elements, such as germanium or antimony, which exhibit crystallization times of a few nanoseconds. In other words, these must be among the worst possible glass formers from a thermal-stability viewpoint. However, the fact that such materials have large opto-electronic property contrasts between metastable crystal (electrically-conducting 'SET' state, {1}) and glass (electrically-resistive 'RESET' state, {0}) means that they can form the basis of new non-volatile electronic (or optical) solid-state memory devices – so-called 'phase-change memory' (PCM). Binary bits of information {0,1} are stored as the structural state of the memory material, rather than as electrons trapped at the floating gate in conventional silicon CMOS flash-memory devices. I will discuss our recent million-atom, device-scale computer simulations of SET and RESET processes in Ge-Sb-Te PCMs using machine-learned interatomic potentials with density-functional-theory (DFT) levels of accuracy.

GOMD S1 - Fundamentals of the glassy state

GOMD S1 S2 Glass Crystallization and Glass-Ceramics III

Room: Pender

Session Chair: Maria Rita Cicconi, FAU - Friedrich-Alexander-Universität Erlangen-Nürnberg

10:20 AM

(GOMD-S1-S2-012-2025) Enhanced upconversion luminescence from oxyfluoride glass ceramic microspheres utilizing rapid crystallization under rapid cooling

K. Shinozaki*¹; Y. Kitagawa¹

1. Sangyo Gijutsu Sogo Kenkyujo Kansai Center, Japan

Glass-ceramics can impart excellent optical functions to the formability and transparency of glass. Recently, our group reported fast fluoride nanocrystal precipitation by designing glass structures similar to crystals. Using this technique, we have also succeeded in synthesizing transparent nanocrystallized glass in a rapid cooling process. In this work, we extend this process to the synthesis of microspheres by developing upconversion glass with precipitated

Er-dope NaYF₄ nanocrystals, which are then laser-melted into microspheres by surface tension. The upconversion luminescence intensity was successfully enhanced more than 20 times by optical confinement and resonance. The mechanism of rapid nucleation and similarity of glass and crystal structure is also investigated.

10:40 AM

(GOMD-S1-S2-013-2025) The crystallization behaviors and mechanical performance evolutions of alkali earth modified Li₂O-Al₂O₃-SiO₂ glass

J. Zhang*¹; C. Zheng¹; J. Xie¹

1. Wuhan University of Technology, China

Alkali earth oxides were introduced into Li₂O-Al₂O₃-SiO₂ glass components. The dependency of alkali earth oxide contents and ratios on the glass structure, crystallization phases and mechanical performance were investigated. With MgO addition into glass components, the glasses show increased glass transition and first crystallization temperatures due to tighter structures. After heat treatment, the main crystal phases change from Li₂SiO₅ and LiAlSi₄O₁₀, to the combination of LiAlSi₂O₆ and MgAl₂Si₄O₁₂, and finally to MgAl₂Si₄O₁₂. The Vicker's hardness of glasses ceramics are highly dependent on MgO/Li₂O ratios in glass components and heat treatment temperatures. CaO was also introduced into glass, the non-linear glass hardness with maximum deviation from end numbers indicates the mixed alkaline earth effect in Li₂O-Al₂O₃-SiO₂ glass. MgAl₂Si₄O₁₂ and SiO₂ crystals were precipitated in Li₂O-MgO-Al₂O₃-SiO₂ glass matrix, and changed to the combination of MgAl₂Si₄O₁₂, LiAlSi₃O₈, and SiO₂, to LiAlSi₃O₈, SiO₂, to LiAlSi₃O₈, SiO₂, ZrSiO₄, and finally to Li₂O-Al₂O₃-7.5SiO₂, SiO₂, ZrSiO₄, due to the changed ion radius and contents, with the increased CaO/(MgO+CaO) ratios. The hardness and Young's modulus of glass ceramics increase at first, from 8.30 to maximum 8.67 GPa, and from 74.00 to 84.20 GPa, with 0.2 CaO/(MgO+CaO) ratio and then dropped.

11:00 AM

(GOMD-S1-S2-014-2025) Simulation of seeded crystal growth with multiple seeds: effects of seed misorientation, separation and crystal growth temperature

R. Thapa*¹; M. E. McKenzie²; V. Dierolf³; H. Jain⁴

1. Lehigh University, Material Science and Engineering, USA
2. Corning Incorporated, Science & Technology, USA
3. Lehigh University, Physics, USA
4. Lehigh University, International Materials Institute for New Functionality in Glass, USA

The growth of lithium niobate crystals in glass, initiated from two preexisting crystal seeds, has been investigated using molecular dynamics simulations. Key parameters explored in the study include seed separation, relative misorientation, and crystal growth temperature. The cation-anion interactions were modeled using the Buckingham potential with a repulsive correction at short separations, combined with long-range Coulomb interactions. A melt-quench approach was used to generate glass models containing 500,000 atoms, with portions of the system fixed as crystalline seeds while the rest equilibrated to high-temperature melt conditions. The system was then annealed at elevated temperatures following a controlled temperature cycle to study the evolution of seed size, the characteristics of the growing crystals, and the changes in the surrounding glass network. Detailed atomistic analyses were conducted to examine the nature of the crystals formed under various parameter combinations and the characteristics of grain boundaries separating them.

11:20 AM

(GOMD-S1-S2-015-2025) SiO₂-rich glasses from the system CaO-Al₂O₃-SiO₂ - Crystallization behavior and thermal stability of beta-cristobalite

C. Thieme^{*1}; K. Thieme¹; S. Selle¹; L. Ortmann²; R. Hahn²; S. Begand³

1. Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS, Germany
2. Qsil GmbH Quarzschmelze Ilmenau, Germany
3. Fraunhofer-Institut für Keramische Technologien und Systeme IKTS - Standort Hermsdorf, Germany

Heating glasses with high SiO₂-concentrations often leads to cristobalite crystallization. During cooling, a phase transition occurs running parallel to a decrease in volume, which deteriorates materials properties. The addition of different oxides to the glasses allows the suppression of this phase transition. Respective materials, which contain solely β-cristobalite, are suitable as thermal shock resistant refractories. An effective way of stabilization is the addition of CaO and Al₂O₃ to the glasses. Such materials can be synthesized from liquid precursors (sol-gel) or with extreme temperatures using arc melting. Both attempts were used to prepare a variety of different compositions within the ternary system. Glasses with higher concentrations of Al₂O₃ and CaO show the formation of a residual phase surrounding the crystals, which can be crystalline or amorphous. Within this paper, the processes leading to the stabilization of β-cristobalite down to room temperature are discussed in terms of micro- and nanostructural analyses. The stability of β-cristobalite depends on the composition of the starting glass and on the heat-treatment, especially on the maximum temperature applied. The results are compared with X-ray diffraction and dilatometry and will give a deeper understanding into the mechanisms of the stabilization of β-cristobalite.

GOMD S1 S4 - Structures-property relation

Room: Saltspring AB

Session Chairs: Jincheng Du, University of North Texas; Shingo Urata, AGC Inc.

10:20 AM

(GOMD-S1-S4-022-2025) Computational study on an anomalous density change between crystalline β-Eucryptite and its glass phase

K. Umemoto^{*1}; S. Nakane²

1. Nippon Electric Glass, Fundamental Technology Division, Japan
2. Nippon Electric Glass, Japan

β-Eucryptite (LiAlSiO₄) is one of important materials as an ingredient of glass ceramics, because of very low volume thermal expansion coefficient over a wide temperature range and negative thermal expansion along the c axis. In addition, it should be noted that the density of the crystalline β-Eucryptite is smaller than that of the glass with the same composition: Li₂O-Al₂O₃-2SiO₂. This density behavior is anomalous, since crystalline phases in usual materials have higher density than their glassy counterparts. In order to design new materials based on LAS glass ceramics, it is fundamental to understand the reason why the anomalous density behavior occurs. In this study, we perform molecular dynamics studies by both first principles and model potentials on β-Eucryptite, another crystalline phase α-Eucryptite, and the glass phase with the same composition. We computationally confirm the density (ρ) relationship: ρ(β-Eucryptite) < ρ(glass) < ρ(α-Eucryptite). Analysis on radial distribution functions and coordination numbers shows that intermediate-range (3~4Å) structures correspond to the anomalous density change.

10:40 AM

(GOMD-S1-S4-023-2025) Criticality of Amorphous-Amorphous Transitions in Compressed Silica Glasses

J. Perradin^{*1}; S. Ispas¹; A. Hasmy¹; B. Hehlen¹

1. University of Montpellier, Lab. Charles Coulomb, France

To investigate the structural mechanisms underlying plastic behaviour and polyamorphism in silica glasses (v-SiO₂), we conducted Molecular Dynamics (MD) simulations using various computational approaches. A recent Density Functional Tight-Binding study demonstrated that structural transformations between LDA and HDA states in v-SiO₂ occur via percolation transitions, which can also explain certain mechanical properties of v-SiO₂. To further study clusters and percolation networks, we used the classical MD simulation approach, which allowed a significant improvement in statistics and access to larger length scales (up to 12 nm). The percolation transitions were successfully reproduced, and clusters spanning several orders of magnitude enabled the extraction of scaling laws for properties like mass, correlation length, and order parameter. The scaling of these properties is linked to critical exponents and the fractal dimensionality of clusters, defining the universality class of the transition. Our analysis of the SiO_n-SiO_m connectivities (n,m=4,5,6) reveals a single universality class and provides a framework to detect amorphous-amorphous transformations upon compression. We have extended this work by simulating liquid SiO₂ to track the evolution of the transitions with temperature and pressure, potentially allowing us to construct a metastable “phase” diagram for v-SiO₂.

11:00 AM

(GOMD-S1-S4-024-2025) Medium-Range Order Structure of Alkali Silicate Glasses

A. Fadavi Firooz^{*1}; R. Christensen¹; C. Biscic²; M. M. Smedskjaer¹

1. Aalborg Universitet, Department of Chemistry and Bioscience, Denmark
2. Aalborg Universitet, Department of Mathematical Sciences, Denmark

Several key questions regarding oxide glasses' medium-range order (MRO) structure remain unresolved. This study analyzes the MRO structure of alkali silicate glasses using both persistent homology and traditional ring analysis. While traditional analysis identifies only chemically bonded rings, persistent homology captures both chemically and non-chemically bonded ring structures. Our analyses rely on atomic configurations obtained through classical molecular dynamics simulations of lithium, sodium, and potassium silicate glasses with varying modifier content. First, we examine the size and shape of chemically bonded rings using persistent homology and investigate their role in contributing to the first sharp diffraction peak (FSDP) of the structure factor. We also show that covalently bonded loops can be directly identified using persistent homology by disregarding the modifiers in the analysis and setting the initial radii for Si and O atoms to zero. Next, we establish that, although chemically bonded rings contribute to the FSDP—particularly at lower modifier contents—considering the nonbonded MRO features is also crucial for a complete understanding of the FSDP.

11:20 AM

(GOMD-S1-S4-025-2025) Atomistic Simulations of Lithium Ion Exchanged Glass

S. Chowdhury^{*1}; S. Goyal¹; C. O'Shaughnessy¹; J. Harris¹; C. Smith¹

1. Corning Incorporated, USA

Ion exchange is an effective and widely used chemical process to strengthen glass products. Smaller ions replaced with larger ions during ion exchange induces compressive stress at the surface of glass articles which suppresses crack propagation and enhances mechanical properties and performances. Since this ion exchange is an atomic length scale phenomenon, it is a challenge to understand the mechanisms through experiments. Molecular dynamics (MD) method is a

good tool to characterize materials at atomistic length scale. In this work, MD simulations are used to study the effects of ion exchange on the structure-property relationships in a lithium aluminosilicate glass. Glass structure is prepared with melt-quench process and smaller lithium ions are replaced with larger sodium ions through atom swapping followed by high temperature thermal annealing to mimic experimental ion-exchange process. The effects of ion exchange on structural changes are quantified with packing density, molar volume, coordination number etc. and the corresponding effects on network dilation coefficient and Young's modulus are examined. Several interatomic force fields such as Pedone, SHIK, Buckingham, and machine learning are explored.

11:40 PM

(GOMD-S1-S4-026-2025) Understanding the Role of Fracture Pathways on the Mechanics of Glasses

V. D. Maksimov^{*1}; A. Potter³; C. Wilkinson²

1. Alfred University, Inamori School of Engineering, USA
2. Alfred University, Glass Science, USA
3. New York State College of Ceramics at Alfred University, Glass Science and Engineering, USA

Conventional linear elastic fracture mechanics (LEFM) assumes that the critical energy release rate (G_c) is a material property, universally dictating fracture propagation. However, this interpretation often oversimplifies the complexities of fracture behavior in brittle materials. This study introduces an algorithm that predicts possible fracture pathways based on input material structures and interatomic potentials, challenging the conventional understanding of G_c . Results demonstrate that G_c varies significantly depending on the crack propagation pathway, establishing it as a path-dependent property rather than an intrinsic material constant. This work highlights the existence of multiple fracture pathways with distinct G_c values under identical loading conditions, revealing the nuanced interplay between material structure, applied stress, and fracture energetics. The developed software enables precise calculations of the elastic contribution to G_c , offering a robust tool for advancing fracture mechanics in brittle materials.

GOMD S1 S7 - Glass under non-ambient conditions I

Room: Moresby

Session Chair: Lawrence Gammond, Corning Incorporated

10:20 AM

(GOMD-S1-S7-001-2025) Structural properties of MgO-SiO₂ liquid and glasses (Invited)

Y. Shuseki^{*1}

1. Kyoto Daigaku, Japan

The MgO-SiO₂ system is important in both glass science and geo science, because MgO-SiO₂ glass is a binary silicate glass system and enstatite (crystalline (c-) MgSiO₃) and forsterite (c-Mg₂SiO₄) are main components of mantle of the earth. Understanding of the structure of both glass and high temperature liquid of MgSiO₃ (high glass forming ability (GFA)) and Mg₂SiO₄ (low GFA) makes it possible to understand the origin of glass formation and magma ocean solidification. The status of density/viscosity measurements at the International Space Station, quantum beam diffraction measurements at SPring-8 and Oak Ridge National Laboratory will be reported and results of DFT-MD simulations will be discussed.

10:50 AM

(GOMD-S1-S7-002-2025) Hot and steamy: The corrosion of transition metal phosphates in steam (Invited)

C. O'Shaughnessy^{*1}; K. T. Hufziger²; N. Stone-Weiss³

1. Corning Incorporated, Inorganic Materials, USA
2. Corning Incorporated, Characterization Science, USA
3. Corning Incorporated, Science and Technology, USA

Phosphate glasses are a favorable host for the incorporation of transition, heavy, and rare-earth metals. Their optical and electrical properties are of particular interest for a wide variety of technological applications, ranging from thermochromic materials to energy storage devices. The main drawback to the adoption of these glasses stems from their poor chemical durability. It is believed that the asymmetry of the [PO₄] tetrahedron is at the origin of their corrosion. A classic 85/85 durability test comprises of using a humidity chamber held at 85 °C and 85% RH for a prolonged period of time. Increasing the pressure and temperature of the steam creates a hostile environment which accelerates and amplifies the alteration at the glass surface. We will be discussing a series of experiments on a suite of ternary transition metal phosphates which have been exposed to a variety of steam conditions. The structure of the pristine glasses and resulting surface alteration after steam exposure have been characterized using Raman and NMR spectroscopy. We will offer some new insight in the debate concerning the hydration and network breakdown reactions which are said to dominate the dissolution of phosphate glasses in aqueous systems.

11:20 AM

(GOMD-S1-S7-003-2025) Effect of physical and chemical pressure onto glasses

M. Ono^{*1}

1. Tohoku Daigaku, Applied Physics, Japan

Hot compression is known to be effective in reducing optical loss in silica glass. In this study, we investigate how the properties of silica glass change under high pressure by using physical pressurization through a hot isostatic pressing (HIP) machine with gas media. As a comparison, we recently discovered that chemical pressurization can be achieved by depositing silica glass onto crystalline substrates. In this presentation, we will explain how both physical and chemical pressurization alter the structure of silica glass and affect its optical, thermal, and mechanical properties.

11:40 AM

(GOMD-S1-S7-004-2025) High Pressure Viscosity of Silica glasses

A. Sarafian^{*1}

1. Corning Incorporated, USA

Viscosity is a critical material property for understanding mass transport and relaxation phenomena. This work uses a falling sphere method at high pressure, >1GPa, using a multi-anvil apparatus to determine the high temperature viscosity of fused SiO₂ glass. Our results are compared to other high silica glasses.

GOMD S2 - Glass and interactions with its environment - Fundamentals and applications

GOMD S2 S2 - Glass Dissolution and Interfacial Reactions I

Room: Saltspring C

Session Chairs: Stephane Gin, CEA; Seong Hyeon Kim, Kongju National University

10:20 AM

(GOMD-S2-S2-008-2025) Incorporating Textual Information for Accurate Prediction of Glass Dissolution (Invited)

N. Krishnan^{*1}

1. Indian Institute of Technology Delhi, Civil Engineering, India

In this study, we compiled a large dataset of over ~2000 glasses from published literature, including composition pH and temperature values. We integrated Machine Learning (ML) with physical and chemical descriptors to develop a universal descriptor-based ML model (DML) for predicting the dissolution rates of any glass composition. However, the DML model demonstrated inadequate accuracy when applied to unseen glass compositions. To enhance the predictive capabilities of the DML model, we incorporated additional variables, including testing and processing conditions alongside composition, pH, and temperature. By employing Natural Language Processing (NLP) techniques, we converted textual data from the literature into numeric features, leading to the development of a new descriptor-based ML model (NLP-DML). Our findings reveal that the NLP-DML model significantly outperforms the DML model in predicting the complex dissolution rate property. Furthermore, we conducted an analysis of the NLP-DML model to elucidate the underlying mechanisms and dependencies of input features on the glass dissolution rate. This understanding can potentially accelerate the discovery of novel glass compositions with tailored properties for sustainable nuclear waste management.

10:50 AM

(GOMD-S2-S2-009-2025) Revisiting the concentration dependent diffusion coefficient (Invited)

A. L. Ogrinc^{*1}; A. Borhan¹; S. H. Kim²

1. Pennsylvania State University, Chemical Engineering, USA
2. Pennsylvania State University, Chemical Engineering & Materials Science, USA

The Doremus model of interdiffusion is a landmark model which has seen widespread use over the last 50 years. It was derived by assuming steady state and utilized a concentration dependent diffusion coefficient to account for structural changes in the glass due to swelling from the ingress of water. In this work, we propose two new models to explain the corrosion behavior of glass in aqueous solutions, which fit for systems with and without the formation of a gel layer. These models are based on the same underlying convection-diffusion equations as originally formulated by Lanford et al., but require neither of the assumptions listed above to fit with experimental data. The model is then used to understand the leaching of sodium from soda lime silica glass into a pH 1 solution that was pre-saturated with NaCl, which provides new insight into the driving force for aqueous corrosion of silicate glass.

11:20 AM

(GOMD-S2-S2-010-2025) Room-temperature aging of bottle glass in solutions of moderate acidity

A. Potter^{*1}; R. J. Pao²; G. Gaustad³; C. Wilkinson⁴

1. New York State College of Ceramics at Alfred University, Glass Science and Engineering, USA
2. Alfred University, Inamori School of Engineering, USA
3. NYS College of Ceramics, Alfred University, Inamori School of Engineering, USA
4. Alfred University, Glass Science, USA

Rising costs of labor and fuel in the United States coupled with rapidly dwindling landfill capacity have driven increased interest in reducing the amount of discarded glass entering the waste stream. For glass packaging, reuse schemes are some of the most effective methods of reducing energy consumption and carbon footprint, many of which are already in place around the world. However, for markets sensitive to impurity, such as the New York State wine industry, organic molecules lodged in the porous aged glass surface create a residual scent. This forms a major technical barrier to the implementation of glass packaging reuse in these markets. To determine the cost and technical feasibility of removing this layer during cleaning, this study used a new infrared spectroscopic technique alongside secondary ion mass spectrometry to compare wine bottles aged from 0.3 to 7.6 years, for dry Riesling wines of similar pH sourced from wineries in the Finger Lakes region of New York State. Alteration layer depths were compared with etch rates predicted for various cleaning temperatures and soap compositions, supporting the feasibility of bottle reuse efforts.

11:40 AM

(GOMD-S2-S2-011-2025) Effects of Weathering on the Failure Characteristics of Ion Exchanged Glasses

R. Grodsky^{*1}; R. Brow¹; J. Kim²; T. Stone²; J. Fenton³

1. Missouri S&T, Materials Sci & Engrg, USA
2. National Nuclear Security Administration Kansas City National Security Campus, Mod/Sim, USA
3. National Nuclear Security Administration Kansas City National Security Campus, Analytical Sciences, USA

The widespread application of ion exchanged (IEX) glass in a variety of environments could result in degradation of the glass surface. Developing a mechanistic understanding of water induced structural changes and their effects on mechanical properties is important to prevent this from happening. Novel techniques were utilized to correlate glass failure with changes in the glass surface chemistry. These included the use of computer vision methods to study the failure characteristics of IEX glasses and characterizing changes in surface chemistry using several techniques including Auger electron spectroscopy and Raman spectroscopy. An FEA simulation was used to assess the potential failure mechanisms and was correlated with ring-on-ring failure strength measurements.

GOMD S3 - Optical and electronic materials and devices - Fundamentals and applications

GOMD S3 S3 - Optical fibers and waveguides, optoelectronic glass-based devices II

Room: Cortes

Session Chairs: Johann Troles, University of Rennes 1;
Thomas Meyneng, Universite Laval

10:20 AM

(GOMD-S3-S3-011-2025) Toward a low-cost SERS probe by ion-exchanged processed optical fibers

D. Kaur^{*1}; D. Farnesi¹; M. De Angelis¹; C. D'Andrea¹; N. G. Boetti¹;
D. Janner¹; G. Nunzi Conti¹; S. Berneschi¹; S. Pelli¹

1. Istituto di fisica applicata Nello Carrara Consiglio Nazionale delle Ricerche, Italy

Ion-exchange process has attracted continue and growing attention as suitable technique in many application fields, from Integrated Optics to glass strengthening up to the enhancement of light source and photovoltaic cell performances. In addition, this method is used in Plasmonic due to the possibility to induce the formation of metal nanoparticles (i.e.: silver nanoparticles, Ag NPs) in the glass matrix by an ad hoc thermal post-process. In the present work, the use of this low-cost procedure for the realisation of a fibre optic probe for SERS applications is reported. As a first step, the ability of ion – exchanged soda-lime glass microrods to work as active SERS substrates is demonstrated. Therefore, from this result, one can move on to the next step: a piece of a multimode optical fibre, loaded at its end with a thin layer of the same soda-lime glass, is potentially able to work - in backscattering - as a SERS probe when Ag NPs are exposed on the same layer by a suitable ion-exchange process. These results pave the way towards the development of low-cost fibre optic SERS probe, alternative to those realised by sophisticated and expensive lithographic processes, for sensing/biosensing applications.

10:40 AM

(GOMD-S3-S3-013-2025) The Effects of BaO on the Thermal, Structural and Optical Properties of Bismuth-Gallo-Germanate Glasses

H. Camici^{*1}; T. Guérineau¹; S. LaRochelle¹; Y. Messaddeq¹

1. Université Laval, Centre d'optique, photonique et laser, Canada

Heavy metal oxide (HMO) glasses have attracted significant interest due to their excellent infrared transmission, high refractive index, rare-earth ion solubility, and low phonon energy compared to SiO₂-based glasses. Among these, GeO₂-based glasses are particularly notable for their higher glass transition temperature, superior thermal stability, and better mechanical strength compared to tellurite glasses. Bi₂O₃-GeO₂ glasses have emerged as promising alternatives to PbO-GeO₂ glasses to reduce lead usage due to its toxicity. In this study, bismuth-gallo-germanate glasses are explored as a strong candidate within the HMO glass family. The effects of BaO on the thermal, structural, and optical properties of these glasses were systematically investigated. Differential scanning calorimetry (DSC) confirmed their outstanding thermal stability, while thermomechanical analysis (TMA) showed low thermal expansion coefficient (CTE). Low phonon energy of these glasses was verified by Raman spectroscopy. Optical characterizations revealed a high refractive index (≈ 2) and low linear absorption coefficients, supporting a broad transmission window extending up to 6 μm . Their excellent thermal stability, combined with superior optical properties, positions bismuth-gallo-germanate glasses as ideal materials for optical fiber fabrication and other photonic applications.

GOMD S5 - Glass manufacturing

GOMD S5 S1 - Manufacturing VI

Room: Saturna Island Ballroom

Session Chairs: Luiz Pereira, Université de Munich (LMU);
Katelyn Kirchner, CelSian

10:20 AM

(GOMD-S5-S1-025-2025) A generic physical model for an accurate prediction of the viscosity of multicomponent glasses

R. Conradt^{*1}

1. uniglassAC GmbH, Germany

The viscosity temperature relation is a key property of a glass forming system. The available calculation schemes for multicomponent glasses are typically based on the statistical evaluation of a large number of experiments and on oxide specific increments derived from them. But these schemes badly fail outside of narrow compositional bounds. In the present contribution, a generic approach to the viscosity of glass forming multicomponent systems is presented. In a first step, the constitutional relations of the isochemical equilibrium system are determined. Entropies of melting and heat capacities of the individual constitutional corner compounds are superimposed to approach the fragility slope of a given composition. The position of T_g is determined by the temperature where the cP curve reaches the Dulong-Petit value of 3R per g-atom, and the high-T limit of viscosity is obtained from Frenkel's approach by the hopping distance bringing about a positional change at the atomic scale. Predictions based on this generic approach yield accurate predictions of viscosity levels better than ± 7 K.

10:40 AM

(GOMD-S5-S1-026-2025) Viscosity and structure of transition metal oxide containing silicate melts (Invited)

S. Sukenaga^{*1}; R. Uchida⁴; I. Takahashi⁴; Y. Onodera²; K. Shinoda¹;
D. Neuville³; H. Shibata¹

1. Tohoku University, Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Japan
2. National Institute for Materials Science, Japan
3. Institut de Physique du Globe de Paris, France
4. Tohoku University, Graduate School of Engineering, Japan

Transition metal oxides are important constituents of silicate melts, which are used in high-temperature industries and formed by natural processes. The viscosity of the transition metal oxides containing melts should be essential to understand the high-temperature phenomena. Previous studies demonstrated that the melt viscosity drastically changes with the addition of transition metal oxides (e.g., Fe₂O₃); however, the viscosities have been scarcely correlated with their oxidation state or local structure near the transition metal cations. The present study shows the effect of the oxidation state of iron and titanium on the viscosity of silicate melts in the range of 10⁻¹–10¹² Pa s. The viscosity of alkali or alkaline-earth iron silicate melts increased with the increasing ratio of Fe³⁺ to total iron. This behavior indicates that Fe³⁺ cations act as a network former, whereas Fe²⁺ cations act as a role of modifier. This tendency is consistent with the structural characterization of the local structure near iron cations using Raman, X-ray absorption spectroscopy, and synchrotron X-ray total scattering. In addition, the viscosity and structure of the titanium oxide-containing system will be presented.

11:10 AM

(GOMD-S5-S1-027-2025) Pressure Dependence of Viscosity of Geological Melts: A Review & Way Forward (Invited)

J. K. Russell^{*1}; K. Hess²; A. Anzulovic³; D. B. Dingwell²

1. University of British Columbia, Earth, Ocean and Atmospheric Sciences, Canada
2. Ludwig-Maximilians-Universität München, Earth and Environmental Sciences, Germany
3. Universitetet i Oslo, Norway

Terrestrial magmatism produces a diverse array of silicate melt compositions comprising 8-10 oxides plus volatile species (H₂O, CO₂). Extensive high-temperature (T) experimentation has elucidated, and allowed for modelling of, melt viscosity as a function of composition (X) and T. Our knowledge of the effects of pressure (P) on the viscosity of geological melts is significantly less due to the sparse experimental database. These melts exhibit complex P-effects including positive or negative, and linear or non-linear P-dependence. Here we review the experimental database for silicate melts and summarize the apparent effects of P. We also summarize the emerging data and insights from molecular dynamic (MD) simulations on the P-dependence of viscosity for geological melts. We then address these questions. Is the P-dependence of terrestrial silicate melts important for answering geoscience questions? If so, for which melt compositions and at what P's are these effects critical? Can we feasibly produce enough data for accurate modelling of viscosity given the technical challenges and inherent uncertainties in measuring melt viscosity at high-P. We suggest that, although there are difficulties involved in comparing experimentally obtained viscosities with MD values, merging the data and insights from these two fields may prove a way forward for the next generation of T-X-P models for melt viscosity.

GOMD S1 - Fundamentals of the glassy state

GOMD S1 S1 - Glass Formation and Structural Relaxation

Room: Cortes

Session Chairs: Katelyn Kirchner, CelSian; Roger Loucks, Alfred University

1:15 PM

(GOMD-S1-S1-001-2025) Connecting mechanical properties of glasses to their topological defects (Invited)

W. Kob^{*1}; Z. Wu²; J. Barrat³

1. University of Montpellier, France
2. Beijing Normal University, China
3. Université Grenoble Alpes, France

Recent studies indicate far-reaching connections between the topological characteristics of structural glasses and their material properties. In this talk I will discuss different possibilities how such defects can be defined, and the pros and cons of the various definitions. Using a particular definition and large scale computer simulations of a prototypical glass-former, I will show that these defects are not distributed uniformly in the glass sample but instead form surprisingly regular patterns. Furthermore it is found that the locations at which the density of these topological defects is high, the sample is likely to yield when sheared, a result which establishes a connection between topological defects and the yielding of the glass sample.

1:45 PM

(GOMD-S1-S1-002-2025) Trends in dynamical heterogeneity in Supercooled Liquids (Invited)

S. Sen^{*1}

1. University of California, Davis, Department of Material Science and Engineering, USA

While the atomistic origin of a stretched exponential relaxation kinetics in supercooled liquids remains a highly debated topic in the literature, it is well-established that the stretching results from a spatio-temporally heterogeneous relaxation with a distribution of relaxation times. The temperature dependence of the stretching exponent β^{shear} for shear relaxation is determined for a wide variety of supercooled strong and fragile liquids using parallel plate rheometry. Contrary to the conventional wisdom, β^{shear} and fragility are observed to be uncorrelated. However, a clear pattern emerges when the variation of β^{shear} is considered as a function of the α -relaxation timescale τ_α . In particular, β^{shear} increases rapidly (slowly) for relatively strong (fragile) liquids with decreasing τ_α upon increasing temperature above T_g . A possible origin of this intriguing trend will be discussed within the frameworks of the energy landscape and the elastic facilitation models of relaxation of supercooled liquids. On the other hand, the stretching exponent β^{hop} for the hopping dynamics of the modifier cations measured by high-temperature NMR spectroscopy is found to be nearly identical to the Haven ratio H for a wide variety of oxide glass-forming liquids. This intriguing equality between β^{hop} and H will be shown to be consistent with the modifier dynamics being controlled by percolation in the energy landscape.

2:15 PM

(GOMD-S1-S1-003-2025) Dynamic Light Scattering in Network-forming Glass Melts (Invited)

D. Sidebottom^{*1}; J. McCown¹; J. Kevill¹; D. Olabode¹; D. White¹

1. Creighton University, Physics, USA

As liquids cool near the glass transition temperature, molecular-level rearrangements slow and viscosity increases. These features are universal to all glass-forming matter, but the rate at which viscosity increases near T_g (known as the fragility) varies tremendously between organic liquids and conventional network-forming oxides. Organic liquids (e.g., glycerol) often exhibit high fragility with a sub-ambient T_g . This makes it convenient to study the dynamics using broadband dielectric spectroscopy. Far less studied are the network-forming oxides (NFOs) for which T_g is well above ambient and the fragility typically lower. Our efforts have focused on the use of photon correlation spectroscopy (PCS) to study these viscous dynamics in high temperature NFO melts. Here, I review some of our efforts to try to connect viscous dynamics with the bonding structure of these networks and I report on recent studies of several "mixed network forming" melts.

2:45 PM

(GOMD-S1-S1-004-2025) On the Origins of Fragility in Sodium Borosilicate Glass and its Influence on Structural Relaxation

A. Bossen^{*1}; J. C. Mauro¹

1. The Pennsylvania State University, Materials Science and Engineering, USA

Angell's concept of fragility (m) has proven invaluable in describing the widely varying behavior of glassforming liquids. However, there remain difficulties in linking this macroscopic property of the liquid to its underlying structure in a systematic way. The Adam-Gibbs (AG) model provides an initial resolution to this issue by connecting viscosity and configurational entropy, but lacks specificity in characterization of the underlying atomic processes driving relaxation. This work seeks to develop a better theoretical description of atomic-scale rearrangements by more rigorously defining a cooperatively rearranging region (CRR). The improved definition is then evaluated through molecular dynamics simulations of sodium borosilicate

(NBS) glass in the isoconfigurational ensemble. The temperature dependence of CRR size is then extracted from MD simulations using dynamic propensity maps and the peak position of the four-point dynamic susceptibility $\chi_4(t)$, which relates back to fragility.

3:30 PM

(GOMD-S1-S1-005-2025) Compositional and temperature dependence of viscosity in model borosilicate-based nuclear waste glasses: An augmented Adam-Gibbs Model Approach

P. Malviya^{*1}; P. Ferkl²; P. Hrma³; A. A. Kruger³; A. Goel¹

1. Rutgers The State University of New Jersey, Material Science and Engineering, USA
2. Pacific Northwest National Laboratory, USA
3. US Department of Energy, USA

This study combines the augmented Adam-Gibbs model with experimental data to investigate the influence of temperature and composition on viscosity, expanding the predictive capability of the model for nuclear waste glasses. The Adam-Gibbs model has predicted viscosity with a promising correlation to literature data for commercial glasses. The predictions demonstrated the influence of constituent oxides on viscosity, suggesting a decrease upon the addition of B₂O₃, Na₂O, CaO, or Li₂O and an increase with ZrO₂, Al₂O₃, or SiO₂. The glass matrix, structured around a centroid composition derived from average HLW and LAW reference compositions, is normalized after excluding minor components. A series of 25 glasses is aimed to be synthesized, encompassing constituent compositional spectrum from the centroid to extreme values, and their viscosities are to be measured using a rotation spindle viscometer, beam bending viscometer, and parallel plate viscometer. This synergistic integration of experimental and modeled data establishes a paradigm for anticipating the response of nuclear waste melters to melt viscosity, aiding in the development of safe and efficient waste immobilization.

3:50 PM

(GOMD-S1-S1-006-2025) Accelerated Low-Temperature Relaxation of Glasses via Thermo-Ultrasonication

L. Tran^{*1}; P. Lynch¹; E. Akirmak-Yamac¹; G. Sop Tagne¹; C. Cano²; P. Marrero³; A. Phillips²; R. Welch¹; D. Wiedeman³; R. Sharma³; K. Richardson³; S. Feller²; W. LaCourse¹; S. Yaniger¹; C. Wilkinson¹; M. Kang¹

1. Alfred University, USA
2. Coe College, USA
3. University of Central Florida, USA

Glasses are characterized by time-dependent relaxation, leading to temporally inconsistent properties. This inconsistency is a substantial issue in the development of optical glasses that require predictive responses to realize highly controlled and uniform optical responses. Such consistency is realized by long period of times at elevated temperature, often presenting issues especially for device fabrication where process time and costs need to be minimized. The process time can be exponentially decreased using a high temperature beyond a glass transition temperature (T_g), but there can be adverse effects associated with excessive viscous flow leading to deformation of the sample. Here, we seek to expedite the relaxation rate using a novel thermo-ultrasonication process. The As₂S₃ chalcogenide glass system is an ideal candidate due to its low T_g and prevalent use as optical materials. The samples were subjected to ultrasonic vibration at an elevated temperature below T_g to accelerate their relaxation. We employ a combined theoretical-experimental approach to study structural and stress glass relaxation via the evolution of refractive index and optical band-edge. By understanding the effects of ultrasonication on glasses, we demonstrate new insights into the nature of relaxation while opening the possibility of developing ultra-stable glasses that can realize optical devices with increased lifespan.

4:10 PM

(GOMD-S1-S1-007-2025) Critical-like slowdown in thermal soft-sphere glasses via energy minimization

R. S. Hoy^{*1}; K. A. Interiano-Alberto¹; P. K. Morse²

1. University of South Florida, Physics, USA
2. Seton Hall University, Physics, USA

Using hybrid molecular dynamics/SWAP Monte Carlo (MD/SMC) simulations, we show that the terminal relaxation times $\tau(\phi)$ for FIRE energy minimization of soft-sphere glasses can decrease by orders of magnitude as sample equilibration proceeds at constant density ϕ and the jamming density ϕ_j slowly increases via “thermal onset”. However, these times always scale as $\tau(\phi) \sim (\phi_j - \phi)^{-2} \sim [Z_{iso} - Z_{ms}(\tau)]^{-2}$, where $Z_{iso} = 2d$ (here d is the spatial dimension) is the average coordination number of marginally-jammed systems and $Z_{ms}(\tau)$ is the average coordination number of particles satisfying a minimal local mechanical stability criterion ($Z \geq d + 1$) at the top of the final potential-energy-landscape (PEL) sub-basin the system encounters during energy minimization. This common scaling allows us to collapse τ datasets that look very different when plotted as a function of ϕ , and to address a closely related question: how does the character of the PEL basins that dense thermal glasses most typically occupy evolve as the glasses age at constant ϕ and T ? We argue that signatures of this aging may be observable in real colloidal and small-molecule glasses’ vibrational spectra.

4:30 PM

(GOMD-S1-S1-008-2025) Revealing the nature of the boson peak using metal-organic framework polymorphs

S. S. Sørensen^{*1}; F. Cao¹; P. Rasmussen¹; J. A. Finkler¹; M. H. Henningsen¹; M. Aouane²; D. Bessas³; J. Bulled³; A. Bossak³; G. Monaco⁴; M. M. Smedskjaer¹

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. ISIS Facility, Rutherford Appleton Laboratory, United Kingdom
3. European Synchrotron Radiation Facility, France
4. University of Padova, Department of Physics and Astronomy ‘Galileo Galilei’, Italy

The boson peak is a vibrational feature observed as an excess of vibrational modes beyond the level expected by the Debye model. This has been showcased in many crystalline and glassy structures of very varying compositions, but its origin remains unclear. Both theoretical and experimental studies suggest that its origin stems from structural disorder, differences in density, and local variations in elasticity, amongst others. However, in most cases, the tested amorphous or glassy polymorphs are less dense than the corresponding crystals, i.e., both density and disorder affect the boson peak intensity and position in a similar manner. To overcome this, we have used inelastic neutron (ISIS) and X-ray scattering (ESRF) to test the boson peak in a metal-organic framework (MOF) system of composition Zn(Imidazolate)₂, as polymorphs with varying density and disorder exist. This includes a very porous and crystalline structure (ZIF-4), which upon heat treatment, first collapses into a high-density amorphous phase (ZIF-HDA) before crystallizing into a structure denser than ZIF-4 (ZIF-zni). Further heating leads to melting and glass formation upon cooling (ZIF-glass). By probing the different polymorphs, we showcase how the boson peak is inherently bound to structural disorder. Our results provide new insights into the nature of boson peak and its correlation with fundamental structural parameters.

GOMD S1 S7 - Glass under non-ambient conditions II

Room: Moresby

Session Chair: Lawrence Gammond, Corning Incorporated

1:15 PM

(GOMD-S1-S7-005-2025) Structure, properties, and chemical strengthening of sodium aluminoborosilicate glasses

L. V. Gammond^{*1}; J. Wu¹

1. Corning Incorporated, USA

B₂O₃ is an important component of many technical glasses, imparting advantageous material properties that facilitate melting, forming, processing, and functionality. However, the inclusion of B₂O₃ in oxide glasses often has a negative impact on the ion exchange processes used to strengthen these materials. In this study, we investigate the structure, properties and chemical strengthening capability of sodium aluminoborosilicate glasses with the compositions (Na₂O)₁₅ (Al₂O₃)₁₅ (B₂O₃)_x (SiO₂)_{70-x} and (Na₂O)₁₅ (Al₂O₃)_{15-x} (B₂O₃)_x (SiO₂)₇₀, where x = 0, 5, 10, and 15. Our results show that boron exists in BO₃ trigonal units or BO₄ tetrahedral units and that knowledge of the speciation between these structural units is crucial for understanding the composition-dependent glass properties. The response of these glasses to a K⁺/Na⁺ ion exchange treatment is strongly dependent on B₂O₃ content, which influences the level of strengthening that can be achieved. Understanding these structure-property-process relationships helps to guide new glass design and highlights the importance of controlling the boron speciation, which can be achieved through e.g. choice of composition, thermal treatments, and high-pressure processing.

1:35 PM

(GOMD-S1-S7-006-2025) Investigation into the impact of pressure-induced densification upon the structure and properties of metaluminous sodium aluminoborosilicate glasses

N. Stone-Weiss^{*4}; S. Kapoor¹; B. Siboczy¹; R. Sun²; F. Lodesani³;

R. Youngman⁴; M. Bockowski⁵; A. Pedone³; L. Huang²; A. Goel¹

1. Rutgers The State University of New Jersey, Materials Science and Engineering, USA
2. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA
3. Università degli Studi di Modena e Reggio Emilia, Department of Chemical and Geological Sciences, Italy
4. Corning Incorporated, Science & Technology Division, USA
5. Instytut Wysokich Cisnien Polskiej Akademii Nauk, Poland

Aluminoborosilicate glasses comprise a large fraction of essential glasses used in both everyday life and for cutting edge-technological applications. These glasses show a wide range of composition-dependent properties which are exploited for applications spanning from ultra-strong cell phone cover glass and thermally resistant glasses to glasses for nuclear waste immobilization. Applying high pressure to glasses near the glass transition has been shown to permanently alter glass structure and properties, where these treatments promote polymorphism in the glass network via densification of the molecular structure. We aim to elucidate the effects that pressure has upon structural transformations in well-connected sodium aluminoborosilicate glasses by utilizing both NMR spectroscopy and MD simulations to quantify short-to-medium range structures of glasses prepared at ambient and 1 GPa pressures. Further, we aim to correlate these structural transformations as a function of glass composition with the mechanical and elastic properties generated for the glasses synthesized at different pressures. Accordingly, we expect to unearth the mechanisms by which well-connected glass networks transform via pressure-based treatments, and in turn, how these changes impact glass performance and characteristics.

GOMD S2 - Glass and interactions with its environment - Fundamentals and applications

GOMD S2 S1 - Glasses, glass-ceramics and glass-based biomaterials

Room: Pender

Session Chairs: Maziar Montazerian, The Pennsylvania State University Department of Materials Science and Engineering; Leena Hupa, Åbo Akademi University

1:15 PM

(GOMD-S2-S1-001-2025) Glass for Healthcare: From Research, Invention to Industrialization (Invited)

Q. Fu^{*1}

1. Corning Incorporated, USA

Bioactive glass, invented in 1960s, was initially targeted for soft tissue or non-loaded hard tissue regeneration. Most recently, research has been conducted to explore their applications in vascularization, wound healing and beyond. To meet the requirements for these emerging applications, glasses in the form of particulates, microspheres, fibers, and porous scaffolds have been developed. However, progress in the commercialization of bioactive glasses have been relatively slow, with the most successful ones being 45S5-based Perioglas[®], Novabone[®] and NovaMin[®]. Exploration and inventions of new glass compositions with a step change in bioactivity and performance are critical to enable new applications. Meanwhile, fundamental understanding of the glass manufacturing attributes, such as melting and forming in an industrial continuous-unit melting system, is important to enable the scale-up and industrialization.

1:45 PM

(GOMD-S2-S1-002-2025) Frontiers of Amorphous Materials: Fabrication of metallic glass thin films, microfibers and bulk systems for biomedical applications (Invited)

E. Sharifikolouei^{*1}; B. Sarac²; E. Yuce³; A. Rezvan³; F. Sourani³; D. Singh³;

A. Calogero Scalia¹; Z. Najmi¹; A. Cochis¹; L. Rimondini¹; J. Eckert³

1. Università degli Studi del Piemonte Orientale Amedeo Avogadro, Health Sciences, Italy
2. ZKW, Austria
3. Erich Schmid Institut für Materialwissenschaft, Austria

Metallic glasses are a revolutionary class of materials where crystallization upon solidification is suppressed, keeping them in a disordered state. Many phenomena such as wear release, or cytocompatibility depend on the surface properties and metallic glasses often have lower surface energies regulating their behavior and their interaction with cells and/or bacteria. We are studying and developing the potential use of metallic glasses as intrinsic antibacterial materials without a need for antibiotic or nanoparticle loading on their surface. In the biomedical field, we have shown that metallic glasses, such as Zr-Cu-Ag thin films, demonstrate ≈95% antibacterial efficiency due to their superhydrophobic surfaces, validated through cytocompatibility studies with human mesenchymal stem cells. In another work, we have shown the potential of bulk Ti-based metallic glasses, free from toxic elements like Cu and Ni, as dental implants showing superior corrosion resistance and significant inhibition of oral biofilm formation compared to conventional Ti-6Al-4V implants. High-resolution characterization techniques, such as HR-TEM and XPS, have further revealed their unique mechanisms, including oxidation resistance, which prevents the formation of hydrophilic oxides associated with bacterial attachment.

2:15 PM

(GOMD-S2-S1-003-2025) The Reaction of Na-Ca-Borophosphate Glasses in Simulated Body Fluids Under Dynamic Flow ConditionsR. L. Blatt^{*1}; R. Brow¹

1. Missouri S&T, Materials Sci & Engrg, USA

Glasses with the nominal molar compositions $20\text{Na}_2\text{O}-20\text{CaO}-x\text{B}_2\text{O}_3-(60-x)\text{P}_2\text{O}_5$ ($0 \leq x \leq 60$) were reacted in simulated body fluid (SBF) at 37°C under continuous flow rate conditions of 1 and 2 mL/hr. Borate and phosphate anions were released to solution, along with sodium and calcium ions, where they reacted to form precipitated calcium phosphate (CP) phases. Inductively coupled plasma optical emission spectroscopy (ICP-OES) was used to characterize the concentration of ions in solution throughout the testing period as well as the final composition of the reacted particles. The glass dissolution rates go through a minimum at $x=20$, with faster reactions occurring under greater flow rates. Reactions with the borate-rich ($x>40$) glass particles initially increased the SBH pH until the glasses were fully dissolved after four days on test. The CP phases that formed on the reacted particles of these more basic glasses were crystalline orthophosphates, hydroxyapatite and brushite, whereas the phases that formed on the more acidic, phosphate-rich ($x \leq 40$) glasses were amorphous calcium phosphates (ACP). Those ACP phases included polyphosphate anions that were released from the glasses, as characterized by high-performance liquid chromatography and Raman spectroscopy. The stability of the ACP phases under these flow conditions will be discussed.

2:35 PM

(GOMD-S2-S1-004-2025) The effect of fluorine on the structure and antibacterial property of CaF_2 -CaO-ZnO- B_2O_3 -SiO₂ glassesJ. Chung^{*1}; m. Hwang¹; J. Kim¹

1. Korea Institute of Ceramic Engineering and Technology, Republic of Korea

This study aims to investigate the effect of fluorine on the antibacterial property in CaF_2 -CaO-ZnO- B_2O_3 -SiO₂ glasses. It was confirmed that the zeta potential of glasses increased and antibacterial property improved with increasing fluorine concentration. The glasses with fluorine showed 99.9% antibacterial activity against *E. coli* and *S. aureus*. The structure of oxyfluoride glasses was analyzed by ²⁹Si and ¹¹B MAS-NMR. It was observed that the amount of non-bridging oxygen decreased with increasing fluorine. Furthermore, as CaF_2 contents were increased, the $[\text{BO}_4]$ ratio increased and the $[\text{BO}_3]$ ratio decreased. We also analyzed the dissolution property of glasses. There was no significant change in the amount of Si^{4+} ions released according to the CaF_2 content. The amount of released Zn^{2+} and Ca^{2+} ions increased with increasing CaF_2 contents. We could conclude that the improvement of antibacterial property of fluorine containing zinc borosilicate glasses was due to the increase of zeta potential and increase of the amount of released Zn^+ ions. We believe that our results will be useful for the analysis of new antimicrobial materials and mechanisms.

2:55 PM

(GOMD-S2-S1-005-2025) Manganese-Doped 85S Mesoporous Bioactive Glasses (MBGs)E. Luna²; M. Fook²; M. Montazerian^{*1}1. The Pennsylvania State University - University Park Campus, USA
2. Universidade Federal de Campina Grande, Brazil

Effective bone regeneration remains a significant challenge in regenerative medicine, particularly for treating large bone defects due to complex fractures, degenerative diseases, and reconstructive surgeries. MBGs have emerged as promising biomaterials because of their ability to promote osteointegration and accelerate bone regeneration. We explored the formulation and characterization of Mn-doped 85S MBG ($85\text{SiO}_2-(15-x)\text{CaO}-x\text{MnO}$ mol%, where $x = 1, 2, 3, 4$). Morphological and structural analyses confirmed the

amorphous and mesoporous structure of the glasses, with an average pore size of 2 nm. Bioactivity was assessed in vitro in simulated body fluid, demonstrating the formation of a hydroxyapatite layer on the scaffold surfaces, as evidenced by X-ray diffraction, Fourier transform infrared spectroscopy, and scanning electron microscopy. The cytotoxicity was evaluated in vitro using the MTT assay, revealing that Mn-doped glasses exhibit no significant cytotoxicity. Antimicrobial and antifungal properties were also tested, resulting in a 100% reduction in bacterial colony-forming units for the 2% Mn, and a 99.70% and 94.09% reduction in fungal activity for the 0% and 1% Mn groups, respectively. These results suggest that both pure (85S) and Mn-doped MBGs hold potential and provide protection against infections.

3:30 PM

(GOMD-S2-S1-006-2025) Preferred Cation-Anion Pairs in Mixed-Cation Sulfate and Sulfophosphate Glasses, as Elucidated by Raman and O-17 SSNMRC. Calahoo^{*1}; P. Zhang²; L. Wondraczek²; J. Zwanziger³; U. Werner-Zwanziger³1. Genics, R&D Glass Division, Canada
2. Friedrich Schiller University, Germany
3. Dalhousie University, Chemistry, Canada

Segregated modifier channels and cation interactions are used to explain the well-studied mixed-modifier effect (MME), a deviation in the physical properties as a function of composition from linearity when two or more unlike modifiers are present in the glass. In the case of ionic glasses, where there are little to no conventional BOs and only anions crosslinked by cations, it is more challenging to define the glass network. Their structure must be dominated by Q^1 -units, such that the glass lacks any 2-d chains. The MME is well studied in phosphate glasses, however, it is possible to synthesize pure sulfate glasses (no conventional network) and high-sulfur containing sulfophosphate glasses with an SP-type structure. The mixed-cation and mixed-former ZnKS, ZnKP, ZnPS, KPS, and ZnKPS glass series were measured and understood in terms of their glass structure, with a focus on ¹⁷O SSNMR. The investigation into these glass samples involves their hygroscopic properties, structural analysis via WDX, XRD, Raman, FTIR, and NMR spectroscopy, and mechanical, thermodynamic, and electrical properties. The synthesis of ¹⁷O-enriched crystalline starting materials K_2SO_4 , ZnSO_4 , KPO_3 , $\text{NH}_4\text{H}_2\text{PO}_4$, and $\text{Zn}_3(\text{PO}_4)_2$ was completed using the conventional enriched H_2^{17}O chemical method.

3:50 PM

(GOMD-S2-S1-007-2025) Structural, luminescent and in vitro studies of europium-doped soda lime phosphate glassesD. Kaur^{*1}; R. Priya²; O. Pandey³; K. Attri³; D. Choudhury³1. Istituto di fisica applicata Nello Carrara Consiglio Nazionale delle Ricerche, Physics, Italy
2. Chandigarh University, Physics, India
3. Thapar Institute of Engineering and Technology (Deemed to be University), School of Chemistry and Biochemistry, India

In this article, we have reported the effect of varying concentration of europium (Eu) in $(50-x)\% \text{P}_2\text{O}_5-25\% \text{Na}_2\text{O}-24\% \text{CaO}-\% \text{Eu}_2\text{O}_3$, where $x = 1, 3, 5$. The glass samples were synthesised via the conventional melt-quench method. The impact of europium ion (Eu^{3+}) on the structural, optical and luminescent properties of phosphate soda lime glasses has been studied using X-ray diffraction (XRD), Fourier-transformed infrared (FTIR) spectroscopy, ultraviolet-visible spectroscopy, scanning electron microscopy coupled with energy-dispersive spectroscopy and photoluminescent techniques. XRD patterns confirmed the amorphous nature of glass samples. FTIR confirmed the presence of various functional groups. The emission spectra of synthesised samples exhibited intense emission peaks corresponding to Eu^{3+} under excitation at 393 nm. The maximum intensity was observed for $^5\text{D}_0 - ^7\text{F}_2$ transition among all the peaks. Furthermore, cytotoxic studies were carried out on normal cell lines of human embryonic kidney cells (HEK-293)

using MTT assay. Results showed that the prepared samples significantly enhanced growth in glass sample-treated cells as compared to control cells. These findings suggest that synthesised glass samples are biocompatible and have potential for applications in display devices and biomedical research areas.

GOMD S2 S2 - Glass Dissolution and Interfacial Reactions II

Room: Saltsping C

Session Chairs: Nicholas Stone-Weiss, Corning Incorporated;
Seong Kim, Pennsylvania State University

1:15 PM

(GOMD-S2-S2-012-2025) Corroded Glass Microstructures: From Historical Perspectives to Modern Insights (Invited)

A. Mir*¹

1. University of Huddersfield, Electron Microscopy and materials Analysis, United Kingdom

Corroded glasses have been studied extensively across fields such as archaeology and nuclear industry. In the nuclear industry, glasses are used for immobilizing radioactive elements, making studies into their corrosion behavior an important aspect of safety case. Under laboratory conditions, glasses exhibit leaching, dissolution, and precipitation, forming microstructures that shed light on fundamental corrosion processes. Studies of naturally corroded, archaeological, and historical glasses—exposed to uncontrolled conditions over extended periods—offer valuable insights that could help validate short-term laboratory experiments. Corroded microstructures thus serve as a unique bridge between archaeology, and nuclear science. The presentation will provide a historical overview of corroded glass microstructures, beginning with Sir David Brewster's 1860s optical microscopy studies, when microstructures were meticulously hand-drawn. It will highlight key contributions by renowned scientists such as Lord Rayleigh and C.V. Raman, who explored phenomena like iridescence and laminae formation, and trace advancements from the mid-20th century to today's nanoscale characterization of simple and complex systems. Finally, the presentation will focus on recent progress in correlative and multi-modal characterization approaches, providing deeper insights into the fundamental processes driving glass corrosion.

1:45 PM

(GOMD-S2-S2-013-2025) Alteration of a borosilicate glass between a few minutes and 27 years - discussion on rate-limiting mechanisms

S. Gin*¹; S. Narayanasamy¹; S. Tiwari¹; J. Delaye¹

1. CEA, DPME/SEME/LEMC, France

In this study, we describe the behavior of CJ2 glass (65SiO_2 , $17\text{B}_2\text{O}_3$, $14\text{Na}_2\text{O}$, $4\text{Al}_2\text{O}_3$) - a simplified version of International Simple Glass - altered for durations ranging from a few minutes to 27 years. The study includes several experiments, all conducted at 90°C and pH 9. The analysis of the solution by ICP-OES, combined with the characterization of the gel at different time points using ToF-SIMS, TEM, TGA, DVS, and SAXS, provide key information to link the glass alteration kinetics to the physical and chemical characteristics of the gel (composition, porosity, pore size, diffusivity). It appears that even for such a simple glass in a simple alteration medium, the mechanisms limiting glass alteration evolve as the reaction progresses. Compared to established knowledge, it appears that gel maturation (evolution of porous network) has a significant impact on long-term alteration rates. To illustrate this phenomenon, other glass compositions altered under the same conditions as CJ2 glass are used. As a whole, this work highlights the important role of B and Al in this maturation process.

2:05 PM

(GOMD-S2-S2-014-2025) Effect of Heavy-Ion Irradiation on Glass Dissolution Rates and Surface Alteration Layer Formation studied by Fluid-Cell Raman Spectroscopy

M. I. Lönartz*¹; L. Stausberg¹; C. Trautmann²; T. Geisler¹

1. Rheinische Friedrich-Wilhelms-Universität Bonn, Geochemistry/Petrology, Germany
2. GSI Helmholtzzentrum für Schwerionenforschung GmbH, Germany

Borosilicate glass is a preferred material for immobilizing high-level nuclear waste due to its compositional flexibility and corrosion resistance in aqueous systems. In a geological repository, the vitrified waste will be exposed to irradiation damage from radionuclides and corrosion from infiltrating groundwater. However, the effect of self-irradiation damage on the structural integrity of the glass and its corrosion behavior is not yet fully understood. For this, borosilicate glass was irradiated with 950 MeV Au ions to induce radiation effects within a layer of $\sim 50\ \mu\text{m}$. Fluid-cell Raman spectroscopic (FCRS) experiments revealed a two to three order of magnitude increase in the initial dissolution rate of the irradiated glass compared to non-irradiated glass, corroded in a 0.5 M NaHCO_3 solution and at temperatures between at $\sim 85^\circ\text{C}$. The thickness of the irradiated layer and the associated depolymerization of the borosilicate network correlated with dissolution kinetics and textural features of the surface alteration layer (SAL), evolving from homogeneous to laminar textures with changes in the effective diffusivity as indicated by D_2O tracer experiments. FCRS provides operando insights into reaction and transport processes, capturing the effect of irradiation damage on the dissolution kinetics and transport properties of the SAL.

2:25 PM

(GOMD-S2-S2-015-2025) Static Dissolution Testing for the Long-Term Performance Evaluation of 24 LAW Glasses

B. Parruzot*¹; J. Neeway¹; S. Kerisit²; J. M. Westman¹; I. Burch¹; J. T. Reiser¹; J. V. Crum¹; G. L. Smith¹; M. Asmussen¹

1. Pacific Northwest National Lab, Energy and Environment Directorate, USA
2. Pacific Northwest National Lab, USA

The understanding of long-term corrosion behavior of glass waste forms and acquisition of long-term static testing data is key for the parameterization of geochemical models used to quantify the glass dissolution and the rate of release of radionuclides from a nuclear waste disposal facility. This presentation will provide updated long-term static dissolution data for 24 high- Na_2O borosilicate nuclear waste glasses (known as the eLAW matrix). These glasses were statistically designed to cover a compositional range relevant to Hanford Low-Activity Waste glasses. Tests were conducted for 1500 to 2000 days at temperatures ranging from 22°C to 90°C at a solution-volume-to-glass-surface-area ratio of $2000\ \text{m}^{-1}$. Certain tests were seeded with a small amount of zeolite Na-P2 to initiate and evaluate Stage III dissolution behavior. The additional data (from previously reported 700 days) will be discussed, including the evolution of the long-term dissolution rates and their temperature dependence and the influence of the addition of zeolite seeds on the long-term rates at lower temperatures (22°C and 40°C). This updated dataset will be discussed in the broader context of the disposal of ILAW glasses in the Hanford Site near-surface Integrated Disposal Facility, a low-level waste and mixed-low-level waste landfill located in Washington State, USA.

2:45 PM

(GOMD-S2-S2-016-2025) Impact of the aluminum coordination on the dissolution kinetics of magnesium aluminoborosilicate glassesA. Jose^{*1}; M. Bertani²; R. Youngman⁷; G. Tricot³; S. Gin⁴; A. Pedone⁵; A. Goel⁶

1. Rutgers University, Material Science and Engineering, USA
2. University of Modena and Reggio Emilia, Department of Chemical and Geological Sciences, Italy
3. Universite de Lille, France
4. CEA, DE2D, France
5. University of Modena and Reggio Emilia, Italy
6. Rutgers University, USA
7. Corning Incorporated, USA

Aluminum is known to exist in four, five, and six coordination in the structure of glasses, where their fraction is governed by the non-frame-work cation-to-alumina ratio and the ionic field strength of the cation. The role of higher-coordinated alumina in the structure of glasses and its impact on their thermo physical properties has been a long-standing point of discussion in the glass community. In this work, we aim to elucidate the effect of aluminum coordination on the dissolution kinetics of magnesium aluminoborosilicate glasses. The melt-quenched glasses have been investigated for their short-to-intermediate range structure via 1D and 2D MAS NMR, and Raman spectroscopy. The dissolution behavior of glasses has been studied at pH = 1 in HCl solution over a period of 3 days followed by the characterization of post-dissolution glasses and liquid aliquots using XRD, MAS NMR spectroscopy, XPS and ICP-OES.

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(GOMD-S2-S2-017-2025) Extension of corrosion kinetic models from simple glasses toward complex multicomponent glassesN. J. Smith^{*1}; E. Barros de Moraes¹; E. Bakowska¹; N. Stone-Weiss²

1. Corning Incorporated, USA
2. Corning Incorporated, Science and Technology, USA

Predicting chemical durability and corrosion properties is a perennial challenge in the development of novel technical glasses for advanced applications such as next-gen displays, cover glasses, advanced optics, and electronic wafer substrates. At Corning, we have set about a multi-year experimental and modeling effort to tackle this problem, largely aimed at understanding the critical principles underlying forward rate behavior from the standpoint of glass structure, and with timeframes and chemistries that impact technical glass products. This level of deep fundamental understanding is often favored by foundational experiments with simplified (3-4 component) glasses whose structures are far less ambiguous, generally obeying established principles of glass material science that make interpretation more tractable. However, it remains an open question how well models based on simple glasses can be extended to more compositionally-complex glasses of realistic commercial importance. In this talk, we discuss an analysis of this question from a long series of accumulated experiments with representative glass families across this spectrum from simple to multicomponent glasses, offering insights that speak to the extensibility of such models.

3:50 PM

(GOMD-S2-S2-018-2025) Influence of glass composition on its dissolution rate in simulated physiological fluids (SPF)S. Gandon^{*1}; Q. Hérault¹; M. Jacquemin¹; S. Gin²; F. Angeli³

1. Saint-Gobain Recherche, France
2. CEA, DPME, France
3. CEA, France

Glass durability is a key property for numerous fields of application, such as nuclear waste vitrification, pharmaceutical and food containers, and insulation fibers. Bio-solubility is especially important for insulation fibers as one of the tests to pass before commercialization is an in-vivo lung dissolution test on rats. To better understand bio-solubility, a possibility is to use in vitro reactor experiments with

glass immersed in simulated lung fluids. This study aims to understand the impact of glass composition on the in vitro solubility of glass fibers in simulated lung fluids. These fluids are neutral (pH 7.4) or slightly acidic (pH 4.5) aqueous solutions. The pH being a key parameter for glass alteration, it is essential that it is fixed and stable, through and between experiments, to observe other impacting parameters. We study the alteration kinetics of glasses experiments to extract the initial rate, interpreted in relation to composition or structural parameters such as boron coordination. We use a design of experiment approach on simplified SiO₂-B₂O₃-Al₂O₃-Na₂O-CaO oxide glasses with a constant silica content. This approach provides a mean for understanding the hierarchy of influence between several factors, including oxides rates, influencing fiber durability to find an optimal formulation that meets regulatory dissolution requirements.

4:10 PM

(GOMD-S2-S2-019-2025) Corrosion Behavior of Sodium Aluminophosphate Glasses under Aqueous ConditionsM. Watanabe^{*1}; R. Sakai²; T. Kawasaki¹; K. Miyatani²; K. Hayashi¹

1. AGC Inc., Materials Integration Laboratories, Japan
2. AGC Inc., Innovative Technology Laboratories, Japan

Phosphate glasses are widely utilized in optical devices due to their distinctive properties and compositional flexibility. However, their susceptibility to water-induced corrosion poses a significant challenge to maintaining long-term device performance. The incorporation of elements such as aluminum, iron, or alkaline earth metals can enhance their resistance. However, the microscopic mechanism responsible for these improvements remains poorly understood. This research investigates the corrosion behavior and its dependence on the structural unit of sodium aluminophosphate glasses by systematically varying the aluminum content. Immersion tests were conducted in distilled water over controlled timescales, ranging from several seconds to a few hours. Subsequent surface compositional analyses using X-ray photoelectron spectroscopy (XPS) enabled us to track the onset and progression of corrosion reactions at the glass-water interface. By elucidating the initial corrosion behavior of phosphate glass, we pave the way for applications that require water resistance, such as advanced optical devices and high-performance lenses.

4:30 PM

(GOMD-S2-S2-020-2025) Dissolvable Phosphate and Nitrate-based Glasses for Growing Media and FertilizerC. Calahoo^{*1}; W. Hammer²; D. Stiling²; A. Patel²; W. Wall¹

1. Genics, R&D Glass Division, Canada
2. University of Regina Faculty of Engineering & Applied Science, Industrial Systems Engineering, Canada

The agriculture industry faces many challenges: Policymakers worldwide are calling for substantial reduction in nutrient loss and fertilizer emissions by 2030. Dissolvable glass fertilizer aims to optimize uptake of nutrients by the plants and limit the environmental damage from nutrient loss to the environment (e.g., phosphates leaching into the local water system or NO_x and NH₃ being released into the air). Glass composition and properties are endlessly tunable to a variety of soil types, growth habits, plants/crops, climates, ecosystems, rhizospheres, and seasons. For field-based agriculture, several nitrate glasses were synthesized and their dissolution behaviour investigated. Nitrate glasses can be either mixed-cation, or mixed-former, while a mixture of the two catalyzes nitrogen loss and/or crystallization. Beads of the different nitrate compositions were tested in the lab, in soil and barley growing experiments, and compared to conventional commercial mineral and slow-/controlled-release fertilizers. Phosphate-based fibres and beads were made and tested in hydroponics and field-based agriculture, respectively. As expected, aluminum, boron, calcium, magnesium, zinc and iron-containing glasses had slower dissolution rates in lab settings; however, in plant trials, the resulting higher ion concentrations in the nutrient solution had some effects on germination and plant growth.

GOMD S3 - Optical and electronic materials and devices - Fundamentals and applications

GOMD S3 S2 - Glasses for energy applications

Room: Saturna Island Ballroom

Session Chair: Caio Bragatto, Alfred University

1:15 PM

(GOMD-S3-S2-001-2025) Balancing the mechanical and electrochemical properties in glassy solid-state electrolytes (Invited)

S. S. Sørensen*²; M. Micoulaut¹; M. M. Smedskjaer²

1. Sorbonne Université, France

2. Aalborg University, Department of Chemistry and Bioscience, Denmark

Solid state electrolytes (SSEs) have the potential to overcome many of the problems associated with liquid electrolytes, including improvements of fire safety, energy density, and battery lifetime. However, SSEs introduce new problems, especially due to the brittle nature of most potential SSEs such as glasses. The constant cycling of ions leads to undesired stresses in the electrolyte, which may ultimately cause fracture of the SSE and device failure. Despite this, the fracture process and its relation to glass structure and electrochemical properties are only vaguely understood. To address this, we here simulate a promising family of SSEs, namely alkali thiosilicate glasses, using classical molecular dynamics simulations based on a recently established force field. We probe the elasticity and fracture mechanics of the glasses as well as the ionic conductivity to establish correlations between electrolytic performance and mechanical stability of the SSEs. We also provide detailed analyses of the ion movement and dynamic heterogeneities in the glasses. Ultimately, our work highlights the need to consider how the propensity for fracture generally increases simultaneously with the increase of conductivity. This calls for future optimizations of glassy SSEs to balance between mechanical stability and electrochemical properties.

1:45 PM

(GOMD-S3-S2-002-2025) The development of a lithium mixed-oxy-sulfide silico-borate glassy solid electrolyte

S. J. Leland*¹; H. Cochran¹; S. W. Martin¹

1. Iowa State University, Materials Science and Engineering, USA

Previous work identified a lithium mixed-oxi-sulfide (MOS) silicate glass as having a high ($> 1 \text{ mS/cm}^2$) ionic conductivity, favorable working range (T_g - T_x) and isothermal stability for thin-film ($< 100 \mu\text{m}$) drawing, and greater electrochemical stability than similar MOS silico-phosphate glasses. However, to maximize power density for lightweight solid-state batteries, a lower density electrolyte is desirable. To achieve a lower density, a eutectic lithium borate compound, $\text{Li}_{2.15}\text{BO}_{2.57}$, was added to the MOS silicate glass, substituting the existing lithium silicate eutectic, $\text{Li}_{3.48}\text{SiO}_{3.74}$, and expanding on the prior composition range. The resulting compositions showed comparable conductivities and electrochemical stability to the base MOS silicate glass. Density consistently decreased with increasing boron content. Increasing boron content decreased working ranges in the glasses but increased the fragility, decreasing the estimated film-drawing temperature. Isothermal DSC measurements confirmed thermal stability at estimated draw temperatures. Structural analysis through Raman and Fourier transform IR spectroscopy confirmed the presence of boron-bearing species. The produced glasses show potential to provide high (1 mS/cm^2) ionic conductivities with an increase in power density compared to the base MOS silicate glass.

2:05 PM

(GOMD-S3-S2-004-2025) Development and Characterization of Sodium Mixed Oxy-Sulfide Glassy Solid Electrolytes for Improved Electrochemical Stability

A. G. Wakefield*¹; N. Riley¹; K. M. Maier¹; S. W. Martin¹

1. Iowa State University, Materials Science and Engineering, USA

Glasses in the $(1-y) \text{Na}_2\text{S} + y [(1-z)\{(1-a) \text{SiS}_2 + a \text{PS}_{5/2}\} + (1-z) \text{NaPO}_3]$ (NaPSiSO) series are promising candidates for the development of solid-state sodium-ion batteries, but lack the electrochemical stability to function long term in a full-cell format. To overcome this obstacle, glasses with $\text{O}/(\text{O}+\text{S}) = 0.125$, $\text{P}/(\text{P}+\text{Si}) = 0.274$, and R-values between 2.0 and 3.0 were analyzed for ionic conductivity, electrochemical stability, and structure to determine the cause of observed side reactions. The source of the instability was determined to be homopolar sulfur bond defects, which react to form Na_2S during cycling. Using Raman spectroscopy to observe the prevalence of homopolar sulfur bonds, the defect's presence was found to be correlated with the glass R-value above $R = 2.5$. Using electrochemical impedance spectroscopy to determine conductivity and Galvanostatic cycling combined with cyclic voltammetry to measure electrochemical stability, an optimal composition of $R = 2.2$ was found. Sulfide defects were further reduced using a heat-treatment procedure, creating an excellent candidate glass for thin-film drawing of electrolytes.

2:25 PM

(GOMD-S3-S2-005-2025) Mixed network former effect on the ion-dynamics of Sodium Alumino-Phospho-Silicate glasses

S. R. Keshri*¹; I. Mandal²; A. Gaddam³; S. Ganisetty⁴; R. Allu⁵;

N. Gosvami¹; N. Krishnan⁶

1. Indian Institute of Technology Delhi, Materials Science & Engineering, India
2. Indian Institute of Technology Delhi, School of Interdisciplinary Research, India
3. University of Aveiro, Materials and Ceramics Engineering, Portugal
4. Aalborg University, Department of Chemistry and Bioscience, Denmark
5. CSIR- Central Glass and Ceramic Research Institute, Kolkata, Energy Materials & Devices, India
6. Indian Institute of Technology Delhi, Civil Engineering, India

Absence of a unified composition-structure-conductivity correlation in glass materials hinders the development of novel glass electrolytes possessing essential RT ionic conductivity ($\sim 10^{-3} \text{ S/cm}$) for solid-state batteries. In that respect, the concentration of two glass formers (SiO_2 and P_2O_5) was varied in $\text{Na}_3\text{Al}_2\text{P}_3\text{O}_{12}$ NASICON glass till 20 mol% SiO_2 addition for P_2O_5 , by keeping the modifier (Na_2O) constant and its effect on the ion-conductivity and other glass properties were evaluated. A mixed glass former effect (MGFE) was observed in the current glass system with the highest DC ionic conductivity of $\sim 9 \times 10^{-6} \text{ S/cm}$ at 473K for 15 mol% SiO_2 substitution. The results from Raman Spectroscopy and MD simulations confirm the formation of isolated orthophosphate units for NAPS 20 glass, which traps the mobile Na^+ ions, thereby reducing the ionic conductivity of this glass composition. Furthermore, ion-dynamics using AC conductivity analysis was assessed to learn that diffusion, and not sub-diffusion within the potential wells, governs the ion-conduction in the as-synthesized glasses. Overall, it was found that the ion-dynamics in the present glass system is composition-dependent, with different factors such as mobile charge carrier concentration, ion mobility, and coulombic forces due to structural modifications, playing the dominant role in different glass compositions.

2:45 PM

(GOMD-S3-S2-006-2025) Highly Temperable Glass for Bifacial Solar Panels (Invited)A. Mitchell*¹; Z. Zheng¹

1. Corning Incorporated, USA

Thermally strengthened, or tempered, soda lime silicate glass (SLG) is ubiquitous in everyday life. Tempered SLG has been optimized to be as inexpensive as possible to manufacture and strengthen. At thicknesses less than ~2.6 mm, however, existing SLG compositions are unable to be fully tempered using conventional tempering equipment. In this talk, a novel glass composition is described that can impart 65-74% more central tension at the mid-plane of the glass than SLG at 1.2-3.2 mm thicknesses. For applications such as bifacial solar panels that use 2.0 mm thick glass, this increase in imparted stress is predicted to allow the glass thickness to be reduced to 1.75 mm at the same strength or to allow for higher strength at 2.0 mm. To understand which glass properties contribute to the final tempering stresses, coupled viscoelastic, thermal-structural, and material models were used to independently predict the tempering stresses obtained via experiment. In order of quantitative importance, it was found that higher α_{liq} , Young's modulus, Poisson's ratio, and α_{glass} all contribute to more stress in the final glass article.

3:30 PM

(GOMD-S3-S2-007-2025) Intermediate Temperature Electrochemical Devices Utilizing Proton Conducting Phosphate Glass for Energy Conversion Toward Carbon Neutrality (Invited)T. Ishiyama*¹; H. Arai¹; H. Nagashima¹; H. Miyamura¹; T. Yamaguchi¹; T. Omata²1. National Institute of Advanced Industrial Science and Technology, Japan
2. Tohoku University, IMRAM, Japan

Energy conversion by electrochemical reactions is a crucial technology for achieving carbon neutrality, as it enables highly efficient energy conversion in principle. Notably, operating at intermediate temperatures of around 300 °C is attracting attention as a means of not only increasing efficiency, but also providing advantages in terms of reaction selectivity and reaction rate. The development of electrochemical devices that work at such intermediate temperatures is expected to have a variety of applications. Our research group has successfully developed phosphate glasses with high proton conductivity designed specifically for this temperature range and is currently using them to develop devices such as fuel cells and electrochemical reactors. In this presentation, a new type of cell with a glass electrolyte formed on a porous electrode substrate will be introduced. The results of fuel cell operation, hydrogen production by steam electrolysis and methane synthesis by CO₂ reduction using this cell will also be presented.

4:00 PM

(GOMD-S3-S2-008-2025) Quantification of chemical replacement zones by means of ToF-SIMS, NRA and nanoindentation (Invited)K. Rein¹; K. Weitzel*¹

1. Philipps-Universität Marburg, Chemistry Department, Germany

Chemical replacement zones in solid state materials have relevance in many fields of material science. The most powerful approach for generating such replacement zones is the electric field assisted ion exchange (EFAIE) which allows to manipulate the physical properties of solid electrolytes, especially near the sample surface. The ion exchange can lead to, among other things, chemical hardening, improvement of antimicrobial properties or the formation of waveguide structures. In this contribution we demonstrate the

formation and the quantification of replacement zones by different techniques. The alkali deuterium substitution (ADS) is a special form of the EFAIE, where Deuterium is converted to D⁺ ions at a thin platinum electrode. An electric field applied drives the D⁺ ions into the sample and induce replacement of the native (and mobile) alkali ions. We present the results of an ADS experiment on an ion conducting D263T borosilicate glass. As a result of the ADS experiment, the native Na⁺ and K⁺ are replaced by D⁺ ions up to a depth of 2 micrometer from the surface. The replacement zones are quantified by means of ToF-SIMS, nanoindentation and Nuclear Reaction Analysis (NRA). We compare the quality of the results of the different techniques. Ultimately, all three techniques arrive at the same width of the replacement zone, however, with complementary information content.

4:30 PM

(GOMD-S3-S2-009-2025) Impact of heteroatom cross-linking in phosphoric acid chains on proton transport in phosphate glassesT. Omata*¹; J. Nishii²; T. Ishiyama³1. Tohoku University, IMRAM, Japan
2. Hokkaido University, RIES, Japan
3. National Institute of Advanced Industrial Science and Technology, Japan

Proton-conducting phosphate glasses, prepared by electrochemical substitution of Na⁺ ions with protons, exhibit high proton conductivity around 300 °C, making them promising materials as electrolytes for intermediate temperature fuel cells. Cross-linking between phosphoric acid chains with heteroatoms such as silicon, germanium, aluminum, and tungsten enhances the glass transition temperature and thermal stability, providing long-term electrolyte durability under fuel cell operating conditions. However, heteroatom cross-linking can either hinder or enhance proton transport properties. For example, silicon cross-linking reduces proton transport, whereas tungsten cross-linking improves it. To achieve both high proton conductivity and thermal stability in glasses at intermediate temperatures, it is essential to understand how heteroatom cross-linking affects proton transport and to design glass compositions accordingly. This talk will present recent understandings about the effects of heteroatom cross-linking on proton transport properties.

4:50 PM

(GOMD-S3-S2-010-2025) Solid-state cation/H⁺ ion exchange of phosphate glasses for an intermediate temperature fuel cellY. Daiko*¹

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Intermediate temperature fuel cells (ITFC), which operate at around 400-500°C, are being investigated as next-generation FC because they do not require expensive electrocatalysts such as platinum, can reduce the cost of components, and have high power generation efficiency through the use of waste heat. High proton conductivity is required for the electrolyte of this type of fuel cell. Phosphate glasses have high polarity, and protons in OH groups dissociate more easily compared with silicate glasses, and we have been promoting their application as electrolyte materials for medium-temperature fuel cells. However, phosphate glasses are typically insufficient in water durability. We have found that 6-coordinated Si is very effective in improving the water resistance of phosphate glass. Phosphate glasses with 6-coordinated Si have excellent chemical durability and hardly dissolve even after immersion in water at 50°C for more than 2000 h. If solid-state ion exchange between cations in glasses and H⁺ (from anode) can be efficiently achieved under the fuel cell operating conditions, the phosphate glasses would be a great candidate for the electrolyte of ITFC. Here, we present the solid-state ion exchange of phosphate glasses in a hydrogen atmosphere.

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