The American Ceramic Society

2024 Glass & Optical Materials Division Annual Meeting

ABSTRACT BOOK

May 20–23, 2024
Las Vegas, NV

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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S3 Optical and Electronic Materials and Devices Fundamentals and Applications

Don’t miss the 2024 GOMD Award lectures:

Monday, May 20, 2024, 8 – 9 a.m.

Stookey Lecture of Discovery: Jas Sanghera

At the Naval Research Laboratory (NRL), we are developing infrared glasses, ceramics and optical fibers for many active and passive applications. The chalcogenide glasses transmit from approximately 1 µm to 12 µm in the important infrared wavelength region. Fibers have been developed for passive applications, including light-pipes for remote chemical sensor systems for environmental pollution monitoring, exo-planet discovery, scanning near field optical microscopy and other applications. Active applications have also been developed to exploit the high optical nonlinearity of the fibers to generate broadband IR supercontinuum sources and Raman wavelength shifters. In addition, rare earth doping has been used to create bright sources in the IR. More recent developments have focused on fabricating hollow core negative curvature fiber with waveguide loss >100X lower than the material loss in the infrared. Additionally, fiber devices and components have been designed and fabricated. Examples include IR fiber combiners utilized to couple the output from several QCLs in the MWIR and LWIR into a single output fiber, thereby enabling efficient power and wavelength scaling. By tailoring the composition of the chalcogenide glasses it is possible to control refractive index and dispersion, as well as diffusion to enable graded optics, thereby enabling many new multiband optical lens materials.

Tuesday, May 21, 2024, 8 – 9 a.m.

George W. Morey Award Lecture: Stephen Garofalini

Although Rahman’s molecular dynamics simulations of a simple Lennard-Jones liquid in 1964 altered the understanding of diffusion in a liquid, more general acceptance of simulations required development of more realistic interatomic potentials to describe functional materials. In 1976, Woodcock, Angell, and Cheeseman published a potential for amorphous silica that included an exponential repulsion and a screened coulomb term that started an increase in simulations of silica and silicates. More complex potentials were added in future simulations to address more complex systems, especially where chemical reactions were involved. Simulations began to provide insight into molecular mechanisms that could only be inferred from experimental data or provided predictions that were subsequently verified via experiment. Often the simulations instigated further experimental studies or the development and application of better microscopies and spectroscopies. Conversely, simulation methods evolved to provide ever more realistic results via design and incorporation of better interatomic potentials or enhanced ab-initio methods. Today’s presentation will discuss our evolving studies of glass surfaces, glass/crystal and glass/water interfaces, nanoconfined phases and the effect each phase has on the other.

Tuesday, May 21, 2024, 12:15 – 1:15 p.m.

Norbert J.Kreidl Award Lecture: Brian Topper

A new approach to quantifying the short-range structural units of glass forming melts has been developed by evolving the classical lever rule. The nodes of the traditional lever rule are reimagined as ‘Short-Range Order Configurations’ (SROCs) that allow for proper accounting of disproportionation and isomerization of chemical species. The simplicity is that only the short-range structure of just a few glasses needs to be determined, then any composition can be considered as a linear combination of the bounding SROCs. The model is first constructed and then applied to the binary zinc borate system over the entire glass forming region. Experimentally, the $x\text{ZnO}-(1-x)\text{B}_2\text{O}_3$ system is investigated with NMR, Raman, and IR spectroscopies along with density and DSC measurements. By finding the meta-, pyro-, and orthoborate SROCs, the short-range structure of binary zinc borate glasses is modeled. Correspondence with experimental data is excellent, with predicted density within 0.1% and N_4 within 1% of experimental values.

Wednesday, May 22, 2024, 8 – 9 a.m.

Darshana and Arun Varshneya Frontiers of Glass Science Lecture: Edgar Dutra Zanotto

Modern glass science defines the glassy state through three key features: structure, relaxation, and crystallization. Understanding how materials vitrify or avoid crystallization requires examining dynamic processes like relaxation and crystallization. Crystallization is the nemesis of vitrification, however, controlled nano or micro-crystallization allows the creation of valuable polycrystalline glass-ceramics. This centrality in hindering and harnessing crystallization makes it the most cited keyword in glass science history.

This lecture focuses on the early stages of crystallization, with a nod to relaxation processes. We will delve into the significant progress made in understanding crystal nucleation in supercooled liquids and glasses, where relaxation plays a critical role. The Classical Nucleation Theory (CNT), the workhorse for analyzing crystallization dynamics for over 70 years, has limitations.

Experimental data reveals significant discrepancies between CNT predictions and observed nucleation rates and their temperature dependence in various glass formers, including metallic, organic, and oxide materials. However, recent MD simulations using simpler models have successfully validated CNT and uncovered intriguing connections between crystal nucleation and dynamic heterogeneities within the material.

Thursday, May 23, 2024, 8 – 9 a.m.

Darshana and Arun Varshneya Frontiers of Glass Technology Lecture: Shibin Jiang

Rare-earth doped phosphate, silicate, germanate, and tellurite glasses and their fibers have been studied and developed for fiber amplifiers and lasers. Many unique lasers and optical components have been developed and successfully commercialized by utilizing these innovative glass fibers. Single frequency CW and pulsed fiber lasers at 1 micron, 1.55 micron and 2 micron wavelengths are widely used for coherent lidar and fiber sening applications. All-fiber isolator could be a critical component of high-power laser system for defense applications. Both nanosecond and picosecond lasers were demonstrated at IR, green and UV wavelengths, which have been used laser materials processing for glass and ceramic industry.

Monday, May 20, 2024

S1 Fundamentals of the Glassy State

Session 2: Glass Crystallization and Glass-Ceramics I

Room: Bel Air II
Session Chairs: Ashutosh Goel, Rutgers University;
Hrishikesh Kamat, James R. Glidewell Dental Ceramics

9:20 AM

(GOMD-S1-001-2024) ZERODUR®: A LAS-glass-ceramic material enabling optical technologies (Invited)

I. Mitra*[1]

1. Schott AG, Germany, Germany

Near-zero expansion is the key-feature of ZERODUR® as a material which enables various technologies. This unique property is based on a crystal phase exhibiting negative thermal expansion. Controlled nucleation and growth of this phase as nano-sized crystals turns the family of lithium aluminosilicate (LAS)-glass-ceramics to a state-of-the-art transparent nanomaterial. Insight will be provided into the origin of these key-properties and their implementation within various technologies ranging from 1960s up today. These materials exhibit near-zero expansion from room temperature to 700°C ensuring high resistance to thermal shock. The use as cooktop panels, fireplace windows and fire-rated doors opened up a broad consumer market. When astronomer requested telescope mirrors, ZERODUR® was especially designed to provide near-zero expansion across harsh and ambient temperatures. In conjunction, newer grades were introduced to cater even tighter tolerances. ZERODUR® is an established material in the field of lithography where alignment and position of stages in production of electronic elements require highest precision. Nevertheless, future processing steps at customer sites might exceed current range of operational temperatures. Consequently, a new LAS glass-ceramic with enhanced near-zero expansion ranges will be needed. An outlook on material development anticipating future demands will be presented.

9:50 AM

(GOMD-S1-002-2024) Nd^{3+} ion doped oxyfluoride silicate glasses and glass-ceramics for NIR laser application

R. Dagupati[1]; J. J. Velazquez Garcia*[1]; G. Galleani[1]; R. Klement[1]; D. Galusek[2]; A. Durán[1]; M. Pascual[1]

1. FunGlass-Alexander Dubcek University, Slovakia
2. Joint Glass Centre of the IIC SAS, TnUAD, and FChPT STU, Trenčín, Slovakia, Slovakia

Rare-earth (RE) doped $NaYF_4$ Oxyfluoride Glass Ceramics (OxGCs) is one of the most efficient hosts for RE ions due to its low phonon energy that increase the luminescence while properties preserving the excellent mechanical properties of the parent glasses. It has two crystalline forms, cubic and hexagonal, which can be changed with each other by setting the glass composition and/or heat treatment conditions. This ability to adjust the crystal phase makes it possible to choose the settings to obtain the most optically favourable hexagonal phase. Thus, development of RE-doped $NaYF_4$ GCs as well as the RE content effects on the crystal precipitation and its structural-optical properties are worth investigating. Here, (0.2-1.0) NdF_3 doped $NaYF_4$ OxGCs (mol%) were prepared by melt-quenching followed by a controlled crystallization of the parent glass. Structural properties were analyzed confirming the hexagonal phase precipitation and Nd ions incorporation in this phase. The absorption shows an increment with the NdF_3 content in the GCs. However, the NIR emissions show an enhancement up to 0.5 mol% of doping, decreasing at higher concentration. Fluorescence lifetimes follow the same behavior, indicating the optimum Nd content for the emission efficiency. According to the extremely strong emission band at 1056 nm, $0.5NdF_3$ doped GCs can be considered as a potential material for NIR laser applications. Acknowledgement: EU′s Horizon 2020 R&I program No 739566 and VEGA project 1/0844/21

10:10 AM

(GOMD-S1-003-2024) SrF2 generation in novel transparent germanate glass-ceramics: a structural and optical study

A. Deslandes*[1]; T. Guerineau[1]; T. Cardinal[2]; Y. Messaddeq[1]

1. Laval University, Center for Optics, Photonics and Lasers, Canada
2. ICMCB-CNRS, France

Oxyfluoride glass-ceramics as well as germanate glasses are widely studied for photonic applications due to their low phonon energy, which enables extended transparency in the vis-IR region. As such, they are broadly studied as hosts for various luminescent ions. This work focuses on a novel glass-forming composition within the GeO_2–BaF_2–SrF_2–In_2O_3 system. XRD measurements on such samples after a crystallization treatment show the formation of SrF_2 crystals, which are reported in the literature as desirable hosts for rare-earth dopants. However, to reduce Rayleigh scattering and ensure optimal transparency in the visible and infrared regions, the crystals formed should be nanometer-sized. Nucleation-growth treatments were thus conducted as part of this study. XRD and TEM measurements coupled with electronic diffraction have been conducted on the obtained transparent samples. Furthermore, UV-visible characterization showed a visible reduction in Rayleigh scattering for crystallized samples doped with Europium. Luminescence studies on these glass-ceramics also showed an absence of Europium segregation in the phase separated domains. As such, tuning of the Eu content in the obtained transparent glass-ceramic enables a direct control of the SrF_2 crystal size. To the author’s knowledge, this is also the first reported instance of SrF_2 generation in a transparent germanate matrix.

10:30 AM

(GOMD-S1-004-2024) Copper-containing glass-ceramic with high antimicrobial efficacy (Invited)

T. M. Gross*[1]

1. Corning Incorporated, New Materials & Processes, USA

Hospital acquired infections (HAIs) and the emergence of antibiotic resistant strains are major threats to human health. Copper is well known for its high antimicrobial efficacy, including the ability to kill superbugs and the notorious ESKAPE group of pathogens. We sought a material that maintains the antimicrobial efficacy of copper while minimizing the downsides - cost, appearance, and metallic properties - that limit application. A copper-containing glass-ceramic material is described that provides controlled release of copper (I) ions resulting in a continuously killing antimicrobial surface. The material consists of two amorphous phases: a continuous matrix phase enriched in silica and a water-sensitive, discontinuous droplet phase enriched in phosphorus and potassium. Cuprite crystals precipitate from within the droplet phase and are accessed through dissolution of the surrounding amorphous material. Latex paint containing the glass-ceramic powder exhibits ≥ 99.9% reduction in S. aureus, P. aeruginosa, K. aerogenes, and E. Coli colony counts when evaluated by the US EPA test method for efficacy of copper alloy surfaces as sanitizer. These results approach that of the benchmark, copper metal.

Session 5: Data-based Modeling and Machine Learning for Glass Science

Room: St. Andrews
Session Chairs: Daniel Cassar, Vitreous Materials Laboratory;
N M Anoop Krishnan, Indian Institute of Technology Delhi;
Xiaonan Lu, Pacific Northwest National Lab

9:20 AM

(GOMD-S1-005-2024) Impacts of Oxygen Doping on Sodium-Ion Diffusion in Solid-State Batteries with Glassy Electrolyte: A Molecular Dynamics Perspective (Invited)

K. Luo[1]; R. Zhou[1]; S. W. Martin[1]; Q. An*[1]

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

As the demand for higher-performance energy storage systems increases, the innovation of high-performance battery technologies has become a vital frontier in modern technology. In this talk, we discuss the atomic-level mechanisms that enhance the performance of sodium-ion solid-state batteries via oxygen doping in Na_3PS_3O glassy solid electrolytes (GSEs). Utilizing machine learning force field (ML-FF) molecular dynamics simulations, we modeled sodium-ion diffusion in amorphous Na-P-S-O GSEs. Our simulations demonstrate that oxygen doping contracts the structure, thereby reducing the diffusion coefficient of Na ions, while simultaneously enhancing sintering densification, leading to a more favorable structure for Na-ion diffusion. This work provides a new perspective on the mechanism previously proposed in experimental studies. Offering a novel atomic-level understanding of oxygen doping's role, our research aids in designing superior sodium-ion solid electrolytes.

9:50 AM

(GOMD-S1-006-2024) Predicting dynamics in glasses using graph neural networks

R. Christensen*[1]; L. Fajstrup[2]; M. M. Smedskjaer[1]

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. Aalborg University, Department of Mathmatical Sciences, Denmark

Understanding the dynamics of atoms in glasses is crucial for unraveling their transport and dynamical properties. However, identifying the structural features controlling atom dynamics in glasses remains challenging. Recent advances in this field have used machine learning models such as graph neural networks (GNNs) to predict long-term dynamics, but prior studies have mostly focused on simulations of model systems like Kob-Andersen-type Lennard-Jones mixtures. This study extends this approach by using GNNs and molecular dynamics simulations to investigate the dynamics of atoms in realistic glass systems (such as sodium silicates) across varying timescales. By harnessing the capabilities of GNNs, our method provides an effective means for predicting the long-term dynamics of ions in glassy systems, based solely on initial particle positions, without relying on handcrafted features. We compare the present results to those of previously proposed methods. Our findings pave the way for understanding how the disordered structure of glasses governs their dynamics.

10:10 AM

(GOMD-S1-007-2024) Predicting Temperature and Frequency-Dependent Dielectric Properties of Oxide Glasses by Physics- and Chemistry-Informed Machine Learning Model

Y. Shih*[1]; B. Lin[1]

1. National Taipei University of Technology, Department of Materials and Mineral Resources Engineering, Taiwan

In our previous work, we successfully demonstrated the ability of machine learning (ML) to predict temperature and frequency-dependent dielectric properties of oxide glasses. To further improve the transferability of the previous ML model, we replaced the descriptors in the chemical composition domain with those in the element physical and chemical properties domain. The newly designed descriptors include stoichiometric, elemental-property-based, valance orbital occupation, and ionicity features. Among the studied ML models, the artificial neural network performs best in predicting the dielectric constant, and the support vector regression performs best in predicting the dielectric loss. The SHAP analysis was used to reveal the importance of the studied features and their correlation with the dielectric properties. The results indicate that the average and deviation of the boiling points of constituting elements exhibit the highest impact on the dielectric constant and loss. The increasing average of the boiling points of constituting elements implies a more difficult ionic motion, leading to a decline in dielectric constant and loss. The growing deviation of the boiling points of constituting elements suggests the higher network former contents, leading to a decreasing dielectric constant and loss. Besides the boiling points, the melting points, heat of formation, and dipole polarizability of constituting elements also significantly influence the dielectric properties.

10:30 AM

(GOMD-S1-008-2024) Property Optimization and Sampling of Atomistic Systems via Latent Space Representation Learning with Variational Autoencoder (VAE)

R. Bhattoo*[1]; B. Wang[1]

1. University of Wisconsin-Madison, Civil Engineering, USA

Atomistic simulations often involve high-dimensional representations of complex systems, posing challenges in efficient exploration, property optimization, and data sampling. This work introduces a novel approach leveraging Variational Autoencoders (VAEs) for latent space representation learning in the context of atomistic configurations. The proposed methodology utilizes the encoder-decoder architecture of VAEs to compress high-dimensional input data into a lower-dimensional latent space, capturing essential features while discarding redundant details. The latent space, characterized by smooth and continuous properties, serves as an effective domain for property optimization, enabling the discovery of configurations that optimize specific atomic properties. Moreover, sampling in the latent space facilitates the generation of diverse and coherent atomistic configurations, providing an efficient means for exploration of new atomic configurations.

10:50 AM

(GOMD-S1-009-2024) Predicting the Dynamics of Atoms in Glass-Forming Liquids by a Surrogate Machine-Learned Simulator

H. Liu[1]; M. Bauchy*[1]

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA

Molecular dynamics (MD) is a workhorse of computational material science. However, the inner-loop algorithm of MD (i.e., numerically solving the Newton's laws of motion) is computationally expensive. This is a key limitation since, as a result, MD simulations of glasses are typically limited to very fast cooling rates. Here, we introduce a surrogate machine learning simulator that is able to predict the dynamics of glass-forming liquid systems with no prior knowledge of the interatomic potential or nature of the Newton's laws of motion. The surrogate model consists of a graph neural network (GNN) engine that is trained by observing existing MD-generated trajectories. We demonstrate that the surrogate simulator properly predicts the dynamics of a variety of systems featuring very different interatomic interactions, namely, model binary Lennard-Jones system, silica (which features long-term coulombic interactions), silicon (which comprises three-body interactions), and copper-zirconium alloy (which is governed by many-body interactions). The development of machine-learned surrogate simulators that can effectively replace costly MD simulations could expand the range of space and time scales that are typically accessible to MD simulations.

11:10 AM

(GOMD-S1-010-2024) Visualizing the energy landscape of glassy systems

V. Bihani*[1]; S. Sastry[2]; S. Ranu[3]; N. Krishnan[4]

1. Indian Institute of Technology Delhi, Yardi School of Artificial Intelligence, India
2. Jawaharlal Nehru Centre for Advance Scientific Research, Theoretical Sciences Unit and School of Advanced Materials, India
3. Indian Institute of Technology Delhi, Department of Computer science and engineering, India
4. Indian Institute of Technology Delhi, Department of Civil Engineering, India

Understanding the energy landscape is key to discovering glasses with targeted properties since the landscape encapsulates a system's complete thermodynamic and kinetic behavior, including its non-equilibrium properties, such as relaxation and metastable phases. However, the curse of dimensionality prohibits one from effectively visualizing the energy landscape—the energy landscape of an N-atom system has 3N dimensions. Here, we propose a method to visualize the complex energy landscape. We demonstrate that the proposed low-dimensional projection aligns well with the curvatures of the actual landscape, validated through Hessian analysis. Further, we show that we can gain interesting insights into the behavior of different gradient-based and machine-learned optimizers using the proposed visualization approach. We hope that the study will enhance the understanding of the energy landscapes that, in turn, will provide both a fundamental understanding of the physics of glassy materials and accelerate their discovery.

11:30 AM

(GOMD-S1-011-2024) Atomistic simulations of seeded growth of lithium niobate crystal in erbium-doped xLNbO3 - (1-x)SiO2 glasses

R. Thapa*[1]; M. E. McKenzie[2]; C. Barker[1]; V. Dierolf[3]; H. Jain[1]

1. Lehigh University, Material Science and Engineering, USA
2. Corning Incorporated, USA
3. Lehigh University, Physics, USA

The growth of lithium niobate crystals in lithium niobosilicate, xLNbO3 - (1-x)SiO2 glasses with x=0, 0.22, and 0.30, undoped and doped with erbium, from preexisting crystal seeds has been studied using molecular dynamics simulations. The interactions of various cations with oxygen anions are modeled using Buckingham potential with repulsive correction at low separations. We created a melt-from-quench model of the glasses with 100,000 atoms fixing a part of the cell as crystalline seed while allowing others to equilibrate to the high-temperature melt conditions. The assembly of atoms without any Er is then quenched to yield a system consisting of a crystal seed surrounded by a glassy matrix. The system is annealed at a constant temperature cycle at elevated temperatures to model the evolution of the size of the seed and changes in its surrounding network. The crystal growth rate has been calculated with predictions made by a machine-learned clustering algorithm trained on the structural and dynamic characteristics of the atoms. The simulations are then repeated for a system doped with erbium. Spatial distribution of the Er atoms in the melt as well as during the seeded crystal growth is determined. The partitioning and state of Er atoms are followed as they incorporate into the growing lithium niobate crystal.

S2 Glass and Interactions with Its Environment Fundamentals and Applications

Session 1: Glasses, Glass-Ceramics, and Glass-Based Biomaterials

Room: Bel Air I
Session Chair: Delia Brauer, Friedrich-Schiller-Universität

9:20 AM

(GOMD-S2-001-2024) Spray-dried bioactive glass microparticles as building blocks for porous scaffolds: structural properties and functionalization (Invited)

G. Vecchio[1]; P. Lagarrigue[1]; S. Le Grill[1]; F. Brouillet[3]; C. Combes[1]; D. Poquillon[1]; A. Bethry[2]; M. Castanié[3]; V. Darcos[2]; J. Soulié*[1]

1. Institut National Polytechnique de Toulouse, France
2. Institut des Biomolécules Max Mousseron, France
3. Université Paul Sabatier, France

Silicate bioactive glass nano/microparticles are of great interest for bone substitution due to their ability to promote osteointegration through the release of active ions and the formation of an apatite layer. Additional pro-angiogenic/antibacterial properties could be provided by Cu-doping. While sol-gel methods are efficient, synthesizing Cu-doped nano/microparticles that poorly aggregate without a secondary CuO phase remains a challenge. This work focuses on an alternative route using a combination of sol-gel and spray-drying processes. In the resulting microparticles, copper is incorporated either as Cu^0 nanoparticles or integrated as Cu^{2+}. Copper impacts the connectivity of the silica network, as calcium and phosphorus are preferentially distributed in the glass network or involved in CaP nano-domains, depending on the doping amount. Additionally, we investigated the functionalization of particles with PDLLA to enhance their potential as building blocks for fabricating freeze-cast porous scaffolds. We demonstrated that both functionalization and doping ratio affect: i) the amplitude of acellular degradation in SBF, ii) the in vitro behavior, and iii) the mechanical properties of freeze-cast scaffolds. These results pave the way for the development of PDLLA/bioactive glass macroporous composites for bone substitution.

9:50 AM

(GOMD-S2-002-2024) Exploring sintering behavior and cohesion quality of phosphate bioactive glass coatings for enhancing Bioglass 45S5 mechanical properties

A. López-Grande*[1]; A. Arafat[2]; D. S. Brauer[1]

1. Friedrich-Schiller-University Jena, Germany
2. University of Wolverhampton, United Kingdom

Phosphate glasses are versatile materials with a wide range of technological applications, including their potential as bioactive materials. Despite their promise, the existing body of literature on the utilization of phosphate glasses for bone regeneration underscores a fundamental challenge: achieving a delicate equilibrium between optimal processing conditions and controlled dissolution. In this study, we focus on understanding the sintering behavior of a specific composition: x K_2O - (18-x) Na_2O - 15 CaO - 22 MgO - 45 (P_2O_5) phosphate bioactive glasses, where x varies (x=0, 2, 9, 18). The primary goal of our investigation is to assess the suitability of these phosphate glasses as coatings for Bioglass 45S5, aiming to enhance the mechanical properties of the latter. This research involves a comprehensive analysis of how the glass composition influences key factors such as sintering behavior, processing windows, and the resultant microstructure of the phosphate materials. By systematically exploring the relationship between composition and these critical properties, we seek to gain insights into the potential of these phosphate glasses for practical applications.

10:10 AM

(GOMD-S2-003-2024) High resolution 3D printing of bioactive glass (Invited)

L. Hambitzer[1]; F. Kotz-Helmer*[1]

1. University of Freiburg, IMTEK, Germany

Porous bioactive glass scaffolds are desirable for bone tissue engineering, as they exhibit rapid bone ingrowth and subsequent replacement with new bone. Mimicking the structure of cancellous bone is a common approach. The geometry influences critical properties such as, cell intrusion, vascularization, tissue ingrowth and mechanical performance. Among various manufacturing techniques, 3D printing has attracted attention for its precise control over the geometry and therefore tailoring the properties of the scaffolds. Yet, previous studies were not able to fabricate structures smaller than 200 μm, limiting the geometric control. Furthermore, most used glass composition are prone to crystallization during sintering. Crystallization should be avoided as it is reducing the bioactivity. To circumvent these issues, this study used DLP printing of a bioactive glass 13-93, which is suitable for sintering. A glass composite was printed, the organic content thermally removed and the glass sintered. The sintered glass was fully densified, remained amorphous and exhibited in vitro bioactivity. Various scaffolds, including cancellous bone structure obtained from μCT data, were fabricated. Features as small as 77 μm were achieved, which corresponds to the smallest struts found in human cancellous bone. As such, our work may allow new insight into the influence of microstructure on bioactive glass scaffolds for tissue engineering.

10:40 AM

(GOMD-S2-004-2024) Effect of different dynamic test conditions on the early stage dissolution behaviour of bioactive glasses

H. Kankova*[1]; L. Bunova[1]; A. Svancarkova[1]; D. Galuskova[1]; D. Galusek[1]

1. FunGlass, Centre for Functional and Surface Functionalized Glass, Alexander Dubček University of Trenčín, Slovakia

To investigate the effect of pH, flow rate and initial sample amount on the leaching process, the 45S5 bioactive glass as a reference material and 45S5 glass doped with zinc were selected. The powder sample was loaded into a cell of approximately 1.5 mL volume through which fresh solutions was continuously flowed. The Ca, P, Si and Zn concentrations as a function of time were directly monitored by the optical emission spectrometer with inductively coupled plasma. Unlike neutral leaching medium, increased concentrations of Ca, P and Zn ions were detected in the input medium with the pH (2-4). At a slow medium flow rate (0.03 mL/min), the measured concentrations of ions were higher than at a faster one (2.6 mL/min). If the input amount of powder was varied, the highest concentrations were measured for the highest amount. When normalized, the tests revealed the highest fraction of respective elements were leached in the experimental arrangement with the lowest initial amount of powder. The tests documented a significant influence of experimental setup on the amounts of elements leached from a bioactive glass under various conditions, indicating a necessity of normalization of invitro leaching tests. Acknowledgement: This item is a part of dissemination activities of project FunGlass. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 739566. The authors would like to acknowledge VEGA 01/0191/20 grant

11:00 AM

(GOMD-S2-005-2024) Zinc-doped bioactive glass nanoparticles for tissue regeneration (Invited)

Z. Neščáková*[1]; J. J. Velazquez Garcia[1]; H. Kankova[1]; M. Michálek[1]; D. Galusek[2]

1. Centre for Functional and Surface Functionalized Glass – FunGlass, Alexander Dubček University of Trenčín, Slovakia
2. Joint Glass Centre of the IIC SAS, TnUAD and FChFT STU, Slovakia

Bioactive glasses (BGs) are widely studied inorganic biomaterials for tissue regeneration. Sol-gel derived BG nanoparticles (BGNs) have attracted interest as promising therapeutic and regenerative agents. By incorporating therapeutic zinc ions, specific biological properties can be moderated. Zinc plays a crucial role in bone formation and development, it is involved in homeostasis, angiogenesis, and has antibacterial and wound healing properties. In this study, the Zn-doped system $62SiO_2$-30CaO-$3P_2O_5$-5ZnO (mol%) was synthesised and characterised for its elemental composition, structural, morphological, and antibacterial properties. The BGNs with a size <80 ± 20 nm with high Ca^{2+} content (up to 30 mol%) were prepared by precise control of the sol-gel processing parameters. Zinc addition did not affect the amorphous nature of glass, and slowed down but did not inhibit the formation of HAp, confirming the bioactivity of BGNs. Biocompatibility with human fibroblasts and antibacterial properties against bacterial and fungal pathogens were confirmed. The antimicrobial activity of BGNs was demonstrated against all tested microorganisms in indirect contact with the elution extracts (10 mg/mL), in a dose-dependent manner reflecting the time of ions leaching (1-28 days). The results indicate the possible use of BGNs as an alternative non-antibiotic treatment for microbial infections associated with implantation procedures. Fund by EU Horizon 2020 R&I program grant agreement No 739566

Session 2: Dissolution and Interfacial Reactions

Room: Turnberry
Session Chair: Nicholas Stone-Weiss, Corning Incorporated

9:20 AM

(GOMD-S2-006-2024) Materials Characterization Center Test 1 Response of Silicate Glass-Based Waste Forms as Functions of Time and Composition (Invited)

J. Vienna*[1]; B. Parruzot[1]; J. T. Reiser[1]; X. Lu[1]; K. Finucane[2]

1. Pacific Northwest National Lab, USA
2. Veolia Nuclear Services, Federal Services, USA

The Materials Characterization Center test number 1 (MCC-1, ASTM C1220) is particularly well suited to evaluate the durability of multiphase silicate waste forms since the test is performed on monolithic samples with representative surface areas of constituent phases. Solution concentration data are used to evaluate the overall waste form release while surface characterization provides information on the contribution of individual phases. The MCC-1 responses of 36 silicate glass-based waste forms were measured for the glasses at 90°C for up to 365 days. A model was generated as a function of glass composition using the 28-d responses combined with 28-d MCC-1 data from previous studies for a total of 194 datapoints. Component effects were discussed in context of glass alteration theory. The extended time data were also evaluated as functions of both time and composition to give insights into longer-term performance.

9:50 AM

(GOMD-S2-007-2024) Durability Testing and Test Method Development on Multiphase Waste Forms

J. T. Reiser*[1]; B. Parruzot[1]; P. D. Sutton[2]; D. Gregg[2]; M. Asmussen[1]; J. M. Westman[1]; G. L. Smith[1]

1. Pacific Northwest National Laboratory, USA
2. Australian Nuclear Science and Technology Organisation, Australia

Multiphase materials such as ceramics and glass-ceramics are increasingly being considered for the stabilization and immobilization of primary and secondary nuclear wastes around the world, due to the potential advantages of multiphase materials over existing waste forms. Although many properties of multiphase materials can make them effective candidate waste forms for the immobilization of challenging nuclear waste types, major research questions need to be addressed. The physical properties, durability behavior, and geochemical relationships are complex due to interactions between phases that are not fully understood. Recently, Pacific Northwest National Laboratory (PNNL) and the Australian Nuclear Science and Technology Organisation (ANSTO) entered a joint research program to investigate chemical durability testing and corrosion modeling of multiphase nuclear waste forms. Durability testing was conducted using variations of numerous methods (e.g., stirred reactor coupon analysis test and static leach tests) to evaluate the performance of waste forms from both institutions. Characterization and data processing approaches were adapted for the multiphase forms to evaluate durability behavior for the bulk waste form and individual phases. The results from this work improve the methods and calculations required to identify and quantify key thermodynamic and kinetic parameters to consider during long-term durability model development of multiphase waste forms.

10:10 AM

(GOMD-S2-008-2024) Using the Stirred-Reactor Coupon-Analysis (SRCA) Technique to Evaluate Forward Dissolution Rate Parameters Impact on Nuclear Waste Glass Disposal

B. Parruzot*[1]; J. T. Reiser[1]; S. Kerisit[2]; J. Neeway[1]; G. L. Smith[1]; M. Asmussen[1]

1. Pacific Northwest National Lab, Energy and Environment Directorate, USA
2. Pacific Northwest National Lab, Physical and Computational Sciences Directorate, USA

The Stirred Reactor – Coupon Analysis testing method allows for measurement of the forward dissolution rate of multiple glasses at once. It was approved as ASTM method C1926 after a round-robin evaluation in 2022. This method was used to measure the forward dissolution rate of a set of 24 statistically-designed low-activity waste nuclear glasses. These rates were used to parameterize the immobilized low-activity waste glass corrosion model for the completion of a performance assessment of a low-activity waste repository located on the Hanford Site in Washington State, USA. After introducing the SRCA technique and providing an overview of the current knowledge on the technique, this presentation will summarize the process followed to derive the forward-rate parameters from laboratory measurements, evaluate realistic sensitivity evaluations based on the correlation between these parameters, and their impact on the waste form evolution in repository conditions.

10:30 AM

(GOMD-S2-009-2024) Elemental releases from enhanced low-activity waste glasses tested by 48-hour room temperature methods

J. Marcial*[1]; J. Neeway[1]; C. Pearce[1]; S. Choi[1]; J. Vienna[1]; J. T. Reiser[1]; J. Hager[1]; D. Kosson[2]; R. Delapp[2]; L. Brown[2]; A. A. Kruger[3]

1. Pacific Northwest National Laboratory, USA
2. Vanderbilt University, USA
3. US DOE Office of River Protection, 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. The use of an autotitrator demonstrated that less acid was required to achieve a desired pH while buffered testing showed lower elemental releases relative to the conventional EPA method 1313.

10:50 AM

(GOMD-S2-010-2024) Waste Glass Corrosion Testing Using EPA 1313, Vapor Hydration, and Stirred Reactor Coupon Analysis

C. Lonergan*[2]; J. Neeway[1]; J. M. Westman[1]; M. Miller[1]; S. Choi[1]

1. Pacific Northwest National Lab, USA
2. Missouri University of Science & Technology, Materials Science and Engineering, USA

Understanding glass corrosion in a disposal facility is often gained through performing laboratory testing to assess the extent of the release of glass components into solution as a function of time. Data from corrosion durability tests were measured and mined from previously published literature for select glass compositions. The tests include the Vapor Hydration Test (VHT), the Stirred Reactor Coupons Analysis (SRCA), and the EPA Method 1313 (EPA1313). As is evident from this work, the steps to perform the tests are quite different as well as the environments to which the glasses are subjected. The VHT data affirm that the test results between replicate samples are not very reproducible, suggesting that this test may not be ideal to control glass compositions during WTP operations. The EPA1313 test is an alternative analysis that was performed to evaluate its reproducibility in comparison to literature values and to assess the ease in which it could be employed as a WTP operations test. The SCRA provides valuable information to support modeling and further data on additional glasses tested here can support that modeling. This presentation will discuss the three tests mentioned above and how the results tie to WTP operations.

S3 Optical and Electronic Materials and Devices Fundamentals and Applications

Session 5: Rare-earth and Transition Metal-doped Glasses and Ceramics for Photonic Applications I

Room: Shoal Creek
Session Chairs: Volkmar Dierolf, Lehigh University; Stuart Gray, Corning Research and Development Corporation

9:20 AM

(GOMD-S3-001-2024) Femtosecond Laser Writing of Er: LiNbO$_3$ Single Crystals for Integrated Quantum Memory

C. Barker*[1]; S. Gray[2]; D. Nolan[2]; H. Jain[3]; V. Dierolf[1]

1. Lehigh University, Physics, USA
2. Corning Incorporated, USA
3. Lehigh University, Institute for Functional Materials and Devices, USA

Sustaining photonic quantum networks creates a need for developing materials to improve certain properties. Materials for a quantum memory in such a network would ideally have a long coherence lifetime and a wide wavelength range to store single photons. The usage of a femtosecond pulsed laser focused within the bulk of a lithium niobosilicate glass enables the fabrication of single crystal $LiNbO_3$ in 3D architectures, allowing the design of an integrated photonic device. Doping this crystal with erbium can act as quantum memory within the telecom wavelength band. In this work electron backscatter diffraction, combined excitation emission spectroscopy, Xray fluorescence mapping, and extended X-ray absorption fine structure (EXAFS) analysis are employed to determine the nature of crystal growth and erbium incorporation within the crystal. This information is correlated with spectral hole burning measurements and absorption spectroscopy to determine how the structure impacts the material's viability for quantum applications. The potential for tuning the crystal's structure and properties via processing parameters is discussed.

9:40 AM

(GOMD-S3-002-2024) Compositional Study of $CsPb(Br/I)_3$ Perovskite Nanocrystal Embedded Germanate Glasses for Red Color Converter

J. Lee[2]; W. Chung*[1]

1. Kongju National University, Division of Advanced Materials Engineering, Republic of Korea
2. Mico Co. Ltd., Republic of Korea

Perovskite nanocrystals (PNCs) based on cesium lead halide ($CsPbX_3$) have been extensively studied due to their prominent color converting properties such as high photo-luminescence quantum yield (PL-QY) and narrow emission bandwidth, which is suitable for high picture quality display applications such as ultra high definition (UHD) TV. However, seriously weak chemical, thermal and photonic stability of colloidal PNCs inhibited their practical applications. PNC embedded glasses (PNEGs) can provide complete inorganic passivation to PNCs and thus overcome those stability issues facilitating extensive studies. In order to fabricate a white LED using InGaAs based blue LED as an excitation source, green and red color converting materials are required. Although $CsPbBr_3$ based green PNEG has been reported with their high PL-QY above 80%, few studies have been reported for red emitting PNEG with high PL-QY under blue excitation. In this study, we fabricated a PNEG containing $CsPb(Br/I)_3$ nano-crystals based on boro-germanate glass system for efficient red color converter. Glass compositions and heat treatment conditions were varied to improve PL-QY up to 70%. The formation of $CsPb(Br/I)_3$ nano-crystals were examined by XTD and HR-TEM. Compositional role on the PNEG was discussed with Raman and XPS analysis. Thermal, photonic and chemical stability of the PNEG was inspected. The PNEG composed a white LED with green PNEG and showed wide color gamut up to 139% of NTSC defined area.

10:00 AM

(GOMD-S3-003-2024) Effect of Na/Al atomic ratio in a germanate matrix on the optical properties of a bismuth dopant

L. J. Henry*[1]; M. Klopfer[2]; K. Richardson[3]

1. Air Force Research Laboratory, Directed Energy Directorate, USA
2. Innovative Employee Solutions, USA
3. University of Central Florida, 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 that displays unique optical properties in oxide glasses. The multi-valent nature of bismuth can serve to stabilize charged defects in the glass matrix and the matrix itself can also work to stabilize bismuth emission sites. The work presented here will show how the optical excitation and emission properties of bismuth change for glass matrices having an atomic excess and deficit of sodium relative to aluminum, across the 1:1 Na/Al ratio. We will also show how the presence of bismuth in a doped glass affects the balance of charge and the formation of matrix defects relative to what is seen in the analogous undoped, Bi-free glass.

10:20 AM

(GOMD-S3-004-2024) Evaluation of bismuth source on resulting valence equilibrium in soda alumino germanate glass

L. J. Henry*[1]; M. Klopfer[2]; K. Richardson[3]

1. Air Force Research Laboratory, Directed Energy Directorate, USA
2. Innovative Employee Solutions, USA
3. University of Central Florida, USA

Bismuth (Bi) is a dopant ion known to exist in multiple reduction states within a material. When melted with the raw materials of a glass matrix, most commonly as an oxide Bi_2O_3 (Bi^{3+}), the glass network impacts the equilibrium valence state of Bi, driving the species via reduction towards metal (Bi^0) and metal ion clusters when melted at higher temperatures and/or for longer melt times. The work presented illustrates that the reduction equilibrium of bismuth established when melting Bi_2O_3 (Bi^{3+}) or Bi metal (Bi^0) with the components of a soda alumino germanate glass matrix in air, does not largely impact the glass' resulting structure or optical properties. This is supported by x-ray photoelectron spectroscopy and luminescent behavior which examines excitation and emission properties of the bismuth emission centers in both glasses. This work demonstrates that the reduction pathway of bismuth can move both toward lower and higher reduction states of bismuth during a melt, impacting the resulting optical behavior of the bismuth dopant within a glass matrix.

S5 Delbert Day Honorary Symposium

Session 5: Delbert Day Honorary Symposium

Room: Peeble Beach
Session Chairs: Qiang Fu, Corning Incorporated;
Kisa Ranasinghe, Kennesaw State University

9:30 AM

(GOMD-S5-001-2024) Delbert Day and the Development of Glasses for Biomedical Applications (Invited)

R. Brow*[1]; S. Jung[2]

1. Missouri S&T, Materials Sci & Engrg, USA
2. MO-SCI LLC, USA

Prof. Delbert Day, his students, and colleagues, developed commercially significant glass-based technologies used for two very different medical applications: chemically stable radioactive rare-earth aluminosilicate (REAS) glass microspheres that are used to treat liver cancer, and fast-reacting borate-based glass fibers used for tissue regeneration, including wound healing, and bone grafts. In this talk, we will review Prof. Day's development of these products, with an emphasis on the materials science behind their compositions and performance characteristics and how these two widely different compositional families are connected through the way they interact in physiological environments. More soluble borate-versions of the chemically inert REAS glasses were first developed to produce resorbable microspheres and this research then led to the development of the family of Ca-releasing borate glass compositions, and on the way sparking the interest of the international glass community in borate bioactive glasses.

10:00 AM

(GOMD-S5-002-2024) Understanding glass crystallization via DSC. A tribute to Delbert Day (Invited)

E. Dutra Zanotto*[1]

1. Federal University of Sao Carlos, Materials Engineering, Brazil

Among his 350+ glass science and technology papers, one of Delbert s favorite topics was crystallization (~30 articles). He has worked with several co-authors, including Chandra Ray, W. Huang, Kisa Ranasinghe, Kenneth Kelton, and others, to study this vital phenomenon using Differential Scanning Calorimetry (DSC) methods they developed. In this talk, I will briefly review their work on DSC techniques and our own contributions to computing different properties: liquidus temperature, crystal nucleation rates, crystal growth rates, and glass stability against crystallization.

10:30 AM

(GOMD-S5-003-2024) Making Glass in Space (Invited)

R. Weber*[1]

1. MDI, USA

Professor Delbert Day pioneered experiments on glass processing in space in the mid-1980s. His work was inspirational to many glass scientists. It laid the foundation for increased activity in low gravity research on glass formation, measurements of the thermophysical properties of supercooled and non-equilibrium liquids, and research on processing of oxide materials in space. This talk will cover ongoing work with NASA using the Japanese Aerospace Exploration Agency (JAXA) Electrostatic Levitation Furnace (ELF). A variety of molten metal oxides are being investigated in experiments on the International Space Station. Low gravity suppresses buoyancy driven fluid motion so that heat and mass transport occur in nearly diffusion-controlled conditions. Containerless processing using the JAXA ELF enables access to deeply supercooled liquids and glass formation from very fragile liquids. The density, surface tension and viscosity of the stable and supercooled liquids is being measured using imaging techniques. Similarities and differences between Earth and space-made glasses will be described. The work will be discussed in the context of developing new types of glass for use on Earth, processing glass materials in space for value added manufacturing, and utilizing locally available materials for human exploration of the Moon, Mars and beyond. Work supportted by NASA under grants 80NSSC19K1288 and 80NSSC18K0059.

11:00 AM

(GOMD-S5-004-2024) What to consider when developing future bioactive glasses? (Invited)

L. Hupa*[1]

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

Bioactive glasses were reported for bone tissue applications in 1969. Since then, myriad compositions within the silicate, phosphate, and borate glass families have been tested for their potential application in tissue engineering. Professor Day has been a pioneer in developing glasses for challenging environments. Only a few compositions have been widely used in clinical applications. However, their long-term behavior in the human body is still to be better understood, especially when applied in product forms and indications not tested before. The current research focuses on doping the glasses with additional elements present as trace elements in the body, including some considered toxic or harmful in other implant materials. This presentation discusses the factors to be considered when tailoring and developing new bioactive glass compositions for specific indications. Special attention is paid to dynamic in vitro tests for an enhanced understanding of the dissolution of glasses. The efforts should favor modeling tools and artificial intelligence to screen the compositions with the best potential and to minimize the clinical tests. Also, early implementation of appropriate regulatory aspects supports the transfer of the results to practice and material industrial production. Finding reliable tools for understanding the properties of bioactive glasses – both the current utilized and new formulations – is central to the sustainable development of new implant materials.

11:30 AM

(GOMD-S5-005-2024) Investigating the Crystallization Kinetics of $Na_2O.B_2O_3$ Glass Embedded with Cerium Oxide Nanoparticles

K. S. Ranasinghe*[1]; E. Manqueros[1]

1. Kennesaw State University, Physics, USA

The effect of CeO_2 doping on the development of Cerium Oxide Nanoparticles on the $Na_2O.B_2O_3$ Glass was investigated. While four main nanoceria structures were observed through Transmission Electron Microscopy, only two crystal growth peaks were identified when the glass was analyzed using Differential Thermal Analysis. The peak points of crystal growth for the parent $Na_2O.B_2O_3$ glass were obtained at 565C. However, upon heat treatment at 150C, the crystallization peaks of the parent glass diminished. Two additional crystal growth curves emerged, reaching peaks at 590C and 630C. Similar behaviors were observed for different heat treatment temperatures indicating structural changes and growth of ceria crystals on $CeO_2(Ce^{4+})$ and $Ce_2O_3(Ce^{3+})$ nanocrystals. Raman spectroscopy shows the development of the B-O-Ce bond within the glass structure, and the crystal formation changes with the ratio of Ce^{3+}/Ce^{4+} nanoparticles.

S1 Fundamentals of the Glassy State

Session 2: Glass Crystallization and Glass-Ceramics II

Room: Bel Air II

Session Chairs: Ashutosh Goel, Rutgers University; Alfonso Pedone, University of Modena and Reggio Emilia

1:20 PM

(GOMD-S1-012-2024) Exploring homogeneous and surface nucleation in silicate glasses: insights from atomistic modeling and the Metadynamics approach (Invited)

F. Lodesani*[1]; A. Pedone[2]; S. Urata[1]

1. AGC, Innovative Technology Laboratories, Japan
2. University of Modena and Reggio Emilia, Italy

Studying crystallization in glass-forming liquids is a challenging yet crucial aspect for controlling the production of high-performance glass ceramic materials and preventing glass devitrification. Nucleation is a key step of the process, which can occur homogeneously in the bulk, heterogeneously at the interface, or from defects within the structure. All the processes occur at a nanoscopic level, and therefore it is experimentally difficult to understand. Molecular dynamics (MD) simulation has emerged as a valuable tool for studying glasses properties and gaining insights into crystallization-related phenomena. By creating models of the glass and crystalline phases, as well as their interfaces or inserting crystalline seeds into a glass matrix, thermodynamic features can be extracted. These findings can be combined with theory to support and clarify experimental observations. However, due to the high viscosity of these systems, MD simulation alone cannot fully uncover the crystallization pathway. To overcome this limitation, Metadynamics has been employed. It involves introducing a bias potential during the simulation to promote a specific process. We have investigated the crystallization of lithium disilicate in the bulk and in the presence of a nucleating agent, P_2O_5. Metadynamics identified different nucleation pathways, and nucleation barriers were estimated.

1:50 PM

(GOMD-S1-013-2024) Machine-learned tracking of Seeded Crystal Growth in glass

R. Thapa*[1]; M. E. McKenzie[2]; E. J. Musterman[3]; J. Kaman[1]; H. Jain[1]; V. Dierolf[4]

1. Lehigh University, Material Science and Engineering, USA
2. Corning Incorporated, USA
3. Brookhaven National Laboratory, USA
4. Lehigh University, Physics, USA

To describe the transformation of glass to crystal fully, a quantification of the degree of crystallinity is required as the system moves from a disordered state to an ordered crystalline phase. Various attempts have been made in this regard with the Steinhardt bond-orientational order parameters being the most common. Before Steinhardt, Mandell et al. used the idea of local structure-function to identify crystalline nuclei. After Steinhardt, ten Wolde et al. extended the idea of bond-orientational order parameters to identify individual solid-like particles. All these parameters are based entirely on the atomic arrangement within the system and contain no information about the dynamics of the ordered and disordered states. Since the crystallization of glasses is a high-temperature phenomenon, the dynamics of the atoms also become an important variable to be considered. We developed a machine-learned (ML) framework for classifying atoms as crystal-like or glass-like based on a set of structural and dynamic characteristics. The Kmeans clustering algorithm is used to determine what cluster an atom belongs to entirely based on the feature vector of that atom. We have used this algorithm to study the seeded crystal growth on lithium niobate crystal in lithium niobate glass. The predictions made by the ML classification scheme helped us determine the crystal growth rate and its dependence on the initial seed size, seed geometry, and the effect of periodic boundary conditions.

2:10 PM

(GOMD-S1-014-2024) Computational study of fracture in lithium aluminosilicate glass-ceramics

D. Sun*[1]; M. M. Smedskjaer[1]

1. Aalborg Universitet, Denmark

Crystals in glass-ceramics can induce crack deflection and diversion to impede crack propagation and consequently improve the fracture toughness compared to that of the parent glass. However, the structural details of these phenomena are not yet fully understood. Here, we simulate the fracture behavior of lithium aluminosilicate glass-ceramics with different crystallinity using molecular dynamics. We analyze the fracture data using a classification-based machine learning method to compute the so-called ’softness’ metric. We find that the tendency of Al atoms to undergo bond switching events increases with the increase in the softness of Al atoms, which is manifested by frequent bond switching and rearrangements of Al ions during the fracture process. Cracks tend to expand along the path of the ’soft’ Al atom distribution. These results can help guide the future design of optimized microstructures of glass-ceramics with high fracture resistant.

2:30 PM

(GOMD-S1-015-2024) ZrO2-SiO2 nanocrystalline glass-ceramics (Invited) *WITHDRAWN*

W. Xia*[1]

1. Uppsala University, Materials Science and Engineering, Sweden

Developing superior materials to replace our damaged teeth is an ongoing challenge. Glass ceramic (GC) is a prominent material extensively utilized in dental restoration. One well-known material is lithium disilicate-based GC, recognized for its balanced strength and translucency; however, there is room for strength improvement. Zirconia full ceramics exhibit superior flexural strength and toughness, but their translucency is less promising. The fundamental question arises: can we discover a material that seamlessly combines the translucency of GC with the robustness of zirconia ceramics? In this study, the GC raw powders were synthesized through a sol-gel process, followed by sintering using different methods, i.e. spark plasma sintering, lasering sintering and ultra-fast high-temperature sintering, for GC samples. It was established that both zirconia concentration and the microstructure of the zirconia/silica GCs played crucial roles in determining translucency and mechanical strength. A threshold of zirconia concentration was identified concerning mechanical strength. The regionally ordered structure was identified as contributing significantly to the outstanding combination of translucency and flexural strength observed in the GCs. Our research unveiled a novel GC incorporating nano zirconia in a silica matrix, demonstrating promising translucency along with high flexural strength and toughness. This suggests a promising amalgamation of GC for dental applications.

Session 5: Data-based Modeling and Machine Learning for Glass Science

Room: St. Andrews
Session Chairs: Daniel Cassar, Vitreous Materials Laboratory; N M Anoop Krishnan, Indian Institute of Technology Delhi; Xiaonan Lu, Pacific Northwest National Lab

1:20 PM

(GOMD-S1-016-2024) Applications of Machine-Learning Potentials for modeling borate glasses (Invited)

S. Urata*[1]

1. AGC Inc., Innovative Technology Research Center, Japan

Recent applications of machine-learning potentials (MLPs) in modeling boron-containing glasses are introduced, and the model accuracies are compared with experiments and available analytical force fields. In addition, we will compare a commercial MLP with our own MLPs for modeling alkaline borate glasses. Specifically, MLPs provide improved estimations of 3 and 4-fold coordinated boron ratios and generate a higher number of three-membered rings compared to analytical force fields. This enhanced accuracies in structural modeling enabled us to observe variations in boron coordination and the generation of three-membered rings during uniaxial tensile and compressive deformations.

1:50 PM

(GOMD-S1-017-2024) Insights Into Glass Element Dissolution Rate: A Machine Learning Approach for Predicting and Interpreting Dissolution Rate of Glass

S. Mannan*[1]; N. Gosvami[3]; M. Bauchy[2]; N. Krishnan[1]

1. Indian Institute of Technology Delhi, Department of Civil Engineering, India
2. University of California, Los Angeles, Civil and Environmental Engineering Department, USA
3. Indian Institute of Technology Delhi, Department of Materials Science and Engineering, India

The long-term chemical resistance of glass is crucial in nuclear waste immobilization. However, understanding the dissolution rate of glass, considering its composition, pH, and temperature, is challenging due to its complex and non-linear relationship. To address this, we have curated a large dataset of approximately ~2100 glass compositions along with corresponding pH and temperature values. Furthermore, we use different machine learning models (Artificial Neural Network and Xg-Boost) to exploit the inherent relationship between composition, temperature, and pH to predict glass dissolution rates. The results show that the Xg-Boost model performs well and predicts the dissolution rate with reasonably good accuracy with a training score R^2 value greater than 0.9. Further, we investigated the composition, pH, and temperature dependency using a game theory-based SHAP approach. In addition, we converted the

composition into different descriptors to train a universal model that allows prediction for completely unseen compositions beyond the training set. It has been demonstrated that descriptor-based models predict as effectively as compositional-based models, suggesting their potential use as a generalized model for predicting dissolution rate. Finally, we derive the functional form of the dissolution rate in terms of different descriptors via symbolic regression to calculate the dissolution rate for any glasses.

2:10 PM

(GOMD-S1-018-2024) Machine Learning simulation of Mg-silicate 29Si NMR spectra for large models

M. Bertani*[1]; A. Pedone[1]; F. Faglioni[1]; T. Charpentier[2]

1. University of Modena and Reggio Emilia, Departement of Chemical and Geological Sciences, Italy
2. CEA, DRF/IRAMIS/NIMBE/LSDRM, France

he simulation of NMR spectra is fundamental for the interpretation of experimental data and can unveil the relation between NMR signal and glass structure. These simulations are based on expensive DFT calculations that limit the application to small systems (~1000 atoms). Machine Learning (ML) algorithms can be used as a valuable tool to overcome this limitation and extend the NMR calculations to larger systems with low computational cost and high accuracy. To do so, the ML model is trained with accurate input-output couples coming from DFT calculations on small structures. The local environment of each Si atom was encoded into the smooth overlap of atomic positions (SOAP) descriptor, whose parameters have been optimized in this work. The ML algorithm applied was a Least Square Support Vector Regression based on a Kernel Ridge Regression (LSSVR-KRR) which exploits the so-called "Kernel trick". The database comprises structures extracted from MD simulations of 5 (Na, Mg)-silicate glasses with different [MgO]/[Na O] ratios. Structures were extracted at 1000, 300, and 0K using three different interatomic potentials. The trained model gave a mean absolute error of 1.46 ppm on the external test set and was successfully applied to simulate the Si MAS NMR spectra of larger simulation boxes containing up to 20k atoms using the full low-temperature trajectory overcoming the possibility of DFT calculations.

2:30 PM

(GOMD-S1-019-2024) Extracting materials tetrahedron of inorganic glasses using natural language processing

M. Zaki*[1]; K. Hira[2]; M. Mausam[2]; N. Krishnan[1]

1. Indian Institute of Technology Delhi, Civil Engineering, India
2. Indian Institute of Technology Delhi, Yardi School of Artificial Intelligence, India

Developing novel glasses for tailored applications requires the application of machine learning (ML) to predict their properties under different processing and testing conditions. However, the major limitation is the availability of such databases. Natural language processing (NLP) is an approach which deals with organizing large amounts of unstructured (e.g. text) and structured data (e.g. tables) into desired formats. In this work, we use NLP tools like language models (MatSciBERT, a materials domain language model), and DiSCoMaT (graph neural network-based pipeline for extracting materials compositions from research paper tables) to autonomously create the largest database of inorganic glasses. We extract ~250,000 material compositions, their properties, processing, and testing protocols from respective research papers published in Elsevier journals. We also compare the extracted information with compositions present in SciGlass and INTERGLAD databases, which are currently the largest databases used by glass researchers for the ML-aided design of tailored glasses. Our proposed approach has resulted in the extraction of ~100,00 unique glass compositions and properties as compared to existing databases. This new database will help the researchers to update and improve the existing ML models for predicting the properties of glasses and facilitate their rational design.

2:50 PM

(GOMD-S1-020-2024) Novel approaches to informatics-driven nuclear waste form design: Dataset curation, surrogate modeling, and sequential learning (Invited)

S. Allec*[1]; V. Hegde[1]; M. Peterson[2]; X. Lu[2]; B. J. Riley[2]; T. S. Mahadevan[3]; J. Kalahe[3]; J. Du[3]; J. Vienna[2]; J. E. Saal[1]

1. Citrine Informatics, External Research Department, USA
2. Pacific Northwest National Laboratory, Energy and Environment Directorate, USA
3. University of North Texas, Materials Science and Engineering, USA

Informatics-driven approaches have demonstrated potential to drastically accelerate next-generation materials design. However, there remain certain families of materials that have not benefited as extensively from such approaches due to their extreme complexity, of which nuclear waste form materials are a prime example. In this case, difficulties in informatics-driven design primarily arise from (i) a vast and complex design space (in terms of chemistry, phase, and microstructure) that spans glasses, ceramics, and glass-ceramic composites, and (ii) a lack of data for a unique set of materials properties related to time-dependent properties (e.g., degradation) and radiation effects. Nonetheless, there is a plethora of literature on informatics-driven glass science that is relevant to nuclear waste form design. While many of these models were trained to predict a single property on a specific family of glasses (e.g., borosilicates), a recently developed multi-task deep neural network model, GlassNet, has been trained on the entire SciGlass database to predict 85 glass properties with high accuracy on most properties. Here, we explore the applicability of GlassNet to potential iron phosphate nuclear waste forms, assessing its ability to predict glass stability as a surrogate property for glass forming ability, as well as the usefulness of its predicted properties as input features for predicting solubility.

S2 Glass and Interactions with Its Environment Fundamentals and Applications

Session 1: Glasses, Glass-Ceramics, and Glass-Based Biomaterials

Room: Bel Air I
Session Chair: Leena Hupa, Åbo Akademi University

1:20 PM

(GOMD-S2-011-2024) Design of bioactive glasses for soft tissue engineering – Challenges and future research directions from the perspective of a materials scientist (Invited)

A. Goel*[1]

1. Rutgers University, USA

The concept of third-generation biomaterials is based on the principle of activating a synchronized sequence of genes at the cellular level to stimulate the regeneration of living tissues. Accordingly, the third-generation bioactive glasses are expected to (1) be fully biodegradable; (2) release functional ions in a controlled manner while matching their dissolution rate with the recovery rate of the injured tissue; and (3) not promote calcification of tissues and cytotoxicity. While considerable effort is being made to design and develop these glasses, there are several challenges – at a fundamental level – that need to be addressed to achieve this goal. The presentation will discuss a few of these challenges and open questions from the perspective of glass science and propose the topics on which future research needs to be directed to accomplish the abovementioned goals.

1:50 PM

(GOMD-S2-012-2024) Glasses and Glass-Ceramics in Dentistry

H. Kamat*[1]

1. Glidewell Laboratories, Research & Development, USA

Glasses and glass-ceramics are widely used in restorative dentistry due to their natural tooth-like appearance, good mechanical strength, and excellent biocompatibility which minimizes allergic reactions. Depending on the intended use, the composition of the base glass, and its heat-treatment cycle, needs to be tailored to nucleate targeted crystalline phases and control the microstructure of the final glass-ceramic. This, in turn governs the optical, mechanical, and thermal properties of the final device. The as-derived glass-ceramic can then be utilized for manufacturing durable permanent restorations, either as all-ceramic or hybrid constructions fused to metal or ceramic. This presentation will delve into the design criteria, encompassing factors like base glass composition and processing techniques, employed in the synthesis of glass-ceramic-based dental restorations. Additionally, glasses and glass-ceramics find utility in accessory dental products such as glaze and stains. These are used to either conceal the opaque appearance of metal/ceramic substructures or impart gloss, color, and translucency gradient to both single as well as multi-unit restorations, including full arches. The presentation will also address challenges encountered during the processing of such glass/glass-ceramic-based glazes and stains, and discuss their work-flow in dentistry.

2:10 PM

(GOMD-S2-013-2024) The Remineralising Ability of a Fluoride-Containing Bioactive Glass Composite for Preventing Recurrent Decay (Invited)

M. Tiskaya*[1]; s. Shahid[1]; R. Hill[1]

1. Queen Mary, University of London, Institute of Dentistry, United Kingdom

Objectives: Recurrent decay is the main cause of failure of white fillings, resin-based dental composites (RBC), due to polymerization shrinkage of the material, resulting in a gap at the tooth-material interface. The aim of this study was to investigate the bioactive properties of an experimental bioactive glass (BAG) containing RBC (BAG-RBC). Methods: Discs of BAG-RBCs were prepared and immersed into artificial saliva pH7 (AS7) and pH4 (AS4) for up to 6 months and characterized post-immersion using ATR-FTIR, XRD and NMR. The ion concentrations in the supernatant solutions were analysed using inductively coupled plasma-optical emission spectrometry (ICP-OES) and an ion selective electrode (ISE). The remineralisation was also assessed on extracted tooth with an artificial decay using X-ray microtomography (XMT). Results: ATR-FTIR, XRD and NMR detected the formation of apatite post-immersion for BAG-RBCs, which increased over time. There was a greater release of therapeutic ions (F^-, Ca^{2+} and PO_4^{3-}) in AS4 compared to AS7. SEM indicated apatite precipitation on the cross section upon immersion and XMT line profiles suggested an increase in mineral density at the carious lesion, suggesting remineralisation. TP did not show any evidence of remineralisation. Conclusions: The studied BAG-RBCs released beneficial ions, neutralized the pH in acidic conditions and the apatite layer formed could potentially occlude the marginal gap to prevent secondary caries and promote remineralization.

2:40 PM

(GOMD-S2-014-2024) Aging Behavior of Copper Oxide-Doped Alumina Toughened Zirconia Ceramic Composites

M. Abbas*[1]

1. Qatar University, Center for Advanced Materials, Qatar

The effects of copper oxide doping on the ageing behaviour alumina-toughened zirconia (ATZ) was investigated. The undoped and doped ATZ composites were conventionally sintered within the temperature range of 1250°C to 1500°C, employing a holding time of 12 minutes. The hydrothermal ageing experiment was conducted under autoclave conditions with distilled water, heated to 180°C at 10 bar, for durations extending up to 100 hours. The tetragonal phase stability and microstructural evolution of the samples were studied. The analysis of X-ray diffraction indicated the stability of the tetragonal phase in samples sintered up to 1450°C, even after 100 hours of exposure. For samples sintered at 1500°C, both undoped and doped samples retained their tetragonal phase for up to 3 hours but experienced a phase transformation after 10 hours. Initially, CuO-doped ATZ showed lower monoclinic content, progressively increasing with aging. In contrast, undoped ATZ exhibited better aging resistance, maintaining around 40% monoclinic content after 100 hours. Microstructural images indicated changes in surface roughness caused by the transformation of tetragonal grains to monoclinic grains. Fracture analysis of the aged samples identified the presence of macrocracks and microcracks on the transformed surface layer. The study's conclusion highlighted that doping with 0.2wt% CuO did not prevent low-temperature degradation (LTD) at elevated temperatures.

Session 2: Dissolution and Interfacial Reactions

Room: Turnberry
Session Chair: Jincheng Du, University of North Texas

1:20 PM

(GOMD-S2-015-2024) Role of Al on the chemical durability of SiO_2-B_2O_3-Al_2O_3-CaO-Na_2O glasses (Invited)

J. Delaye*[1]; K. Damodaran[1]; S. Tiwari[1]; M. Taron[1]; S. Gin[1]

1. CEA Marcoule, DPME, France

It has been shown experimentally that Al_2O_3 has a great impact on the chemical durability of SiO_2-B_2O_3-Al_2O_3-CaO-Na_2O glasses In glasses with a low Al_2O_3 content, a rapid release of Si into the solution is observed, followed by a sudden stop of the glass alteration. Conversely, glasses with a higher Al_2O_3 content exhibit a longer period before the Si and B releases into the solution diminish. To gain deeper insights into these experimental findings, classical molecular dynamics (MD) simulations were conducted using potentials fitted to simulate SiO_2-Al_2O_3-CaO-Na_2O glasses in contact with water. Employing the Potential Mean Force method to simulate hydrolysis processes enabled us to explain the impact of Al on glass durability. Specifically, we noted that an increase in the Al_2O_3 content in the glass composition resulted in a substantial augmentation of hydrolysis energies within the Si local environments. Simultaneously, the energy required to reform the Si-O bonds decreased. Utilizing a new Monte Carlo approach capable of simulating glass alteration by modeling both water diffusion within the glass and hydrolysis mechanisms, various alteration scenarios were explored in SiO_2-B_2O_3-Al_2O_3-Na_2O glasses. The calculations suggest that a rapid release of Si into the solution can result in the formation of a Si-enriched and dense external layer, contributing to a quick reduction of the alteration rate.

1:50 PM

(GOMD-S2-016-2024) Impact of the aluminum coordination on the dissolution kinetics of magnesium aluminoborosilicate glasses *WITHDRAWN*

A. Jose*[1]; Q. Qin[1]; R. Youngman[2]; G. Tricot[3]; A. Goel

1. Rutgers University, USA.
2. Corning Incorporated, USA
3. LASIR - Laboratoire de Spectrochimie Infrarouge,France.

Aluminum is known to exist in four, five and six coordination in the structure of glasses, where their fraction is governed by the non-framework 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 longstanding point of discussion in the glass community. In this work, we aim to elucidate the impact 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 behaviour of glasses has been studied at pH = 2 in HCl solution over a period of 21 days followed by the characterization of post-dissolution glasses and liquid aliquots using XRD, MAS NMR spectroscopy, XPS and ICP-OES.

2:10 PM

(GOMD-S2-017-2024) Role of B on borosilicate glass dissolution (Invited)

S. Gin*[1]; S. Narayanasamy[1]; M. Taron[1]; J. Delaye[1]

1. CEA - University of Montpellier, ISEC/DPME, France

In borosilicate glasses, boron preferentially forms Si-O-B bonds over B-O-B bonds. Furthermore, these bonds are more hydrolysable than Si-O-Si bonds. It has long been recognized that the addition of boron to a silicate glass tends to decrease its chemical durability. In the initial dissolution regime, the effect of boron depends on its content in the glass as well as its coordination, with trigonal boron being more hydrolysable than tetragonal boron. In the residual rate regime, characterized by the formation of more or less passivating alteration layers, boron plays a crucial role. It is responsible for the majority of the gel's porosity, contributes to the reorganization of the gel through the condensation of silanol groups, and exhibits slow diffusivity within the gel. Consequently, under certain conditions, boron may be trapped in nanoporosity, leading to an enhanced passivation effect of the gel. Based on a study of ISG glass, it has been suggested that the residual dissolution rate of the glass is limited by the hydrolysis of Si-O-B bonds in a pH range from 3 to 9. In this presentation, we discuss this hypothesis by comparing glasses with different B contents. An analytical model is currently being developed to account for glass passivation by the gel, incorporating the effect of boron.

2:40 PM

(GOMD-S2-018-2024) The Current Understanding of Stage III Behavior on Long-Term Glass Corrosion

J. V. Crum*[1]; B. Parruzot[1]; S. Kerisit[1]; J. T. Reiser[1]; R. Daniel[1]; J. Neeway[1]; G. L. Smith[1]; M. Asmussen[1]

1. PNNL, USA

Stage III glass corrosion behavior is caused by the formation of secondary phases, typically zeolites, and occurs in long-term static corrosion tests as an increase of the corrosion rate after the glass has reached pseudo-equilibrium with solution. Secondary phase formation consumes components from the static dissolution system, which disrupts the pseudo-equilibrium (alteration layers and solution chemistry) that naturally slows the corrosion rate of glass with time. Stage III behavior has been observed to rapidly corrode glass during static dissolution testing at 70°C and 90°C and vapor phase hydration testing > 150°C. The sink phases formed in these tests are like those observed at lower test temperatures and in natural low-temperature systems. For this reason, Stage III behavior is an uncertainty that must be captured when predicting the long-term performance of glass in a low-temperature disposal environment. We will present the results of static dissolution tests seeded with P2 zeolites versus glass composition and temperature (22°C - 90°C). Results include corrosion rates, durations of Stage III behavior, final alteration products, and identification of alteration products responsible for Stage III behavior. These seeded static dissolution test results will also be compared to past vapor phase hydration test results. Lastly, we will discuss how the magnitude and sustainability of seeded Stage III behavior are affected by glass composition and reaction temperature.

S3 Optical and Electronic Materials and Devices Fundamentals and Applications

Session 5: Rare-earth and Transition Metal-doped Glasses and Ceramics for Photonic Applications II

Room: Shoal Creek
Session Chairs: Doris Möncke, Alfred University;
Volkmar Dierolf, Lehigh University

1:20 PM

(GOMD-S3-005-2024) Using the luminescence of Nd^{3+} and Eu^{3+} to understand local stress and density in glass (Invited)

D. de Ligny*[1]; M. Bergler[1]; F. Werr[1]; A. Veber[3]; K. Cvecek[2]; M. Schmidt[2]

1. University Erlangen-Nürnberg, Materials Sciences and Engineering, Germany
2. Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Photonische Technologien, Germany
3. Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Although usually considered to be insensitive to their environment, the luminescence of rare earth elements shows significant changes in their emission with pressure and temperature when their local environment is modified by elastic or plastic deformation. It is then an unexpected possibility to use them as local structural probes or pressure gauges if appropriate calibration curves are available. A new series of soda-lime glass, naturally doped with Nd and doped with 0.2 wt% Eu_2O_3, was densified to 21 GPa in a multi-anvil press. In parallel, samples with different fictive temperature were prepared. The densities of all these millimetre-sized samples were accurately measured using a floatation method. Complementary experiments using a uniaxial press and a hot stage allowed the dependence of luminescence on pressure and temperature to be determined in the elastic regime. All samples were characterised by Eu3+ and Nd3+ emission as well as by Raman and Brillouin spectroscopy. The evolution of the spectra was evaluated using integration methods to reduce error bars. The luminescence versus density curves obtained show very good discrimination between elastic and plastic behaviour as well as between thermal and pressure induced evolutions. The Nd^{3+} emission was found to be the most sensitive calibration. These new calibration curves are finally used to characterise glass under extreme processing conditions such as tempering, aerosol deposition, laser writing or laser cutting.

2:00 PM

(GOMD-S3-006-2024) Spectroscopic studies of rare-earth titanate glasses

B. Topper*[1]; A. Neumann[3]; S. K. Wilke[2]; A. Al-Rubkhi[2]; M. Pettes[4]; D. Möncke[6]; A. Mafi[5]; R. Weber[2]

1. Clemson University, USA
2. Materials Development, Inc., USA
3. Center for High Technology Materials, USA
4. Center for Integrated Nanotechnologies, Materials Physics and Applications Division, USA
5. University of Kansas, USA
6. Alfred University, USA

Lanthanum titanate glasses have been studied in detail with fluorescence spectroscopy spanning the visible to mid-infrared. Erbium has been studied extensively in singly doped as well as co-doped systems with Nd^{3+} or Pr^{3+}. The introduction of a small amount of Pr^{3+} effectively removes the bottleneck of the lower laser level, yielding a promising outlook for a MIR Er^{3+} based laser. Ytterbium fluorescence at 1-micron was studied as a function of temperature as well as excitation wavelength, yielding the variation in the Stark splitting of the Yb^{3+} ion in the $17La_2O_3$-$83TiO_2$ host. Nonlinear refraction and absorption were investigated in the undoped base glass with 550 picosecond pulses at 532 nm with variable intensities between 0.25-2.5 GW/cm^2. An effective nonlinear refraction coefficient of 85 x 10^{-13} esu and two-photon absorption coefficient of 2.2 cm/GW were measured. The stimulated Raman gain of the base glass is approximately 60 times higher than that of silica (suprasil) at 532 nm. Vibrational spectroscopies (Raman, infrared) are used to probe influence of rare-earth type and quantity on the glass structure.

2:20 PM

(GOMD-S3-007-2024) Radiation response properties of strontium fluoride translucent ceramics with a luminescence center

N. Kawano*[1]; T. Kato[2]; R. Conner[3]; L. G. Jacobsohn[3]; K. Ichiba[2]; K. Okazaki[2]; Y. Takebuchi[2]; D. Nakauchi[2]; T. Yanagida[2]

1. Akita University, Japan
2. Nara Institute of Science and Technology, Japan
3. Clemson University, USA

Radiation dosimetry technology has been intensively used to determine ionizing radiation dose in diverse applications, including in the form of imaging plates. It often utilizes luminescence materials that can absorb incident ionizing radiation followed by thermally-stimulated luminescence (TSL) or optically-stimulated luminescence (OSL) readout using thermal or optical energy external stimulation, respectively. Recently, transparent ceramics have gained research attention for use as luminescent materials since they tend to show more intense TSL and OSL signals than their single crystal counterparts. In this work, we fabricated strontium fluoride translucent ceramics by the spark plasma sintering method with Tb^{3+} as the engineered luminescence center. Their scintillation and dosimetry properties were evaluated, revealing these ceramics to have efficient TSL and OSL signals related to the 4f-4f transitions of Tb^{3+} ions.

2:40 PM

(GOMD-S3-008-2024) Processing and properties of neodymium doped alumino-phosphate laser glasses

C. Guillet[1]; M. Muñoz-Quiñonero[1]; J. Azkargorta[2]; I. Iparraguirre[2]; R. Jiménez-Riobóo[3]; J. Fernández[4]; R. Balda[2]; F. Munoz*[1]

1. Institute of Ceramics and Glass, CSIC, Spain
2. University of Basque Country, Applied Physics, Spain
3. Institute of Materials Science of Madrid (CSIC), Spain
4. Donostia International Physics Center, Spain

One of the most important drawbacks for the preparation of high-quality phosphate laser glasses lies in their ability to retain water during the melting process. We have managed this issue through a preparation procedure that consists of a second melting under a constant flow of N_2 using a graphite crucible, that allows the preparation of glasses with very low final water contents and a high degree of homogeneity. In this work, we present the results of the dehydroxylation processing in alumino-phosphate glasses by studying factors such as melting temperature, time or mass of remelted glass. The study of the processing parameters of the dehydroxylation method used for these glasses agrees with a linear decrease of the water content with the melting temperature and shows to depend on the diffusion coefficient of the water in the melt through the viscosity. Furthermore, the spectroscopic properties of Nd^{3+} ions as well as the main thermomechanical properties of glasses of the system Na_2O-K_2O-BaO-Al_2O_3-P_2O_5-Nd_2O_3 with increasing contents of Al_2O_3 will be shown.

S5 Delbert Day Honorary Symposium

Session 5. Delbert Day Honorary Symposium

Room: Peeble Beach
Session Chairs: Kisa Ranasinghe, Kennesaw State University; Qiang Fu, Corning Incorporated

1:20 PM

(GOMD-S5-006-2024) Development of Bioactive Borate Glasses for Biomedical Applications (Invited)

M. N. Rahaman*[1]

1. Missouri University of Science & Technology, Materials Science & Engineering, USA

This presentation will provide a brief historical account of research into the development of bioactive borate glasses for biomedical applications, an area in which Delbert Day has had a significant impact. Topics that will be discussed include the conversion of borate glasses into biologically useful materials such as hollow hydroxyapatite microspheres; formation of borate-based glasses into scaffolds having appropriate porosity, strength and degradation rate for healing bone defects; use of borate glass microfibers in wound healing; and incorporation of borate glass particles into appropriate hydrogels to form injectable multifunctional implants.

1:50 PM

(GOMD-S5-007-2024) A New Network Connectivity Model for Predicting the Properties of Acid Degradable Silicate Glasses Containing Intermediate Oxides (Invited)

R. Hill*[1]

1. Queen Mary University of London, DPS, United Kingdom

Network Connectivity (NC) which is the average number of bridging oxygens per silicon has been used to predict the ability of bioactive glasses to dissolve and form apatite. More recently a modified NC model was developed to account for the presence of orthophosphate in bioactive glasses. This was called the Modified Network Connectivity or Split Network model. These models are now widely used in the literature. The present paper aims to further expand network connectivity models to glasses containing intermediate oxides that result in acid hydrolysable bonds within the glass. Here the NC is defined as the average number of bridging oxygens per silicon minus the average number of acid hydrolysable bonds. In the first instance the model will be applied to acid degradable calcium alumino-silicate glasses used to form dental cements using existing published data. In these glasses there are both non-bridging oxygens and acid hydrolysable Al-O-Si bonds. It will be shown the new NC model predicts the cement properties well. The new model will then be applied to conventional bioactive glasses containing ZnO that is thought to act like Al_2O_3 as an intermediate oxide. The model will be shown to predict the dissolution behaviour under both neutral and acidic conditions. Finally the advantages of this approach will be discussed with regard to the design of new degradable glasses.

2:20 PM

(GOMD-S5-008-2024) Bioactive Glasses for Regeneration of Large Segmental Bone Defects and Volumetric Muscle Loss (VML)

Q. Fu*[1]

1. Corning Incorporated, USA

Injuries to either hard (bone) or soft (skin and muscle) tissues have profound consequence in healthcare. Regeneration of large segmental bone defects and volumetric muscle loss (VML) remains a challenge for materials and medical sciences. Here we show that, through the use of bioactive glasses, effective bone healing and defect bridging can be achieved in a rabbit femur segmental defect model without growth factors or stem cells. We further demonstrate that faster muscle regeneration can be achieved in a VML model in rats. Considering these promising results, bioactive glass may serve as a potentially simple, novel, and safe means to regenerate damaged bone and muscles.

2:40 PM

(GOMD-S5-009-2024) Day Quixhote – Reintroducing a versatile material to a skeptical industry (Invited)

J. V. Ryan*[1]

1. Pacific Northwest National Lab, USA

In the United States, borosilicate glasses have been deemed the “best available technology” for nuclear waste immobilization. Did you know, though, that phosphate glasses were among the first vitreous materials studied for this application? Despite this early research, complications involving synthesis discouraged further study of what was a promising material. Later, when other persistent issues were experienced using borosilicate systems, Dr. Day saw the potential for phosphate glasses to solve many of the problems. While many of the key applications for phosphate glasses depend on their inherent solubility, particularly in medicine and bioengineering, Dr. Day led the charge to reintroduce these versatile compositions to the suite of durable wasteform options. This talk will explore the history of phosphate glass use in the nuclear industry and Dr. Day’s key role in advancing the science of these exceptional materials.

S1 Fundamentals of the Glassy State

Session 2: Glass Crystallization and Glass-Ceramics III

Room: Bel Air II
Session Chairs: Ashutosh Goel, Rutgers University;
Alfonso Pedone, University of Modena and Reggio Emilia

3:40 PM

(GOMD-S1-021-2024) Complementary scanning x-ray diffraction and fluorescence mapping for glass-ceramic characterization

E. J. Musterman*[2]; C. Barker[3]; K. J. Veenhuizen[4]; V. Dierolf[3]; H. Jain[1]; A. M. Kiss[2]

1. Lehigh University, Materials Science and Engineering, USA
2. Brookhaven National Laboratory, National Synchrotron Light Source II, USA
3. Lehigh University, Physics, USA
4. Lebanon Valley College, Physics, USA

Devitrification of glass can follow complex crystallization pathways producing a myriad of chemically and structurally distinct phases. Controlling these pathways can be used to engineer glass-ceramic microstructures with tailored mechanical, thermal, and optical properties, but predicting and characterizing the final microstructures can prove difficult. In this presentation, we will describe recent progress developing scanning x-ray diffraction mapping capabilities at the Submicron Resolution X-ray Spectroscopy beamline at the National Synchrotron Light Source II as a tool for characterizing glass-ceramic microstructures. These developments will be demonstrated with example laser-fabricated crystal architectures in glass. Structural characterization such as phase and orientation mapping with x-ray diffraction is complemented by simultaneous chemical mapping with x-ray fluorescence. This correlative approach further offers increased sensitivity relative to electron-microscopy based techniques which we demonstrate by mapping elemental gradients in and around the laser-fabricated crystal microstructures and by mapping changes in orientation across individual crystal grains. Simultaneous mapping of microstructure with relatively routine x-ray diffraction and fluorescence techniques at imaging and microscopy beamlines offers several benefits for understanding and optimizing crystallization of glass.

4:00 PM

(GOMD-S1-022-2024) Effect of nucleation crystal growth and incorporation of P_2O_5 and ZrO_2 in lithium disilicate dental glass ceramics

S. Abdelmaseh*[1]; M. Cicconi[1]; D. de Ligny[1]

1. Friedrich-Alexander-Universityet Erlangen-Neurnberg, Institute of Glass and Ceramics, Germany

The crystallization kinetics for four different glass compositions in the lithium silicate binary system, with SiO_2 content of ~ 60, 63, 67, 71 mol%, was investigated using non-isothermal techniques by DSC. The incorporation of 1 mol% of P_2O_5 was found to play an important role in improving the glass stability and stabilizing the crystallization of $Li_2Si_2O_5$. However, it was observed that P_2O_5 has no role as a nucleating agent since the crystallization of Li_3PO_4 starts at higher temperatures than $Li_2Si_2O_5$ and Li_2SiO_3. The incorporation of Zr_2O with different concentrations ~ 2, 4, 6, 8 mol% was carried out to study their effect on the crystallization mechanism and the microstructure. The glass structure and evolution of the crystalline phases were inspected using In-situ Raman spectroscopy and XRD. The integrated Raman-Brillouin-Calorimeter (ARABICA), in-house equipment, was used to simultaneously follow the effect of nucleation time and temperature on the phase stabilization and the evolution of the crystal phases, crystal size, and volume fraction, and therefore the elastic and mechanical properties. Optical analysis using SEM was employed to observe the microstructure and evaluate the crystallized volume fraction. The hardness and toughness were estimated using the Vickers indentation method. The results showing the crystallization kinetics, the effect of the nucleation process, and the main role of P_2O_5 and Zr_2O incorporation will be presented.

4:20 PM

(GOMD-S1-023-2024) Ultrafast crystallisation of lithium disilicate glass systems for dental application *WITHDRAWN*

J. V. Campos*[1]; I. R. Lavagnini[1]; A. Rodrigues[1]

1. Federal University of Sao Carlos, Materials Engineering, Brazil

This presentation introduces the innovative technique of “Flash Crystallization,” a novel approach that combines controlled electric fields and temperature to achieve ultrafast crystallization of lithium disilicate (LS2) glass systems, with promising applications in dentistry. Glass compositions resembling commercial Ivoclar e.max®CAD were melt-quenched into parallelepipedal moulds, and subsequent crystallized using both conventional and our novel approach. It was shown that LS2 can be rapidly crystallized to the disilicate phase at a furnace temperature of only 300 °C (even below the glass transition of 470 °C) within a few seconds. However, the conventional application of this method yielded unstable sample shapes due to hotspot formation during thermal runaway. “Power Ramp Flash Crystallization,” developed through finite element analysis, controls power injection as a ramp, preventing overheating and maintaining the original shape. Optimized crystallization parameters resulted in LS2 with small crystals (approx. 100 nm), Vicker’s hardness of 742 HV, and fracture toughness of 1.26 MPa m0.5.

Impedance spectroscopy, SEM, and XRD characterized the material. Results highlight the efficacy of Flash Crystallization in producing high-quality dental biomaterials. Its rapid processing and lower temperature needs position it as a promising method for dental prosthetics crystallization.

4:40 PM

(GOMD-S1-024-2024) Fast Crystallization below the Glass Transition

P. Lucas*[1]; W. Takeda[1]; J. Pries[2]; M. Wuttig[2]

1. Univ of Arizona, USA
2. RWTH Aachen University, Germany

Some glassy solids as fundamental as water or as technologically important as phase change materials do not exhibit a calorimetric phase transition when heated a conventional rates. The inability to observe a clear glass transition has in some cases led to controversies as in the case of water. Here we show that some poor glass-formers that have been hyperquenched undergo crystallization far below the glass transition fast enough to prevent calorimetric measurements of T_g as in the case of phase change materials and water. We present experimental evidence and modeling results to explain how these systems crystallize prior to reaching the glass transition. We note that this behavior is often observed in systems exhibiting a fragile-to-strong transition.

5:00 PM

(GOMD-S1-025-2024) Effects of Ion-Exchange on Soda-Lime Silicate Glass-Ceramics

Y. Shih*[1]; T. Huang[1]

1. National Taipei University of Technology, Department of Materials and Mineral Resources Engineering, Taiwan

The hardness of soda-lime silicate glass is significantly improved by the surface crystallization and the following ion-exchange process. In this work, the $0.15Na_2O-0.15CaO-0.7SiO_2$ soda-lime silicate (SLS) glass was crystallized after nucleation and growth. The surface crystallization with the major phase devitrite ($Na_2Ca_3Si_6O_{16}$) and the minor phase cristobalite was observed at the SLS glass ceramics (SLS-GCs). The SLS-GCs exhibit higher hardness than the pristine SLS glass; moreover, the hardness of SLS-GCs increases with increasing crystallinity, which was controlled by the duration of growth. The hardness of SLS-GCs was further improved by the ion exchange process with molten KNO_3 bath. The XRD patterns of chemically strengthened SLS-GCs indicate that the exchange of Na^+ and K^+ ions mainly occurred in the glassy phase. Meanwhile, the hardness increments of the chemically strengthened SLS-GCs are higher than that of the chemically strengthened SLS glass. The chemically strengthened SLS-GCs maintain at least 70% of the transmission under the visible light wavelength range, which is promising for the applications of electronic screens.

5:20 PM

(GOMD-S1-026-2024) Pores plague glass-ceramic

O. Peitl*[1]

1. Federal University of Sao Carlos, Materials Science Engineering, Brazil

Bubbles appear sometimes in glass-ceramics and degrade most properties, especially light transmission and fracture strength. In this work, we deduced microstructural conditions that trigger bubble genesis during crystallization of bubble-free glasses. We related bubble formation to some microstructural parameters in two model glass compositions that exhibit internal crystallization: $1.07Na_2O.2CaO.3SiO_2$ (1.07N2C3S) and $Li_2O.2SiO_2$ (L2S). In this way, we constructed bubble maps – experimental diagrams showing a region of bubble nucleation and growth in a crystal size versus crystallinity plot. Both glass-ceramics show bubbles having similar geometry that emerge from crystal/liquid interfaces and propagate into the residual liquid. These diagrams show that holes of the order of the crystal size tend to form in glass-ceramics containing a high-volume fraction crystallized (>50%) and relatively large crystal size (>10 μm). Mass spectroscopy experiments revealed that bubble formation in the 1.07N2C3S system is caused by O_2. We believe the knowledge generated by this work and resulting maps provide a very useful tool for the design of bubble-free glass-ceramics.

Session 5: Data-based Modeling and Machine Learning for Glass Science

Room: St. Andrews
Session Chairs: Daniel Cassar, Vitreous Materials Laboratory;
N M Anoop Krishnan, Indian Institute of Technology Delhi;
Xiaonan Lu, Pacific Northwest National Lab

3:40 PM

(GOMD-S1-027-2024) Waste Glass Formulation with Machine Learning: Optimization and Experimental Validation

X. Lu*[1]; J. Vienna[1]; V. Gervasio[1]; P. Ferkl[1]; M. Peterson[1]; L. Gunnell[2]; J. Hedengren[2]

1. Pacific Northwest National Lab, Energy and Environment Directorate, USA
2. Brigham Young University, Department of Chemical Engineering, USA

The US Department of Energy manages Hanford Site's nuclear waste, processing it into low-activity waste (LAW) and high-level waste fractions through vitrification methods. Previously, algorithms for LAW glass formulation were developed using traditional methods such as partial quadratic mixture (PQM) models. Since machine learning (ML) has been successfully used to predict glass properties, the objective of this study is to develop capability and evaluate the use of ML in waste glass formulation. In this proof-of-principle study, Gaussian process regression (GPR) models were fitted to glass properties (viscosity, chemical durability, etc.). GPR models with comparable performance to PQM models were obtained. An optimization program was then developed to formulate glass compositions to maximize waste loading while satisfying property constraints within model prediction uncertainties. Slightly higher waste loadings were achieved using the ML-based method. Experimental characterizations were conducted to validate the GPR property models, where the results were then used to update the models. Compared to the previous glass design framework, the ML-based optimization methods offer improved glass designs and a streamlined approach to generation of optimally designed data and near real-time updates. Through this approach, substantial manual effort can be reduced and improved model predictions can be achieved following the incorporation of additional data by experimental validation.

4:00 PM

(GOMD-S1-029-2024) Structures and properties of sodium phosphate and iron phosphate glasses from molecular dynamics simulations

J. Du*[1]; J. Kalahe[1]; N. Marchin[1]; X. Lu[2]; J. Vienna[2]; B. J. Riley[2]

1. University of North Texas, Materials Science and Engineering, USA
2. Pacific Northwest National Lab, USA

Phosphate glasses draw considerable recent attention due to their applications in biomedicine, nuclear waste disposal, laser glass and low melting sealing glasses. The properties of phosphate glasses can be tailored by addition of modifier oxides and properties such as chemical durability modified for different applications. In this talk, I will present our recent studies to understand the structural changes of phosphate glasses due to addition of sodium oxide and iron oxide by using molecular dynamics simulations with two-body and three-body potentials with effective charges. Physical properties such as glass transition temperature and elastic moduli were calculated. Comparison with experimental results was performed and differences discussed. The results provide insights on the short and medium range structures of phosphate glasses that help to understand their composition-property relations.

4:20 PM

(GOMD-S1-030-2024) Method of Dimensionality Reduction of Labelled Data and an Application to Nuclear Waste Glass Nepheline Crystallization

N. A. Mecholsky*[1]; K. Gilbo[2]; I. Pegg[1]

1. The Catholic University of America, Vitreous State Laboratory and Department of Physics, USA
2. The Catholic University of America, Vitreous State Laboratory, USA

Data sets with a high-dimensional domain are increasingly important in today's data-rich world. However such high-dimensional data sets provide an obstacle for analysis since visualization is, for the most part, restricted to a few dimensions. A good example is data for crystallization of nepheline ($Na_3KAl_4Si_4O_{16}$) upon slow cooling (i.e., Canister Centerline Cooling) of nuclear waste glasses, which comprises labeled glass compositions where nepheline either crystalizes or does not crystalize when cooling. In this work we explore new methods including utilizing coordinatizations of the Grassmannian to find easily separable low-dimensional representations of this labeled data in order to find a low-dimensional predictive model, such as a Support Vector Machine, to classify and predict nepheline formation in unclassified glasses.

Session 8: Chalcogenide and phase change materials: Theories, electronic, and thermal properties

Room: Bel Air I
Session Chair: Shuai Wei, Aarhus University

3:40 PM

(GOMD-S1-031-2024) A machine-learning interatomic potential for the $Ge_2Sb_2Te_5$ phase change compound (Invited)

O. Abou El Kheir[1]; L. Bonati[2]; M. Parrinello[2]; M. Bernasconi*[1]

1. University of Milano-Bicocca, Materials Science, Italy
2. Italian Institute of Technology, Atomistic Simulations, Italy

In the last fifteen years atomistic simulations based on density functional theory (DFT) have provided useful insights on the structural and functional properties of chalcogenide alloys of interest for applications in phase change memory devices. However, several key issues such as the effect of confinement and nanostructuring on the crystallization kinetics, just to name a few, are presently beyond the reach of DFT simulations. A route to overcome the limitations in system size and time scale and enlarge the scope of DFT methods is the exploitation of machine learning techniques trained on a DFT database to generate interatomic potentials for large scale molecular dynamics simulations. In this talk, we report on the generation of an interatomic potential for the $Ge_2Sb_2Te_5$ compound within the neural network framework implemented in the DeePMD-kit package. The interatomic potential allows simulating several tens of thousands of atoms for tens of ns at a modest computational cost. The validation of the potential and its application to the study of the crystallization kinetics of the amorphous phase and of the properties of the supercooled liquid will be discussed.

4:10 PM

(GOMD-S1-032-2024) Electronic defects and charge trapping in phase-change telluride materials (Invited)

S. Elliott*[1]

1. University of Oxford, Physical and Theoretical Chemistry Laboratory, United Kingdom

Telluride materials, including the canonical GST composition, $Ge_2Sb_2Te_5$, exhibit unique behaviour (nanosecond crystallization times, large opto-electronic property contrasts between glassy and crystalline phases) which enable them to function as non-volatile memory materials, in which digital information is stored as the atomic-structural state rather than as stored electronic charge, as in conventional Si CMOS (flash) memory. Intermediate memory states, i.e. partially crystalline and glassy, can also be programmed, thereby allowing more than 1 bit to be stored in each memory cell. However, such multilevel operation is compromised by 'resistance drift' in the glassy state, whereby the electrical resistance increases with time after a RESET voltage pulse producing the glassy state. The origin of resistance drift remains obscure. In this talk, I will outline computer-simulational work that we have undertaken to study the nature, and behaviour, of structural defects in models of glassy GST and other phase-change materials, which give rise to shallow- and deep-lying localized electronic states in the bandgap of the materials. In particular, I will describe results obtained from simulations of charge-trapping by such defects, as well as the effects of applied high electric fields. The implications for resistance drift will also be discussed.

4:40 PM

(GOMD-S1-033-2024) Thermodynamics and kinetics of the crystallization of phase change materials from simultaneous nanocalorimetry and in situ microscopy

I. McGieson[2]; T. D. Koledin[1]; J. Ciston[4]; F. Yi[3]; D. A. LaVan[3]; M. K. Santala*[1]

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

The thermodynamics and kinetics of crystallization are key to understanding the stability of glass-forming materials, including poor glass formers such as phase change materials (PCMs). The crystal growth rate, u, has been directly measured from the glass transition, T_g, to the melting temperature for good glass formers owing to their low u. In contrast, u in PCMs can exceed 10 m/s. Thus, it is challenging to measure u directly with microscopic methods, because the small grain sizes demand high spatial resolution and the grains impinge rapidly. This has led to the use of indirect methods to study PCM crystallization such as differential scanning calorimetry (DSC). In this work nanocalorimetry with high-frame-rate transmission electron microscopy (TEM) imaging was used to investigate the thermodynamics and kinetics of the crystallization of $Ag_3In_4Sb_{76}Te_{17}$ and GeTe above T_g. The PCMs were deposited on individually-calibrated nanocalorimeters designed to be operated in a TEM. Direct electron detectors capture the crystal growth in the milliseconds before impingement enabling direct measurement of u. The enthalpies of crystallization are calculated from nanocalorimetry measurements. Classical models for nucleation and growth are fit against these data and models that predict the growth rate solely from DSC data are compared to the direct growth rate measurements.

5:00 PM

(GOMD-S1-034-2024) Crystallization kinetics and beta-relaxations in GeTe

A. Makareviciute*[1]; S. Wei[1]

1. Aarhus University, Department of Chemistry, Denmark

Phase-change materials (PCMs) like Ge–Sb–Te and Sb-rich alloys may undergo reversible and rapid phase transitions between crystalline and amorphous phases for memory device applications. Recent studies showed that crystallization kinetics of $Ge_{15}Sb_{85}$ can be slowed down substantially by suppressing the beta relaxations in the glassy state via thermal annealing. However, it remains unclear how thermal annealing affects the crystallization of Te-containing phase-change materials. In this work, we studied the crystallization kinetics of amorphous GeTe using differential scanning calorimetry and demonstrated that thermal annealing slows down crystallization.

The in-situ synchrotron X-ray diffraction experiments revealed that although annealing of GeTe has introduced some partial crystallization in the sample, the crystallization rate of annealed GeTe is slower than that of as-deposited samples, as the crystal growth dominates the process. The local structures related to Peierls-like distortions are analyzed with respect to the suppression of the beta-relaxations in GeTe. This work may help better understand the crystallization kinetics in the partially crystallized PCMs.

5:20 PM

(GOMD-S1-035-2024) Novel wide-bandgap chalcogenide optical phase change materials enabled by high-throughput combinatorial studies

C. Lee*[1]; Y. Huang[1]; H. Sun[1]; C. Lian[1]; J. Frantz[2]; I. Takeuchi[1]; C. A. Ocampo[1]

1. University of Maryland, Materials Science and Engineering, USA
2. Office of Naval Research, USA

Chalcogenide-based optical phase change materials (OPCMs) exhibit a significant contrast in refractive index when reversibly switched between their stable amorphous and crystalline states. OPCMs have rapidly gained attention due to their versatility as nonvolatile amplitude or phase modulators in photonic integrated circuits, plasmonic structures, optical thin-film coatings, metamaterials, etc. Given that each application or optical device requires a tailored set of optical properties, developing high-throughput methods to expand the current OPCM library driven by specific performance metrics is paramount. As an example, one of the open challenges for OPCMs is achieving reliable response and transparency spanning into the visible spectrum, a combination of properties in which current broadband OPCMs (Ge2Sb2Se4Te1, Sb2Se3, or Sb2S3) fall short. Here, we tackle this challenge by leveraging the reliable response of Sb2Se3 and doping with silicon following a combinatorial sputtering study We demonstrate that Si-doped Sb2Se3 leads to a larger bandgap in both states, with transparency down to 800 nm and throughout the near and mid-infrared. Furthermore, we study the functional properties and microstructure of different OPCM combinatorial spaces using high-throughput characterization and data processing techniques. Our findings pave the way for broadband OPCMs for scalable nonvolatile photonics and propose a framework to discover novel alloys with multiple performance targets.

S2 Glass and Interactions with Its Environment Fundamentals and Applications

Session 2: Dissolution and Interfacial Reactions

Room: Turnberry
Session Chair: Stephane Gin, CEA

3:40 PM

(GOMD-S2-019-2024) Glass Corrosion Kinetics at Liquid and Frozen Conditions (Invited)

R. Schaut*[1]; S. A. Tietje[1]; E. Bakowska[2]; D. Ragland[1]

1. Corning Incorporated, S&T, Glass Research, USA
2. Corning Incorporated, Characterization Science, USA

Glass is the preferred material for packaging of pharmaceutical solutions, primarily due to its low chemical reactivity. Relative to other glass applications (food packaging, architecture, or handheld electronics), pharmaceutical packaging uses more chemically durable glass compositions, lower storage temperatures, more neutral pH, and lower surface area-to-volume ratios and accordingly produces lower elemental concentrations in the test solution. With such low signal, characterizing chemical performance can be challenging. Pharmaceutical solutions are generally stored at room temperature or refrigerated, where the solution remains liquid and reaction kinetics are slow, but continue to follow Arrhenius relationships. However, certain COVID vaccines and emerging biologics require frozen conditions for storage, occasionally at -80°C or even -180°C. Here we will discuss corrosion experiments conducted between -80 and +40°C to elucidate whether reactions continue when the solution is a frozen solid. Results for both borosilicate and aluminosilicate vials will be compared to understand the influence of heterogeneities on the kinetics of release.

4:10 PM

(GOMD-S2-020-2024) Dissolution and Precipitation Reactions of Na-Ca-Borophosphate Glasses in Simulated Body Fluid (Invited)

R. Brow*[1]; R. L. Blatt[1]; R. Youngman[2]

1. Missouri S&T, Materials Sci & Engrg, USA
2. Corning Incorporated, USA

When Na-Ca-borophosphate glasses dissolve in water, the resulting solution pH can range from acidic to basic depending on the phosphate-to-borate ratio in the glass and in vitro tests show that borophosphate glass compositions that create pH-neutral conditions promote cell viability. In simulated body fluid, borophosphate glass dissolution rates and the nature of the calcium phosphate (CP) phases that form on the glass surfaces also depend on composition and the molecular-level glass structure. Glasses with the greatest fraction of $B(OP)_4$ sites in the glass network react most slowly, and dissolution rates increase with increasing fractions of hydrolysable B-O-B bonds [1]. Acidic phosphate-rich glasses dissolve congruently without the immediate precipitation of CP phases whereas amorphous CP phases precipitate on the surfaces of the pH-neutral borophosphate glasses and crystalline CP phases form on the surfaces of the alkaline borate-rich glasses. Polyphosphate anions released from the pH neutral borophosphate glasses are incorporated into the amorphous CP layers, inhibiting the formation of crystalline phases like hydroxyapatite. This effect is particularly evident in precipitation layers on glasses reacted under dynamic conditions.

4:40 PM

(GOMD-S2-021-2024) Relating the structure to the aqueous dissolution behavior of P_2O_5-substituted sodium aluminosilicate glasses

N. Stone-Weiss*[1]; H. McMahon[1]; N. J. Smith[1]; J. B. Yehl[1]; J. L. Tubbs[1]; B. J. Rice[1]; E. Bakowska[1]

1. Corning Incorporated, Science and Technology, USA

Aluminosilicate glasses are relevant to several technological applications, including cover glasses for mobile electronic devices, glass substrate sheets for LCD displays, and vials for pharmaceutical applications. Further, P_2O_5 has shown to have significant impacts upon the structure and properties of aluminosilicate glasses, which can be advantageous for the advent of new glass technologies. However, the impact of P_2O_5 on the chemical durability of aluminosilicate glasses has been relatively unexplored in the literature and can in turn have significant impacts upon glass chemical processes. The present work investigates P_2O_5-substituted aluminosilicate glasses, particularly aiming to identify the effects that phosphate additions have upon the glass network structure and dissolution rates. Accordingly, the chemical durability of these glasses was carefully investigated in dilute static environments with controlled pH conditions, across a range of aqueous media. Through careful analyses of dissolution products via ICP-OES and the glass structure via MAS NMR, we aim to build a comprehensive understanding of the relationships between glass network structure and dissolution behavior.

5:00 PM

(GOMD-S2-022-2024) Aqueous CO_2 Adsorption on Amorphous Calcium Silicate Hydrate and Tobermorite

J. Harvey[1]; J. M. Rimsza*[1]

1. Sandia National Laboratories, Geochemistry Department, USA

Global production of cement accounts for ~5% of the carbon emission budget. However, sequestration of CO_2 can occur via reaction between CO_2 and concrete. Therefore, it is feasible to design carbon neutral buildings by optimizing the material for CO_2 sequestration. Calcium-silicate-hydrates (CSH) are the primary phases of ordinary Portland cement (OPC) and are primarily responsible for concrete strength. CSH carbonation has been studied extensively using experimental techniques, including formation of calcium carbonate and de-calcification of the CSH, and how the Si/Ca ratio affects the carbonation have been explored. The initial carbonation process begins via adsorption of CO_2 at the CSH interface. Yet, CO_2 adsorption is largely a molecular process that is rapid and therefore difficult to observe experimentally. Herein, we have used a reactive classical force field to probe the adsorption of CO_2 on amorphous CSH surfaces, as well as the crystalline analog (tobermorite). The energetics of adsorption have been explored as a function of hydration level as well as Si/Ca ratio. Insights on the adsorption and CO_2 reaction mechanism will be provided. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

S3 Optical and Electronic Materials and Devices Fundamentals and Applications

Session 5: Rare-earth and Transition Metal-doped Glasses and Ceramics for Photonic Applications III

Room: Shoal Creek
Session Chairs: Dominique de Ligny, University Erlangen-Nürnberg; Brian Topper, University of New Mexico

3:40 PM

(GOMD-S3-009-2024) Erbium doped transparent ceramics for quantum information storage (Invited)

S. Gray*[1]

1. Corning Research and Development Corporation, USA

Rare-earth-ion-doped solids are promising candidates for storing quantum photonic information due to the relatively long coherence times of the 4f-4f transitions. In particular, erbium doped materials are expected to play a key role in future long-distance quantum networks because of the transition at 1.53 um that is compatible with the low loss window of silica optical fibers. While long coherence lifetimes of rare-earth transitions have been observed in single crystal host materials, transparent ceramics offer several potential advantages such as ease of manufacturing and device fabrication. Here we describe our work on the characterization of erbium doped yttrium oxide fabricated using nanoparticle sintering. We use photon echo techniques to determine the coherence lifetime as a function of the sintering parameters and optimize the process to achieve the longest coherence time and maximum transparency. We also investigate femtosecond laser processing and Lanthanum co-doping as methods of modifying the refractive index to create waveguide structures suitable for integrated photonic devices and determine the impact on the coherence lifetime of the erbium ions.

4:20 PM

(GOMD-S3-010-2024) Structural, thermal, and luminescent properties of gadolinium(III) containing phosphate glasses

J. A. Jiménez*[1]; M. Thomas[1]

1. Georgia Southern University, Biochemistry, Chemistry, and Physics, USA

Gadolinium-containing glasses emitting narrowband ultraviolet (UV) type B light attractive for photodynamic therapies were synthesized and characterized comprehensively for various physical, structural, thermal, and luminescent properties. The glasses were prepared by melting with $50P_2O_5$-$(50 - x)BaO$-xGd_2O_3 (x = 0, 1, 2, 3, 4, 5 mol %) nominal compositions, and studied by density, X-ray diffraction (XRD), Raman spectroscopy, differential scanning calorimetry (DSC), dilatometry, and photoluminescence (PL) spectroscopy measurements. The densities of the Gd^{3+}-containing glasses were found to increase with Gd_2O_3 content, whereas XRD supported the amorphous nature of the glasses. The Raman spectra evolution was indicative of glass depolymerization being induced by Gd^{3+} ions. DSC results showed that the glass transition temperatures increased with Gd^{3+} concentration while the glasses exhibited decreased susceptibility for crystallization. Dilatometry ultimately revealed a steady decrease in the coefficient of thermal expansion for the Gd^{3+}-containing glasses indicating tighter networks were realized. The PL evaluation showed that the intensity of the UVB emission at 312 nm attractive for phototherapy lamps increased linearly with Gd^{3+} concentration. The $^6P_{7/2}$ emitting state dynamics evaluation however indicated that some energy migration occurs at high Gd_2O_3 content in the glasses.

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(GOMD-S3-011-2024) Controlled UV emission from $MgAl_2O_4$:Gd

R. Conner[1]; D. Van der Heggen[2]; D. Poelman[2]; P. Smet[2]; L. G. Jacobsohn*[1]

1. Clemson University, Materials Science and Engineering, USA
2. Ghent University, LumiLab, Belgium

$MgAl_2O_4$ stands out as a wide band gap optical material that can accommodate numerous activators, including rare earths. It has been investigated as a scintillator and luminescence dosimeter, but limited attention has been paid to engineering its UV emission. $(Mg_{1-x}Gd_x)Al_2O_4$ with x = 0, 0.01, 0.05, 0.075, 0.1 and 0.2 were prepared by the co-precipitation method followed by 2hr-long calcination at 900 °C in air. The powders were characterized by XRD, SEM/EDX, XPS, and evaluated in their photophysical properties by diffuse reflectance, radioluminescence (RL) under X-ray excitation from room temperature (RT) to 450 °C, and by photoluminescence emission (PL), excitation (PLE) and lifetime measurements. XRD indicated a single phase and progressive structural disorder as per the broadening of the diffraction peaks for higher x values. RL showed UV emission at 314 nm due to the $Gd^{3+6}P_{7/2} \rightarrow {}^8S_{7/2}$ transition, with the x = 0.075 material having the most intense emission. Lifetime measurements revealed two lifetimes, ca. 1.7 and 4.9 ms, whose relative contributions vary as a function of the Gd content. This behavior was tentatively attributed to the existence of Gd with different chemical bonds as shown by XPS. The UV emission intensity showed a linear decrease as a function of the temperature, being 70% of the RT intensity at 200 °C. This material is based upon work supported by the National Science Foundation under Grant No. DMR-1653016.

Poster Session

Room: Grand 1 and 4

6:00 PM

(GOMD-P001-2024) Relaxation and crystal nucleation interplay in supercooled germanium and water

A. Tipeev[1]; E. Dutra Zanotto*[1]

1. Federal University of São Carlos, Department of Materials Engineering, Brazil

A well-designed study of the relationship between crystal nucleation and relaxation processes in supercooled liquids can clarify some critical issues in condensed matter science. Using MD simulations, we obtained the self-diffusion coefficient D and the shear viscosity η in supercooled germanium and water, described via a Stillinger-Weber model. Then, we determined three relaxation times within the (0.7–0.9)T_m temperature range, where T_m is the equilibrium melting temperature, via i) the shear viscosity, τ_η; ii) the incoherent intermediate scattering function, τ_α; and iii) the self-diffusion coefficient, τ_D. We found that $\tau_\alpha(T) \approx \tau_D(T)$ and $\tau_\eta(T)$<spanlt;$\tau_\alpha(T)$, corroborating the findings of recent experimental and computational studies with other substances. The birth times of the first critical crystal nucleus at steady-state conditions, $\tau_1(T)$, were obtained from the seeded and unseeded nucleation simulations and calculations via the Classical Nucleation Theory. A relevant finding is that the $\tau_\alpha(T)$ and $\tau_1(T)$ curves cross over for germanium and water, confirming the existence of a kinetic spinodal T_{KS} for both liquids. Finally, we demonstrate that if the Kauzmann temperature T_K existed, it would be located well below the T_{KS}; hence, crystallization would intervene in the cooling path before these supercooled liquids could reach T_K, thus averting the Kauzmann entropy paradox. The research was supported by FAPESP grant 2022/05837-5, CNPq and FAPESP contract CEPID 2013/07793-6.

(GOMD-P002-2024) Physics-informed Machine Learning for Sodium-Ion Conductive Glasses

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1. Indian Institute of Technology Delhi, School of Interdisciplinary Research, India
2. Indian Institute of Technology Delhi, India

Solid-state electrolytes based on ceramic materials face hurdles like dendrite formation and erratic sodium movement, limiting their application. This study focuses on sodium ion conductive glasses, aiming to overcome these challenges with grain-boundary-free structures. Utilizing a dataset of 56 experimentally prepared Na_2O-P_2O_5-AlF_3-SO_3 glasses, machine learning (ML) models were constructed. Each glass specimen provided conductivity values at varying temperatures (323 K, 423 K, and 523 K) were utilized as outputs for the ML models. The input features for the ML model comprised six distinct glass components. A neural network model integrated with the Arrhenius equation exhibited exceptional performance, achieving a remarkable 99% goodness of fit for conductivity across diverse temperatures. Furthermore, this ML model accurately estimated activation energy (AE) and pre-exponential components (PEC) of conductivity. Notably, the model's robustness was tested beyond the confines of the training and testing dataset, successfully predicting conductivity at different temperatures, AE, and the PEC with a striking similarity to experimentally measured data. In addition to the ML model, SHAP (SHapley Additive exPlanations) analysis was leveraged to elucidate the impact of various glass components on AE and PEC. This approach provided invaluable insights into enhancing glass conductivity and designing glasses with lower AE.

(GOMD-P003-2024) Fracture behavior of barium titanosilicate glass-ceramics: Role of bond switching and stress fields

D. Sun*[1]; T. Du[1]; M. M. Smedskjaer[1]

1. Aalborg Universitet, Denmark

Fracture toughness of oxide glasses can be improved through controlled crystallization, resulting in so-called glass-ceramics. However, to fully exploit their potential, a deep understanding of the fracture mechanism is needed. In this work, we investigate the structural origin of the variation in fracture toughness of barium titanosilicate glass-ceramics with varying crystallinity by combining experiments and molecular dynamics simulations. Generally, the glass-ceramics exhibit improved hardness, elastic modulus and fracture toughness compared to the precursor glasses. The simulation results of 40BaO-20TiO_2-40SiO_2 glass-ceramics revealed that the differences can be attributed to a large extent of titanium bond switching events, namely, the change of the titanium coordination number under stress to dissipate mechanical energy. We also show that by tuning the content and aspect ratio of the formed fresnoite crystals, the fracture behavior of the glass-ceramics can be modified due to the redistribution of the stress field before fracture, which in turn controls the fracture path.

(GOMD-P010-2024) Physical properties of low dielectric glass fibers at gigahertz frequency range for high speed PCB applications

J. Lee*[1]; J. Kim[1]

1. Korea Institute of Ceramic Engineering and Technology (KICET), Republic of Korea

Borosilicate glasses were prepared with a composition of x Li_2O-(14-x) CaO-21B_2O_3-57SiO_2-8Al_2O_3 where x= 0,1,3,5 and 7 mol%. Each composition was melted in an alumina crucible under atmosphere condition at 1600 °C for 2 h. Clear glasses with a transmittance exceeding 85% were fabricated. Their optical, thermal, and physical properties, such as dielectric constant, density and glass transition (T_g) were studied. The results demonstrated that dielectric constant was between 3.8 and 4.6 at 15GHz. As the Li_2O content increased, the glass transition temperature of the fiber glass decreased from 608°C to 564°C. It succeeded in manufacturing low dielectric glass of less than a dielectric constant of less than 5.5, and confirmed the commercialization of multi-layer PCB substrate materials

(GOMD-P011-2024) Assessment of the durability of cement with waste glass aggregates using machine learning and texture analysis methods

R. Dzierzak*[1]; D. Barnat-Hunek[2]

1. Lublin University of Technology, Department of Electronics and Information Technology, Poland
2. Lublin University of Technology, Department of General Construction, Poland

Combining image texture analysis with ML methods enables the development of increasingly effective predictive models. Using high-quality images, it becomes possible to examine the texture of materials and assess their overall condition. In the current study, this approach was used to evaluate the durability of cement with waste glass aggregates. Textural features were extracted from images acquired through a scanning microscope. Throughout the investigation, eight supervised learning methods were employed for utilizing the texture features. These methods included Support Vector Machine with the C regularization parameter, Support Vector Machine with the nu parameter controlling the number of support vectors, K-Nearest Neighbors, Decision Tree, Multi-Layer Perceptron, Random Forest, Gradient Boosting, and Adaptive Boosting. The model generated using the Support Vector Machine method with the nu parameter exhibited the highest recognition accuracy for the tested samples, achieving an accuracy rate of 82%. This outcome suggests a significant correlation between the effectiveness of hydrophobic coatings in cement with waste glass aggregates and the surface images captured through scanning microscopy. The results obtained highlight the potential of machine learning methods in conducting strength diagnostics for building materials. This underscores the utility of integrating image texture analysis with ML approaches for robust predictive modeling in materials engineering.

(GOMD-GP-P001-2024) Investigation of the first sharp diffraction peak in GeO_2 glass based on persistent homology analysis and machine learning techniques

K. Matsutani*[1]; S. Kasamatsu[1]; T. Usuki[1]

1. Yamagata University, Faculty of Science, Japan

The intermediate-range order (IRO) in network-forming glasses has been suggested to play an important role in determining their properties, but the atomistic details of the IRO remain unclear. This is because X-ray or neutron diffraction experiments on disordered materials can only provide one-dimensional structural information, such as total structure factors and corresponding pair distribution functions. Therefore, computer simulation methods, such as reverse Monte Carlo analysis and molecular dynamics, have been widely employed to obtain three-dimensional real-space structural information on amorphous materials. However, even if reliable three-dimensional structures could be obtained, it would be difficult to interpret the IRO using conventional methods. Recently, a mathematical method from the field of topology called persistent homology has been used with some success to extract geometric features in glass structures. In this study, the IRO in GeO_2 glass is characterized by applying persistent homology analysis to various structures generated by reverse Monte Carlo, hard-sphere Monte Carlo, and molecular dynamics methods. Machine learning models are constructed to reproduce the first sharp diffraction peak (FSDP) using persistence diagrams as structural descriptors. The models are then interpreted to reveal the real-space IRO that leads to the formation of the FSDP in GeO_2 glass.

(GOMD-GP-P002-2024) DFT study on chemical bonding network in amorphous BNTe chalcogenides

D. Kim*[1]; T. Lee[1]

1. Kyungpook National University, Electronics Materials Science and Engineering, Republic of Korea

Ovonic threshold switches (OTS) based on Te-rich amorphous chalcogenides are used in high-speed memory for their essential role as selector switches. These devices require high thermal stability for rapid switching and data integrity during repetitive crystallization. To enhance these properties, Te-rich based OTS materials were doped with various elements such as Ge, Si, As, B, and N. In this study, we focused on the amorphous BNTe, a promising candidate for OTS. Experimental results demonstrated enhanced thermal stability with increasing nitrogen doping level. To elucidate underlying mechanisms of these effects, we have conducted ab initio molecular-dynamics (AIMD) simulations on BNTe models and assesed variations in chemical-bonding properties with different nitrogen doping levels of 0%, 5%, and 10%. In our investigation, we analyzed the chemical bonding network using electron localization function, maximally localized Wannier functions, and crystal orbital Hamiltonian population. From this analysis, we conclude that the peculiar structural units composed of Te atoms shows intimate correlation with the configuration of the BN clusters which determines the crystallization behavior of this materials. Consequently, our findings reveal how the BN clusters crucially influences the thermal stability of the materials during repetitive crystallization. The observed correlations will help in designing Te-rich OTSs materials with improved thermal stabilities.

(GOMD-GP-P003-2024) A machine-learning potential to model multi-component oxide glasses

R. Kayano*[1]; T. Ohkubo[1]; R. Mastubara[2]; K. Ishida[2]

1. Chiba University, Graduate School of Engineering, Japan
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Machine-learning potentials (MLPs) have recently been widely used in modeling various materials. The MLP approach can accurately reproduce First-Principles Molecular Dynamics (fpMD) while enabling large-scale simulations using classical Molecular Dynamics (CMD). In this study, MLPs were used for modeling multi-component oxide glasses. We developed MLPs to describe several systems: SiO2-Na2O, Al2O3-SiO2, B2O3-Na2O, and SiO2-B2O3-Al2O3-Na2O. We performed fpMD on multi-component and binary glasses in the molten state to generate training data. The glass structures were prepared by melting and quenching using CMD with the MLPs and were compared with experimental data such as 11B NMR and X-ray structure factor. The well-known four-coordinated B fraction in the Na2O-B2O3 system and the X-ray structure factor of the multi-component system derived from MD with MLPs agreed well with the experimental data. In addition, various B superstructures, which were difficult to reproduce with conventional CMD, were successfully generated. In conclusion, MLPs provide a route to represent the potential of multi-component glasses with more complex compositions.

(GOMD-GP-P004-2024) Deciphering the structural origin of disorder-induced ion conduction in $NaFePO_4$ glasses

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Current battery technologies rely on solid-state crystalline cathode materials, however, it is becoming evident that various crystals are limited by the low ionic conductivity of their most stable phases. Interestingly, one such crystal, maricite $NaFePO_4$, has been found experimentally to improve its rate capability through disordering (amorphization). However, experimental characterization of amorphous cathode materials remains a major challenge. This study therefore employs molecular dynamics simulations to investigate the structural and dynamical properties of $NaFePO_4$ glasses as cathode materials. We investigate the effects of composition and structure on sodium diffusion coefficients and energy barriers, revealing the influence of short and medium-range order structural features on sodium-ion migration. These results present promising avenues for developing high-performance glassy cathodes for next-generation batteries.

(GOMD-GP-P006-2024) SiO_2-Al_2O_3-CaO-MgO Glass Ceramics as a High Temperature Sealing Material for Solid Oxide Fuel Cells Sealing

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SOFC (Solid Oxide Fuel Cell) has been widely studied since it can generate electricity by the electrochemical reactions using hydrogen. It requires an appropriate sealing material with a high glass softening point and a coefficient of thermal expansion (CTE) similar to those of the SOFC components. To satisfy the high glass softening point as well as high CTE, sealing materials containing BaO were mostly studied. However, the reaction of Ba ions with the metal components forms $BaCrO_3$ phases which seriously ruins SOFC stability. In order to identify suitable sealing materials devoid of Ba, the glasses of SiO_2-Al_2O_3-CaO-MgO system were modified to adjust high CTE and flowability by the formation of a diopside phase through crystallization. Various glass compositions were prepared by conventional melt-quenching techniques and subjected to heat treatment around the sealing temperature to examine their flow properties and crystallization behaviour. Differential thermal analysis (DTA) and thermomechanical analysis (TMA) were employed to characterize thermal properties. X-ray diffraction (XRD) inspected crystal formation of the heat-treated glass samples. Adhesion properties were examined and potential interactions between the sealing material and components were explored using scanning electron microscopy equipped with energy dispersive spectroscopy (SEM-EDS).

(GOMD-GP-P007-2024) Low temperature Sealing Materials Based on CaO-ZnO-B_2O_3-SiO_2 Glass Ceramics for Solid Oxide Electrolyzer Cells

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SOEC (Solid Oxide Electrolyzer Cell) can generate hydrogen and oxygen by decomposition of water at high temperature. However, it requires a proper sealing material which has high glass softening point as well as high coefficient of thermal expansion (CTE) similar to those of the SOEC components. Conventional high temperature sealing materials mostly contain BaO to meet the high glass softening point and CTE. However, BaO can react with Cr ion of the interconnect to form $BaCrO_3$ which can cause delamination of the cell. In this study, we investigated a CaO-ZnO-B_2O_3-SiO_2 quaternary glass system which can expect high CTE with hardystonite phase after crystallization excluding Ba. Various glass compositions were synthesized via conventional melt-quenching and heat treated at sealing temperature to examine its flow property and crystallization behavior. The thermal properties were inspected by DTA (Differential Thermal Analysis) and TMA (Thermomechanical Analyzer). The heat-treated samples were examined by XRD (X-ray Diffraction) to determine the crystal formation within the glass. Adhesion property to the SOEC components such as YSZ and FC460 has been examined and possible reaction between the sealing material and components was inspected with a scanning electron microscopy (SEM) equipped with an energy dispersive spectroscopy (EDS).

(GOMD-GP-P008-2024) Impact of pressure on the chemical bonding and material properties of amorphous chalcogenides

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Understanding amorphous chalcogenide materials has been a significant challenge in the field of glass science. A diversity of their properties cannot be comprehensively elucidated by conventional chemical bonding theories. Therefore, a new type of chemical bonding, i.e., multi-center hyperbonding, has been proposed recently. In this study, to improve the hyperbonding theory, we have performed in-depth study on the amorphous (a-) state of Te, the prototypical anion element for electronic memory devices, using ab initio molecular-dynamics (AIMD) simulations based on the density functional theory (DFT). We have examined the correlations between the chemical-bonding properties and induced pressure on a-Te. Furthermore, we have analyzed changes in optical and electronic properties. To understand the dependence of hyperbonding tendency on material characteristics, the chemical bonding properties of a-S and a-Se as a function of pressure were also investigated and compared with those of a-Te. We expanded our study for binary and ternary amorphous chalcogenides. Manipulating the density of amorphous chalcogenides has allowed us to explore the dynamics of hyperbond formation and annihilation, and associated correlations with material properties. Moreover, this study opens a new avenue for studying many other properties of amorphous materials.

(GOMD-GP-P009-2024) Machine learned Gaussian approximation potentials for amorphous tellurium and its applications for large model simulations

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Amorphous chalcogenides exhibit unique chemical bonding characteristics, enabling widespread use in a diversity of applications, including phase-change memory and photocatalysis. Ab initio molecular-dynamics (AIMD) simulations based on density functional theory (DFT) have been intensively utilized for accurate simulations of these materials. However, its high computational cost and finite size effects limit its applicability. Here, we have employed a Gaussian approximation potential (GAP) trained on extensive DFT data for simulating large chalcogenide models with high accuracy comparable to DFT results. Our GAP potentials were validated by comparing many static and dynamic properties of GAP models with those of DFT models. The good agreement with DFT results confirms the accuracy of the GAP simulations. By using the generated GAP potential, we have analyzed multi-center hyperbonding characteristics of a-Te, the unique bonding mechanism in amorphous chalcogenides, thereby providing valuable insights into the complicated network structure of the a-Te models. This study demonstrates the reliability of our GAP models for a-Te, and paves the way for efficient simulations for other chalcogenide materials or physicochemical properties that require large system sizes and/or fast MD simulations, including crystallization phenomena or thermal transport property of amorphous chalcogenides.

(GOMD-GP-P010-2024) Network depolymerization in Na_2S-GeS_2 superionic glasses and its relationship with ion conduction

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The properties of xNa_2S-$(100-x)GeS_2$ glasses, which represent promising systems for all-solid-state batteries, are thoroughly investigated from a variety of experimental and theoretical techniques. The ionic conduction measured as a function of composition reveals a powerlike behavior with a threshold composition found at low Na content. Three particular compositions (0%, 33%, and 66% Na_2S) are characterized by a combination of x-ray diffraction and density functional based molecular dynamics. Different structural properties are measured and calculated, such as structure factors, pair distribution functions, angular distributions, coordination numbers, and neighbor distributions. The comparison with experiments reveals a rather good agreement in real and reciprocal space. The short-range order is found to consist of a base network made of $GeS_{4/2}$ tetrahedra (with Ge and S coordination numbers being of about 4 and 2) that are progressively depolymerized upon Na addition that also leads to a breakdown of the ring structure. Na coordination numbers are loosely defined, especially at high Na content. Typical features of alkali-modified silicates are also found, such as the presence of channel-like dynamics, a bond-length distribution that is different between Ge and bridging or nonbridging sulfur, a distribution Q^n of Ge tetrahedra having n bonding sulfur, and a decoupling at low temperatures between network species (Ge, S) and Na dynamics.

(GOMD-GP-P014-2024) Toughening of soda-lime-silica glass by nanoscale phase separation

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The low fracture toughness of oxide glasses (generally <1 MPa $m^{1/2}$) entails that they are prone to fracture, which remains a limitation for their applications. Nanoscale phase separation is a potential toughening strategy, as the formation of a heterogeneous nanostructure can alter the fracture behavior, while the important transparency of the glass can be retained. Using atomistic molecular dynamics simulations, we study the fracture of soda lime silica glasses with either homogeneous or heterogeneous nanostructures, the latter mimicking phase-separated glasses comprised of silica-rich nanodroplets in a modifier-rich matrix. We observe phase separation-induced toughening, as seen from increased fracture toughness, and find a stronger effect of larger droplets. Furthermore, we identify multiple mechanisms that cause the observed toughening. That is, the crack propagation is impeded by direct crack-particle interactions, i.e., crack arrest, deflection, and diversion. Moreover, the nanoscale heterogeneity in chemical composition, hence also in mechanical properties, leads to crack propagation in a less brittle matrix phase, ultimately causing toughening through more stress dissipation. Finally, we show how the droplets of higher stiffness alter the stress field, potentially shielding the crack from high stress.

(GOMD-UP-P001-2024) Layered Hybrid Germania-Silica Nanoparticle Sol-Gel Synthesis for use in 3D-printing Glass Optics

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Glass products play an essential role in everyday life and are essential to advancing common technologies. The development of new chemical approaches to fabricate glass materials is vital to enabling innovative, additive manufacturing of 3D-printed glass technologies. This project aims to examine the fundamental sol-gel chemistry needed to synthesize various nanoparticle structures composed of germania and silica. This report summarizes our exploration of various hybrid silica-germania nanoparticles designed in layer-by-layer compositions through multiple methods of analysis. Particle size and morphology data and analysis were done using atomic force microscopy (AFM), with further data collected using backscatter detection (BSD) on a scanning electron microscope (SEM), and from dynamic light scattering (DLS). The chemical composition of these particles was determined by using energy-dispersive X-ray spectroscopy (EDS) and Fourier transform infrared radiation spectroscopy (FTIR). Findings from this project could help reimagine the fabrication of glass materials and ultimately aim to enable the design of freeform optics and innovate optical system design.

(GOMD-UP-P002-2024) Effects of Thermal Processing on Network Evolution and Microstructure of Glasses Derived from Hybrid Sol-gel Particles

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Hybrid sol-gel nanoparticles (NPs) play a central role in advancing the additive manufacture, or 3D printing, of glass materials in compositions and geometries inaccessible by conventional melt quench techniques. In this presentation, we investigate how glass materials from different weight percent GeO2-SiO2 NPs change over the heat treatment process. Our study explores the range of weight ratios possible for two different architectures of NP materials that have undergone eight different heat treatment schemas. By varying the maximum and dwell temperatures and times experienced by the NPs, the opacity and structure of the finished glass can be optimized for each NP composition. NP shape, size, and morphology were analyzed using scanning electron and atomic force microscopy. The chemical composition of the NPs was probed by energy-dispersive X-ray spectroscopy, Raman, and Fourier-transform infrared spectroscopies to study chemical structures and bonding in the resulting NPs and glass networks. Ongoing research seeks to link NP structure, glass network formation, and glass quality (i.e., transparency).

(GOMD-UP-P003-2024) Investigating Polyols for Germania Nanoparticle Growth Control for Use in 3D-Printed Glass

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Germania is a well-known glass former with several desirable properties for use in glass optics. In comparison to silica, germania has higher refractive capabilities and k-dielectric properties. Additionally, it has a wider optical transparency window and a higher linear coefficient of thermal expansion. The use of germania in 3D printed glass optics has been limited due to the chemical challenges with synthesizing small (sub-50 nm), stable, amorphous germania nanoparticles. Here, we investigate the use of polyol surfactants, such as mannitol, to tune germania nanoparticle growth. Replicate samples were grown at various temperatures and times of addition. Dynamic light scattering (DLS), atomic force microscopy (AFM), and infrared spectroscopy (IR) measurements were acquired to elucidate the size and structure of the sol-gel nanoparticles. Results show the potential for polyol to act as a surfactant and inhibit germania particle growth. Studies investigating the point of addition and the stoichiometric equivalents of polyol are ongoing

(GOMD-UP-P004-2024) Revisiting The Time-Dependent Nucleation Rate in Lithium-disilicate Glass

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Lithium disilicate was employed to reexamine the investigation into the time-dependent nucleation rate. The total number of nuclei was determined using the differential thermal analysis (DTA) method. During heat treatment for shorter durations, ranging from 1 to 10 hours, the number of nuclei rapidly increased, reaching what was previously perceived as a steady state nucleation rate. However, upon extending the heat treatment to longer durations, a decrease in the rate at which the nuclei developed was observed. These data suggest that the previously presumed steady-state nucleation may not have attained the transient nucleation.

(GOMD-UP-P005-2024) Synthesis and refinement of $Li_2S + SiS_2 + Li_{3.48}SiO_{3.74}$ based glassy solid-state electrolytes

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Glassy solid electrolytes in the $Li_2S + SiS_2$ system are strong contenders for use in solid-state batteries due to their high ionic conductivities, electrochemical stability, and processability. However, the binary systems do not have the processability required for thin film drawing. To rectify this, $Li_{3.48}SiO_{3.74}$ was added. Its incorporation introduced a strong glass former and oxygen into the system while maintaining a high lithium content to increase the processability and conductivity of the glass. As the lithium concentration in these glasses increases, the ionic conductivity is expected to rise. An iterative series including all three components was synthesized. These compositions were tested using differential scanning calorimetry (DSC), Raman spectroscopy, Fourier transform infrared spectroscopy (FTIR), and electrochemical impedance spectroscopy. After extensive investigation, it was determined that $(0.5)Li_2S + (0.45)SiS_2 + (0.05)Li_{3.48}SiO_{3.74}$ had the best thermal properties of the series. Further work was done to refine the lithium silicate precursor by modifying starting materials and processing parameters. Iterations of the precursor were tested utilizing X-ray diffraction before being incorporated into glasses for further testing and verification before scaling production.

(GOMD-UP-P006-2024) Non-exponential Relaxation in Metaphosphate Glass Melts measured by Photon Correlation Spectroscopy

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Photon correlation spectroscopy was conducted on a series of metaphosphate glass melts to measure the liquid's dynamic structure factor near the glass transition and thereby characterize the degree of non-exponentiality in its time decay. Each metaphosphate consists of long, polymeric chains of $[PO_4]^{-1}$ monomers interspersed by a variety of modifying cations (Ag^+, Ba^2, Ca^{2+}, Sr^{2+}) which can potentially form inter-chain crosslinks via ionic bonding. Our results show that the non-exponentiality of the α-relaxation decreases monotonically with increasing field strength of the cation-oxygen bond as the oxide structure evolves from purely polymeric to a continuous 3d network.

(GOMD-P006-2024) Multilinear Regression Models to Estimate Time to Resumption and Resumption Corrosion Rate of Low Activity Waste Glasses

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This study addresses the challenges of predicting the long-term behavior of Low Activity Waste glasses that are intended for safe storage for hundreds of thousands of years. The interaction of such glasses with water involves numerous chemical processes during the various stages of alteration. When relatively insoluble glass components (e.g., Al, Fe, and Si) accumulate in the bulk solution, zeolite subgroup minerals can precipitate. Depending on the type of glass and alteration phases that form, this can casue the glass-water reaction to transition from the residual rate regime and return to an elevated rate, which is termed "Stage III corrosion" or resumption. This transition complicates predictive modeling of the long-term behavior. An objective of the present work was to develop a model that estimates the time to the resumption stage in the glass alteration process as well as to analyze the most influential glass components and significant interactions that affect the time to onset of "Stage III". Data from 182 leaching experiments were analyzed using connected piecewise linear regression where two lines are representative of Stage II and Stage III separated by a time-to-resumption breakpoint (Tr). Tr as a function of the glass composition was then analyzed by Multilinear regression methods. The results indicate that ZrO_2 is the largest influencer that delays Tr followed by P_2O_5, TiO_2, SO_3, and Al_2O_3, while Li_2O, Na_2O, and K_2O decrease Tr.

(GOMD-P007-2024) Developing a Method to Determine Sulfur Saturation of Hanford Low Activity Waste Glasses – Past, Present, and Future

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Within the past decade, Pacific Northwest National Laboratory (PNNL) has been refining experimental methods to determine the sulfur solubility in Hanford waste glasses. Sulfate is one of the critical constituents that limit waste loading for many tank waste glasses. Melter feeds with unacceptably high sulfur concentrations are subject to salt segregation in the melter which hinders melter operation by corroding components and shortening the melter life. Previous studies evaluated various methods (e.g., salt saturation, bubbling) and conditions (e.g., temperature, time) to achieve complete sulfur saturation, leading to the implementation of the three-time saturation method. However, further improvements to the current method are under investigation to reduce cost and time required to test and analyze each glass. Additionally, sulfur is partially volatile which complicates the measurement of sulfur solubility and mass balance calculations between the glass and sulfate salt phases. This work provides an overview of past progress, present findings, and future questions towards refining a method to experimentally determine sulfur saturation.

(GOMD-P008-2024) Laser-induced modification of transition metal ions doped sodium phosphates

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Microstructural changes caused by localized melting and solidification of $Na_2FeP_2O_7$ and $Na_4Ni_3(PO_4)_2P_2O_7$, which are promising cathode active materials for sodium-ion batteries, were evaluated by infrared laser light irradiation. Glass formation, crystallization, and foaming due to melting and solidification in the micro melt pool were confirmed depending on the laser power and scanning speed. This method contributes to the small heat capacity. It enables the formation of a dense glassy cathode layer, which can be adhere to solid electrolyte and is effective for fabricating all-solid-state batteries.

(GOMD-P004-2024) Analyzing lithium-ion conduction in thiophosphate glassy electrolytes via machine learning

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Glasses such as lithium thiophosphates (Li_2S-P_2S_5) show promise as solid electrolytes in lithium-ion batteries, but a poor understanding of the impact of the disordered structure on lithium transport properties limits the further development of glassy electrolytes. Here, we simulate glassy Li_2S-P_2S_5 electrolytes with varying fractions of polyatomic anion clusters using classical molecular dynamics. Based on the determined variation in ionic conductivity, we use a classification-based machine learning metric termed "softness" – a structural fingerprint that is correlated to the atomic rearrangement probability – to unveil the structural origin of lithium-ion mobility. To derive a real-space origin of the machine-learned softness metric, we analyze the energy barrier of softness-coded lithium ions migrating between two sites, showing that soft lithium-ion migration requires a smaller energy barrier to be overcome relative to that observed for hard lithium-ion migration.

(GOMD-P012-2024) Fabrication technology and luminescence properties of the lithium-vanadate-borate glass

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The development of glass compositions for the creation of new efficient luminescent glass and glass-ceramic materials is an important practical task as such materials are used in light-emitting devices, sensors, laser technologies, etc. The main component of the developed in this work glass-ceramics is boron oxide, which is characterized by a wide glass-formation range of concentrations. The addition of some network modifiers, usually alkali metal oxides, can lead to an increase of the coordination number of the boron from 3 to 4, changing the properties of borate glass. This phenomenon, known as the "borate anomaly" can improve mechanical and spectroscopic properties of the glass matrices. In the present study, we use lithium oxide for this purpose. The xLi_2O-yV_2O_5-$(100-x-y)B_2O_3$ glass samples synthesized by melting quenching technique are characterized by wide band photoluminescence (PL) with a maximum at around 570 nm. Its intensity is increasing considerably with the increase of Li_2O concentration. The samples without V_2O_5 component have

no PL. An assumption is made that the observed wideband PL can appear as a result of recombination processes with the participation of self-localized holes in 4-coordinated borate networks and electrons trapped on the broken and recharged vanadate groups. The EPR analysis has revealed an increase of the $V^{5+} \rightarrow V^{4+}$ transformation with the increase of the Li concentration, that supports the made assumption.

(GOMD-GP-P005-2024) Compositional study on Lead-Free Perovskite Nanocrystal-Embedded Germanate Glass system for LED Applications

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$CsPbX_3$ (X=Cl, Br, I) halide perovskite nanocrystals showed promising potential in optoelectronics, specifically for applications in solar cells and LEDs, owing to their narrow emission spectrum and high quantum efficiency. However, their Pb content, a heavy metal with environmental concerns, poses challenges. Additionally, susceptibility to degradation from air and light restricts their commercial viability. Recently, many studies aimed to discover Lead-Free Metal Halide Perovskite (LFMHP) nanocrystals. However, these studies, relying on wet chemical processes, face limitations in thermal and chemical stability. To ensure stability, there have been also various exploration of Pb-free perovskite nanocrystal incorporation within a glass matrix. In this study, to achieve LFMHP nanocrystals replacing Pb from $CsPbBr_3$ within the previously reported germanate glass composition, PbO was substituted with alternative materials. Among various compositions, a luminescence under UV excitation was detected from a glass containing Cs_2ZnBr_4 nanocrystals. In order to improve emission intensity, composition of the glass was changed and heat treatment conditions such as heat treatment temperature and duration time were varied. Cs_2ZnBr_4 nanocrystals within the glass matrix was verified using X-ray Diffraction and Transmission Electron Microscopy. Photoluminescence and photoluminescence quantum yield were measured and demonstrated the potential of the material for LED applications.

(GOMD-GP-P011-2024) The optical and thermal properties of GeO_2-based mid-infrared transmission glasses

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Recently, there has been growing interest in infrared (IR) optical systems owing to their widespread use in optics. These optical systems utilize electromagnetic radiation from the atmosphere in the mid-IR region, typically ranging from 3 to 12 μm. Germanium oxide-based (GeO_2) systems have been recently highlighted for mid-IR-transmitting glasses because of their high refractive index of approximately 1.7, wide transparency in the IR region, and relatively low glass-transition temperature between 500–600 °C. Furthermore, they exhibit higher chemical and thermal stabilities compared to other chalcogenide and heavy-metal oxide glass systems. We fabricated novel $BaO\text{-}TiO_2\text{-}Ga_2O_3\text{-}TeO_2\text{-}GeO_2$ glasses and analyzed the relationship between glass compositions and optical properties. The refractive indices increased with increasing TeO_2 and BaO concentrations, owing to the increase in the electronic polarizability of oxygen and density of the oscillators. The Abbe number decreased with increasing TeO_2 concentration because the resonance wavelength of the oscillator shifted to a longer wavelength, indicating a decrease in the optical bandgap energy. By substituting TeO_2 and BaO for GeO_2, the cutoff wavelength of the IR region shifted to a longer wavelength. Furthermore, thermal-expansion coefficient values of the glass samples developed in this study ($9.45–11.58 \times 10^{-6}$/K) were lower than those of commercial optical glasses.

(GOMD-GP-P012-2024) Spectroscopy Study of Mn^{5+} in High Basicity Glasses: A Raman Resonance Effect

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Turquoise Mn^{5+} was stabilized in high basicity $40Cs_2O\text{-}10BaO\text{-}50SiO_2$ glasses. While Mn^{4+} is unstable in these glasses, the blue Mn^{5+} cation was unambiguously identified using optical spectroscopy, electron paramagnetic resonance, photoluminescence, Raman, and X-ray photoluminescence spectroscopy. Subsequent observations, showed an interesting Raman resonance effect, giving a sharp, narrow high-intensity Raman signal at 798 cm^{-1} for even samples with only as low as 0.5 mol% MnO content. Typical for Raman resonance, the better the symmetric stretching mode overlaps with the optical absorption of the charge transfer transition of the same polyhedron, the signal can be enhanced by varying the excitation laser wavelength. As described earlier, for aqueous $Mn^{(IV+)}$, a CT band is hidden under the d-d transitions that give the turquoise blue color of Mn^{5+} leading to the observed Raman resonance. Such an effect had also been reported earlier in glasses for the Ti-O band in ULE glasses. In this study, in addition to presenting spectroscopical evidence for stabilizing Mn^{5+} in high optical basicity glass, we focus on reporting the interesting observed Raman resonance phenomenon for Mn^{5+}.

(GOMD-GP-P013-2024) Investigation of Bonding Glass Surfaces Using Ultrafast Laser Pulses *WITHDRAWN*

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Since the early 2000s, advances have been made toward bonding transparent and nontransparent materials but have since made little advance in fundamental science and few novel results. There are even fewer results in bonding of larger surfaces of glass substrates, leading to the focus of our study. Femtosecond lasers use short bursts of laser pulses to create a laser-modified molten region which is quenched immediately after the molten material is ejected into the gaps of the top stacked substrate, eliminating the need for adhesives. The bonds created between the two substrates have the capability of being as strong, if not stronger than bonds created using adhesives. We have used femtosecond as well as nanosecond laser pulses to study bonding in float glass compositions. We will present an overview of the state-of-the-art of the field along with early results of our study. Our results will reveal potential composition effects on bonding surfaces leading to a better understanding of the response of the substrates to the laser radiation for optimizing bonding methods. These results will provide a basis for further completing a full analysis, using terahertz time-domain spectroscopy (THz-TDS), ultraviolet-visible-near infrared (UV-Vis-NIR), Fourier transform infrared (FTIR), and Raman spectroscopies, among others, of the bonds created across the entire surface of stack glass substrates, constructing a double layer of glasses with strong bonds.

(GOMD-UP-P007-2024) Electrical Characterization of Sodium-containing Germanium Selenide Amorphous Thin Films

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High lithium cost, limited resources, and flammability of available organic electrolytes pose a significant concern on the future of rechargeable lithium-ion batteries in power storage applications. Increasing demand for large capacity rechargeable power storage devices in electric vehicles and robotics requires development of safe, low-cost all-solid-state batteries, which would prevent leakage, volatilization, or flammability. Rechargeable sodium-ion batteries are perspective candidates that can satisfy these requirements in the near future, provided appropriate materials are found for cathode and solid-state electrolytes. Germanium selenide glasses show potential due to their wide glass-forming range, covalent type of bonding, and large amount of free volume proper to their structure. In present work, amorphous thin films of Na-containing germanium selenides have been successfully prepared using thermal evaporation in vacuum method. The obtained films are characterized with scanning electron microscopy and impedance spectroscopy. The electrical characterization was performed in the range of 4 Hz to 8 MHz frequencies using HIOKI LCR meter and temperature controlled LINKAM stage. Temperature and frequency dependences of measured electrical parameters were used to calculate complex plain dependences. Possibility to use this material as solid-state electrolyte for sodium transport is discussed. [This work was supported by National Science Foundation (grant OISE-2106457)]

(GOMD-UP-P008-2024) Structure-property relationships of LiPON doped glassy solid electrolytes (GSEs): 58 Li2S + 42[(1-x) SiS2 + (x) {(1-y) LiPO3 + (y) LiPON}]

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Glassy solid electrolytes (GSEs) are currently a strong contender for the future of solid-state batteries due to their insulative ability and high ionic conductivity. However, within these glasses it's important to optimize the electrochemical stability of the glass to maintain prolonged lifespan of the electrolyte. To improve the ionic conductivity and electrochemical stability, nitrogen is incorporated via the doping of LiPON into the glass. In previous research it has been found that the incorporation of LiPON has caused a steady increase and then a rapid decrease in ionic conductivity, however the previous series of glasses spanned a short varying range of x and y values. This series is meant to expand on the previous series and elucidate the trend in ionic conductivity with increasing values of LiPON. Raman and Fourier transformation infrared spectroscopy are used to analyze the local short range order glass structure, Electrochemical impedance spectroscopy is used to analyze the ionic conductivity, and Differential Scanning Calorimetry is used to analyze the changes in glass transition and crystallization temperatures.

(GOMD-UP-P009-2024) Instrumentation and application of a measurement system for high-frequency investigations of glassy-solid-state-electrolytes

C. S. Martin*[1]; A. G. Wakefield[1]; S. W. Martin[1]

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

In certain highly ionically conductive glass species, deviations from expected Arrhenius conductivity exist in elevated temperature and frequency regions. These effects serve as a point of interest, potentially as theoretical conductivity limits for ionically conductive glasses applied in glassy solid-state electrolytes (GSSEs). To highlight this, the Keysight RF E4991A analyzer was proposed to measure conductivities across temperature ranges and up to frequencies of 3 GHz. Serving as a low-loss dielectric, PTFE was implemented as a calibration standard. First, permittivity measurements were conducted to ensure the system's accuracy in a parallel plate capacitor between system electrodes. Next, sputtered PTFE was placed in AG7 coin cells, allowing for the thickness-dependent stray capacitance of the coin cell to be determined. Using these calibrations, high-frequency measurements of conductive, air-sensitive glasses can be made, and non-Arrhenius behavior can be investigated.

(GOMD-P009-2024) Surface free energy and frost resistance of concrete with of waste glass aggregate

D. Barnat-Hunek*[1]

1. Lublin University of Technology, Department of General Construction, Poland

The study on the physical properties of concrete with waste glass aggregate was presented. Its basic characteristics: absorbability, density, porosity, compressive strength, frost resistance were defined. Five concrete mixtures were prepared, using: Portland cement CEM I 42.5 R, coarse aggregate 2-16 mm, sand, water, superplasticizer and waste glass aggregates, the quantity of which varied in percentage (0; 5; 10; 15; 20%). For the highest glass aggregate content of 20%, the compressive strength is reduced by 10% for the standard concrete. Wetting properties of concrete were determined by measuring the contact angle (CA) of their surfaces using water and glycerine. On this basis, surface free energy (SFE) were defined using the Owens-Wendt method. The highest CA (97°) with water was obtained by concrete with the largest addition of waste glass. This concrete is characteristic of the lowest porosity, absorptivity and the lowest SFE (2.45 mJ/m^2) among the tested materials. After 180 cycles of freezing-thawing, no cracks in the concrete with glass aggregate were observed. The concretes are characterized by an insignificant mass change due to freezing-thawing processes in the case of the control concrete – 4%, samples with 20% waste glass – 0.3%. The glass aggregate increased the hydrophobicity of the concrete.

(GOMD-P013-2024) Recycling of colored waste cullet from glass bead production

A. Klouzkova*[1]; P. Dvoráková[1]; M. Kolárová[1]

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

The paper focuses on treatment of colored glass waste from the production of glass beads. The red-colored glass cullet chosen for the study was analyzed by XRF and sorted into several size fractions. Treated cullet was subsequently mixed with waste material from kaolin mining. Waste mixtures were homogenized together with a suitable temporary binder. The samples were prepared by pressing and subsequent firing by different temperature regimes at temperatures 800-1000°C. The final material was characterized by X-ray methods to determine chemical and mineralogical composition. In addition, mass absorption, porosity, shrinkage, mechanical properties and coefficient of thermal expansion were measured. Proposed glass wasted treatment process brings material with good mechanical properties having bending strength up to 40 MPa, which may be used for production of tiles and other decoration artefacts.

(GOMD-P014-2024) Everglass: The new role of glass in a sustainable society. Technology for the integral recycling of glass

A. Durán[1]; M. Pascual*[1]

1. Instituto de Ceramica y Vidrio (CSIC), Glasses, Spain

Glass recycling uses mature technology limited by high energy consumption to melt tons of glass and the inflexibility of a heavy-duty system. Current technology only allows the recycling of certain glasses and a very small amount of waste generated. A new technology is required to allow the integral recycling of all types of glass, drastically reducing the carbon footprint. EverGLASS proposes to develop a radically new technology called "glass laser transformation" for on-site glass recycling and the generation of customized or technical products. The vision is ambitious, as it aims to bring to the consumer market a novel technology to enable virtually infinite reuse of glass. It proposes an alternative approach to the traditional centralized recycling process (particularly where this model is not possible, generating thousands of tons of glass waste annually taken to landfills). Therefore, EverGLASS has the potential to revolutionize recycling as a concept. It also addresses one of the main problems with recycling, user participation, in an innovative way by allowing the personalization of recycled items of different use. This project brings together experts from advanced laser technologies (UVIGO, Spain), glass and ceramics science (ICV-CSIC, Spain), glass processing and engineering (TnUAD, Slovakia), risk and impact assessment (ACTALIA, France), Social Sciences (ESCI, Germany) and numerical simulation (ITWM, Germany).

(GOMD-UP-P0010-2024) Chemical and Physical Effects of Particle Size and Surface Chemistry on Direct Ink Write Glass Printing

N. Tobin*[1]; J. F. Destino[1]

1. Creighton University, Chemistry & Biochemistry, USA

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 through a nozzle 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 solvent formulation, specifically, the relative ratios of conventional DIW solvents (propylene carbonate and tetraglyme) and silica particle surface area, chemistry, and charge. Qualitatively, ink formulations were screened based on the maximum solids loading achievable and the ability to extrude through an 18-gauge nozzle under 200 N. From these results, the rheology of select formulations was characterized. Initial results indicate that polar silica particles disperse best (i.e., achieve a higher solid loading) in majority propylene carbonate solvent mixtures, and non-polar silica particles disperse best in majority tetragylme solvent mixtures. Furthermore, particles with a greater surface area more readily sinter to transparency.

Tuesday, May 21, 2024

S1 Fundamentals of the Glassy State

Session 3: Structural Characterizations of Glasses and Melts

Room: Turnberry
Session Chairs: John McCloy, Washington State University; Dominique de Ligny, University Erlangen-Nürnberg

9:20 AM

(GOMD-S1-036-2024) A review on the structure of oxynitride phosphate glasses and a thermodynamic approach to their study (Invited)

A. López-Grande[2]; F. Munoz*[1]

1. Institute of Ceramics and Glass, CSIC, Spain
2. Otto-Schott Institute for Materials Research, Germany

Oxynitride phosphate glasses were originally explored because of the higher chemical resistance they offered in comparison with the one of phosphate ones. Most of their interest was on the application as sealing glasses; however the increase of the electrical conductivity in lithium phosphates after nitridation gave rise to a research field focused on exploring the possibilities of utilization as solid electrolytes. The structure of the oxynitride phosphate glasses can be represented by the PO_4, PO_3N and PO_2N_2 groups with modifier cations coordinated by the non-bridging oxygens, and where nitrogen atoms are bonded to either two or three phosphorus. An important aspect of the nitridation reaction is that the same chemical rules apply to any composition, though the final structure has shown to depend strongly on the type of modifier cations. Furthermore, some recent studies suggest that the effect of composition could also lead to different degrees of segregation in oxide and oxynitride domains within the phosphate network. In this talk, the evolution of the most important experimental findings on the structure of this kind of glasses will be reviewed, and we will also present the most recent research on the nitridation of alkali phosphates that has allowed us to make a relationship between the structure of the oxynitride glass network and the formation energies of the crystalline oxynitrides within the given system of composition.

9:50 AM

(GOMD-S1-037-2024) Structure-property correlations in RE-doped fluoride-phosphate glasses sought by magnetic resonance and electronic spectroscopies (Invited)

A. de Camargo*[1]

1. BAM Federal Institute for Materials Research and Testing, 5.6 - Glass, Germany

As the development of optimized glass compositions by traditional trial-and-error methods is laborious, expensive, and time consuming, it is desirable to gather fundamental understanding of structure and to develop structure-property relation models, which allow best and faster choices. Particularly, when it comes to optical applications of glasses doped with emissive trivalent rare earth ions (RE), the chemical environmental around the ions will have a direct influence on the radiative/non-radiative emission probabilities. The vibrational environment and the chemical nature of the bonds in the first coordination sphere of the ions can be tailored, to some extent, based on structural information given by magnetic resonance (NMR and EPR) techniques associated to Raman and photophysical characterization. For the past 5 years we have been researching fluoride-phosphate glasses for promising high energy radiation detection. The glasses are based on the compositional system $(Ba/Sr)F_2$-$M(PO_3)_3$-MF_3-$(Sc/Y)F_3$ where M = Al, In, Ga, and the phosphate component is substituted by the fluoride analogue in 10-30 mol%, using Sc^{3+}, Y^{3+}, and the Eu^{3+} and Yb^{3+} dopants, as structural probes. Through this exemplary study, the aim of this presentation is to show how powerful the combination of NMR, EPR, Raman and PLE spectroscopies can be to provide structural information and to present the perspectives for their introduction in the research agenda of Div. 5.6 - Glass at BAM, in Germany.

10:20 AM

(GOMD-S1-038-2024) Plutonium oxide melt structure and bonding

S. K. Wilke*[1]; C. J. Benmore[2]; O. L. Alderman[3]; G. Sivaraman[4]; M. Ruehl[5]; K. Hawthorne[5]; A. Tamalonis[6]; D. A. Andersson[7]; M. A. Williamson[5]; R. Weber[1]

1. Materials Development, Inc., USA
2. Argonne National Lab, X-ray Science Division, Advanced Photon Source, USA
3. Rutherford Appleton Laboratory, ISIS Neutron and Muon Source, United Kingdom
4. University of Illinois at Urbana-Champaign, Chemical & Biomolecular Engineering, USA
5. Argonne National Lab, Chemical and Fuel Cycle Technologies Division, USA
6. Tamalonis Technologies, USA
7. Los Alamos National Lab, Materials Science and Technology Division, USA

Plutonium oxides are important components in mixed oxide nuclear fuels (MOX) and vitrified nuclear waste. Because of experimental radiotoxicity hazards, the structure and properties of Pu-containing oxides are typically drawn from computational modeling. Yet, the ability to validate these models is limited by the scarcity of experimental data, especially at high temperatures. We report on the atomic structure of PuO_{2-x} over the temperature range 1300-3000 K, including through its melting transition. A technique combining aerodynamic levitation, laser beam heating, and X-ray total scattering provides the first structural data for PuO_{2-x} melts. Using levitation gases with different oxidation potentials provides access to compositions spanning much of range between Pu_2O_3 and PuO_2. Structural models consistent with the X-ray data indicate that the melts contain mixtures of mostly 5-, 6-, and 7-coordinate Pu-O polyhedra. The melts are also found to be isomorphous with molten CeO_{2-x}, a commonly used non-radioactive surrogate, if differences in Pu and Ce oxidation potentials are addressed. Pu-O bonding exhibits some degree of covalency, based on electronic structure calculations. These data provide useful constraints for material models pertinent to MOX and nuclear reactor design, including planning for hypothetical accidents.

10:40 AM

(GOMD-S1-039-2024) Pb Coordination Environment and its connectivity in Lead Silicate Glasses: Results from 2D 207Pb NMR

S. Sen*[1]; R. Lancelotti[2]

1. University of California, Davis, Department of Material Science and Engineering, USA
2. Federal University of São Carlos, Graduate Program in Materials Science and Engineering, Brazil

The Pb-O coordination environment in binary $(PbO)_x(SiO_2)_{100-x}$ glasses with $30 \leq x \leq 70$ is probed using two-dimensional ^{207}Pb nuclear magnetic resonance (NMR) isotropic-anisotropic correlation spectroscopy. The isotropic ^{207}Pb NMR spectra show little composition dependent evolution of the Pb-O nearest neighbor coordination environment. The systematic variation of the chemical shift tensor parameters offers unique insight into their local site symmetry and suggests the presence of pyramidal PbO_3 and PbO_4 sites with sterically active electron lone pairs, and with Pb-O bond lengths ranging between 0.23 and 0.25 nm. The PbO_3:PbO_4 ratio shows a small but monotonic increase from ~ 70:30 to 80:20 as the PbO content increases from 30 to 70 mol%. When taken together, the isotropic and anisotropic ^{207}Pb NMR spectra suggest that the majority of the PbO_n ($3 \leq n \leq 4$) pyramids in these glasses are connected to the SiO_4 tetrahedra via Pb-O-Si linkages. Significant fraction of Pb-O-Pb linkages, where the oxygen is linked only to Pb atoms, appears only in glasses with PbO ≥ 60 mol%. These oxygen atoms appear to be corner-shared between the PbO_n pyramids in the structure and no evidence for edge-sharing between these pyramids is observed in this composition range. We hypothesize that a substantial fraction of the constituent PbO_n pyramids start to participate in edge-sharing only at higher PbO contents (> 70 mol%), which diminishes the glass forming ability of the network.

11:00 AM

(GOMD-S1-040-2024) Comparative Structural Study of Al_2O_3-SiO_2 Glasses and Amorphous Thin Films

L. Cormier*[1]; S. Ben Khemis[1]; E. Burov[2]; H. Montigaud[2]; P. Florian[3]

1. Sorbonne University - CNRS, IMPMC, France
2. CNRS/Saint-Gobain Research Paris, Surface du Verre et Interfaces, France
3. CNRS - U. Orleeans, CEMHTI, France

Non-crystalline (nc) materials can be prepared by a large number of processing routes that often lead to specific properties or structures. Usually, a highly viscous liquid is rapidly cooled down, allowing the elaboration of bulk glasses. Alternatively, nc thin films can be prepared from various chemical and physical vapor deposition (CVD and PVD) methods, chemical reactions such as atomic layer deposition (ALD) or sol-gel methods. The structure of binary aluminosilicate films is complex and remains poorly understood. In this paper, we focus our study on the impact of alumina doping on the evolution of the structure of thin film in comparison to that of bulk Al_2O_3-SiO_2 glasses. Emphasis will be placed on determining the atomic scale structure using NMR, Raman spectroscopy and X-ray diffraction. In thin films and bulk glasses, the addition of Al_2O_3 is accompanied by an increase in the mean Si-O-T angle and an evolution of the ring statistics with a decrease in the proportion of small rings. We evidenced structural differences between sputtered films and fused bulk glasses. Sputtered Al_2O_3-SiO_2 thin films are about 6-7% denser than their equivalent Al_2O_3-SiO_2 bulk glasses. This was mainly due to a change in ring statistics with the formation of small rings within the sputtered thin films. These structural differences on the atomic structural organization highlight the impact of the synthesis conditions.

11:20 AM

(GOMD-S1-041-2024) Physical and structural properties of R_2O_3–SiO_2 glasses prepared by a levitation technique

A. Masuno*[1]; K. Yoshida[2]; S. Sasaki[2]; Y. Yanaba[3]; H. Inoue[3]

1. Kyoto University, Graduate School of Engineering, Japan
2. Hirosaki University, Graduate School of Science and Technology, Japan
3. The University of Tokyo, Institute of Industrial Science, Japan

Transparent xR_2O_3–$(100-x)SiO_2$ binary glasses (R = rare earth element) were synthesized using an aerodynamic levitation technique. It was found that the minimum x value increased with a decrease of the ionic radius of R^{3+}. The density increased as the R_2O_3 content increased. The packing density increased with a decrease of the ionic radius of R^{3+}. Young's modulus E were greater than 100 GPa and it further increased to 130 GPa with an increase of the ionic radius of R^{3+}. The optical band gap was larger than 5.5 eV that was estimated from UV-vis transmittance spectrum. Local structural analyses were performed by using Raman scattering spectroscopy, ^{29}Si MAS NMR, and XAFS. It was found that the Si–O–Si networks were largely broken by the addition of R_2O_3.

11:40 AM

(GOMD-S1-042-2024) Structure and properties of glasses and melts in the CaO-Al_2O_3-SiO_2 system

D. R. Neuville*[1]

1. IPGP-CNRS-UPC, Géomatériaux, France

The structure and properties of glasses and melts in the CaO-Al_2O_3-SiO_2 (CAS) systems play an important role in Earth and material sciences. Aluminum has a crucial influence in these systems, and its environment is still questioned. We report on results using XANES and Raman spectroscopy and ^{27}Al nuclear magnetic resonance on CAS glasses obtained by the conventional quenching method. We propose an Al/Si tetrahedral distribution in the glass network in different Q^n species for Si and essentially in Q^4 for Al at high silica content. At low silica content, Al can be distributed in more complex Q species. $^{[5]}Al$ and $^{[6]}Al$ show a clearly increase with Al_2O_3. How does this increase in $^{[5]}Al$ affect properties? In particular, how does it influence the mixing between Si and Al in four-fold coordination? We'll try to discuss all this to better understand how structure and properties vary in this diagram.

Session 8: Chalcogenide and phase change materials: Phase transtions and dynamics

Room: Bel Air I

Session Chair: Shuai Wei, Aarhus University

9:20 AM

(GOMD-S1-043-2024) Non resonant phase switching in the chalcogenide SnSe (Invited)

A. Lindenberg*[1]

1. Stanford University, USA

We report on a novel type of phase-change induced by non-resonant, below gap photo-excitation. Typically, light-induced phase-changes are induced through the imaginary part of the dielectric function, associated with above-gap or resonant excitation. Here we show that below gap, mid-infrared excitation can drive novel types of switching in the chalcogenide SnSe, mediated by the real part of the dielectric function. Using time-domain Raman scattering, optical reflectivity measurements, and time-resolved x-ray diffraction we show that a higher symmetry state is induced with dramatic and long-lived modulations in the optical properties. This work defines new routes towards novel types of phase-change materials with reduced energy consumption and ultrafast switching speeds.

9:50 AM

(GOMD-S1-044-2024) Probing relaxation dynamics in fragile liquids with split-pulse x-ray photon correlation spectroscopy at the Linac Coherent Light Source (Invited)

Y. Sun*[1]

1. SLAC National Accelerator Laboratory, USA

The generation of nearly fully transversely coherent femtosecond x-ray pulses by x-ray free electron laser (XFEL) sources, such as the Linac Coherent Light Source (LCLS) has enabled the direct measurement of atomic-scale dynamics in complex systems at their native time scales. A primary methodology to extend dynamic light scattering to angstrom and femto-/picosecond is the so-called split-pulse x-ray photon correlation spectroscopy (sp-XPCS) technique, where the sample dynamics are encoded in the intensity fluctuations in the coherent scattering from rapidly successive XFEL pulses. In the presentation, I will first introduce the x-ray split-delay system. It generally consists of an optical arrangement capable of splitting and recombining x-ray beams after introducing a delay, thus generates double x-ray pulses in rapid succession from a single XFEL pulse. I will summarize our decade-long developments at the LCLS, which have culminated in the production of picosecond-separated near-identical double x-ray pulses. To explain the sp-XPCS methodology, I will show a demonstration experiment that utilizes the pulse pairs from the split-delay system to reveal the sub-picosecond structural relaxation in a model system, i.e., $Ge_{15}Te_{85}$ in its fragile state. Finally, I will discuss various promising aspects of the technique, including accessing dynamics in transient states initiated by an optical laser pulse and exploring heterogeneous fluctuations through higher order time correlations.

10:20 AM

(GOMD-S1-045-2024) Pressure-induced reversal of Peierls-like distortions elicits the polyamorphic transition in GeTe and GeSe (Invited)

T. Fujita*[1]; Y. Chen[2]; Y. Kono[3]; S. Takahashi[4]; H. Kasai[4]; D. Campi[5]; M. Bernasconi[5]; K. Ohara[6]; H. Yumoto[7]; T. Koyama[7]; H. Yamazaki[7]; Y. Senba[7]; H. Ohashi[7]; I. Inoue[7]; Y. Hayashi[7]; M. Yabashi[7]; E. Nishibori[4]; R. Mazzarello[2]; S. Wei[1]

1. Aarhus University, Chemistry, Denmark
2. Sapienza University of Rome, Department of Physics, Italy
3. Ehime University, Geodynamics Research Center, Japan
4. University of Tsukuba, Department of Physics, Faculty of Pure and Applied Sciences and Tsukuba Research Center for Energy Materials Science (TREMS), Japan
5. University of Milano-Bicocca, Department of Materials Science, Italy
6. Shimane University, Faculty of Materials for Energy, Japan
7. RIKEN SPring-8 Center, Japan

While polymorphism is well known in crystalline states, the polyamorphic transition in amorphous states has not been well understood in various types of glasses. Recently, direct evidence of a liquid-liquid transition has been reported in the supercooled liquid of phase-change materials (PCMs), where temperature induces Peierls-like distortions (PLD) that play a key role in the transition. On the other hand, influence of the other factors such as pressure on PLD is still not identified in the polyamorphic transitions. Here we investigated the structural changes of amorphous GeSe and GeTe under in-situ high pressure conditions by 100 keV X-ray diffraction experiment. The analysis of structural factors and pair distribution functions shows clear evidence that pressure can reverse the PLD that elicits a polyamorphic transition. This is supported by our molecular dynamics simulations based on a neural-network potential. A higher transition pressure in GeSe than that in GeTe can be rationalized in terms of PLD. The high-pressure state is characterized by vanishing PLD, a larger coherence length, and a lower compressibility. In addition, the reversed PLD implies a closing of the pseudo-bandgap, which may result in a semiconductor-to-metal transition. Our work highlights PLD as an essential feature of many amorphous octahedral systems including most PCMs, which might be controlled by pressure and chemical components for designing properties in PCM applications.

10:50 AM

(GOMD-S1-046-2024) Revealing phase transitions in fragile supercooled liquids by femtosecond X-ray diffraction (Invited)

P. Zalden*[1]

1. European XFEL, Germany

The supercooled state of fragile liquids is inherently difficult to investigate experimentally due to its short lifetime, limited by crystallization. Femtosecond X-ray diffraction at a free electron laser enables measurements of the atomic structure on the relevant timescale, using the ability to perform PDF-like analysis based on a single femtosecond X-ray pulse. We employed this technique to investigate the supercooled liquid state of phase-change materials. These materials are employed as active elements in novel electronic memory technology. The common materials Sb_2Te (with few % of Ag and In added) and $Ge_{15}Sb_{85}$ are found to undergo a structural transition upon quenching, driven by the onset of a Peierls distortion mechanism toward lower temperatures. This structural transition is consistently observed in the experimental diffraction data as well as in ab-initio molecular dynamics simulations. It coincides with an increase of the activation energy of atomic diffusivity that was previously reported based on fast calorimetric measurements. It constitutes a promising approach to explaining the origin of the fragile-to-strong transition reported earlier. The Peierls distortion localizes charge in the shorter bonds, thereby increasing their covalency and causing more rigid bond angles.

11:20 AM

(GOMD-S1-047-2024) Supercooled liquid tellurium: Water's distant relative? (Invited)

P. Sun*[1]

1. University of Padova, Department of Physics and Astronomy "Galileo Galilei", Italy

Water is known to exhibit many thermodynamic anomalies, earning it the name "the most anomalous liquid". Recent studies have provided strong support for the existence of two forms of liquid water—a phenomenon generally known as "liquid polymorphism"—as the mechanism behind these anomalies. Meanwhile, thermodynamic anomalies which hint at liquid polymorphism have been found in several other systems, including liquid tellurium (Te) where experimental input is relatively lacking. In our recent work, simultaneous small- and wide-angle X-ray scattering measurements are performed on liquid Te supercooled from its melting point to more than 130 K below. We observe clear maxima in its thermodynamic response functions around 615 K, suggesting the possible existence of liquid polymorphism. The wide-angle scattering data further allow us to uncover the structural evolution accompanying the thermodynamic maxima. They reveal a development of intermediate-range order upon cooling, which we attribute to bond-orientational ordering. Comparing our findings to those on water, striking similarities can be found, despite the lack of hydrogen-bonding and tetrahedrality in Te. Therefore, our results indicate that water-like anomalies may be a general phenomenon among liquid systems with competing bond- and density-ordering, which is consistent with the predictions of the two-state model.

S2 Glass and Interactions with Its Environment Fundamentals and Applications

Session 3: Glass Surfaces, Interfaces, and Coatings

Room: St. Andrews
Session Chair: Albert Fahey, Corning Incorporated

9:20 AM

(GOMD-S2-023-2024) Density Functional Theory Modeling of Silicate Glass Surface Structure and Dissolution Mechanisms (Invited)

J. D. Kubicki*[1]

1. University of Texas at El Paso, Earth, Environmental & Resource Sciences, USA

Density functional theory (DFT) calculations have the ability to predict structures, thermodynamics, spectroscopic properties, rates and mechanisms of chemical reactions. Applying DFT to understand interfaces between silicate glasses and aqueous solutions can provide insights beyond experiment data alone. However, the simulation results should be carefully benchmarked against observation wherever possible to ensure that the models are realistic and the computations accurate. This talk will focus on two types of simulations – periodic and cluster models – to shed light on potential mechanisms of T-O-T hydrolysis and glass dissolution. The former can provide details on the nanoscale structure of the interface and the latter can be used to produce accurate spectroscopic parameters and reaction mechanisms. The presentation will start with a experimentally-determined reaction rates of silica glass dissolution as impacted by solution composition and link this with recent spectroscopic observations of the interface. Periodic DFT links the two types of observations and provides an explanation for enhanced dissolution rates in high ionic strength solutions. The second part of the talk will focus on ring structures in silicate glasses and their potential role in dissolution.

9:50 AM

(GOMD-S2-024-2024) Particle-glass interactions: Impacts of pretreatment, aging condition, and glass composition

G. Agnello*[1]; N. J. Smith[1]; A. Antony[1]; C. V. Cushman[1]; H. Kaya[1]; G. Stone[1]; J. Banerjee[1]; H. Park[1]

1. Corning Incorporated, USA

The physics and chemistry that dictate particle-glass interactions under different conditions are important to consider throughout the glass manufacturing process all the way to end-product application. Everything from the process used to clean the glass to what materials it is packed with can have critical impact on field performance, and as such, decisions relating to finishing processes of record (POR) must be informed by rigorous experimentation and fundamental understanding to satisfy today's stringent product specifications. Recently, our group has presented results from several relevant experiments where relationships between particulate transfer to glass surfaces (as well as removal efficiency from said surfaces) and chemical pretreatment have been discussed. Here, we continue this discussion by considering several additional factors, most notably aging environment (i.e. relative humidity) and glass composition (Corning Eagle XG® and Corning® Gorilla® Glass 2). The data provides additional support for the hypothesis that glass composition, chemistry used to treat the surface and the type of contacting material are all critical factors for how different types of particles interact with glass as they age in contact with one another.

10:10 AM

(GOMD-S2-025-2024) Causes and consequences of interaction of soda-lime-silica glass surface with superheated steam

B. Roy*[1]; A. Rosin[1]; T. Gerdes[1]

1. University of Bayreuth, Keylab Glass Technology, Germany

WITHDRAWN

Glass surfaces are vulnerable to the interaction with any atmosphere they are exposed to. The unsatisfied dangling bonds on the surfaces are one of the root causes of their inevitable tendency to interact with any atmosphere. This study was an attempt to discover a novel approach of enhancing the mechanical properties of soda-lime-silica (SLS) glasses by exposing the surface to superheated steam. We discovered that the SLS surface undergoes a silicate network rear-rangement during its interaction with sub-T_g superheated steam, facilitating the diffusion of molecular water into the inter-tetrahedral voids within the silicate network. The stuffing of the voids was the cause of a substantial enhancement in subsurface hardness by 30% up to a depth of 300 nm below the glass surface. The drawback of this approach was linked to the vulnerability of the surface to atmospheric degradation in the first instance. The hardness deteriorated on exposure of the steam-treated surface to the ambient atmosphere for a week. This was due to the condensation of vicinal silanols accompanied by the loss of the entrapped water molecules. One of the approaches to prevent the degradation of hardness on ageing was to bombard the steam-treated surface by N^+ ions. The effect of ion-implantation to stabilize the hardening effect caused by super-heated steam will be presented.

10:30 AM

(GOMD-S2-026-2024) Glass Composition Dependence of Incongruent Release and Surface Leached Layer Formation

N. J. Smith*[1]; E. Barros de Moraes[1]; D. C. Allan[1]; T. Dimond[1]; R. Schaut[1]

1. Corning Incorporated, USA

The interaction of technical glasses with aqueous solutions is important and ubiquitous in commercial applications, glass manu-facturing, and product finishing. Depending on exposure conditions, it is not unusual to observe formation of a hydrated, leached layer on the glass surface—especially in strongly acidic chemistries. The presence of such layers has important ramifications on surface prop-erties, from optical response and haptic feel, to wetting, reactivity, and mechanical response. Their formation under dilute conditions is generally attributed to a reactive interdiffusion mechanism between H^+/H_3O^+ in solution exchanging with leachable elements in the glass network, often in tandem with dissolution of the glass matrix at the outermost interface. Kinetics of this two-moving-interface problem have been historically difficult to predict as a function of glass composition. Here, we summarize work to numerically solve the relevant set of diffusion equations with concentration-dependent diffusivities by finite-difference methods, enabling model fits against solution-concentration data from a host of experiments on simpli-fied glasses in acidic media. Results are validated by comparison with direct elemental depth profiles of H-enriched leached layers on the same glasses measured by SIMS. These studies enable new insights into glass-composition-based drivers for leaching kinetics, paving the way for prediction of this important attribute in glass chemical durability models.

10:50 AM

(GOMD-S2-027-2024) The chemical diffusion through the interface between float glass and an amorphous thin film

E. Burov*[1]; S. Ben Khemis[1]; H. Montigaud[1]; L. Cormier[2]

1. Saint-Gobain, Laboartoire Mixte Saint-Gobain/CNRS, France
2. IMPMC, Sorbonne University-CNRS, France

Chemical diffusion plays an important role at all stages of flat glass processing, and in particular controls interaction between the glass surface and thin films during heat treatments (tempering, bending) above the glass transition temperature of the substrate. The diffusion of alkalis from glass (particularly sodium) within all or part of the stack has been identified as the most common phenomenon. This contribution may be required for certain processes, but it often leads to degradation of the optical, electrical or mechanical properties of thin-film stacks. Silica layers with different types of doping partially reduce the migration of alkalis to the functional layers. The migration of elements from glass to the silicates thin films depends in a complex way on the temperature and composition of the glass and layers. It due to the couplings between species during the movement of ions within a highly polymerized structure. The challenge of studying the diffusive properties of thin films deposited by magnetron sputtering of alumina-doped silica used as a barrier layer lies in the thin thicknesses and amorphous nature of the silica films, which required specific developments for their characterization. In this study, the qualitative diffusion profiles in the films obtained by SIMS (Secondary Ion Mass Spectroscopy). The impact of the films and substrate glass composition has been analyzed. The obtained results are correlated also with the structure of the thin films.

11:10 AM

(GOMD-S2-028-2024) Two-dimensional material-based coatings for next-generation damage-resistant glasses

S. Sahoo*[1]; O. P. Khatri[2]; Z. Khan[3]; S. Mannan[4]; D. Thakur[5]; Z. Ye[6]; V. Balakrishnan[5]; N. Krishnan[4]; N. N. Gosvami[1]

1. Indian Institute of Technology Delhi, Department of Materials Science and Engineering, India
2. CSIR - Indian Institute of Petroleum, India
3. National Institute of Technology Srinagar, Department of Metallurgical and Materials Engineering, India
4. Indian Institute of Technology Delhi, Department of Civil Engineering, India
5. Indian Institute of Technology Mandi, School of Engineering, India
6. Miami University, Department of Mechanical and Manufacturing Engineering, USA

The ubiquitous presence of glasses in our daily lives underscores their importance, yet susceptibility to contact damage, such as indents and scratches, remains a significant mechanical drawback. Conventional glass coatings often face limitations related to their transparency, adhesion, or durability. This work explores the burgeoning potential of atomically thin two-dimensional materials as a new paradigm for protective glass coatings. For macro-scale contacts, an in situ dispersion-derived graphene oxide film is shown to mitigate cracks and wear in water by minimizing the frictional shear stresses. At micro-scales, the deposition of few-layered graphene is demonstrated to suppress dry scratch damage and mechanochemical wear in humid conditions. Such excellence of graphene coatings is owed to its super-lubricity, out-of-plane stress shielding, and chemical impermeability towards aqueous corrosion. Finally, the study explores the viable large-area growth of WS_2 films via chemical vapor deposition to extend the superior scratch performances toward higher scales. The experimental data are complemented with atomistic simulations to reveal the tribochemical bonding and deformation mechanisms under rigid contacts. Overall, this work paves the way for a new era of damage-resistant glasses holding immense promise for diverse applications, from smartphone screens to advanced optical lenses and next-generation electronics.

11:30 AM

(GOMD-S2-029-2024) Thickness determination of thick polymer coatings with spectroscopic ellipsometry

H. Kaya*[1]; A. Li[1]

1. Corning Incorporated, USA

Polymer coatings are implemented on glass surfaces for variety of applications. Reliable methods for non-destructive characterization of such films are few, especially when the refractive index of the coating is like that of the glass. Spectroscopic ellipsometry (SE) is a widely used technique for thinner films, typically less than ~5 μm, though as the layers become thicker, SE analysis becomes less straightforward. Couple this with low index of refraction contrast between the substate and thin film(s) and the task becomes even more challenging. Here, we report on the feasibility of using SE for analyzing thick polymer layer coatings (>10 μm) on glass. Limitations of SE as well as comparison of the results with the results obtained from other techniques will be presented.

11:50 AM

(GOMD-S2-030-2024) Probing the Outer Monolayer of Aluminosilicate Glass Surfaces with Low-Energy Ion Scattering (LEIS)

R. Thorpe*[1]; N. J. Smith[2]; C. V. Cushman[2]; G. Agnello[2]; J. Banerjee[2]; A. Antony[3]

1. Lehigh University, Institute for Functional Materials and Devices, USA
2. Corning Incorporated, Science & Technology Division, USA
3. Corning Incorporated, Manufacturing, Technology, and Engineering Division, USA

The outermost atomic layer of a glass has significant implications on properties such as electrostatic charging, wetting, and adhesion. This surface layer may not be well approximated by the bulk composition, and most spectroscopic techniques are unable to isolate the signal from such a thin layer. Low-energy ion scattering (LEIS) is considered the most surface sensitive spectroscopic technique and is a powerful tool to probe glass surfaces at the atomic scale. Building upon prior LEIS studies with ternary Ca-aluminosilicate glass compositions, we explore the impact of glass modifier ion identity on LEIS signals through a series of simple aluminosilicate glasses (e.g., $15R_xO$-$15Al_2O_3$-$70SiO_2$, where R = Ca, Mg, Sr, Na), examining fresh fracture surfaces created under high-vacuum. We then extend these studies by examining potential effects of ion beam damage or in vacuo exposure of the fracture surface to atomic oxygen or water vapor. Results show substantial differences in behavior between alkali and alkaline-earth glasses at the outermost monolayer, the former showing much greater sensitivity to effects of beam damage and surface preparation. These observations cast doubt on the ability to accurately characterize alkali-containing glasses with commercial importance. However, they also highlight the potential promise of understanding alkaline-earth glass surfaces at this scale.

Session 4: Materials for Waste Immobilization

Room: Shoal Creek
Session Chair: Joseph Ryan, Pacific Northwest National Lab

9:20 AM

(GOMD-S2-031-2024) Predicting Long-Term Aqueous Corrosion of Immobilized Low-Activity Waste Glass (Invited)

S. Kerisit*[1]; J. Neeway[1]; X. Song[1]; Y. Fang[1]; B. Parruzot[1]; J. V. Crum[1]; S. K. Cooley[1]; M. Asmussen[1]; G. L. Smith[1]

1. Pacific Northwest National Lab, USA

The immobilized low-activity waste (ILAW) glass corrosion model (IGCM) was initially developed in the late 1990s in the context of a performance assessment (PA) of the Integrated Disposal Facility (IDF), a low-activity waste repository located on the Hanford Site in Washington State, USA. The IGCM has recently undergone several changes in terms of the functional forms used in the model, the approaches used for parameterization, and the glass composition space for which it has been parameterized. This presentation will describe the resulting quantitative improvements in the ability of the IGCM to predict the long-term aqueous corrosion of ILAW glass. We will focus on predicting the concentrations of dissolved glass components in static dissolution tests at multiple temperatures and in pressurized unsaturated flow tests, which simulate the hydraulically unsaturated conditions expected in the IDF. Additionally, recent work has emphasized understanding and quantifying the impact of glass composition on IGCM parameters through the development of composition–parameter correlation (CPC) models. We will discuss how CPC models can be used to predict the long-term corrosion rates of ILAW glass and how glass corrosion rates correlate to the release rates of contaminants of concern from the bottom of the IDF.

9:50 AM

(GOMD-S2-032-2024) Glass Formulations to Expand Hanford High-Level Waste Processing to Composition Regions Appropriate for Minimal Pretreatment

J. Vienna*[1]; X. Lu[1]; V. Gervasio[1]; J. T. Reiser[1]; M. Peterson[1]; N. L. Canfield[1]; J. Lang[1]; J. C. Rigby[1]; J. George[1]; N. Lumetta[1]; J. M. Westman[1]

1. Pacific Northwest National Lab, USA

Alternative options are being considered for the startup of the Hanford High-Level Waste (HLW) Vitrification Facility. One option is the direct feeding of HLW tank waste to the Facility with no leaching and minimal or no washing. Fifteen glasses were formulated for a range of potential direct-feed HLW (DFHLW) waste composition estimates using glass property-composition models developed for pretreated Hanford HLW. The glasses were fabricated and tested to determine if the previous models were appropriate for use with currently proposed DFHLW feeds. It was found that most models could sufficiently predict glass properties while other models need significant adjustments. This talk will describe the formulation and test results for the glasses along with adjustments made to existing models to enable reliable DFHLW flowsheet evaluations.

10:10 AM

(GOMD-S2-033-2024) Accounting for Reaction Progress in Simulation of the Long-Term Aqueous Corrosion of Nuclear Waste Glass

S. Kerisit*[1]; J. Neeway[1]; B. Parruzot[1]; J. V. Crum[1]; M. Asmussen[1]; G. L. Smith[1]

1. Pacific Northwest National Lab, USA

A portion of the low-activity waste (LAW) inventory at the Hanford Site will be immobilized through vitrification and disposed of on site at the Integrated Disposal Facility (IDF). The performance assessment (PA) for the IDF analyzes the long-term performance of the planned disposal system, including the release of contaminants 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 the parameterization of the glass dissolution and IEX components using static test data collected over two years for a matrix of 24 ILAW glasses that provides statistical coverage of several major components in the ILAW glass composition space expected to be produced at the Hanford Waste Treatment and Immobilization Plant (WTP). This work evaluated constant, time-dependent, and time- and pH-dependent functional forms of the IEX component of the IGCM. While adding a pH-dependent term had little impact on the goodness of fit due to pH not changing significantly over the two-year test period, the addition of a time-dependent term significantly improved agreement with measured concentrations (B, Na, and Si). This work thus demonstrates that a time-dependent IEX term is a simple means to complement the chemical affinity term in accounting for the glass-water reaction progress.

10:30 AM

(GOMD-S2-034-2024) Modeling of Secondary Phases to Account for Incongruent Glass Dissolution

J. Neeway*[1]; J. V. Crum[1]; J. T. Reiser[1]; S. Kerisit[1]; B. Parruzot[1]; M. Asmussen[1]; G. L. Smith[1]; D. Swanberg[2]; R. Skeen[2]

1. Pacific Northwest National Lab, USA
2. Washington River Protection Solutions, USA

As glass dissolves, elements from the glass are released into solution. Typically, boron is used as the tracer of matrix dissolution because it is highly soluble and it is typically not retained in glass alteration layers. However, the release of other glass components is incongruent due to solubility considerations and glass structural factors. For this reason, a suite of secondary phases with an appropriate log K matrix is needed for glass corrosion models to accurately account for the release of a range of elements besides boron. This presentation discusses the Incongruent Dissolution Representation (IDR), a suite of secondary phases established to accurately predict the solution concentrations of a wide range of elements as a function of reaction progress. The IDR was established by minimizing the root mean square logarithmic error between model and experiment from static dissolution tests at 40 °C and 90 °C of a compositional matrix of 24 statistically-designed glasses. In addition to the assigned secondary phases, we also present the use of retention factors to eliminate coupled effects resultant of solution chemistry and the application of kinetic rate constants that control the rate of secondary phase formation once thermodynamic saturation is achieved. Collectively, the IDR and retention factors drastically improves the agreement between model predictions and experimental results.

10:50 AM

(GOMD-S2-035-2024) Sensitivity of Long-term Modeling of Glass Corrosion to Model Parameters in Arid, Shallow Subsurface Disposal

M. Asmussen*[1]; S. Kerisit[1]; J. Neeway[1]; X. Song[1]; Y. Fang[1]; B. Parruzot[1]; J. V. Crum[1]; J. T. Reiser[1]; G. L. Smith[1]; P. D. Meyer[1]

1. Pacific Northwest National Lab, Energy and Environment Directorate, USA

The immobilized low activity waste (ILAW) glass to be generated at the Hanford site will be disposed of at the Integrated Disposal Facility (IDF). The IDF is a shallow subsurface disposal facility locatedat Hanford where arid conditions are prominent. In performance assessment modeling simulations of the IDF, glass corrosion is estimated with the ILAW Glass Corrosion Model (IGCM) in reactive transport modeling. Various parameters are used in the IGCM to represent the glass and combined with inputs of near field processes (e.g., mineral precipitation) occurring during disposal. Predictions of the release rates of contaminants of concern from the IDF into the subsurface are sensitive to the various IGCM parameters and overall model framework. The IGCM parameters have varying levels of uncertainties due to the experimental approaches used to determine them, and they have different extents of correlation to glass composition. This presentation will discuss glass corrosion simulations that quantify the sensitivity of predictions of glass dissolution rates and contaminant release rates to various IGCM parameters (e.g., pseudo-equilibrium constant, ion-exchange rate). Sensitivity test cases will be presented from modeling efforts and compared against examples of sensitivity responses from laboratory tests predicting contaminant release in both saturated and unsaturated conditions along with field data from a lysimeter test of glass waste forms.

11:10 AM

(GOMD-S2-036-2024) Borosilicate vitrification of zeolites and geopolymers for long-term immobilization of cesium and strontium

T. R. Elumalai*[1]; A. Farrant[1]; A. Krishnamurthy[1]; S. Kroeker[1]

1. University of Manitoba, Chemistry, Canada

The safe trapping of radioactive waste products such as $^{135/137}$Cs and ^{90}Sr remains a critical issue with the continued use of nuclear fission as a carbon-neutral power source. The bioaccumulation of Cs and Sr from contaminated groundwater or food sources can have dire consequences on health due to radioactive decay. Naturally occurring zeolites such as clinoptilolite (CPT) can selectively adsorb Cs and Sr ions from aqueous environments, however low ion-retention capacity hinders their use in long-term disposal. Geopolymers (GP) have been proposed as an encapsulation matrix for Cs- and Sr-loaded CPT, however, they suffer from poor chemical durability, resulting in a material that is not entirely amorphous.

Our approach improves on these partial solutions by adapting the highly durable borosilicate glasses used in immobilizing high-level liquid waste. Waste-loaded zeolites and geopolymers are combined with glass-forming components and melted to form a homogeneous borosilicate "geoglass". The incorporation of B_2O_3 into the aluminosilicate networks of CPT and GP improves the melting characteristics and amorphous character of the glass, thus increasing its durability. The aim of this study is to understand the incorporation of waste ions into the network structure of these vitrified wasteforms with the help of solid-state NMR spectroscopy, and to optimize compositions to maximize waste loading and chemical durability, leading to durable, high-volume radioactive wasteforms

11:30 AM

(GOMD-S2-037-2024) The effect of alkali metal and alkaline earth cations on the dissolution behaviour of UK High Level Waste glass

J. Ayling*[1]; R. J. Hand[1]; M. T. Harrison[2]; C. L. Corkhill[3]; C. L. Thorpe[1]

1. The University of Sheffield, United Kingdom
2. National Nuclear Laboratory, United Kingdom
3. The University of Bristol, School of Earth Sciences, United Kingdom

During the operational lifetime of a geological disposal facility, groundwater of variable composition may ingress and interact with vitrified radioactive waste, leaching elements. The rate of this dissolution process is understood to be influenced by elements dissolved in the solution; however, since groundwater is a complex mix of many elements, elucidating the mechanism by which these elements influence dissolution is challenging. A series of MCC-1 tests were used to investigate the effect of single groundwater cations on the residual dissolution rate of simulant UK high level waste glass. Glass monoliths were reacted in solutions containing chloride salts of lithium, sodium, potassium, magnesium, calcium, and strontium for up to 540 days. The dissolution rates were measured by ICP analysis of the solutions and compared as a function of each cation element. The alteration layers were imaged by Scanning Electron Microscopy (SEM) and the thickness measured, and the location of elements characterised by Electron Probe Microanalyzer (EPMA) and laser ablation mass spectroscopy (LA-MS) to infer their role in dissolution.

S4 Outreach Glass Technology Manufactury Recycling & Cross-Cutting Topics

Session 1: STEM Outreach

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

9:20 AM

(GOMD-S4-001-2024) From magnetic, glowing and light bending Glasses, the Sound of Breaking Glass & The Long Night of Science - STEAM outreach in Alfred and beyond (Invited)

D. Möncke*[1]

1. Alfred University, New York State College of Ceramics, USA

Outreach, mostly to school children and prospective students, has a long tradition at Alfred University (AU) and can take many forms, involving faculty, graduate students, admission and recruitment (in no specific order). We are always improving our glass collection, adding new and often surprising, interactive samples that invite questions and show the wide field of applications – materials from our labs to industrial products from AU Alumni. A large, hands-on museum collection is being processed for display for the university and visitors. Our "Sound of Breaking Glass" routine (we invite the audience to break safety glass panes and Prince Rupert's drops) is a hit with any audience, prospective students and parents, or when we visit local High Schools – or they visit us. Our graduate students even took it to ACerS events in Columbus 2023 and Pittsburgh 2022. Our newest experiment was inspired by the European "Long Night of Science", opening all labs for a day to the public, inviting families with kids of all ages. For the inaugural event, we ended up with impressive 500 visitors. Several teachers who attended were inspired to schedule a separate visit with their classes afterwards, interested in the experiemnts we offered. Learning from the Art department, some project-based classes do not sit for a final written exam but invite the public to a show where the students present their synthesis, failures and success, research by showing samples, videos as well as posters.

9:50 AM

(GOMD-S4-002-2024) Ceramic and Glass Industry Foundation Outreach Program: How You Can Help Impact the Next Generation of Professionals (Invited)

L. Houghton*[1]

1. The American Ceramic Society, CGIF, USA

This presentation will discuss the outreach efforts of the Ceramic and Glass Industry Foundation (CGIF), to bring materials science education to students and communities, and align with the foundation's mission, "to attract, inspire, and support the next generation of ceramic and glass professionals." Additionally, the presentation will focus on the importance of volunteerism, specifically within the materials science community. The CGIF has a wide range of support to provide individuals and sections of the American Ceramics Society, who wish to serve in their communities. The support to be provided will be discussed in detail, as well as sharing the impact results of an event supported by CGIF through a recently awarded section grant.

10:20 AM

(GOMD-S4-003-2024) Innovations in K-12 Ceramic and Glass Initiatives at Missouri S&T

K. Wilkerson*[1]; C. Lonergan[1]

1. Missouri S & T University, USA

The Materials Science and Engineering (MSE) Department at the Missouri University of Science and Technology (S&T) is dedicated to ceramic education in the form of K-12 student outreach and engagement through interactive programs and hands-on activities. The recent addition of the Kummer Center for STEM Education on the S&T campus, which aims to provide equal access and opportunity to underserved, underrepresented, and rural communities in Missouri, has provided the MSE department with opportunities to reach hundreds of K-12 students. The department's dedication to creating a supportive learning environment and fostering a sense of community contributes to student success, academically and personally, enriching the current undergraduate experience, while showcasing the passion they have for ceramics and glass. Some of the key outreach activities include hosting both a teachers' camp and high school student camp on materials science in collaboration with the ASM Materials Education Foundation, and hosting multiple sessions during the University's flagship Jackling Introduction to Engineering Camp. Specifically, the ceramic engineering program has put glass at the forefront of several demonstration efforts to show case the intersection of art, science, and engineering with our hot glass shop, utilizing cotton candy to demonstrate glass fiber fabrication (along with a tasty treat!), 3D printing for biomedical applications and more.

10:40 AM

(GOMD-S4-004-2024) Connecting to Students Through the Science of Everyday Materials

H. Smith*[1]

1. Swarthmore College, USA

We have designed a series of hands-on materials science activities centered on helping middle-school students ask science questions about the materials they encounter in their everyday lives, such as the concrete sidewalks they walk on, the steel playground equipment they play on, and the window glass they look through. These activities have been implemented as a series of laboratory investigations in the 'Science for Kids' (SFK) program at Swarthmore College. SFK is an academic part of the Chester Children's Chorus (CCC) summer camp programming. The CCC is a community outreach program run by Swarthmore College to support the academic achievement and personal development of children from Chester, an underserved community about 15 min from Swarthmore, Pennsylvania. This series of laboratory investigations engages students in science by exploring the properties of materials they encounter on a daily basis, and makes extensive use of kit materials and curriculum provided by the Ceramic and Glass Industry Foundation. SFK participants have the opportunity to do experimental science and engage with concepts including: making predictions, forming a hypothesis, collecting data, interpreting their results, and making conclusions. This talk will discuss the design of the curriculum around the core themes of predicting, testing, reflecting, lessons learned, and the impact of these activities on the SFK students.

11:00 AM

(GOMD-S4-005-2024) Clear Futures: Rethinking Education for Advanced Manufacturing of Glass in the US

S. Cooper*[1]

1. Celsian Glass USA, USA

The glass manufacturing industry currently grapples with significant workforce challenges as most manufacturers cite difficulties in filling roles, cultivating specialized knowledge, and retaining talent as the top challenge they face. Traditional education systems, geared towards bachelor's degrees and above, have left a knowledge gap in areas of manufacturing that do not require 4-year degrees. To maintain global competitiveness, it is crucial that the US reevaluate its approach to educating the manufacturing workforce. Glass-focused programs from other countries will be compared to successful domestic manufacturing programs in other industries to paint a picture of what continuous education in the US glass industry could look like. Furthermore, the session will explore the potential of digital platforms in facilitating non-traditional education pathways. Through these comparisons, the goal is to formulate actionable ideas for enhancing glass manufacturing education in the US, addressing the immediate needs of the industry while ensuring long-term global competitiveness.

11:20 AM

(GOMD-S4-006-2024) Empowering Tomorrow's Workforce: ACerS' Workforce Development Initiatives

A. Engen*[1]

1. The American Ceramic Society, USA

This talk highlights The American Ceramic Society's (ACerS) enhanced efforts in workforce development within the ceramics and glass research and manufacturing communities. ACerS employs a multifaceted strategy to workforce development that incorporates educational opportunities, networking, mentoring, and cutting-edge research dissemination. The Society provides these continuous learning experiences through conferences, online and in-person short courses, webinars, and publications.

11:40 AM

(GOMD-S4-007-2024) Full STEAM ahead: Alfred University's efforts to recruit and train ceramic and glass professionals (Invited)

G. Gaustad*[1]; L. Lake[2]; W. LaCourse[1]; R. Welch[1]

1. NYS College of Ceramics, Alfred University, Inamori School of Engineering, USA
2. Alfred University, School of Art and Design, USA

Significant effort is required on an on-going basis to educate the general public, particularly pre-college students and their parents, that ceramics and glass is neither simply pots and windows nor a niche technical career. This talk will highlight a variety of specific recruiting efforts underway at Alfred University along these goals including High School Summer Institutes in glass, ceramics, and digital fabrication, our Night of Science & Art for elementary and middle school students, the Ring of Fire, high school focused social media campaigns, and our gallery and museum events. The New York State College of Ceramics uniquely blends our recruiting and education across both the School of Engineering and the School of Art & Design; examples of cross-discipline efforts in STEAM will be highlighted.

S1 Fundamentals of the Glassy State

Session 1: Glass Formation and Structural Relaxation

Glass Formation and Structural Relaxation

Room: Bel Air II
Session Chair: Collin Wilkinson, Alfred University

1:20 PM

(GOMD-S1-048-2024) Structure of silicate glasses under pressure (Invited)

W. Kob*[1]; Z. Zhang[2]

1. University of Montpellier, France
2. Chengdu University of Technology, China

Many features of the short range order of glasses are reasonably well understood. Much less is known about the medium range order (MRO), i.e., structure on length scales between 5-20 Angstroms, since experimentally this range is difficult to access. In this talk we will present the results from large scale molecular dynamics computer simulations in which we investigated this MRO in sodium silica glasses under hydrostatic pressure, covering a pressure range between 0 and 200 GPa. For pressures above 20 GPa we find that the density increases logarithmically with pressure, and this independent of the Na concentration. For silica we find that the local structure, if characterized by the position of the nearest and second nearest neighbor peaks in the Si-Si pair correlation function, is non-monotonic as a function of pressure. In contrast the peaks at larger distances shift their positions continuously to smaller distances if pressure is increased. By investigating the size of the Si-O-rings as a function of the number of links we find that these rings are fractal objects with a dimensionality that is surprisingly independent of the pressure. The distribution of the particle density in three dimensional space allows to extract a correlation length scale of the positional order. We find that this scale is non-monotonic as a function of pressure and has a maximum at around 10GPa, thus signaling the presence of a special pressure at which silica has a pronounced structural order.

1:50 PM

(GOMD-S1-049-2024) Understanding the Fragile-to-Strong Transition in Silica from Microscopic Dynamics (Invited)

B. Wang*[1]; Z. Yu[2]

1. University of Wisconsin-Madison, USA
2. University of Illinois at Urbana-Champaign, Chemistry, USA

The fragile-to-strong transition (FTS) is an intriguing phenomenon as it signifies a fundamental shift in the dynamical behavior in a glass-forming liquid without compositional changes. Understating FTS may inform us the origin of the fragility of glass forming systems. Here we studied the FTS in the simulated BKS silica, utilizing machine learning to link atomic structure and dynamics. The FTS is found to originate from a change in the temperature dependence of the microscopic activation energetics. Furthermore, results suggest there are two diffusion channels with different energy barriers in BKS silica. The fast dynamics at high temperatures is dominated by the channel with small energy barriers, which is controlled by the short-range order. The rapid closing of this diffusion channel when lowering temperature leads to the fragile behavior. On the other hand, the slow dynamics at low temperatures is dominated by the channel with large energy barriers controlled by the medium-range order. This slow diffusion channel changes only subtly with temperature, leading to the strong behavior. The distributions of barriers in the two channels show different temperature dependences, causing a crossover at around 31000 K. This transition temperature in microscopic dynamics is consistent with the inflection point in the configurational entropy, suggesting there is a fundamental correlation between microscopic dynamics and thermodynamics.

2:20 PM

(GOMD-S1-050-2024) Effect of physical aging on the structure of lithium disilicate and lead metasilicate glasses

R. F. Lancelotti*[2]; S. Sen[1]; E. Dutra Zanotto[2]

1. University of California, Davis, Materials Science and Engineering, USA
2. Federal University of Sao Carlos, Brazil

Glass is a non-crystalline, thermodynamically unstable material that spontaneously relaxes towards the supercooled liquid state. While the kinetics of the relaxation process can be obtained by tracking a property variation, the experimental determination of the atomic-scale structural rearrangements by which glass relaxes remains elusive. Therefore, in this work, we investigated the medium-range order structural rearrangements occurring during relaxation in lithium disilicate and lead metasilicate glasses using Raman and Nuclear Magnetic Resonance spectroscopies. Our findings reveal that the structural relaxation of these glasses involves the Q-species disproportion reaction: $Q^{n-1} + Q^{n+1} \rightarrow 2Q^n$. This reaction tends to shift towards the right as the fictive temperature decreases. The concomitant rearrangement of the network can be consistent with the increase in the refractive index, density, and enthalpy recovery upon glass annealing, providing valuable insights into the structural changes during glass relaxation.

2:40 PM

(GOMD-S1-051-2024) Study of the a-relaxation in mixed network forming glass melts by photon correlation spectroscopy

D. Sidebottom*[1]

1. Creighton University, Physics, USA

We report a dynamic light scattering investigation of the α-relaxation in $(GeO_2)_x(NaPO_3)_{1-x}$ glass melts where two network forming materials are being mixed together. The addition of GeO_2 results in increased numbers of bridging oxygen bonds formed in the oxide network which is seen to monotonically increase the glass transition temperature but result in more complex changes to the glass forming fragility which initially decreases with increasing GeO_2 but increases again at higher GeO_2 contents. In our analysis, we have re-applied a coarse-graining strategy previously applied in sodium germanate glasses to arrive at a proposed resolution to the odd fragility behavior. Also observed in the light scattering measurements is a secondary relaxation, several orders of magnitude slower than that of the α-relaxation, which we have tentatively attributed to diffusive gel-like dynamics of the Ge crosslinks formed between phosphate chains.

3:00 PM

(GOMD-S1-052-2024) The Origin of the Imaginary Heat Capacity in Temperature Modulated Differential Scanning Calorimetry: A Role of Dynamic Heterogeneity

W. Takeda*[1]; P. Lucas[1]

1. University of Arizona, Materials science and engineering, USA

Temperature-modulated differential scanning calorimetry (TMDSC) has been used extensively in glass science despite the lack of concrete understanding of what it probes. The confusion arises from the interpretation of the imaginary part of the complex heat capacity C_p". The meaning of C_p" during glass transition has been debated since the early development of TMDSC. In this study, we investigate what exactly C_p" probes during modulated heating. We employ a recently developed phenomenological model, which accounts for dynamic heterogeneity in undercooled liquid and glass. We show that the simulated C_p" is not the direct measure of enthalpy fluctuation before the modulated heating. Instead, C_p" probes the dynamic evolution of enthalpy fluctuation during heating.

Session 3: Structural Characterizations of Glasses and Melts

Room: Turnberry
Session Chairs: Daniel Neuville; Andrea de Camargo,
Physics Institute of Sao Carlos, University of Sao Paulo

1:20 PM

(GOMD-S1-053-2024) Boroxol ring dissolution in molten and glassy B_2O_3 by neutron diffraction, x-ray diffraction and difference methods (Invited)

O. L. Alderman*[1]

1. STFC, ISIS Neutron and Muon Source, United Kingdom

The structure of $^{11}B_2O_3$ boron oxide glass and its liquid have been measured over a wide temperature range by pulsed neutron diffraction, from T = 14 K up to 1100 K. Contrary to prior neutron scattering results in the literature, thermal expansion of the B–O bond is resolved, with a coefficient of $\alpha_{BO} = 3.2(6) \times 10^{-6}\ K^{-1}$, in quantitative agreement with the result derived by high-energy x-ray diffraction. Exploiting the scattering contrast between neutrons and x-rays, difference functions are derived which eliminate contributions due to O–O pairs, revealing, for the first time, the nearest-neighbour B–B peak in the pair distribution function. This peak occurs at $r_{BB} = 2.430(1)$ Å in B_2O_3 glass, consistent with a mean B-O-B bond angle $\beta = 124^o$ and a large boroxol ring fraction. In the liquid, a much larger $r_{BB} = 2.54$ Å, and $\beta = 134^o$, are indicative of either a much lower ring fraction, a larger non-ring B-O-B bond angle, β_{NR}, or a combination of both. The latter scenario is supported by comparison to a range of molecular dynamics models with varying boroxol ring fractions.

1:50 PM

(GOMD-S1-054-2024) Evolving the lever rule: SROCs and their application in modeling Zn borate glasses

B. Topper*[1]; D. Möncke[2]; R. Youngman[3]; E. I. Kamitsos[4]; C. Varsamis[5]

1. Clemson University, USA
2. Alfred University, USA
3. Corning Incorporated, USA
4. National Hellenic Research Foundation, Greece
5. University of West Attica, Greece

A new approach to quantifying the short-range structural units of glass forming melts has been developed by evolving the classical lever rule. The nodes of the traditional lever rule are reimagined as 'Short-Range Order Configurations' (SROCs) that allow for proper accounting of disproportionation and isomerization of chemical species. The simplicity is that only the short-range structure of just a few glasses need to be determined, then any composition can be considered as a linear combination of the bounding SROCs. The model is first constructed and then applied to the binary zinc borate system over the entire glass forming region. Experimentally, the $xZnO-(1-x)B_2O_3$ system is investigated with NMR, Raman, and IR spectroscopies along with density and DSC measurements. By finding the meta-, pyro-, and orthoborate SROCs, the short-range structure of binary zinc borate glasses is modeled. Correspondence with experimental data is excellent, with predicted density within 0.1% and N_4 within 1% of experimental values.

2:10 PM

(GOMD-S1-055-2024) New Perspectives on the Structural Evolution of Borosilicate Glasses and Crystals (Invited)

B. Moulton*[1]

1. Alfred University, Glass Science and Engineering, USA

Although the glass structure is known to control the properties of oxide glasses generalizable predictive relationships are few and far between. Current models often require a priori knowledge of the coordination of the network formers to work. The connectivity changes resulting from a change in the availability of oxygen to the network formers often comes from Raman spectroscopy. Given the pervasive use of Raman spectroscopy, renewed efforts to compare isochemical glasses with crystals where ab initio simulations can reproduce the mode frequencies and their relative intensities. Evaluation for crystalline barium silicates and lithium borates are presented. These results confirm and challenge some 'well-established' band assignments and point to new directions for understanding the structural evolution in their amorphous counterparts. Informed by the Raman interpretations above, the ternary barium-borosilicate glasses have been fully treated. The coordination and connectivity are linked to show that the oxygen packing is a perfectly linear function between end-member binaries $MO-SiO_2$ and $MO-B_2O_3$. This approach requires only the composition and density be known. The consequences of these relationships are discussed including the limit in the invert glass region as well as that of phase separation. It follows that density-dependent properties should be able to be predicted with a high degree of accuracy for oxide glasses, if these relationships hold.

2:40 PM

(GOMD-S1-056-2024) Structural dynamics in soda-lime silicate glasses driven by synchrotron X-ray-induced charging field

Q. Ma*[1]; D. T. Keane[1]

1. Northwestern University, Northwestern Synchrotron Res. Center, USA

Silica-based glasses are used in a wide range of applications and contribute immensely to social and economic progress. Throughout human history a large body of knowledge has been accumulated through glass-smith apprenticeships and modern-days research efforts. Here we present our recent studies of structural dynamics in soda-lime glasses driven by intense synchrotron X-ray-induced charging fields. The X-ray absorption and scattering measurements simultaneously carried out show that under the charging fields, the first-neighbor structures undergo distortion (the extent of which depends on bond strengths, local dielectric properties, and the field strength) while the medium-range structures, up to ~10 Å, counter-intuitively evolve towards more ordered states. The nominal O_h symmetry of Ca^{2+} polyhedra is lowered likely because of off-center Ca^{2+} displacements, analogue to those found in ferroelectric systems such as perovskite $CaTiO_3$ and $BaTiO_3$. In contrast, the changes in the first-neighbor structures around Si^{4+} ions are weak. The ordered medium-range structures allow estimates of bond angles and dihedral interactions as well as provide a rare glimpse of the dynamical interplay between the local structure and glassy network. These field-driven changes are "reversable" and should be interesting to beam-matter interaction and structure-property relationship communities.

3:00 PM

(GOMD-S1-057-2024) Structural order analysis based on ring shape for network-forming materials

M. Shiga*[1]; A. Hirata[2]; Y. Onodera[3]; H. Masai[4]

1. Tohoku University, Japan
2. Waseda University, Japan
3. National Institute for Materials Science (NIMS), Japan
4. National Institute of Advanced Industrial Science and Technology (AIST), Japan

Rings comprising chemically bonded atoms are essential topological motifs for the structural ordering of network-forming materials. Quantification of such larger motifs beyond short-range pair correlation is essential for understanding the linkages between the orderings and macroscopic behaviors. We recently proposed two quantitative analysis methods based on rings. The first method quantifies rings by two geometric indicators: roundness and roughness. These indicators revealed the linkages between highly symmetric rings and crystal symmetry in silica and that the structure of amorphous silica mainly consists of distorted rings. The second method quantifies a spatial correlation function that describes three-dimensional atomic densities around rings. A comparative analysis among the functions for different degrees of ring symmetries revealed that symmetric rings contribute to the local structural order in amorphous silica. Another analysis of amorphous models with different orderings revealed anisotropy of the local structural ordering around rings; this contributes to building the intermediate-range ordering.

3:40 PM

(GOMD-S1-058-2024) Fluorine in complex alumino-boro-silicate glasses: insight into chemical environment and structure

J. Bussey*[1]; J. McCloy[1]; N. Smith-Gray[1]; N. Stone-Weiss[2]; R. Youngman[2]; D. Neuville[3]; M. Dixon Wilkins[1]

1. Washington State University, School of Mechanical and Materials Engineering, USA
2. Corning Incorporated, USA
3. Université Paris Cité, Institut de Physique du Globe de Paris, France

Fluorine incorporation into silicate glasses is important for technical fields as diverse as geophysics, extractive metallurgy, reconstructive dentistry, optical devices, and radioactive waste management. In this study, we explored the structural role of fluorine in alkaline alumino-borosilicate glass, with increasing amounts of fluorine up to 25 mol% F while maintaining the molar ratios of the other components. Glasses were characterized by X-ray diffraction (XRD), ^{27}Al and ^{19}F nuclear magnetic resonance (NMR) spectroscopy, and electron probe microanalysis. Results showed that essentially all F was retained; however, between 12-15 mol% F (~3.6-4.5 wt.% F), excess fluorine partitions to CaF_2 then NaF and Na-Al-F crystalline phases. Even prior to crystallization, there exist five distinct F environments; three of which evolve into F sites in crystalline phases. The two persistent glassy sites likely involve Al-F-Ca/Na local structures. We propose a general understanding of the expected chemical shift of ^{19}F NMR in systems containing Al, Ca, and Na. Further,

the authors have an accepted proposal to conduct F K-edge X-ray absorption spectroscopy (XAS) on these samples, likely to be scheduled before GOMD. We are unaware of any previous literature regarding F K-edge XAS on glassy materials and believe that this data can complement the current structural understanding.

4:00 PM

(GOMD-S1-059-2024) Cl and F incorporation in aluminoborosilicate glass and effect on sulfate retention, salt formation, and other properties (Invited)

J. McCloy*[1]; J. Bussey[1]; N. Smith-Gray[1]; N. Stone-Weiss[2]; R. Youngman[2]; S. Karcher[1]; D. Neuville[3]

1. Washington State University, School of Mechanical and Materials Engineering, USA
2. Corning Incorporated, USA
3. University of Paris, Insitut de Physique du Globe, France

Volatiles in silicate melts, including F^-, Cl^-, and SO_4^{2-}, play a vital role in materials and processes including volcanism, optical materials, bioglasses, electrofining, and nuclear waste vitrification. In magma, volatiles impact viscosity, explosivity, and metals transport. In nuclear waste vitrification, volatiles play a significant role in inducing salt formation, which is deleterious to melter operations and waste form durability. Two series were synthesized with progressive additions of F and Cl in Na-Ca-Al-B-Si-O glasses, with SO_4^{2-} added to examine any anionic interactions. Cl saturated around 3 mol%, then, at higher concentrations, partitioned into the vapor phase then liquid salt. Cl decreased SO_4^{2-} retention, decreased density, and increased T_g. Salt formation removed Na from the melt, increasing glass network polymerization. By contrast, F saturated ~13 mol%, before partitioning into sub-micron salt crystals (CaF_2 most favorable, then NaF and Na-Al-F crystals), with only slight losses to a vapor phase. F did not affect single melt SO_4^{2-} retention and, in concert with crystallization, decreased T_g and density. Structural data from Raman, NMR, viscosity, and differential thermal analysis is provided. The behavior of Cl and F in low-activity waste type glasses with sulfate additions is significantly more complex than the traditional models. These results will help refine the models for sulfate retention in waste glass as it relates to simultaneously present halides.

4:30 PM

(GOMD-S1-060-2024) Effect of Molybdenum Incorporation on the Network Structure of Sodium Aluminoborophosphate Glasses

A. Krishnamurthy[1]; J. Perillo[1]; P. Florian[2]; S. Kroeker*[1]

1. University of Manitoba, Chemistry, Canada
2. CEMHTI, France

Understanding the incorporation of high-valent cations into oxide glasses has stimulated much research on the structure of multicomponent glasses. Originating from the importance of immobilizing nuclear waste ions such as Mo^{6+}, S^{6+}, Cr^{6+} and P^{5+} by vitrification, increasingly detailed structural studies have presented opportunities to refine existing models and better account for the observed properties. Whilst nuclear magnetic resonance (NMR) spectroscopy has played a key role in describing the local environments of cations in amorphous systems, structural resolution generally decreases with greater compositional complexity, resulting in indeterminate structural models. In this work, high-field ^{27}Al, ^{11}B and ^{95}Mo NMR spectra are interpreted in the light of Pauling bond-strength analysis, bond-valence theory and relevant crystal structures, prompting a re-evaluation of conclusions based on previous NMR data. New information about the influence of Mo^{6+} on network connectivity in aluminoborophosphate glasses will be presented, along with insights into its mechanism of structural integration, and its relationship with changes in properties. In situ high-temperature ^{23}Na and ^{31}P NMR are used to probe ionic mobility and reorganization to the glass network structure at temperatures mimicking those of early-stage vitrified radioactive wasteforms.

Session 8: Chalcogenide and phase change materials: Glass structure and properties I

Room: Bel Air I
Session Chair: Pierre Lucas, Univ of Arizona

1:20 PM

(GOMD-S1-061-2024) Tailoring chemical bonds to design unconventional chalcogenide glasses (Invited)

M. Wuttig*[1]; C. Schön[1]; C. Bichara[2]; C. Gatti[3]; J. Raty[4]

1. RWTH Aachen University, Germany
2. CNRS, France
3. Istituto Lombardo, Italy
4. University of Liege, Belgium

Glasses are commonly described as disordered counterparts of the corresponding crystals; both usually share the same short-range order, but glasses lack long-range order. Here a quantification of chemical bonding in a series of glasses and their corresponding crystals is performed, employing two quantum-chemical bonding descriptors, the number of electrons transferred and shared between adjacent atoms. For popular glasses like SiO_2, $GeSe_2$ and GeSe, the quantum-chemical bonding descriptors of the glass and the corresponding crystal hardly differ. This explains why these glasses possess a similar short-range order as their crystals. Unconventional glasses, which differ significantly in their short-range order and optical properties from the corresponding crystals are only found in a distinct region of the map spanned by the two bonding descriptors. This region contains crystals of GeTe, Sb_2Te_3 and $GeSb_2Te_4$, which employ metavalent bonding. Hence unconventional glasses are only obtained for solids, whose crystals employ theses peculiar bonds. We can thus employ the map to identify crystals which possess glasses with rather different properties. The map even predicts systematic trends for the property change and speed of crystallization, which helps to tailor the properties of the glasses.

1:50 PM

(GOMD-S1-062-2024) Boson Peaks In Amorphous Phase Change Materials

J. Moesgaard*[1]; S. Wei[1]

1. Aarhus University, Chemistry, Denmark

The Boson peak is a universal phenomenon in amorphous solids. It can manifest as an anomalous contribution to the low-temperature heat capacity from excess vibrational modes. Amorphous phase-change materials (PCMs) such as Ge-Sb-Te are a family of poor glass formers with fast crystallization kinetics, being of interest for phase-change memory applications. So far, whether the Boson peaks exist in PCMs are unknown and, if they do, their relation to PCM properties is unclear. Here, we investigate the thermal properties of the pseudo-binary compositions on the tie-line between $Ge_{15}Te_{85}$ and $Ge_{15}Sb_{85}$ from a few Kelvin to the crystallization temperatures. Our results demonstrated the pronounced Boson peaks in the low-temperature heat capacity for the amorphous phase of each composition. By fitting the data to a Debye model with excess Einstein modes, we can extract the Debye temperature Θ_D, the excess fraction of the Einstein modes n_{exc}, and the mean Einstein temperature Θ_E. Θ_E corresponds to a characteristic vibrational frequency related to the dynamic defects. We find that both n_{exc} and Θ_E correlate with the width of exothermic relaxation in the heat flow of the glassy state. This suggests that a larger volume fraction of dynamic defects with a higher vibrational frequency in the amorphous solids is closely related to stronger enthalpy and structural relaxations just below the glass transition in PCMs. The latter helps elucidate the thermal stability for PCM memory applications.

2:10 PM

(GOMD-S1-063-2024) Characterization of the Glass Transition in As_3Se_2 Glass

D. P. Bayko*[1]; W. Takeda[1]; P. Lucas[1]

1. University of Arizona, USA

The arsenic – selenium binary is a staple composition of chalcogenide glasses with many uses in infrared optics. While many studies examine the stoichiometric composition As_2Se_3, relatively few studies have been performed on the As rich side, which displays sharp Raman features associated with the growth of molecular units in the form of As_4Se_3 as well as other structural units that have so far remained controversial. Therefore, Raman spectroscopy and modulated differential scanning calorimetry (MDSC) were utilized to characterize the structural dynamics during the glass transition and identify the influence of the molecular units. Simultaneously, molecular dynamic simulations were performed to identity the nature of the molecular units present in the glass structure. Raman spectroscopy reveals modification in intensities of various network components during the glass transition while MDSC and standard DSC reveal a complex bimodal dynamic across the glass transition indicative of structural heterogeneity. Molecular dynamics models further reveal the presence of As_4 units embedded in the glass network. Overall, the As_3Se_2 composition providing useful insights into the boundary between network and molecular glasses.

2:30 PM

(GOMD-S1-064-2024) Prism Coupling Refractometry as a Quality Control Measure for Chalcogenide Glass Compositions

A. Howe*[1]; R. M. Gaume[1]; K. Richardson[1]

1. University of Central Florida, USA

Withdrawn

Refractive index control is an important part of quality control for Chalcogenide glasses. The index change from boule to boule must be characterized for these materials to be adopted for the highest precision techniques. At the same time, access to reliable sources of raw materials for these glass compositions has become challenging. Many refractometry techniques are time-consuming or can only be used at one wavelength. This is a limitation in an age where dual band performance is often required of many infrared optics. In this work, we report on an upgraded refractometry instrument that can be used to access index variability both across material and between different boules. It is a broadband system that can be used to monitor the refractive index throughout the infrared. Furthermore, because it does not require prior knowledge of the composition it can be used in situations where techniques such as ellipsometry give rise to ambiguity in the measured index. We then demonstrate that it has the necessary precision to be used to study optical materials where the index needs to be controlled to the fourth decimal place.

S2 Glass and Interactions with Its Environment Fundamentals and Applications

Session 3: Unconventional glass surfaces

Room: St. Andrews

Session Chair: Nicholas Smith, Corning Incorporated

1:20 PM

(GOMD-S2-038-2024) Manipulating Glass Time with Entropy (Invited)

Z. Fakhraai*[1]; H. Wang[1]; Y. C. Chen[1]

1. University of Pennsylvania, Chemistry, USA

Glass transition, the process of falling out of equilibrium for a supercooled liquid, has long been a topic of intense theoretical work. A key factor in this process is rapidly increasing relaxation times in supercooled liquids, which is related to the rapid loss of configurational entropy. However, structure/property relationships are difficult to directly predict in glassy systems as controlling entropy is non-trivial. In most existing studies, intermolecular interactions are used to control the local glass structure and dynamics. Here we demonstrate that configurational entropy can be strongly varied under extreme nanoconfinement. In these conditions, the entropic (intra-molecular) and enthalpic (interactions with interfaces) degrees of freedom for a supercooled liquid can be controlled independently, leading to a better understanding of the effect of entropy on relaxation times. Extreme nanoconfinement is achieved through confining polymers or molecular glasses in densely packed nanoparticle films of various sizes. These composite materials also have interesting functional properties such as resistance to thermal and UV degradation, improved mechanical properties, and improved adhesion to glass, which can all be achieved through the manipulation of entropy.

1:50 PM

(GOMD-S2-039-2024) Revealing the superior scratch resistance of CVD-grown WS_2-coated silica glasses

S. Sahoo*[1]; D. Thakur[2]; Z. Ye[3]; V. Balakrishnan[2]; N. Krishnan[4]; N. N. Gosvami[1]

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2. Indian Institute of Technology Mandi, School of Engineering, India
3. Miami University, Department of Mechanical and Manufacturing Engineering, USA
4. Indian Institute of Technology Delhi, Department of Civil Engineering, India

The fracture strengths of glasses critically depend on surface flaws, to which glasses are prone right from their production to usage. Inhibiting such contact-induced defects requires alleviation of the normal and shear stresses generated around the glass-countersurface contact. In this regard, two-dimensional (2D) materials, such as graphene and tungsten disulfide (WS_2), are promising for glass coatings due to their inherent load-bearing nature and extremely low shear strength, although their large-area and high-quality deposition on glasses is challenging. In this study, we demonstrate chemical vapor deposition (CVD) as a viable technique to grow WS_2 monolayers on silica glass and examine the damage resistance with atomic force microscopy (AFM) scratch tests and atomistic simulations. The phase and the quality of the WS_2 layers were characterized by fluorescence, micro-Raman, and X-ray photoelectron spectroscopies. Nanoscale AFM scratch tests against hard diamond tips highlight the robustness and excellent lubricity of the WS_2 films that render the glass more resistant to plastic wear. Furthermore, the mechanisms and extent of elastic-plastic deformation of the WS_2-silica glass assembly were investigated with atomistic simulations. Altogether, the experimental and simulation results demonstrate the potential of 2D material-based coatings for developing superior scratch-resistant glasses.

Session 3: Special Tutorial Session on Glass Surface Analysis

Room: St. Andrews

Session Chair: Nicholas Smith, Corning Incorporated

2:10 PM

(GOMD-S2-040-2024) X-ray photoelectron spectroscopy of glasses (Invited)

J. Shallenberger*[1]

1. Pennsylvania State University, Materials Research Institute, USA

X-ray photoelectron spectroscopy is a powerful, surface sensitive analytical technique that has various attributes that make it ideal for studying the chemistry of glass surfaces and interfaces. This talk will discuss the principle of the technique and the unique combination of advantages that XPS possesses for probing chemical structure of the outer 1-10 nm of materials. When combined with ion sputtering some, but not all, of the advantages of XPS can be extended hundreds or thousands of nanometers below the surface. XPS also can be applied to probing bulk chemical structure of glass via in situ fracture preparation. I will highlight the advantages and limitations of XPS via case studies of glass materials including organic and inorganic coatings, corrosion, adhesion and related surface-related phenomena.

2:30 PM

(GOMD-S2-041-2024) Analyzing Glass Fracture Surfaces with Monolayer Precision Using HS-LEIS (Invited)

R. Thorpe*[1]

1. Lehigh University, Institute for Functional Materials and Devices, USA

High-sensitivity low-energy ion scattering (HS-LEIS) is considered the most surface sensitive spectroscopic technique in existence. Briefly, a beam of He or Ne ions is directed at a sample, and the energies of the backscattered ions are measured by a detector. Most ions that penetrate the outermost atomic layer of the sample are neutralized and cannot pass through the analyzer lens. Consequently, the majority of the signal in a LEIS spectrum comes from just the top monolayer of atoms. This unique quality makes LEIS an attractive technique for the analysis of glasses, where the surface composition can often be dramatically different from the bulk. This talk will discuss recent work in measuring the composition of vacuum-fractured aluminosilicate glass surfaces, with a particular focus on the practical aspects of this analysis. LEIS is a relatively new experimental technique, and the best practices for acquiring and analyzing LEIS data are still being developed. The choice of calibration samples, experimental procedures, energy correction, and peak fitting parameters all have major implications on the quality of LEIS data, but recent studies have provided a roadmap towards reliable characterization of glasses at a length scale that has never before been accessible.

2:50 PM

(GOMD-S2-042-2024) The Use of Secondary Ion Mass Spectrometry for Glass Surface and Near-Surface Analysis (Invited)

A. Fahey*[1]

1. Corning Incorporated, Microscopy and Surface Analysis, USA

Secondary ion mass spectrometry (SIMS) has developed as a staple analysis method for the semiconductor industry, arguable beginning ~40 years ago. It has been applied to the analysis of organic thin films with the advent of Time-of-flight SIMS (ToF-SIMS) and has spurred the development of numerous ion beams for sputtering that produce ionization enhancements for some species and can sputter slowly and in some cases with little molecular damage to reveal ultra-thin features in inorganic depositions and surfaces to producing molecular depth profiles of polymer films tens of micrometers thick. SIMS has become impressively sensitive to surfaces and low concentrations and effective in characterizing a wide range of inorganic materials in some cases detecting elements present at the ppm-level. This tutorial talk will cover analyses of mostly minerals, oxide particles, ceramics, and glasses. It will cover methods that preserve the fidelity of surface and depth-profile analyses, especially for mobile species such as alkali elements. We will also touch on methods of quantification, which are still somewhat unexplored for glass and oxide analysis. Difficulties and approaches to quantification will be explored with proposed methods and hypotheses for furthering quantification. In addition, we'll also broach the topic of molecular signals from inorganic materials and these signals may, or may not be telling us about the structure of the materials we're analyzing.

Session 4: Materials for Waste Immobilization

Room: Shoal Creek
Session Chair: Joseph Ryan, Pacific Northwest National Lab

1:20 PM

(GOMD-S2-043-2024) Future challenges in the vitrification of nuclear waste in the UK (Invited)

M. T. Harrison*[1]

1. National Nuclear Laboratory, WM&D, United Kingdom

The treatment of high-level radioactive waste (HLW) from the reprocessing of used nuclear fuel been carried out in the UK for over 30 years using vitrification to form a durable glass product suitable for long-term storage and disposal. Recently, a new Ca/Zn-based borosilicate glass has been deployed on the vitrification plant at Sellafield, which will be used for the immobilisation of Mo-rich feeds expected from the future wash-out of highly-active storage tanks. Although Ca/Zn glass has been underpinned for a range of standard and wash-out HLW blends, there are some uncertainties about the timing and strategy for the remaining feedstock. This presentation will describe experiments designed to inform decisions and provide options to allow the continued operation of the vitrification plant. In addition, vitrification is also being considered for some intermediate-level radioactive wastes (ILW) in the UK where it offers several advantages over the existing cement-based encapsulation process. These include volume reduction, destruction of organics, reactivity removal and improved product quality. In parallel to some engineering-scale trials by Sellafield Ltd, NNL is developing the R&D capability to support future ILW vitrification plants in a series of R&D trials. These on-going projects, which are focussed on active processing and product quality analytical techniques, will also be outlined in this presentation.

1:50 PM

(GOMD-S2-044-2024) Effect of Al-source on the retention of rhenium during vitrification of nuclear waste

R. Pokorny*[1]; J. Klouzek[1]; P. Cincibusova[1]; L. Lowy[1]; M. Eret[1]; J. George[2]; P. Hrma[3]; A. A. Kruger[4]

1. University of Chemistry and Technology Prague, Czechia
2. Pacific Northwest National Lab, USA
3. AttainX, USA
4. US Department of Energy, Office of River Protection, USA

Volatilization of technetium-99 is of concern during the conversion of low-activity waste (LAW) feed to glass. Although this is commonly resolved by using recycle loops, this can lead to other problems, such as sulfate phase formation. Thus, ensuring high single-pass retention of Tc (or Re, its non-radioactive surrogate) is required to enable high waste-loading formulations. In our previous study, we observed that the Re retention was significantly higher in a low-activity waste (LAW) melter feed containing gibbsite as alumina source than in a compositionally similar LAW feed containing kyanite. To investigate this effect, we prepared a representative LAW feed with different Al-sources – kyanite, gibbsite, boehmite, and corundum – and measured the Re retention in the produced glasses. We found that the Re retention is highest in the boehmite feed, closely followed by gibbsite, while it is significantly lower in the kyanite and corundum feeds. This is likely because gibbsite and boehmite produce nano-crystalline γ-alumina on heating that, as Xu et al. suggested (J. Nucl. Mater., 483 (2017) 102-106), adsorbs the sulfate-perrhenate melt remaining in the reacting melter feed after the nitrate-nitrite-carbonate melt decomposed.

2:10 PM

(GOMD-S2-045-2024) Investigation of the mixed-alkali effect on crystallization of SnO_2 in LAW glasses for WTP

A. J. Lere-Adams*[1]; J. McCloy[1]

1. Washington State University, Materials Science and Engineering Program, USA

A simulant low-activity waste (LAW) base glass with equal mole fractions of Al_2O_3 and Na_2O (primary modifier- thus charge balancing aluminate tetrahedra in glass), and comparatively low molar amount of smaller cations as well as oxyanions is systematically investigated to understand the deviation in crystal fractions of SnO_2 (that can form when melter temps drop below 1100°C) by gradually replacing one alkali/alkaline earth cation by another (in this case Na with Ca). The forced crystallization of Al containing phases is projected resulting in a residual glass more enriched with less-durable components (alkali and borate) in the starting melt. Powder x-ray diffraction (XRD) is used in quantifying the target phase fraction while critical transition temperatures (T_g, T_c) are measured using differential scanning calorimetry (DSC). From the series of melts, down selected glasses are isothermally heat treated to induce phase formation and canister centerline cooling (CCC) to model melter process at the Waste Treatment and Immobilization Plant (WTP). The bond structure in the crystallized phases is investigated with Raman spectroscopy. A durability test (Vapor Hydration test) is conducted to track the effect of SnO_2 formation on corrosion rate and alteration thickness.

2:30 PM

(GOMD-S2-046-2024) Structural investigation of alkali aluminoborosilicate glass containing MoO_3 for vitrification of nuclear waste

S. Kim*[1]; T. Yeo[2]; J. Cho[1]

1. Pohang University of Science and Technology(POSTECH), Division of Advanced Nuclear Engineering, Republic of Korea
2. Pohang University of Science and Technology(POSTECH), Graduate Institute of Ferrous & Eco Materials Technology, Republic of Korea

Molybdenum (Mo), a significant fission product in high-level radioactive waste, exhibits low solubility in aluminoborosilicate glasses. The high concentration of MoO3 in such glasses presents challenges due to its low solubility and high crystallization tendency. Controlled formation of Mo-containing crystal phases like Na2MoO4 and CaMoO4 during the cooling of the melt is critical to minimize their detrimental effects on the long-term properties of nuclear waste glasses. This study investigates the effects of incorporating various alkali cations (Li, Na, K, Cs) into Mo-containing aluminoborosilicate glasses. The results show that incorporation of larger alkali cations promotes a more polymerized glass network, consequently impeding the crystallization of Mo-containing phases. The spectroscopic results reveal that the nature of Mo units varies with the increasing size of the alkali cation, presenting primarily in two forms: (1) distorted octahedral geometry (MoO66-), and (2) MoOx (x = 4–6) featuring Mo reduction species (Mo5+ or Mo4+). In both scenarios, the structural configurations facilitate a direct connection to the silicate network (Mo-O-Si), in accordance with Pauling's stability rule. The formation of direct linkage between Mo and the silicate network is expected to not only improve the solubility of Mo in aluminoborosilicate glasses, but also disrupt the MoO42--rich depolymerization region, thereby inhibiting molybdenum crystallization.

S4 Outreach Glass Technology Manufactury Recycling & Cross-Cutting Topics

Session 2: Challenges in Manufacturing I

Room: Peeble Beach
Session Chairs: Irene Peterson, Corning Incorporated; Katelyn Kirchner, The Pennsylvania State University

1:20 PM

(GOMD-S4-008-2024) Observation of glass synthesis and reactivity by in-situ high temperature ESEM (Invited)

R. Podor*[1]; J. Lautru[1]; Z. Nabyl[2]; R. Pokorny[3]; F. O. Mear[4]; S. Schuller[2]

1. ICSM, Microscopy, France
2. CEA, France
3. University of Chemistry and Technology Prague, Czechia
4. UCCS, France

The elaboration of glass from primary components is a complex process, the complete description of which requires the use of various characterization techniques. The use of global analysis techniques such as differential thermal analysis and/or thermogravimetric analysis (DTA-TGA) provides thermal information, but does not describe the chemical processes involved. A technique often used is to heat treat samples at different temperatures, soak them at room temperature and then identify the phases formed by XRD, SEM, etc. This technique is time consuming and tedious. It can lead to biases that are linked to the sample quenching (crystallization of molten phases, amorphous phases not identified by XRD...) or to the choice of the quenching temperatures (some rapid transformations or those taking place in a narrow temperature range may not be identified). To overcome these limitations, it may be necessary to implement in-situ characterization techniques, where the analysis is carried out during the heat treatment. In-situ high temperature Environmental Scanning Electron Microscopy, ESEM, possibly coupled with EDS analysis, is a technique that is particularly interesting for identifying the chemical reactions and various transformations taking place between the primary components and then between the different phases formed. This technique can also be used to observe glass reactivity at high temperature such crystallization, glass foam formation, self-healing properties.

1:50 PM

(GOMD-S4-009-2024) A Coupled Phase Diagram Study and Thermodynamic Database Development for the Li_2O-Na_2O-Al_2O_3-SiO_2-ZrO_2 system (Invited)

J. Lee*[1]; I. Jung[1]

1. Seoul National University, Material Science and Engineering, Republic of Korea

Zirconium oxide ceramics are widely used in glass-making process, pyrometallurgical process, and dental industry owing to their excellent corrosion resistance, mechanical strength and low thermal conductivity. In particular, glass-making and pyrometallurgical processes involve very complex multi-phase chemical equilibria in the multicomponent systems of SiO_2, Li_2O, Na_2O, K_2O, CaO, MgO, Al_2O_3, ZrO_2, etc. at high temperature. Therefore, understanding the chemical interactions of ZrO_2 with various oxide components are essential to understand the corrosion of zirconia containing refractory in such high temperature processes. In order to provide accurate thermodynamic calculations for complex chemical reactions and phase diagrams, CALPHAD type thermodynamic database can be employed. In the present study, a coupled phase diagram study and thermodynamic modeling approach was taken to develop the thermodynamic database for the Li_2O-Na_2O-Al_2O_3-SiO_2-ZrO_2 system. In particular, experimental phase diagrams of several key binary and ternary systems containing alkali oxide and ZrO_2 were successfully obtained by employing a sealed Pt capsule technique to overcome the experimental challenges for alkali oxides containing system. The resultant database can be used for practical calculations related to melting, refining and refractory corrosion in glass-making process, and for new glass composition design.

2:20 PM

(GOMD-S4-010-2024) Understanding the impact of hydrogen burners on glass melting (Invited)

E. Sarafian*[1]; C. Fekety[1]

1. Corning Incorporated, USA

Corning is investigating hydrogen burner technology as a path toward more sustainable glass manufacturing. This process change could impact glass melt volatilization in the melter, which is dependent on many factors including the imposed combustion atmosphere. Any changes to volatilization might impact crown refractory corrosion, flue condensate, dust particulate emissions, and volatilization related defects. A thermochemical study was completed to compare glass melt volatilization under methane gas-oxy combustion and hydrogen gas-oxy combustion. The results show that volatilization of each component depends on the pH_2O of the imposed atmosphere according to its speciation in the gas phase. Predicted changes to glass melt volatilization, as well as several other key glass characteristics properties, are being validated in a research-scale continuous flow melting system using a simulated hydrogen burner atmosphere. Results from the first continuous flow experiment suggest that glass melt volatilization, batch melting reactions, glass melt redox, glass melt blister chemistry, and tank refractory corrosion under hydrogen gas-oxy combustion do not significantly change. While additional experimentation is underway, the thermochemical and initial experimental results suggest hydrogen burner technology is a viable path toward more sustainable glass products.

2:50 PM

(GOMD-S4-011-2024) Dynamics of bubbles, crystals, and droplets in silicate melts: industrial and natural applications (Invited)

L. Pereira*[1]; F. Wadsworth[2]; D. R. Neuville[3]; D. Dingwell[1]

1. University of Munich (LMU), Germany
2. Durham University, United Kingdom
3. IPGP, France

Silicate systems in industrial or volcanological contexts comprise a continuous silicate liquid suspending bubbles, crystals, and/or droplets. The presence and amount of these suspended secondary phases affect the fluid-dynamics of these materials at high-temperature. In industrial settings, the suspended phases directly control the efficiency of the high-temperature processes and the quality of the final product. In natural volcanic scenarios, the suspended phases exert a first-order control on eruption style: explosive or effusive. In this seminar, a wide-range of experimental and numerical results about silicates containing bubble, crystals, and droplets (or a mix of them) in both nuclear waste vitrification and volcanological contexts are collated and presented. The key conclusions of this compilation of studies are that (i) surface energies of the suspended phases play a key role in the rheological response and dynamics of silicate systems; (ii) crystal aggregation can induce a large increase in viscosity; and (iii) during the formation of these suspended phases, the melt matrix is chemically modified such that polymerisation is a key metric to constrain further. These three crucial results have a direct impact on both industrial nuclear waste vitrification processes and our understanding of volcanic phenomena on Earth and other planets.

S1 Fundamentals of the Glassy State

Session 1: Glass Formation and Structural Relaxation

Glass Formation and Structural Relaxation

Room: Bel Air II
Session Chair: Collin Wilkinson, Alfred University

3:40 PM

(GOMD-S1-065-2024) Accelerated Structural Relaxation of Chalcogenide Glasses via Thermo-Ultrasonication

P. Lynch*[1]; G. Sop Tagne[1]; R. Welch[2]; R. Sharma[3]; K. Richardson[3]; S. Yaniger[1]; W. LaCourse[1]; C. Wilkinson[1]; M. Kang[1]

1. Alfred University, New York State College of Ceramics, USA
2. Pennsylvania State University, Department of Materials Science and Engineering, USA
3. University of Central Florida, CREOL, College of Optics and Photonics, USA

A novel approach to manipulating the fictive temperature of chalcogenide glasses using a combination of sonic and thermal stimulation is introduced. Glasses exhibit time-dependent structural relaxation, often leading to temporally inconsistent response under post treatments such as direct laser writing. This inconsistency is a substantial issue in the development of novel materials for optical phase change platforms or gradient refractive index media since their optical contrast needs to be maintained over a long period of time. In order to tackle this issue, we employ a novel experimental approach which involves the usage of thermo-ultrasonication, to expedite the relaxation of chalcogenide glasses towards the super cooled liquid state and enable a consistent optical response. Here, we present the use of As_2S_3 and Ge-As-Pb-Se chalcogenide bulk glasses to test the effects of thermo-ultrasonication on relaxation kinetics. These samples were chosen due to the low glass transition temperatures (T_g) and their prevalent use as optical materials. The samples were subjected to ultrasonic vibration at an elevated temperature slightly below T_g to accelerate the structural relaxation rate. We discuss improved kinetics of their structural relaxation in terms of fictive temperature, mass density, and refractive index as well as our process' applicability to a broader range of glass system.

4:00 PM

(GOMD-S1-066-2024) Experimental Measurement of Configurational and Vibrational Entropy in Metallic Glasses

H. Smith*[1]; W. Zhang[1]

1. Swarthmore College, USA

Liquid fragility characterizes how quickly viscosity decreases above the glass transition in glass-forming liquids. This property is fundamental to glass physics and of critical importance for engineering applications. Competing theories have suggested that vibrational properties may play a role in describing fragility by contributing vibrational entropy to the large excess entropy of the undercooled liquid over the crystal above the glass transition. We performed the first in situ inelastic neutron scattering measurements of metallic glasses in the undercooled liquid phase and reported that at most 5% of the entropy of the glass transition originates from vibrational entropy in $Cu_{50}Zr_{50}$ and $Cu_{46}Al_{46}Zr_8$. We have extended this work to include two extremely fragile Pt-based metalloid glasses [3]. In situ measurements of the phonon densities of states were performed with inelastic neutron scattering during constant heating through the glass transition and above the crystallization temperature. This talk will discuss the correlation between excess vibrational entropy in the undercooled liquid and liquid fragility. Our results will be considered in the context of a universal understanding of vibrational contributions to the thermodynamics of the glass transition.

Session 8: Chalcogenide and phase change materials: Glass structure and properties II

Room: Bel Air I
Session Chair: Pierre Lucas, Univ of Arizona

3:40 PM

(GOMD-S1-067-2024) Density functional simulations of Ag migration in a conductive bridging random access memory cell (Invited)

J. Akola*[1]

1. Norwegian University of Science and Technology, Department of Physics, Norway

We have performed density functional/molecular dynamics (DF/MD) simulations to investigate the drift of Ag atoms in an amorphous GeS_2 solid-state electrolyte between Ag and Pt electrodes in the presence of a finite electric field. The model structure of 1019 atoms represents a conductive bridging random access memory (CBRAM) device. Simulations under an external electrostatic potential show Ag migration and the formation of percolating single-atom Ag wires through the solid-state electrolyte. The electronic structure analysis of selected snapshots shows that dissolved Ag atoms become markedly cationic, which changes when Ag clusters form at the Pt electrode. Sulfur becomes more anionic during the migration as a result of Ag-S bonding, and the effect is most pronounced near the active (Ag) electrode. The formation of conductive filaments requires a percolating network of Ag clusters to grow from the Pt interface, and the weakest links of this network appear at the Ag electrode. We also presents result for our latest electronic structure analyses of the prototypical phase-change material $Ge_2Sb_2Te_5$. Hybrid DF simulations have enabled us to pinpoint electron/hole localization effects with local geometrical motifs both in the amorphous and re-crystallized phases.

4:10 PM

(GOMD-S1-068-2024) Optical phase change materials: chalcogenides and beyond (Invited)

J. Hu*[1]

1. Massachusetts Institute of Technology, USA

Phase change materials (PCMs) are a unique class of compounds that demonstrate gigantic contrast in electronic and optical properties upon a nonvolatile structural transition between their amorphous and crystalline phases. In addition to their established use in electronic memories, applications of PCM in optics have attracted significant interest in recent years, which motivates the development of emerging PCM alloys specifically tailored for photonic integration. In this talk, I will review design, synthesis and characterization of broadband infrared transparent PCMs, in particular cycling response of these materials to elucidate their degradation mechanisms in photonic devices. I will also discuss our recent efforts on chalcohalide PCMs targeting low losses in the visible bands.

4:40 PM

(GOMD-S1-069-2024) Probing the ultrafast structural relaxation dynamics of amorphous GeTe and GeSe using MeV ultrafast electron diffractions

S. Wei*[1]

1. Aarhus University, Chemistry Department, Denmark

The femtosecond (fs)-laser excitation was shown to induce a ultrafast structural transition in a crystalline phase-change material (PCM) $Ge_2Sb_2Te_5$. However, it is unclear how the local structure in amorphous PCMs responds to fs-photoexiations. Here we study the structural relaxation dynamics of the isoelectronic systems amorphous GeSe and GeTe using high-repetition ultrashort electron pulses with the pump-probe scheme using the MeV ultrafast electron diffractions (UED) at LCLS, SLAC. While both materials are p-orbital bonded, they are characterized by different extents of Peierls distortions. We measured the electron diffraction patterns with delay times after fs-laser excitations during the relaxation process. By comparing the structural relaxation dynamics between GeTe and GeSe, we find that the even in the amorphous phases, the relaxation dynamics in GeTe at certain Q-range is substantially faster than that in GeSe. We rationalize the different relaxation behaviors in terms of their different bond softness (or covalency or metallicity) and the extents of Peierls distortions of the local octahedral structures.

5:00 PM

(GOMD-S1-070-2024) The development of a mixed-oxy-sulfide silicate glass as a thin film glassy electrolyte

S. J. Leland*[1]; H. Cochran[1]; J. Wheaton[1]; S. W. Martin[1]

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

Initial explorations of the lithium and silicon sulfide systems yielded ionically conductive glass chemistries potentially suitable for usage in solid-state batteries. A methodology was then developed to characterize the thermal behaviors of existing chemistries to evaluate their viability for thin film processing through the glass redraw process. While the ionic conductivities of each system were high, their thermal properties were too poor for thin film processing. A new system was then chosen, aiming to maintain the ionic conductivities while improving drawability. To achieve the desired properties, a eutectic lithium silicate compound was added to the system in small quantities in the form of $Li_{3.48}SiO_{3.74}$. The high lithium content of the addition was predicted to increase the ionic conductivity, while the silicon and oxygen were predicted to improve the thermal properties. The resulting composition was synthesized and tested, demonstrating improved properties in both areas. The glass and lithium silicate compounds were then synthesized repeatedly to verify properties and prepare a large batch for thin-film drawing. Work was conducted to explore the effects of different starting materials on synthesizing the lithium silicate compound, and each newly synthesized glass was tested for its thermal and electrochemical properties.

5:20 PM

(GOMD-S1-071-2024) Impact of polysulfide impurities on the thermal properties of mixed glass former mixed oxy-sulfide sodium and lithium glasses

J. Wheaton*[1]; M. P. Olson[1]; J. Ryner[1]; N. Riley[1]; S. W. Martin[1]

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

Mixed oxy-sulfide (MOS) glasses, where a sulfide glass is doped with a small concentration of oxygen, are currently being researched for use as solid-state electrolytes in both sodium and lithium solid-state batteries due to their easily tunable compositions, high ionic conductivities, and unique processability. Despite the improved properties, both sulfide and MOS glasses often exhibit polysulfide impurities as evidenced by a peak at ~472 cm^{-1} in the Raman spectra. These impurities seem to be present from the impurity These polysulfide impurities can impact the properties of the glass, particularly the thermal and electrochemical properties, possibly counteracting the benefits provided by added oxygen. Continuing from previous work on mixed glass former mixed oxy-sulfide SSEs, several samples of a sodium ionic conductor and a lithium ionic conductor, NaPSiSO and LiPSiSO, were investigated using Raman spectroscopy. LiPSiSO glasses exhibited polysulfide concentrations between 0 to 1.6 wt%, while the NaPSiSO glasses exhibited polysulfide concentrations from 0.9 to 9.8 wt%. The glass transition temperature, crystallization temperature, and fragility index were determined using differential scanning calorimetry. The impact of polysulfide impurities on these thermal properties was investigated through linear regression.

S2 Glass and Interactions with Its Environment Fundamentals and Applications

Session 4: Materials for Waste Immobilization

Room: Shoal Creek
Session Chair: Joseph Ryan, Pacific Northwest National Lab

3:40 PM

(GOMD-S2-047-2024) Impact of transition metal ions on the structure and sulfur solubility in borosilicate-based model nuclear waste glasses

R. Saini*[1]; X. Xu[1]; A. Goel[1]

1. Rutgers University, USA

The addition of transition metal ions has been long known to alter the sulfur (as SO_4^{2-}) solubility in borosilicate-based model nuclear waste glasses. However, the mechanism governing this effect is still unknown. To answer this question, V_2O_5, Cr_2O_3, and Fe_2O_3 have been added to borosilicate-based model nuclear waste glasses and these glasses have been characterized for their short-to-intermediate range structure and the redox chemistry using ^{11}B, ^{27}Al, ^{51}V MAS NMR, Raman, UV-Visible, XPS and Mössbauer spectroscopic techniques. The sulfur solubility in glasses has been determined by the ICP-OES. The results obtained from these investigations shall be presented.

4:00 PM

(GOMD-S2-048-2024) Understanding Composition-Driven Metastability in High-Level Nuclear Waste Glasses via Materials Informatics

I. Sargin*[1]

1. Middle East Technical University, Department of Metallurgical and Materials Engineering, Turkey

High-level waste (HLW) glasses are prone to nepheline crystallization during slow canister cooling. The detrimental effects of nepheline to the glass durability compels precautions to either limit or to avoid its formation. A priori models to predict nepheline formation based on glass composition has been an on-going task for at least a decade. However, the compositional complexity of HLW glasses encumbers this task. Our recent study has showed an overlapping region between nepheline forming and not forming compositions obstructs more general, robust, and predictive models. In this study, we have investigated the reasons for the existence of overlapping region. We have developed two successive models, first to identify the glasses within the overlapping region, and then a model for differentiating between nepheline formers and not nepheline formers. These models not only increase the predicting accuracy but also provides insights on the existence of this overlapping region based on thermodynamics and physical basis of the metastability.

4:20 PM

(GOMD-S2-049-2024) Predicting the nepheline amount in high-level nuclear waste glasses by machine learning

E. Ardic*[1]; I. Sargin[1]

1. Middle East Technical University, Metallurgical and Materials Engineering, Turkey

Vitrification is widely used to immobilize high-level nuclear waste. Nepheline formation stands as a barrier to reaching higher waste loading because its presence can degrade the chemical durability of nuclear waste glass. On the other hand, eliminating all compositions that form nepheline may result in rejecting the potential compositions that allow high waste loadings while providing adequate durability. The prediction of the amount of nepheline may open the door to higher waste loading without affecting the durability since nepheline will be detrimental to the durability if it is above 10 volume percent. By utilizing informatics tools, this study develops models to predict the nepheline amount in high-level waste glasses. The data set of 155 nepheline-forming glass compositions, i.e., individual oxide amounts and structural and complex compositional features, are used for predicting relative nepheline volume. Feature selection was followed by hyper-parameter tuning. The success of the models is evaluated by mean absolute error. The regression model that gives the best results predicts the amount of nepheline with a mean absolute error of less than 10% of the mean nepheline amount of the glasses in the dataset.

4:40 PM

(GOMD-S2-050-2024) MD simulations of QSPR analysis of iron phosphate glasses for nuclear waste disposal

J. Kalahe*[1]; X. Lu[2]; J. Vienna[2]; B. J. Riley[2]; J. Du[1]

1. University of North Texas, Materials Science and Engineering, USA
2. Pacific Northwest National Lab, USA

Iron phosphate glasses, known for their exceptional chemical durability and applicability in nuclear waste management, have gained significant attention over the years. This study uses molecular dynamics simulations (MD) to study the structures of sodium iron phosphate(NFP) glasses and their relationship with glass properties. The structures and QSPR analysis of over 30 NFP glasses in the ternary system were studied using MD simulations with effective partial charge potentials. A modified F_{net} structure descriptor with energy factors such as bond strength in diatomic molecules, cations, and enthalpy of fusion was used in QSPR analysis. Densities exhibited a strong correlation with all energy factors with higher R^2(0.820-0.993), while F_{net} with bond strength in the diatomic cations descriptor showed excellent fitting qualities for mechanical properties. Additionally, correlations between experimental dissolution rates and coefficients of thermal expansion were studied using derivatives of F_{net} and other MD descriptors, including P-O-P and P-O-Fe #/nm^3, effectively correlated with experimental properties. Dissolution rates exhibited positive and negative correlations with P-O-P and P-O-Fe #/nm^3. Notably, the energy factor, enthalpy of fusion yields better correlations for thermophysical properties. However, dissolution rates considerably rely on the glass network connectivity. Proper descriptor refinements enhance efficiency and statistical accuracy in QSPR fitting.

S4 Outreach Glass Technology Manufactury Recycling & Cross-Cutting Topics

Session 2: Challenges in Manufacturing II

Room: Peeble Beach
Session Chairs: Irene Peterson, Corning Incorporated;
Jong Han, Owens Corning

3:40 PM

(GOMD-S4-012-2024) Viscosity of transient glass-forming melt and its relation to foaming during glass batch melting

R. Pokorny*[1]; J. Kunc[1]; J. Klouzek[1]; M. Vernerova[1]; P. Cincibusova[1]; P. Ferkl[2]; J. George[2]; P. Hrma[3]; A. A. Kruger[4]

1. University of Chemistry and Technology Prague, Czechia
2. Pacific Northwest National Lab, USA
3. AttainX, USA
4. US Department of Energy, Office of River Protection, USA

Primary foam affects the heat transfer into the glass batch and the final glass quality, yet remains one of the least understood phenomena of glass melting. Primary foam occurs when a sufficient quantity of transient glass-forming melt evolves with viscosity low enough to close the open porosity of the reacting glass batch. To better understand how the fraction of transient melt and its viscosity affect the primary foam temperature range of a waste glass melter feed, we determined, with x-ray diffraction, the fraction and composition of the transient glass-forming melt in a heated melter feed as a function of temperature. Then we prepared a set of transient melts that occurred within the foaming temperature interval and measured their viscosities with spindle and falling sphere viscometers. The results agree with the Adam-Gibbs and VFT viscosity-composition models, even for transient melt compositions outside of the compositional A-G and VFT validity ranges. As silica and other refractory particles dissolved in the predominantly borate transient melt while temperature increased, viscosity increased from the initial value of ~1200 Pa s at the onset of foaming (~650 °C) to a maximum of 2005 Pa s when silica dissolution was almost complete (~700 °C). As temperature increased further, transient melt viscosity decreased to ~540 Pa s (~850 °C) when the primary foam collapsed.

4:00 PM

(GOMD-S4-013-2024) The oxidation states of Fe and S in natural glasses (Invited)

M. Brounce*[1]

1. University of California, Riverside, Earth and Planetary Sciences, USA

Iron and sulfur are two important multi-valent elements in natural silicate magmas on Earth, Moon, and Mars. Major advances in our understanding of the oxidation states of these elements has occurred in the last 15 years with the application of synchrotron-source X-ray absorption near edge structure (XANES) spectroscopy, offering an order of magnitude increase in precision and a decrease in the analytical volume to ~microns. Iron is typically present in these magmas as Fe2+ and Fe3+ and the proportion of Fe3+ relative to total Fe ranges from ~10% to ~30%, though some lavas from the Moon contain Fe0. Sulfur is present in these magmas as S2- and S6+ (as sulfate) and the proportion of S6+ relative to total S ranges from 0% to 100%. The proportions of oxidized to reduced species of both elements in magmas are initially set by the fugacity of oxygen of the deep interior of these planetary bodies. Then, during migration and storage in the magma chambers of volcanoes, both Fe and S redox compositions change during a variety of magmatic processes including crystallization, volcanic degassing, and eruption. In this talk, I will highlight the importance of XANES analyses to our understanding of redox chemistry of natural silicate magmas and their quenched glasses, summarize what we have learned from these measurements, and highlight major outstanding questions that remain.

4:30 PM

(GOMD-S4-014-2024) Iron Redox and Sulfate Fining in Soda-lime Glass: A Study on Replicating Production Furnace Conditions in the Laboratory

Y. Shiozawa*[1]; T. Maehara[1]

1. AGC inc., Innovative Technology Laboratories, Japan

The hue of flat glass is known to be influenced by the redox state of transition metals, such as iron ions. In glass manufacturing, the iron redox is controlled by adjusting the amount of oxidants, including fining agents, and reducing agents. Iron's redox reaction (1) and the decomposition reaction of sulfate, as a fining agent (2), interact via oxygen dissolved in the glass melt. Consequently, the iron's redox state and the concentration of residual sulfate in the glass cannot be changed independently. Furthermore, the oxygen dissolved in the glass melt is influenced by the varying atmospheric compositions in different places of the furnace, making it challenging to replicate these phenomena in the laboratory. $SO_4^{2-} = SO_2+1/2O_2+O^{2-}$ (1) $Fe^{3+}+1/2O^{2-} = Fe^{2+}+1/4O_2$ (2) Our objective was to melt the batch recipe used in the actual production furnace in the laboratory and obtain glass with the same iron redox and residual sulfate as those in the product. It was achieved through a simplified protocol based on the oxygen concentration of each places actually measured in an actual furnace and the surface layer temperature of each area calculated by CFD.

4:50 PM

(GOMD-S4-015-2024) Modeling cold cap behavior in joule-heated waste vitrification melters (Invited)

P. Ferkl*[1]; P. Hrma[2]; V. C. Leite[3]; D. P. Guillen[3]; J. Klouzek[4]; M. Hall[1]; A. A. Kruger[5]; R. Pokorny[4]

1. Pacific Northwest National Lab, USA
2. AttainX, USA
3. Idaho National Laboratory, USA
4. University of Chemistry and Technology Prague, Czechia
5. US Department of Energy, Office of River Protection, USA

The legacy nuclear waste currently stored at the Hanford site in the U.S. will be mixed with glass-forming and modifying chemicals and subsequently vitrified using all-electric joule-heated melters. The melter feed is introduced from the top, forming a layer of reacting materials known as the cold cap. The cold cap floats on the surface of the molten glass and is where the feed to glass conversion occurs. This endothermic process consumes thermal energy during water evaporation, conversion reactions, and sensible heating. Since most of the heat is transferred to the cold cap from the glass melt below, maximizing this heat transfer is crucial for enhancing the glass production rate. The melting rate can be augmented by increasing the bubbling rate to promote melt convection, formulating glass with lower viscosity or higher thermal conductivity, or optimizing the melter feed to prevent the development of a primary foam that remains stable at high temperatures. Developing mathematical models of the conversion processes within the cold cap enables us to quantify the effects of feed composition and operating conditions on melter behavior.

5:20 PM

(GOMD-S4-016-2024) Effect of shear stress induced by the melt flow on stability of primary foam under the cold cap

P. Hrma*[1]; P. Ferkl[2]; R. Pokorny[3]; A. A. Kruger[4]

1. AttainX, USA
2. Pacific Northwest National Lab, USA
3. University of Chemical Technology Prague, Czechia
4. Office o River Protection, USA

The cold cap bottom temperature is an internal boundary condition for the heat transfer from the melt pool to the cold cap, affecting the rate of melting in electric glass melters. As the bottom of the cold cap consists of a foamy layer called primary foam, it is located at the temperature at which the primary foam is collapsing. The primary foam stability is a function of the transient melt viscosity and the presence of dissolving silica and other refractory particles that destabilize or stabilize the foam according to whether they are located in the foam cell lamellas or in the Plateau borders. The flow in the melt pool is driven by buoyancy and stirring—typically by pneumatic bubbling of gas. The stress imposed on the cold cap bottom by the velocity gradient destabilizes the primary foam by stretching the bottom foam cells and breaking their lamellas. Consequently, the primary foam stabilizes at a higher transient foam viscosity, hence, at a lower cold cap bottom temperature. As a result, the melter feed-to-glass melt conversion kinetics rebalances and more heat is delivered to the cold cap, resulting in a higher rate of melting.

Session 3: Additive Manufacturing of Glass

Room: St. Andrews
Session Chair: Rebecca Dylla-Spears, Lawrence Livermore National Laboratory

3:40 PM

(GOMD-S4-017-2024) Laser-based additive manufacturing of silica-based specialty fibers (Invited)

P. Maniewski*[1]; T. Worman[1]; R. Bannerman[2]; M. Brunzell[1]; F. Laurell[1]; C. Holmes[2]; V. Pasiskevicius[1]

1. KTH Royal Institute of Technology, Applied Physics, Sweden
2. Optoelectronic Research Centre, United Kingdom

Traditional fiber fabrication is cumbersome for prototyping or creating small fiber batches designed for a specific application. In our work, we study laser powder deposition (LPD) for additive manufacturing of high-performance optical fibers. LPD utilizes a combination of mid-infrared CO_2 laser and discrete power jets to sinter and deposit oxide powder. In LPD, arbitrary glass structures with customized compositions can be obtained. In the case of fibers, the printed doped glass rods can be further processed using lasers into preforms, that are then drawn into fibers. Laser-based fabrication techniques have several advantages over conventional glass manufacturing methods, while the confined CO_2 laser-induced hot zone enables an exciting regime for glass manufacturing. The benefits of LPD in glass-making include high deposition rates, high densification, practically no shrinkage, and low built-in stress. The extended versatility of our laser-based system enables the fabrication of unconventional glass fiber preforms through multi-material additive manufacturing, polishing and finally welding of prefabricated components. The LPD-obtained fibers and glass samples showed high-doping profiles (>10 wt%), low transmission loss (<<1 dB/m), low rare-earth clustering (τ_{rad}>10 ms), high gain and photosensitivity utilized for fiber Bragg gratings. The work presented here reveals the great potential of LPD, aiming for fast material customization.

4:10 PM

(GOMD-S4-018-2024) 3D printing and injection molding of transparent fused silica glass (Invited)

F. Kotz-Helmer*[1]

1. University of Freiburg, IMTEK, Germany

Fused silica glass is an outstanding material in terms of its thermal, chemical as well as optical properties. Unfortunately, high-resolution structuring of fused silica glass is quite challenging. We have therefore developed a novel approach to shape fused silica glass using photocurable as well as thermoplastic nanocomposites, which can be shaped like a polymer using high-resolution 3D printing as well as high-throughput injection molding. After the shaping process the nanocomposites are converted to fused silica glass using thermal debinding and sintering. The fabricated microstructured fused silica glass components can be used as templates in metal casting to fabricate microstructured metal-inserts for injection molding with smooth surfaces in metals like bronze, brass and cobalt-chromium. The process has been commercialized by the company Glassomer and finds its application e.g. in optics, photonics and microfluidics

4:40 PM

(GOMD-S4-019-2024) Colloidal Sol-gel Feedstocks for Fabricating Additively Manufactured Glass Materials (Invited)

J. F. Destino*[1]; N. Tobin[1]; R. M. Vires[1]; A. R. Carr[1]; R. M. Wayne[1]; S. Luna[1]

1. Creighton University, Chemistry & Biochemistry, USA

Over the past decade, 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 germania-silica binary feedstocks because as traditional melt-quenches of the same composition exhibit desirable optical properties, with improved optical transmission and a tunable refractive index. We report multiple sol-gel approaches for synthesizing silica-germania 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 controls. Furthermore, we present a recent effort to AM transition-metal-doped stained glasses

5:10 PM

(GOMD-S4-020-2024) 3D Printing of Glass Optics: Shaping the Future of Precision Optical Systems (Invited)

R. Liang*[1]; Z. Hong[1]; P. Ye[1]; D. A. Loy[1]

1. University of Arizona, USA

In this presentation, I will highlight the recent progress our laboratory has made in advancing the frontiers of 3D-printed glass optics. The talk will begin with an overview of the evolution of 3D printing technologies within the field of optics. We will then delve into the unique properties and advantages of our newly developed materials and printing processes. These innovations demonstrate how we are overcoming traditional limitations and opening new avenues in optical manufacturing. The presentation will feature practical applications of these advancements, focusing on their transformative impact on devices such as microscopes, endoscopes, and hyperspectral imaging systems. This will underline the significant potential of 3D-printed glass optics in enhancing the performance and versatility of biomedical imaging technologies. Finally, the talk will address the current challenges in 3D-printed glass optics and share our vision for the next generation of 3D-printed optical components and systems.

Wednesday, May 22, 2024

Award Lectures

Darshana and Arun Varshneya Frontiers of Glass Science Lecture: Edgar Dutra Zanotto

Room: Peeble Beach

8:00 AM

Unlocking crystal nucleation in supercooled liquids and glasses

E. Dutra Zanotto[1]

1. Federal University of São Carlos, Brazil

S1 Fundamentals of the Glassy State

Session 1: Glass Formation and Structural Relaxation Glass Formation and Structural Relaxation

Room: Bel Air II
Session Chair: Sabyasachi Sen, University of California, Davis

9:20 AM

(GOMD-S1-072-2024) The Glass Transition: Kinetics and Thermodynamics (Invited)

S. Simon*[1]

1. North Carolina State University, Chemical and Biomolecular Engineering, USA

The kinetics and thermodynamics associated with the glass transition and structural recovery will be described, new dilatometric and calorimetric data presented, and the shortcomings of the empirical KAHR/TNM models of structural recovery discussed. Nanocalorimetry is exploited to create high-fictive temperature glasses and to fully demonstrate Kovacs' three signatures of structural recovery in enthalpy space. Pressure dilatometry is used to examine the kinetics of structural recovery of pressure-densified and, for the first time, pressure-expanded glasses. Both glasses show early devitrification on heating, indicating that these glasses have more mobility, compared to the conventional isobarically-formed glass. Modification of the KAHR/TNM model, allowing the departure from equilibrium to initially depend on the liquid state that the glass came from and to evolve towards the state that the glass is going to, improves the ability of the model to predict the early devitrification for the pressure-densified glass. Another modification of the model, allowing the temperature and pressure perturbations to relax independently of one another, results in effectively capturing the increased thermal expansion coefficient of glass lines during heating, as well as a 'memory'-like aging behavior, for the pressure-densified glass. The influence of nanoconfinement, cooling rate, and aging temperature on physical aging will also be discussed in the context of current debates.

9:50 AM

(GOMD-S1-073-2024) A New Approach for Interpreting Glass Forming Behavior Consistent with Transition State Theory (Invited)

C. Beg[1]; J. Kieffer*[1]

1. University Of Michigan, USA

The temperature dependence of viscosity is at the heart of glass formation and reflects the structural developments that occur in the supercooled liquid as it passes through the glass transition regime. We have demonstrated that the high-frequency complex mechanical modulus determined using Brillouin light scattering yields the same values for the viscosity as a function of temperature as zero-frequency rotating cylinder viscometry when interpreted using a modified Maxwell-Wiechert model that is based on the assumption of a correlative activation free energy (CAFE) for the viscous dissipation process. Accordingly, both the activation energy and entropy vary with temperature, which implies that the free energy landscape topography evolves along with the molecular structure as the material transitions from a liquid to a glass.[1] Conversely, we can determine the activation energy and entropy by fitting viscosity data using our CAFE model. We have analyzed the viscosity data for 849 glass compositions, confirming the robustness of our model and yielding results that enable deeper insights into structural relaxation mechanisms. We elaborate on the relationship between the rate of change of the energy landscape and fragility, the importance of activation entropy, and the influence of materials chemistry. (Acknowledgement: NSF-DMR 1610742) 1. Beg, C., Kieffer, J. Non-Cryst. Solids: X 14 (2022).

10:20 AM

(GOMD-S1-074-2024) Exploring the Mixed-Alkali Effect in Supercooled Oxide Liquids Through Dynamic and Thermodynamic Measurement Analysis

T. Yeo*[1]; J. Cho[1]; S. Sen[2]

1. Pohang University of Science and Technology (POSTECH), Republic of Korea
2. University of California, Davis, Materials Science and Engineering, USA

The mixed-alkali effect (MAE) on the viscosity, fragility, and glass transition in supercooled borate and phosphate liquids was investigated through dynamic and thermodynamic measurements. In mixed-alkali borates, the greatest negative deviation in T_g always occurs at equal alkali proportions, consistent with the matrix-mediated coupling model. This deviation varies non-monotonically with the alkali size difference, suggesting an interplay between the strength and reorientation likelihood of mechanical dipoles linked to alkali hopping. Heat capacity measurements in mixed-alkali phosphate glasses indicate that the fragility index's negative deviation might not correlate with alkalis' configurational entropy mixing. We propose that the bond scission-renewal dynamics in the network, which facilitate viscous flow, are accelerated by the alkali mechanical dipoles' reorientation in mixed-alkali liquids. This results in reduced activation energy for viscous flow, significantly lowering the fragility index in mixed-alkali liquids compared to single-alkali counterparts. The significance of this catalytic effect lessens at higher temperatures, where thermal contributions to activation barrier crossing predominate, eventually nullifying the MAE on viscosity above a critical temperature

10:40 AM

(GOMD-S1-075-2024) Amorphous silica possessing topology of siliceous zeolite

H. Masai*[1]; S. Kohara[2]; T. Wakihara[3]; Y. Shibazaki[4]; Y. Onodera[2]; Y. Sakai[5]; J. Haines[6]; D. Keen[7]; M. Azuma[8]

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2. National Institute for Materials Science, Center for Basic Research on Materials, Japan
3. The University of Tokyo, Institute of Engineering Innovation, Japan
4. High Energy Accelerator Research Organization (KEK), Photon Factory, Institute of Materials Structure Scienc, Japan
5. Kanagawa Institute of Industrial Science and Technology (KISTEC), Japan
6. Université de Montpellier, ENSCM, Institut Charles Gerhardt Montpellier, CNRS, France
7. Rutherford Appleton Laboratory, ISIS Facility, United Kingdom
8. Tokyo Institute of Technology, Laboratory for Materials and Structures, Japan

Non-equilibrium oxide materials, such as glasses and zeolites, possess nanosized cavities that are specific to their functions. In materials with such large cavities, thermodynamically metastable structures can be formed semipermanently or transiently by applying a much higher pressure than the ambient pressure while simultaneously heating. Densified samples fabricated at high pressures exhibit completely different functions from those fabricated under ambient pressure. In this study, we show that siliceous zeolite (SZ) single crystal cold-compressed at 20 GPa yields permanently densified glassy silica (GS), while cold-compressed SZ powder and densified GS are metastable. Moreover, the topology of the densified amorphous SiO_2 fabricated from SZ retains that of crystalline SZ. After thermal annealing, structure of amorphous SiO_2 from SZ single crystal is different from pristine GS, whereas the densified GS relaxes to pristine GS. These results indicate that it is possible to design new functional amorphous materials by tuning the topology of the initial zeolitic crystalline phases.

11:00 AM

(GOMD-S1-076-2024) Investigation of structural origin of boson peak in glass-forming materials using heterogeneous elasticity theory

T. Mori*[5]; S. Kitani[1]; H. Hijiya[2]; Y. Fujii[4]; S. Kohara[3]; S. Oh[5]; D. Kyotani[5]

1. Tokyo Institute of Technology, Japan
2. AGC Inc., Japan
3. National Institute for Materials Science (NIMS), Japan
4. Ritsumeikan University, Japan
5. University of Tsukuba, Japan

We evaluated the boson peak (BP) dynamics, which is a universal excitation in the THz region of glass-forming materials, based on the heterogeneous elasticity theory. In this study, we utilezed the coherent potential approximation (CPA) for spatially fluctuating shear modulus. By solving the CPA equation numerically, we extracted the local mechanical properties of glasses, and investigated the relationship between determinant factor of BP and medium-range order of glasses.

11:20 AM

(GOMD-S1-077-2024) From the Roman Empire to the present day, just one viscosity curve?

D. R. Neuville*[1]; L. Cormier[3]; N. Schibille[2]

1. IPGP, géomatériaux, France
2. IRAMAT CNRS, France
3. IMPMC, France

One can imagine that mankind has been interested in glass because of its transparency, brilliance and hardness, and has increasingly mastered the material over the course of time. Glassmaking techniques have travelled far and wide and have been the subject of much research and innovation. However, the art of glassmaking is characterized its tremendous longevity. Although working conditions, tools and types of production have evolved considerably since antiquity, glassmaking techniques have adapted without undergoing substantial change. Glassmaking techniques originating in the Middle East have travelled the world, but have remained almost unchanged for over 3000 years. The processes include the shaping of hot glass and enable the manufacture of utilitarian objects such as tableware, lighting, interior decoration and scientific research. But several questions remain: - why have these manual glassmaking techniques not changed over time? - what are the constraints on these techniques? - how do the compositions change in order to maintain the same glassmaking techniques? Three questions that summarize many others, but to which we provide some answers to understand how glass is gathered, shaped and annealed. We will describe in detail the viscosity curve as a function of time and temperature from the liquid state into the relaxation range. We will also discuss the equations that can be used to fit this variation.

Session 6: Mechanical Properties of Glasses I: Rate dependence of mechanical responses

Room: Bel Air I
Session Chair: Timothy Gross, Corning Incorporated

9:20 AM

(GOMD-S1-078-2024) Issues Involving the Nanoindentation Measurement of the Mechanical Properties of Inorganic Glasses at High Strain Rates (Invited)

B. Hackett*[1]; G. Pharr[1]

1. Texas A&M University, USA

As a technique for instrumented indentation testing, nanoindentation occupies a unique role in generating constrained stress fields that promote plastic deformation, even within materials characterized by high levels of brittleness. By circumventing catastrophic fracturing typically encountered during conventional bulk testing, nanoindentation enables the investigation of mechanical deformation properties that would otherwise remain largely inaccessible. With the recent advent of nanoindenters capable of acquiring load and displacement data at higher sampling rates (> 1.25 MHz), measurement capabilities have expanded to include high strain rate deformation behavior. However, the introduction of these advanced tools has also brought a new set of challenges to characterizing materials, particularly inorganic glasses. In this work, the strain rate sensitive mechanical properties of borosilicate, soda-lime silicate, and fused silica glasses are explored using nanoindentation across six orders of magnitude from 10^{-2} to 10^{4} 1/s with an emphasis on the methodological limitations exacerbated by high strain rates.

9:50 AM

(GOMD-S1-079-2024) Strong or fragile? Viscoplastic flow of silicate glasses at room temperature and its strain rate dependance

M. Bourguignon[1]; G. A. Rosales-Sosa[2]; S. Sao-Joao[3]; G. Kermouche[3]; Y. Kato[2]; E. Barthel*[1]

1. CNRS/ESPCI, SIMM, France
2. Nippon Electric Glass, Japan
3. Mines Saint-Etienne, Univ Lyon, CNRS, LGF, Centre SMS, France

We have measured the viscoplastic response of silicate glasses under electron irradiation as a function of electron flux at room temperature. Glass micropillars were fabricated via reactive ion etching and uniaxially compressed with an in situ nanoindenter under electron irradiation inside the scanning electron microscope. The morphology and structure of the samples before and after plastic deformation were investigated by microscopic and Raman observations as a function of electron flux to quantitatively assess the impact of electron irradiation on plastic flow through finite element modelling. We evidence a similar impact on both yield pressure and flow stress. Based on the collection of stress vs strain rate curves at different fluxes, we also show that, in analogy with polymers, a time/flux equivalence holds so that we can build a master curve over 6 orders of magnitude in strain rate. With this wide range of dynamics, a strong contrast appears between pure amorphous silica, which exhibits a single regime, and alumino boro silicate and soda lime silica glasses which display a transition between two regimes. These results parallel the strong/fragile behaviors for viscosity above the glass transition and point to the specific role of the modifiers in the plastic dynamics of silicate glasses at room temperature. The mechanism for electron irradiation on plastic deformation of glass will also be discussed.

10:10 AM

(GOMD-S1-080-2024) In-situ Observation of Deformation and Fracture Behavior of Glass subjected to High-Velocity Impact of a Small Blunt Object

M. Nagano*[1]; Y. Kobayashi[3]; T. Kajihara[2]; S. Sawamura[1]; S. Yoshida[1]

1. AGC Inc., Material Integration Laboratory, Japan
2. AGC TECHNO GLASS Co.,Ltd., Japan
3. Innovative Technology Laboratories, Japan

Fracture of glass subjected to high-velocity impact of small objects is a long-standing problem in various application fields. However, quantitative evaluation is still insufficient due to difficulty of observation and analysis of the high-speed phenomenon. In this study, we conducted "in-situ" observation with 1 Mfps or above, to clarify the fracture process of glass impacted by a 1.37 g WC-Co conical impactor whose tip radius is 0.2 mm and angle is 120 deg, and velocity ranges from 20 to 80 km/h. We also conducted Finite Element Analysis (FEA) to estimate dynamic stress distributions that dominate crack initiation and propagation. As a result, it is found that fracture behavior of glass during the impact with the above conditions can be divided into three major stages. At first, a crowd of fine cracks (or shear lines) appear just after formation of densified or flowed region. In the second stage, a median crack emerges from the crowd of fine cracks. Finally, in the third stage, the median crack propagates with a notable change in velocity around the neutral axis of the ply. In some cases, the median crack stops around the center of thickness, but in other cases, it reaches the backside of the ply and grows into large radial cracks. Combined with FEA results, it is suggested that these fracture phenomena are closely related to the local deformation (indentation and bending) which are affected by non-equilibrium stress fields generated during the high-velocity impact.

10:30 AM

(GOMD-S1-081-2024) Rate Dependence of Indentation-Induced Deformation and Cracking in Glass

S. Yoshida*[1]

1. AGC Inc., Japan

The indentation test is a simple and easy technique to evaluate hardness and cracking behaviors in glass and other brittle materials. Although it has been long used for comparing mechanical properties among various glass compositions, mechanisms of permanent deformation, especially shear flow, and microscopic origin of crack nucleation are still unclear. In addition, there are very limited information on rate-dependent deformation and cracking behaviors in glass. From industrial point of view, it is of primary importance to gain knowledge on mechanical response of glass during impact, machining, or sliding wear to develop and to design high-strength glass products. In this study, dynamic indentation hardness and cracking behavior of glass were evaluated using a lab-made dynamic indenter and using two types of trigonal pyramid indenters whose face angles (between the loading axis and an indenter face) are 65° for Berkovich and 75° for the blunter indenter. The blunt indenter enabled us to create the indentation imprints without any severe cracks and to measure the size of the imprints. In addition, the cracking behavior of glass was evaluated using the Berkovich indenter and the fracture patterns were compared for quasi-static and dynamic indents.

10:50 AM

(GOMD-S1-082-2024) Elucidating the link between strain rate, ductility, and indentation size effect through thermal annealing

P. Shrestha[1]; K. Jardine[1]; M. Bauchy[2]; M. M. Smedskjaer[3]; C. G. Hoover*[1]

1. Arizona State University, School of Sustainable Engineering and the Built Environment, USA
2. University of California Los Angeles, Civil and Environmental Engineering, USA
3. Aalborg University, Department of Chemistry and Bioscience, Denmark

Soda-lime Silicates (SLS) have always shown sensitivity to different loading and strain rates as well as Indentation Size Effects (ISE), where the indentation hardness () decreases with increasing applied force. In this study, we perform micro-indentation to measure hardness using two protocols which are Constant Loading Rate (CLR), resulting in a nonlinear strain rate, and Constant Strain Rate (CSR), resulting in a nonlinear loading rate through the depth of the indent. We previously showed the link between ISE and ductility, such that increase in peak force resulted in decrease in Hardness and increase in ductility. In this work, we use an AFM and annealing technique as proposed by Yoshida et. al. to quantify the volumes associated with inelastic deformation for all 42 families to confirm and further strengthen our findings. The indents were scanned with an AFM to determine the indentation cavity and pile-up volumes before and after annealing. The annealing process results in recovery of all densified material, allowing for calculation of the recovery ratio as well as the densified and the plastically deformed volume. Preliminary results from AFM scans show that initial volume of pile up evolves as an increasing power law trend in function of peak force for both CLR and CSR protocols.

11:10 AM

(GOMD-S1-083-2024) How to mitigate the Indentation Size Effect? Evidence of an intimate link between Size Effect, Strain Rate and Ductility in Soda-lime Silicate

P. Shrestha*[1]; M. M. Smedskjaer[3]; M. Bauchy[2]; C. G. Hoover[1]

1. Arizona State University, School of Sustainable Engineering and the Built Environment, USA
2. University of California Los Angeles, CIVIL AND ENVIRONMENTAL ENGINEERING, USA
3. Aalborg University, Department of Chemistry and Bioscience, Denmark

Many glasses exhibit the so-called Indentation Size Effect (ISE), where the indentation hardness () depends on maximum applied force. Many inorganic silicate glasses have also demonstrated sensitivity to different loading and strain rates. Here, we seek to uncover the connection between the ISE and strain rate in Soda-lime Silicate (SLS) glass. We perform micro-indentation to measure using both a constant loading rate (CLR), resulting in a nonlinear strain rate through the depth of the indent, and a non-linear loading rate that gives a constant strain rate (CSR) vs depth profile. For each protocol, we perform 6 ISE curves, each at a different strain rate, using the same 7 peak loads making a total of 42 families. A modified Bernhardt Size Effect Law was used to determine the extent of the ISE and load-independent hardness. We also determine the ductility for each family and demonstrate that a small increase in ductility can largely mitigate the extent of the ISE while slightly reducing the load-independent hardness. We further demonstrate that the amount of ductility can be increased by either switching from a CLR to CSR protocol or by increasing the applied rates.

S2 Glass and Interactions with Its Environment Fundamentals and Applications

Session 4: Materials for Waste Immobilization

Room: Shoal Creek
Session Chair: Joseph Ryan, Pacific Northwest National Lab

9:20 AM

(GOMD-S2-051-2024) Overview of the UK HLW Programme

O. Stagg*[1]

1. NWS, United Kingdom

In the UK there is a legacy of radioactive waste which is destined for deep underground disposal in a geological disposal facility. To this end, the UK has been studying the vitrification of high-level radioactive wastes for over 60 years, beginning with the development of a single-stage 'in-can' batch process in the 1960s, to the eventual adoption of a continuous process based on induction melter technology. In this presentation, the development of the UK High Level Waste (HLW) glass programme will be discussed. In particular, due to the reprocessing of Magnox fuel, UK HLW glass contains a distinctive Mg-rich composition, which required a targeted experimental programme to support disposability assessments. Research has also been conducted in anticipation of future post-operational clean-out operations, which will contain higher Mo concentrations, requiring a new base glass formulation to be developed. This presentation will therefore provide an overview of the development and current status of our knowledge of vitrified UK HLW, and the programme of future work that is in development to support its disposal in the UK Geological Disposal Facility.

9:40 AM

(GOMD-S2-052-2024) Characterization of Alkali-Iron Phosph Waste Glasses by Structural, Thermal, and Durability Analyses

C. Lonergan*[2]; H. Werth[3]; B. J. Riley[1]; K. Carlson[3]

1. Pacific Northwest National Lab, USA
2. Missouri University of Science & Technology, Materials Science and Engineering, USA
3. University of Nevada Reno, USA

Dehalogenated salt iron phosphate glass forms (DPFs) are promising materials to immobilize salt waste produced from the electrochemical reprocessing of used nuclear fuel. Over 10 glasses were prepared by mixing phosphoric acid with a simulated, chloride-based salt waste and heating to temperatures between 300-600 C, depending on level of desired dehalogenation. Iron oxide was combined with the dehalogenated product and vitrified. Dehalogenation and DPF synthesis were performed in air and argon while the glass melting was performed in air. After preparation, the glasses were characterized with various analytical techniques including liquid chromatography, calorimetry, and Mossbauer spectroscopy for iron redox. The collected data was used to develop composition-property models, as well as property and composition constraints. This information is critical to advance the phosphate-based dehalogenation approach towards a higher Technology Readiness Level.

10:00 AM

(GOMD-S2-053-2024) Alteration of glasses in complex natural environments

C. L. Thorpe*[1]; G. Manifold[1]; C. Lenting[2]; S. Creasey-Gray[1]; C. L. Corkhill[3]; R. J. Hand[1]

1. University of Sheffield, Materials Science and Engineering, United Kingdom
2. University of Cologne, Institut fuer Geologie und Mineralogie, Germany
3. University of Bristol, School of Earth Sciences, United Kingdom

The short-term alteration of nuclear waste type glasses can be estimated in the laboratory using static, sterile tests conducted in simple solutions and often at elevated temperatures. For validation, these tests are compared with long-term, low temperature alteration of natural and man-made glasses exposed to more complex natural environments. Interesting and potenitially significant differences are observed between chemistry and mineralogy of alteration layers formed in natural environments and those altered in the laboratory. In particular, elements present at low concentrations, or with low solubilities, are shown to accumulate over long time periods when glasses are exposed to an open system rather than a closed laboratory system. Glasses altered in both seawater and terrestrial sediments will be compared to demonstrate the accumulation of Fe, P and Ca along with heavy metals and rare earth elements. Secondary minerals observed are discussed in terms of their ability to sequester and retain radionuclides and their potential to form in a repository environment.

10:20 AM

(GOMD-S2-054-2024) Study of inorganic reductants on the conversion behavior of Hanford nuclear waste melter feeds

J. Marcial*[1]; J. C. Rigby[1]; M. Miller[1]; S. Choi[1]; S. Davidson[1]; D. Dixon[1]; A. A. Kruger[2]

1. Pacific Northwest National Laboratory, USA
2. US DOE Office of River Protection, USA

Conventional formulations of Hanford low-activity waste melter feed include the addition of sucrose to mitigate excessive foaming which acts as a barrier between the molten glass pool and the feed. Sucrose enhances processing rates originally diminished by excessive foaming by means of an exothermal reaction of sucrose and nitrates. However, products of incomplete combustion of sucrose are known to produce acetonitrile in off-gas system condensate that may exceed bounding limits, leading to increased cost of processing of the condensate. Limiting the addition of organics, by removing sucrose, reduces the acetonitrile produced by up to 90%. However, without a reducing agent in the feed, excessive foam production from nitrate decomposition during melting resumes. This work proposes the use of boron nitride (BN), carbon coke, vanadium diboride (VB2), and silicon carbide (SiC) as alternatives to sucrose. Feeds were designed with these inorganic reductants and characterized for their material properties, foaming behavior, and gas evolution.

10:40 AM

(GOMD-S2-055-2024) Assessing Reductant Additions to Nuclear Waste by Scaled Melter Processing

D. Dixon*[1]; J. Lang[1]; M. Hall[1]; S. A. Luksic[1]; C. Stewart[1]; D. Cutforth[1]; W. C. Eaton[1]

1. Pacific Northwest National Lab, 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. A small-scale melter system has been designed by Pacific Northwest National Laboratory to investigate specific aspects of the nuclear waste vitrification process. The continuous laboratory-scale melter (CLSM) uses an externally heated, metal vessel designed to operate under radioactive conditions or with non-radioactive simulants. This gives it the ability to

*Denotes Presenter

vitrify actual tank waste and gain information about melter feed processability, the partitioning of components of interest, and validation of simulants used in testing. A simulant of a low-activity waste (LAW) melter feed using sucrose as a reductant was spiked with ^{99}Tc at a level anticipated in Hanford LAW (~4 ppm) and processed in the radioactive CLSM. The melter feed was split into two portions and the sucrose reductant was added at two different concentrations to assess its effect on LAW processing. The production rates and partitioning of ^{99}Tc in the glass and offgas are compared with other melter feeds and reductant conditions.

11:00 AM

(GOMD-S2-056-2024) Redox Effects on Crystallization during Vitrification of High-Chromium HLW

K. Matlack*[1]; I. Pegg[1]; H. Gan[1]

1. Catholic University of America, Vitreous State Laboratory, USA

Various Hanford high level waste (HLW) streams contain sufficiently high concentrations of chromium for it to become the waste loading limiting component in the waste. Chromium has relatively low solubility in borosilicate glasses and leads to the formation of various crystal phases including spinels. The extent of crystal formation must be managed to prevent operational issues and potential premature melter failure that can result from excessive accumulation of crystals in the melter. The form of chromium in the waste and the redox conditions can also affect the extent of crystallization and, therefore, the waste loadings that are achievable. To investigate these effects, a series of continuously fed joule heated melter tests conducted were with simulated Hanford HLW containing different forms of chromium (Cr_2O_3, $Cr(NO_3)_3.9H_2O$, $Cr(OH)_3$, and $FeCr_2O_4$) that are amongst those reported to be present in Hanford HLW. Differing levels of crystallization were measured in the product glasses depending on the form of chromium processed and the concentrations of oxidants in the feed. In addition, crystallization varied with the shifting of local chromium redox equilibrium. Comparison with results from crucible melt tests shows that the relatively slow chromium redox reaction kinetics in comparison to the melter residence time can be beneficial in limiting crystallization, as also can feed additives to control redox, thereby allowing higher waste loadings to be achieved.

11:20 AM

(GOMD-S2-057-2024) Determination of Surface Tension Parameters for Nuclear Waste Glasses

D. P. Guillen*[1]; D. Yankura[2]; Z. Guo[2]; S. A. Luksic[3]; T. Jin[3]

1. Idaho National Laboratory, Materials Science and Engineering, USA
2. Idaho National Lab, USA
3. Pacific Northwest National Lab, USA

Image analysis was performed on sessile droplets to determine the surface tension and contact angle of seven simulant nuclear waste glasses on two different substrates (Monofrax K3 refractory and platinum). Glass pellets were batched and placed into a furnace where they were heated from room temperature to temperatures up to 1000C. Images were acquired during melting using high speed photography. An algorithm was developed to process the images to determine the contact angle, surface tension, and adhesion force for each glass-substrate combination as a function of temperature. Additionally, geometric parameters, such as droplet width and height, used in the calculations are reported. A custom algorithm was developed to automate the processing of the images without the need for labor-intensive manual processing methods. The images were cropped, filtered, converted to grey-scale and thresholded to obtain a crisp outline of the droplet edges. The base of the image is determined by finding the minimum y-value of the threshholded droplets. Challenges encountered when processing high temperature, flatter droplets were overcome using image processing techniques. An iterative approach is used to solve the set of ordinary differential equations and capillary constant. Validation was performed using known liquids and cross-checking results with literature.

S4 Outreach Glass Technology Manufactury Recycling & Cross-Cutting Topics

Session 2: Challenges in Manufacturing III

Room: Peeble Beach
Session Chairs: Scott Cooper, Celsian Glass USA;
Irene Peterson, Corning Incorporated

9:20 AM

(GOMD-S4-021-2024) Influence of atomic surface structure on nepheline crystallization in glass (Invited)

E. Maeda*[1]; R. Welch[2]; F. Lodesani[1]; J. C. Mauro[2]

1. AGC Inc., USA
2. Pennsylvania State University, Materials Science and Engineering, USA

Surface crystallization is an important issue for the mass production and utilization of glass. Although there have been many studies on glass crystallization, there are few reports on surface crystallization, especially as related to the surface glass structure since it is difficult to evaluate. In a previous study, we investigated the possibility of predicting surface crystallization trends in nepheline ($NaAlSiO_4$) by combining molecular dynamics (MD) calculations and the Toy Landscape Model (TLM). From these calculations, it was found that the contact angle between the interface of the crystal and the glass may have little effect than expected on modeling the glass surface nucleation. On the other hand, the results of MD simulations suggested that network modifiers such as sodium tend to aggregate on the surface. Here we consider the possibility that the aggregation of these alkali modifiers may create a compositional environment near the surface that facilitates crystallization. We report MD simulations of anorthite compositions with different Ca/Na ratios to evaluate the compositional ratios and structures of the glass components. The analysis shows that both the compositional ratio and the intermediate-range atomic distances closely resemble the crystal structure up to 10 Å from the surface of the glass. We would like to discuss the effect of structural similarity for surface crystallization.

9:50 AM

(GOMD-S4-022-2024) Determination of the SiO_2 liquidus in the alkali oxide (Li_2O, Na_2O, K_2O)-SiO_2 systems and applications to vitreous silica production

J. Lee*[1]; P. Lauriano[2]; I. Jung[1]

1. Seoul National University, Material Science and Engineering, Republic of Korea
2. École D'ingénieurs Ensil-Ensci, France

Vitreous silica is used for many applications such as optical fibers, astrological mirror, and halogen lightening owing to its high chemical resistance, low thermal expansion coefficient, and superior ultraviolet transparency. One of the methods to produce vitreous silica is to melt and cool high purity silica above its melting temperature of ~1725 °C. In the production of vitreous silica, the existence of small impurity components can drastically affect the melting temperature and melting kinetics of high purity SiO_2. Therefore, accurate phase diagram information for the liquidus of SiO_2 varied with small oxide impurities like alkali oxides is essential to understand the process. Experimentally, due to extremely high viscosity of the SiO_2-rich oxide melt, the accurate phase diagram measurement in the SiO_2-rich region (above 0.95 mole fr. of SiO_2) is rarely available. In this study, the changes in the SiO_2 liquidus by Li_2O, Na_2O, and K_2O in SiO_2-rich region were successfully measured at 1550 to 1650 °C by classical equilibration (10 - 21 days) and quenching method using sealed Pt crucibles followed by X-ray diffraction phase analysis and electron probe micro-analysis. The present experimental data were also compared with the available literature data and the phase diagrams calculated using FactSage^{TM} oxide database. The implication of the present experimental results for vitreous silica production is discussed based on the SiO_2 network modification by alkali oxides.

10:10 AM

(GOMD-S4-023-2024) Advancements in multimaterial glass Volumetric Additive Manufacturing (Invited)

R. Walton*[1]; D. H. Porcincula[1]; L. Myers[2]; M. de Beer[1]; J. Schwartz[1]; A. Troksa[1]; D. Melchert[1]; R. J. Dylla-Spears[1]

1. Lawrence Livermore National Lab, USA
2. Penn State, USA

Gradient refractive index (GRIN) glass has the capability to simplify lens designs, condense camera designs, and offer additional flexibility in optical systems. Current methods to produce GRIN lenses are limited in the gradient shape, maximum change in refractive index, and size of the gradient. Multimaterial direct ink writing (DIW) has been developed to produce fused silica lenses with Ti and Ge gradients to change the refractive index as a function of radial location in the lens. While this method has produced single composition lenses up to 4 cm in diameter and can print gradients of arbitrary sizes and shapes, blending the gradient between print lines presents a challenge due to the high viscosity of the DIW ink. For this reason, we have been developing a layerless 3D printing method, volumetric additive manufacturing (VAM), that will produce transparent fused silica. This begins with formulation of a clear UV-active organic resin with dispersed fumed silica nanoparticles to act as the glass former. Due to the need to pour off unreacted resin, VAM resins are much lower viscosity than DIW inks, which allows for improved diffusion to smooth out dopant particle gradients deposited by DIW. This work will focus on the development of a robust glass VAM ink formulation and methods to process prints to glass, incorporation of compositional gradients in the VAM vial prior to printing, advanced methods of metrology, and outlining the currently achievable geometry space.

10:40 AM

(GOMD-S4-024-2024) Bulk Metallic Glasses can be formed like Oxide Glasses (Invited)

J. Schroers*[1]

1. Yale, USA

The metastable nature of BMGs has imposed a barrier to broad commercial adoption, especially where the processing requirements of these alloys conflict with conventional metal processing methods. Research on the crystallization of BMG formers has uncovered novel processing opportunities using thermoplastic forming (TPF), which utilizes the dramatic softening exhibited by a BMG as it approaches its glass transition temperature. Fabrication processes based on TPF decouple the rapid cooling required to form a glass from the forming step, mitigate the effects of heterogeneities on crystallization, and overcome geometrical limitations associated with casting. This talk introduces such techniques that are unique among metals. For example, through TPF based blow molding of BMGs, geometries can be achieved that were preciously unachievable with any other metal processing method. Due to the absence of an intrinsic size limitation and a phase transition first order during solidification, BMGs can be precision net-shaped on the micro, nano and even atomic length scale. Within TPF, BMGs can be considered high strength material that can be processed like oxide glasses or thermos-plastics. This talk with introduce the specific techniques, suggest opportunities and point at challenges that have to be overcome for a wide spread use of BMGs as a material that combines properties of metals with processing of thermos-plastics and oxide glasses.

11:10 AM

(GOMD-S4-025-2024) A numerical simulation study for optimizing tempering process in hollow glassware production (Invited)

B. Renklioglu*[1]

1. SISECAM, R&D, Turkey

Glass manufacturers aim to enhance furnace efficiency, minimize energy consumption, and meet stringent emission standards in the pursuit of zero carbon driven by the increasing demand for superior and innovative glass products. While significant advancements have been made in furnace designs and combustion technologies that align with these objectives, it holds equal significance to conduct thorough research in exploring the further optimized conventional production processes. Thermal tempering process, a common post-forming treatment, poses challenges due to factors like glass thickness, composition, edge quality, optical distortions, cooling rates, energy consumption, and process control. Manufacturers must carefully consider these factors to determine the feasibility of using thermal tempering for glass applications, balancing performance requirements with the challenges posed by the tempering process. Optimizing the tempering process is one of the essential steps in attaining sustainable glass production. In this context, a comprehensive numerical simulation study focuses on examining the tempering of hollow glassware will be discussed. In this study, the detailed cooling air flow and resulting temperature and stress fields in the glass are computed for various tempering conditions. The insights from the simulations enhance control over the tempering process, contributing to the industry's pursuit of sustainability goals.

11:40 AM

(GOMD-S4-026-2024) Viscoelastic Calculation of Laminate Glass Stress

Z. Zheng*[1]; J. Wu[1]; T. M. Gross[1]

1. Corning Incorporated, USA

Multiple ways of stress prediction for the glass laminate are studied, including classical elastic equations, integration methods of the CTE (Coefficient of Thermal Expansion) difference between core and clad glass, and full-blown viscoelastic FEA (Finite Element Analysis) model. The stress predictions have been compared with the experiment measurement. The integration methods are derived based on the viscoelastic theory. Viscoelastic model and integration methods agree well and show better prediction than the classical elastic equations. A universal temperature T_set, corresponding to the proximity of 10^11 poise viscosity of the softer glass between core and clad, is discovered for the integration temperature range.

Session 3: Additive Manufacturing of Glass

Room: St. Andrews
Session Chair: Joel Destino, Creighton University

9:20 AM

(GOMD-S4-027-2024) Advances in 3D printed glass for gradient compositional control (Invited)

D. Nguyen*[1]; T. Yee[1]; M. Ellis[1]; T. Fears[1]; R. Walton[1]; J. Ha[1]; O. Herrera[1]; V. Vuppuluri[1]; N. Dudukovic[1]; K. Sasan[1]; R. J. Dylla-Spears[1]

1. Lawrence Livermore National Laboratory, USA

The ability to 3D print transparent glass has enabled the creation of complex optics as well as intricate glass structures. Using a direct ink writing approach (DIW), we enable the formation of a variety of glass-based materials, ranging from solid monolithic structures to open mesh geometries all with the capability of including compositional control. The fundamentals behind how to accurately print compositionally controlled glass are of special importance as it is necessary for enabling the formation of gradient refractive index (GRIN). Several challenges in the realm must be addressed, including controlling the rheology of mixing, improving mixing homogeneity under low Reynolds number conditions, and intelligently designing toolpaths that are optimized for compositional control. Here we present the state-of-the-art in DIW methods of glass AM and strategies towards achieving accurate compositional control. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 within the LDRD program 22-ERD-012. LLNL-ABS-858306

9:50 AM

(GOMD-S4-028-2024) Laser-Based Additive Manufacturing of Glass Structures (Invited)

J. Bernardin*[1]

1. Los Alamos National Lab, Engineering Design and Technologies Div, USA

Additive Manufacturing (AM) technologies have grown considerably over the past decade. The associated processing of polymers, metals, and composites have found many useful applications and are beginning to rival traditional manufacturing for rapid prototyping, production of small lots, the creation of difficult-to-produce geometries, etc. The success of glass AM has lagged these other materials, primarily because of the difficulty in manipulating the glass feedstock during printing as well as obtaining desired mechanical and optical properties of the finished parts. The Glass Laser Additive Manufacturing System (GLAMS) at Los Alamos National Laboratory was established in 2017 to explore methods to synthesize and process glass using direct energy deposition with a CO2 laser heat source combined with either glass rod or fiber feedstock. This presentation will summarize the progress made in the GLAMS machine design including laser heat sources, feedstock delivery system, robotic motion controllers, and operational diagnostics. The development of a multi-physics thermal model, glass property characterization at processing temperatures, and an on-machine feedback control system will complement this discussion. Finally, examples will be provided to show the current ability of the GLAMS machine to additively manufacture custom glass structures out of borosilicate and fused silica glasses.

10:20 AM

(GOMD-S4-029-2024) Multi-material printing of glass via direct ink writing

T. Yee*[1]; T. Fears[1]; R. Walton[2]; J. Ha[1]; O. Herrera[1]; V. Vuppuluri[2]; N. Dudukovic[2]; K. Sasan[1]; R. J. Dylla-Spears[1]; D. Nguyen[2]

1. Lawrence Livermore National Laboratory, Materials Science Division, USA
2. Lawrence Livermore National Laboratory, Materials Engineering, USA

3D printed glass can enable functional capabilities previously inaccessible through conventional methods, such as gradient refractive index (GRIN) optics with arbitrary refractive index profiles. One technique that can achieve such a design is through direct ink writing (DIW), in which a viscoelastic glass slurry, or ink, is extruded through a nozzle to build a part layer-by-layer with compositional control. Afterwards, the print is heat treated to achieve fully dense glass. Developing printable glass requires fine tuning both the inks and post processing steps to strike a balance between multiple properties such as printability, processibility, and final transparency. To achieve spatial control over composition (and subsequently refractive index), multiple inks are fed into a mixing chamber immediately before extrusion. However, this additional complexity causes the material and processing tuning windows to become significantly tighter. Here, we discuss strategies for developing 3D printed glasses, additional considerations in fabricating GRIN optics, and strategies for mitigating such challenges. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 within the LDRD program 22-ERD-012. LLNL-ABS-857830.

10:40 AM

(GOMD-S4-030-2024) Fragile Liquids – Structure, Properties and Potential Opportunities for Additive Manufacturing

R. Weber*[1]; S. K. Wilke[1]; C. J. Benmore[2]

1. MDI, USA
2. Argonne National Lab, Advanced Photon Source, USA

Glass is often made from supercooled liquids that become sufficiently viscous to avoid crystallization. Glasses produced on a large scale are typically made from strong liquids that are quite easy to vitrify even when they are cooled slowly. This research is investigating fragile liquids that are difficult to vitrify. By exploring compositions outside the traditional glass families, new properties, structure and potentially performance can be evaluated. The practical challenge is to maintain the desirable performance characteristics while making larger scale products. Glasses made from fragile liquids have a small working range and are prone to crystallization. This means that traditional processing methods often don't work. This talk will cite some examples of structure/properties of aluminate- and titanate-based fragile liquids and glasses made from them. The results will be discussed in the context of potential new methods such as additive processing from powders. The overall goal of the talk is to provide details of example materials and highlight the challenges and opportunities in processing fragile liquids into bulk glass products.

11:00 AM

(GOMD-S4-031-2024) Transparency on Demand: Additive Manufacturing of Precision Glass Elements

Z. Hong*[1]; P. Ye[1]; D. A. Loy[2]; R. Liang[1]

1. University of Arizona, James C. Wyant College of Optical Sciences, USA
2. University of Arizona, Department of Chemistry & Biochemistry, USA

Glass is ubiquitous in modern society due to its exceptional optical, mechanical, and chemical properties. Additive manufacturing (AM) technologies, such as 3D printing, provide an alternative approach that can significantly reduce material waste and enable the production of complex glass structures with high accuracy. However, current 3D printing techniques for glass elements suffer from limited control over their transparency, which highly limits the potential applications of 3D-printed glass components that require precise optical components with controlled transparency. The proposed study enables future manufacturing by developing a method for 3D printing glass with controlled transparency, allowing for the on-demand production of optically functional parts. This could have significant implications for the manufacturing of complex optical components for a variety of industries. Furthermore, the ability to print locally defined transparencies could lead to new design possibilities.

11:20 AM

(GOMD-S4-032-2024) 3D printing glass micro-optics from silsesquioxanes

P. Ye*[1]; Z. Hong[1]; D. A. Loy[2]; R. Liang[1]

1. The University of Arizona, Wyant College of Optical Sciences, USA
2. The University of Arizona, Chemistry & Biochemistry; Material Science and Engineering, USA

We report on the advances in glass manufacturing through the two-photon polymerization of various silsesquioxanes. Our first report of TPP glass printing utilized a solvent-free, partially condensed silsesquioxane called liquid silica resin (LSR), enabling the fabrication of high-precision glass micro-optics with controlled isotropic shrinkage (down to 17%), micrometer resolution, and minimal surface roughness (< 5nm). Building on this, we further explored and optimized the LSR with different crosslinking densities. We demonstrated the potential of our printing strategy by fabricating micro-optics with complex structures including multi-lens objective, gratings, Alvarez lens pair, waveguide array, etc. To overcome the moisture sensitivity problem of LSR, we then utilized a solvent-free polymeric silsesquioxane to fabricate micro- or nano-sizes glass objects. Nanostructures with sub-80 nm feature sizes are achieved. The shrinkage caused by thermal treatment was minimized due to the solvent-free feature. We further explored tuning the refractive index of glass obtained from this polymeric silsesquioxane. In addition, the self-welding behavior of this polymeric silsesquioxane during pyrolysis allows the building of micro-optics containing multi-components with different refractive indices. Together, we believe these studies offer possibilities to shape the future of glass optics and microstructures.

S6 Mark Davis Honorary Symposium

Session 6: Mark Davis Honorary Symposium

Room: Turnberry
Session Chairs: Bill James, Schott Germany; Ina Mitra, Schott, Germany

9:20 AM

(GOMD-S6-001-2024) A new method to infer the diffusivity controlling crystal nucleation in oxide glasses (Invited)

E. Dutra Zanotto*[1]

1. Federal University of Sao Carlos, Materials Engineering, Brazil

It is rather difficult to measure directly the effective diffusivity (D) of the “structural units” of supercooled liquids and glasses during crystal nucleation. Two common methods to infer D are based on viscosity ($D\eta$) or nucleation time-lags ($D\tau$). However, these methods likely underestimate D below the T_g, as recent work has shown that the experimental steady-state nucleation rates (I_{st}) in this T range are much higher than the predictions of the Classical Nucleation Theory (CNT) using any of these two proxies. In this work, we tested another method--based on crystal growth velocity data (Du)--which assumes that nucleation and growth are controlled by the same mass transfer process. We used two stoichiometric silicate glasses as model systems, and measured their nucleation rates, growth velocity, and viscosity using samples of the same glass batches. We found that using very long experimental nucleation times, the experimental temperatures of maximum nucleation rates are much higher than previously reported. Also, the ultimate steady-state nucleation regime was prevented by extensive crystallization in some cases. The most important outcome of the work is that the CNT fitted the experimental $I_{st}(T)$ data much better when using Du instead of $D\eta$, indicating that crystal growth is indeed a good proxy for nucleation diffusivity.

9:50 AM

(GOMD-S6-002-2024) Is glass-ceramic simply a collection of a large number of tiny single crystals? (Invited)

H. Jain*[1]; V. Dierolf[1]; E. J. Musterman[1]; R. Thapa[1]

1. Institute for Functional Materials and Devices, Lehigh University, USA

Glass-ceramics were discovered accidentally by Stookey in 1953; numerous applications followed based on their understanding as a consequence of nucleation and growth of suitable crystalline phase(s) from unstable glass. The rates of nucleation and crystal growth were controlled to yield the desired microstructure and properties semiempirically by heat treating a sample uniformly, resulting in numerous applications. It was implicitly assumed that for all such applications, the glass transformed to glass-ceramic as individual nuclei grew independently following the classical model of crystal growth from a supercooled liquid phase. Recently, it has been possible to grow isolated single crystals in glass using laser heating. These laser-fabricated single crystals exhibit complex lattices often rotating at a predictable rate, presumably because the higher density of crystal than glass produces stresses at the growth front. With many nuclei growing close to each other in a glass-ceramic, these stresses will interact raising the title question. We will explore its answer and attempt to get an insight into the atomic structure of glass-ceramics based on experimental observations and atomistic simulations of single crystal growth in model glass systems.

10:20 AM

(GOMD-S6-003-2024) Oriented Surface Crystallization in Glasses

S. Reinsch*[1]; R. Müller[1]

1. Bundesanstalt für Materialforschung und -prüfung (BAM), Materials Engineering, Germany

Up to now, oriented surface crystallization phenomena are discussed controversially, and related studies are restricted to few glasses. For silicate glasses we found a good correlation between the calculated surface energy of crystal faces and oriented surface nucleation. Surface energies were estimated assuming that crystal surfaces resemble minimum energy crack paths along the given crystal plane. This concept was successfully applied at the Institute of Physics of Rennes in calculating fracture surface energies of glasses. Several oriented nucleation phenomena can be herby explained assuming that high energy crystal surfaces tend to be wetted by the melt. This would minimize the total interfacial energy of the nucleus. Furthermore, we will discuss the evolution of the microstructure and its effect on the preferred crystal orientation.

10:40 AM

(GOMD-S6-004-2024) Surface crystallization of sodium alumino borate glass

T. Honma*[1]; S. Kido[1]

1. Nagaoka Univeristy of Technology, Department of Materials Science and Bioengineering, Japan

$Na_3Zr_2Si_2PO_{12}$ (NZSP) and $NaAl_{11}O_{17}$ (β-alumina) are well-known as sodium ion conductors. Na_3BO_3 is also used as a sintering aid. This study examined the crystallization of Na_2O-Al_2O_3-B_2O_3 glasses to explore new sodium ion conducting oxides. When 33.3 Na_2O-33.3Al_2O_3-33.3B_2O_3 glass was heat-treated, $Na_2Al_2B_2O_7$ of the same composition of glass crystallized on the surface. The thickness of the crystals depended on the heat treatment temperature and time; in both cases, crystal growth was found to proceed from the surface to the bulk interior.

11:00 AM

(GOMD-S6-005-2024) Nano Scale Amorphous Phase Separation and Its Role in Subsequent Crystal Nucleation

R. Hill[1]; s. Shahid*[1]; R. Mansouri[1]

1. Queen Mary University of London, DPS, United Kingdom

Crystal nucleation via prior Amorphous Phase Separation (APS) occurs in many glasses. In most cases it is often inferred from nucleation of the primary crystal phase occurring just above the glass transition temperature (Tg) in the absence of any obvious crystal nucleant phase. SiO_2-Al_2O_3-P_2O_5-CaO-CaF_2 glasses have been shown to undergo APS prior to crystallising to fluorapatite (FAP), however in the compositions studied to date the APS process takes place during quenching. Recently we have found a glass that is single phase initially, but undergoes APS on holding at temperatures above Tg. This glass exhibits one Tg by DSC, as prepared, but two Tgs upon heat treatment (HT) at Tg+X where X is from 10 to 70. The two Tgs provide evidence for APS. The presence of one glass phase prior to HT, but two glass phases after HT is supported by Small Angle Neutron Scattering (SANS) studies, where a peak in I(q) is found for the glasses held at Tg+X with a phase size of 10 to 60nm. APS has a pronounced influence on subsequent crystal nucleation and the optimum nucleation temperature correlates with the observation of two Tgs and APS observed by SANS, which is the first time this has been observed.

11:20 AM

(GOMD-S6-006-2024) Investigating the crystallization of ZERODUR® using DTA methods –working together with Mark Davis

I. Mitra*[1]

1. Schott AG, R&D, Material Development, Germany

Differential thermal analysis (DTA) experiments are commonly used to characterize the crystallization behavior of glasses. In industrial research and development, rapid and easy methodologies are required to determine the parameters for thermal treatments to control the transformation of glass into glass-ceramic. As the development of a new procedure requires validation and benchmarking with already established techniques, new methodologies necessitate the use of state-of-the-art / reference materials and compositions. With this as the underlying motivation, we tested the applicability of DTA methods with a multicomponent and commercially relevant glass-ceramic, ZERODUR®. The procedures of experimental work and discussion with Mark Davis will be presented in order to shed light on his profound interests in unravelling crystallization phenomena that have left a lasting legacy in the field of glass-ceramic development.

S1 Fundamentals of the Glassy State

Session 4: Atomistic simulations and predictive modelling of Glasses

Room: Bel Air II
Session Chair: Alfonso Pedone, University of Modena and Reggio Emilia

1:20 PM

(GOMD-S1-084-2024) Applying the Funnel Theory of Crystallization to Glass (Invited)

C. Wilkinson*[1]

1. Alfred University, Glass Science, USA

Recent progress has been made in the science of nucleation, with new simulation and experimental techniques supporting classical nucleation theory (CNT) and generating new insights into the nature of nucleation. Despite this process, the predictability and underlying physics remain opaque. The difficulty of nucleation is associated with the kinetic function, the non-steady-state nature of nucleation, and the challenge of knowing the surface tension. Conversely, recent progress in the protein literature has shown that funnel-like energy landscapes, have predictive power when discussing preferred protein folding pathways. Here we will consider first principles routes to computing CNT variables and compare the results to the funnel theory of energy landscapes. Testing the funnel like nature of glass forming system's energy landscapes will also be discussed.

1:50 PM

(GOMD-S1-085-2024) Prediction of Nepheline crystallization from MD simulations. A new QSPR-based predictive model

M. Bertani*[1]; A. Pedone[1]

1. University of Modena and Reggio Emilia, Departement of Chemical and Geological Sciences, Italy

Crystallization from glasses has been extensively studied, especially for compositions with minimum devitrification tendency. Crystallization can also be exploited in many technological fields such as glass-ceramic. In particular, nepheline glass-ceramic gained a lot of interest for their mechanical properties while other applications, like nuclear waste confinement, require no nepheline crystallization as it can lower the durability. Many studies have been performed to investigate the relationship between composition, processing, and crystallization and some predictive models have been developed, requiring large experimental databases. This study aims to relate the composition and the crystallization tendency using the simulated structure of the glasses. We started from the assumption that glass can more likely crystallize if the environment of its atoms is similar to the crystal one. We performed MD simulations on several (Na, Ca, Li)-aluminoborosilicate glasses using a state-of-the-art classical potential and, after a structural check, we used the homemade Cluster code, to quantify the similarity between the oxygen environment in the glasses and the nepheline crystal. From these data, we constructed a model able to predict if a glass is likely to crystallize nepheline as the primary phase based on simulation only, with an economic and environmental gain by avoiding glass synthesis.

2:10 PM

(GOMD-S1-086-2024) Diffusion Derived from Energy Barriers: Unveiling the Role of Non-random Walk in Orchestrating Dynamic Slow-down in Glasses

A. Annamareddy*[1]; D. Morgan[1]

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

The diverse local atomic environments manifested in the glassy state renders a wide distribution of activation barriers for atomic rearrangements. While diffusion is the accumulation of many of these local rearrangements, it is not clear how the activation barrier for diffusion is related to the rearrangement barriers. Here, we study a model metallic-glass and show that the non-random walk or non-Brownian motion of atoms plays a major role in obtaining diffusion from the barriers. Specifically, we calculate the correlation factor, quantified as the ratio of random walk to non-random walk diffusion, and show that it is large and follows an Arrhenius behavior in the glassy state. Thus, the diffusion barrier in the glass can be considered as the sum of the activation energies of random-walk diffusion and correlation factor. We demonstrate that non-random walk motion of atoms is partly due to the asymmetric barriers seen by atoms during rearrangements. We believe that by coupling rearrangement barriers and correlation effects we can form a quantitative connection between the atomic scale rearrangement energetics and diffusion, taking us a step closer to having a full atomistic understanding of macroscopic kinetics.

2:30 PM

(GOMD-S1-087-2024) Establishment of an empirical force-field for crystalline and amorphous Li_2S-SiS_2 electrolytes

L. Poitras*[1]; M. Micoulaut[1]

1. Sorbonne Université, France

An empirical force-field of Buckingham type is derived for crystalline and glassy Li_2S-SiS_2 binary alloys using fractional charges, short-range repulsion, and long-range attractive dispersion interactions. Parameters are fitted on low-temperature equilibrium polymorphs Li_2SiS_3, and permit to recover typical bond distances, cell lengths, and to predict elastic properties. We then use classical molecular dynamics to study the structural properties of corresponding glasses and a very good agreement is found with corresponding data obtained from neutron and x-ray scattering. The resulting glasses are composed of fourfold tetrahedral Si and twofold sulfur, whereas Li atoms experience a more complex environment, partially in defective octahedral or tetrahedral geometry with a coordination number close to three. Unlike the base SiS_2, the resulting glass network does not contain edge-sharing tetrahedra and displays a rather broad distribution of tetrahedral species that are quantified using the usual Q^n formalism. Physical Review B 107, 214205 (2023).

2:50 PM

(GOMD-S1-088-2024) Structural simulations of MgO-B_2O_3 and CaO-B_2O_3 glasses by the first principle molecular dynamics technique

H. Inoue*[1]

1. The University of Tokyo, Institute of Industrial Science, Japan

In this study, I investigated the difference in atomic arrangement between MgO-B_2O_3 and CaO-B_2O_3 glasses by structural models using molecular dynamics simulations. The structural model was created using classical molecular dynamics methods by melting and quenching, and then first principle molecular dynamics techniques were used to optimize the strucftural models. For some compositions, the total correlation functions were calculated and compared with the experimental total correlation functions obtained from X-ray diffraction measurements. As for structural characteristics, for example, the N_4 values in the structural models for MgO-B_2O_3 system were from 0.26 to 0.29, which was lower than 0.33 to 0.39 for the CaO-B_2O_3 system. Furthermore, the number of the six-membered ring (B_3O_3) was smaller in the MgO-B_2O_3 system than in the CaO-B_2O_3 system. Furthermore, the formation of triborate groups, pentaborate, and diborate was confirmed in the structure models for the CaO-B_2O_3 systems.

3:10 PM

(GOMD-S1-089-2024) Theoretical Insights into 27Al NMR Parameters of Binary Aluminosilicate Glass and Their Relationship to Atomic and Electronic Structure

T. Ohkubo*[1]; A. Masuno[2]; E. Tsuchida[3]; S. Ohki[4]

1. Chiba University, Faculty of Engineering, Japan
2. Graduate School of Engineering, Kyoto University, Japan
3. National Institute of Advanced Industrial Science and Technology (AIST), Japan
4. High Field NMR Group, National Institute for Materials Science (NIMS), Japan

An accurate atomic structure of 60Al2O3-40SiO2 was modeled using ab initio molecular dynamics (AIMD) simulations containing 418 atoms and employing the melt-quenching route with 15 K/ps. This simulation approach reproduced X-ray diffraction data better than classical molecular dynamics simulations. The structure of the polyhedra formed by O bonded to Al was quantitatively analyzed by evaluating bond-angle distributions and the degree of symmetry using spherical harmonic functions. The relationship between chemical shifts and charge-balancing mechanisms was explored through the analysis of electronic structures obtained from AIMD-derived structures. Interestingly, the Al partial charge and the spatial electron distribution of Al--O bonds were independent of Al coordination number, implying that valence electrons are not localized to specific atoms but are rather distributed throughout the glass network. The theoretical distribution of 27Al NMR parameters was obtained through statistical analysis from theoretically calculated NMR parameters for 100 AIMD-derived structures. By comparing the experimental 27Al NMR data with the theoretical distribution, the previously unclear relationship between 27Al NMR parameters and local structure was elucidated.

Session 6: Mechanical Properties of Glasses II: Current challenges in experiments and modelling of fracture

Room: Bel Air I
Session Chair: Emily Aaldenberg, Corning Incorporated

1:20 PM

(GOMD-S1-090-2024) Phase Separated SiO_2-B_2O_3-Na_2O Glasses: Linking Stress Corrosion Cracking to Mesoscale Structures (Invited)

W. Feng[1]; D. Bonamy[1]; F. Célarié[2]; L. Chomat[1]; A. A. Deshkar[3]; P. C. Fossati[3]; S. Gossé[3]; P. Houizot[2]; C. L. Rountree*[1]

1. Université Paris-Saclay, CEA, CNRS, SPEC, France
2. Université Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, France
3. Université Paris-Saclay, CEA, Service de la Corrosion et du Comportement des Matériaux dans leur Environnement, France

During 2023, the global flat glass and smart glass market was nearly $140 billon, and it is estimated to nearly double by 2032. In parallel, governments are calling for circular economies, which includes extending the lifetime of products. This means that glasses need to be evermore resistant to a variety of damage (everyday use, stress corrosion cracking, sand storms, external irradiations, high temperatures, etc.). Moreover, minor amounts of stress (including residual stresses) can cause small-scale damage to interact with environmental parameters (humidity, temperature, etc.) leading to the subcritical crack growth (stress corrosion cracking, SCC) and premature failure. Making glasses less reactive to SCC, tougher (increasing their fracture toughness, K_c) and lighter, while maintaining other properties, is a fundamental issue plaguing glass scientists and researchers. The works presented herein alters the mesoscale of SBN (SiO_2-B_2O_3-Na_2O) glasses, and then studies how these alterations affect the stress corrosion cracking behaviour. To do this, the chemical composition of the glasses was selected to be in the theoretical three-phase section of the SBN ternary glass system. After fabrication, annealing samples provoked the formation of amorphous phases separated glass systems. The presentation will focus on stress corrosion cracking and how it varies with the mesoscale amorphous phase separation in the SBN glasses.

1:50 PM

(GOMD-S1-091-2024) Challenges of statistical modeling of mechanical lifetime of silicate glass in the near-threshold regime (Invited)

S. Grutzik*[1]; T. Diebold[2]; K. T. Strong[2]

1. Sandia National Laboratories, Materials and Failure Modeling, USA
2. Sandia National Laboratories, Materials Mechanics and Tribology, USA

The stochastic nature of brittle material reliability is commonly characterized using Weibull statistics. In addition, lifetime is often estimated in terms of subcritical crack growth. In practical application many restrictive assumptions are often employed in order to combine these approaches, such as the assuming that subcritical flaw population evolution does not change the strength distribution or stress state does not change in time. In this work, we present a method to allow the strength distribution to evolve over time to account for subcritical crack growth effects in a unified, probabilistic manner while allowing for time-varying stress. Model predictions are compared to measured time to failure under static four-point bending and bending at varying stress rate for alumina ceramic and Schott S8061 glass in a controlled atmosphere at 50% and 95% relative humidity. In particular, we note that it is very difficult to predict long lifetimes at low load levels due to crack growth threshold effects. Some strategies to deal with this issue, including alternate load histories during experiments, are discussed.

2:20 PM

(GOMD-S1-092-2024) From Thermodynamics to Fracture Mechanics: Integrated Modeling Framework for Studying Mechanical Properties of Phase Separated Glasses

E. Barros de Moraes*[1]; X. Xu[1]; N. Prakash[1]; J. Harris[1]; C. Smith[1]

1. Corning Incorporated, USA

Microstructured materials (composites, ceramics, glass ceramics) can have higher fracture toughness than homogeneous materials such as polymers or glasses. Phase-separated glasses, where the microstructure is comprised of two dissimilar amorphous glasses, potentially have higher fracture toughness compared to homogeneous glasses. Phase separation leads to three-dimensional microstructures from droplet formation or spinodal decomposition and could be capable of toughening mechanisms, such as crack deflection, crack bowing and pinning, that are generally absent in traditional amorphous homogeneous glasses. Computational models of phase-separated microstructures are convenient tools to understand microstructure formation and resulting mechanical properties. In this talk, we discuss the development of phase-field models to simulate the phase-separation process in binary systems towards a tridimensional microstructure which is later used as the input for mechanical simulations. We use Peridynamics fracture mechanics modeling to study the effect of phase-separation in the resulting fracture toughness under different conditions. We show results of phase-separation and crack propagation simulations in two-phase spinodal systems and compare modeling and experimental results of phase-separated SiO2-Na2O glass.

2:40 PM

(GOMD-S1-093-2024) Silicate glass fracture surface energy calculated from crystal structure and bond-energy data

M. S. Holzer*[1]; T. Waurischk[1]; J. George[2]; R. Maaß[2]; R. Müller[1]; A. S. de Camargo[1]

1. BAM Federal Institute for Materials Research and Testing, Glass, Germany
2. BAM Federal Institute for Materials Research and Testing, Germany

The search for stronger and tougher oxide glasses is still one of the most challenging tasks to overcome in glass research. Due to the materials inherent brittleness and fracture toughness experiments in such materials being complicated and time-consuming, models for predicting the fracture toughness, K_{Ic}, via the fracture surface energy, γ, are of high value. In this work, we present a novel method to predict γ of isochemically crystallizing silicate glasses using readily available crystallographic structure data of their crystalline counterpart and tabled diatomic chemical bond energies, D_0. The method assumes that γ equals the fracture surface energy of the most likely cleavage plane of the crystal. Calculated values were in excellent agreement with those calculated from glass density, network connectivity and D_0 data in earlier work. This finding demonstrates a remarkable equivalence between crystal cleavage planes and glass fracture surfaces.

3:00 PM

(GOMD-S1-094-2024) Fracture behavior of LATP glass-ceramic electrolytes: A molecular dynamics study

Z. Chen*[1]; T. Du[1]; N. Krishnan[2]; M. M. Smedskjaer[1]

1. Aalborg University, Denmark
2. Indian Institute of Technology Delhi, India

Understanding the mechanical behavior of solid-state electrolytes is crucial for the development of all-solid-state batteries. Through molecular dynamics simulations, we here show that $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) glass-ceramics, as a promising solid-state electrolyte, exhibit enhanced bond-switching characteristics at the composite glass-crystal interface. In turn, this improves the fracture energy. We find that the LATP fracture behaviour is strongly influenced by the nanocrystal grain size and its proximity to the pre-crack location, with the complexed interface being susceptible to localized shear deformation. The fracture energy of LATP glass-ceramics is enhanced when the grain size is larger, as these grains have a larger contact area with the glass phase, resulting in a larger complexed interface. Structural analysis during the tensile process reveals a higher occurrence of bond-switching events at the complex interface, dissipating strain energy associated with the fracture process. This enhancement significantly improves the fracture energy of LATP glass-ceramics as cracks tend to propagate along the interface.

Session 9: Metallic Glasses

Room: Shoal Creek
Session Chairs: Jan Schroers, Yale; Isabella Gallino, Technical University Berlin

1:20 PM

(GOMD-S1-095-2024) The effect of composition on the thermodynamics, structure and atomic motion of (Pd-Pt)$_{42.5}$Cu$_{27}$Ni$_{9.5}$P$_{21}$ alloys (Invited)

N. Neuber[1]; O. Gross[1]; B. Ruta[3]; I. Gallino[2]; R. Busch*[1]

1. Saarland University, Chair of Metallic Materials, Germany
2. Technical University Berlin, Chair of Metallic Materials, Germany
3. Institut Néel, CNRS UPR2940, France

According to basic hard sphere models Pt should replace Pd in the $Pd_{42.5}Cu_{27}Ni_{9.5}P_{21}$ alloy. But $Pt_{42.5}Cu_{27}Ni_{9.5}P_{21}$ shows significant structural differences compared to the Pd based alloy. To study the differences, we prepared a series of $(Pd\text{-}Pt)_{42.5}Cu_{27}Ni_{9.5}P_{21}$ alloys replacing Pd by Pt. We assess the thermodynamic functions revealing that the driving force for crystallization increases with the increase of the Pt content, which is in line with the decreasing critical casting thickness. The Pt-richer alloys are thermodynamically more fragile than the Pd-rich alloys, which is revealed by a larger specific heat capacity and a faster drop of the configurational entropy in the Pt-richer alloys. We conclude that the structure of the Pt rich alloys is dominated by its change in medium range order whereas the Pd-rich alloy is dominated by extraordinary short range. Since the two alloys show similar kinetic fragilities but different thermodynamic and structural fragilities we used XPCS to study the atomic dynamics of the two extreme cases of the series, namely the alloy $Pd_{42.5}Cu_{27}Ni_{9.5}P_{21}$ and the alloy $Pt_{42.5}Cu_{27}Ni_{9.5}P_{21}$ as a function of temperature and wave vector.

1:50 PM

(GOMD-S1-111-2024) Size dependent vitrification in metallic glasses (Invited)

I. Gallino*[1]; D. Cangialosi[2]

1. . Technical University Berlin, Materials Science and Engineering, Germany
2. Donostia International Physics Center, Spain

By means of fast scanning calorimetry (FSC) we have observed up to 40 K reduction in the glass transition temperature of bulk metallic glasses in samples with sizes below 10 µm. We have investigated different compositions in a wide range of time scales in terms of vitrification kinetics via the cooling rate-dependence of the fictive temperature. We have observed a pronounced size dependent vitrification kinetics, which is more evident at low cooling rates. The important implication of this outcome is that mild reductions of the sample size in metallic glasses allow exploring thermodynamic states, in terms of fictive temperature, deep down in the energy landscape.

2:20 PM

(GOMD-S1-113-2024) Size-effects in tensile fracture of rejuvenated and annealed metallic glass

G. Kumar*[1]

1. University of Texas, Dallas, USA

Metallic glass samples with diameters ranging from sub-100 nm to 100 µm were subjected to cryogenic rejuvenation and annealing above glass transition temperature before tensile loading at room temperature. Shear-localized failure with no ductility is observed in large samples whereas the smaller diameter specimens show ductile necking irrespective of the structural state of metallic glass. With decreasing sample diameter, the fracture surface changes from vein pattern to featureless in the shear-localized samples and the ductility increases in the necked samples. Despite similar size-dependent trends, the changes in deformation mode and fracture morphology occur at different diameters in as-cast, rejuvenated, and annealed samples. The critical diameters for transitions from shear localization to necking and from vein pattern to smooth fracture surface shift to larger values in cryogenically rejuvenated samples whereas annealing has the opposite effect. Structural rejuvenation suppresses shear localization on and catastrophic tensile failure in nanoscale metallic glasses.

3:00 PM

(GOMD-S1-099-2024) Densification effects on the thermodynamic and dynamic properties in a ZrTiCuNiBe metallic glass *WITHDRAWN*

J. Shen*[1]

1. Institute of Neel, France

The glass stability is crucial for applications and the understanding of glass formation. Here, the thermodynamic and kinetic stability during the glass-to-liquid transition process has been investigated for metallic glasses (MGs) subjected to hydrostatic densifications. We discovered that the thermodynamics of $Zr_{46.25}Ti_{8.25}Cu_{7.5}Ni_{10}Be_{27.5}$ metallic glass (MG) after densification is significantly dependent on the densification protocols. As undergoing the high-pressure cooling (HPC, pressurization above the glass-transition temperature, T_g), a MG exhibits a lower fictive temperature, while following a short period of the high-pressure annealing (HPA, pressurization below T_g), it displays a higher fictive temperature. X-ray phonon correlation spectroscopy revealed an acceleration of atomic motions with more pronounced stress dominance after both the HPC and HPA, while the acceleration factor of HPC is more pronounced. The distinction is attributed to different densification mechanisms in tuning the atomic-scale local structures for the liquid and glass. This work highlights two distinct densification pathways tuning the intrinsic state of MGs with distinct stabilities and may expand it into a new landscape with unique properties.

Session 10: Sol-Gel and MOF Glasses

Room: St. Andrews
Session Chairs: Lisa Klein, Rutgers University;
Yuanzheng Yue, Aalborg University

1:20 PM

(GOMD-S1-100-2024) Melt-quenched Carboxylate Metal-Organic Framework Glasses (Invited)

H. Moon*[1]

1. Ewha Womans University, Republic of Korea

Although carboxylate-based frameworks are commonly used architectures in metal-organic frameworks (MOFs), liquid/glass MOFs have thus far mainly been obtained from azole- or weakly coordinating ligand-based frameworks. This is because strong coordination bonds of carboxylate ligands to metals block the thermal vitrification pathways of carboxylate-based MOFs. In this talk, we present the first example of carboxylate-based melt-quenched MOF glasses comprising Mg^{2+} or Mn^{2+} and an aliphatic carboxylate ligand, adipate. These MOFs have a low melting temperature (T_m) of 284 °C and 238 °C, each, compared to zeolitic-imidazolate framework (ZIF) glasses, and superior mechanical properties in terms of hardness and elastic modulus. The low T_m may be attributed to the flexibility and low symmetry of the aliphatic carboxylate ligand, which raises the entropy of fusion (ΔS_{fus}), and the lack of crystal field stabilization energy on metal ions, reducing enthalpy of fusion (ΔH_{fus}). This research will serve as a cornerstone for the integration of numerous carboxylate-based MOFs into MOF glasses.

1:50 PM

(GOMD-S1-101-2024) Structural descriptors for zeolitic imidazolate framework glasses

M. M. Smedskjaer*[1]; T. Du[1]; Y. Yue[1]

1. Aalborg University, Department of Chemistry and Bioscience, Denmark

The glassy state of metal-organic frameworks (MOFs) offers unique features, such as combining nano-porosity with lack of grain boundaries. Zeolitic imidazolate frameworks (ZIFs) are an important subset of MOFs, some of which can be vitrified to glass through melt-quenching, but their structure-property relations have not yet been fully understood. Based on a developed deep learning force field for molecular dynamics simulations, which is able to reproduce both the structure and mechanical properties of ZIF glasses, we study the structural origins of phase transitions and composition dependence of mechanical properties. Specifically, we discuss the role of various structural descriptors, such as ring orientation index and local entropy and volume of metal ions, in capturing these variations. The development of suitable structural descriptors is crucial for the future design of MOF glasses with improved performances.

2:10 PM

(GOMD-S1-102-2024) High Temperature Insulation Based on Silica Aerogels and Fillers

M. Buttgereit[2]; A. Schoeffler[3]; P. Hidalga[4]; T. Siddarthan[1]; L. C. Klein*[1]

1. Rutgers University, MS&E, USA
2. Rutgers University, C&BE, USA
3. Rutgers University, I&SE, USA
4. Rutgers University, BME, USA

Thermal insulation has relied on the same materials for the past half century, with most structures using mineral wool and fiberglass insulation. Aerogels are a class of insulating material that can replace these materials while providing thinner, dust-free insulation. Aerogels are highly porous, fragile, amorphous solids made from a variety of silica precursors. Their high porosity gives them very low thermal conductivity. The aerogels studied here were silica-based, derived primarily from tetraethyl orthosilicate (TEOS), dimethyldiethoxysilane (DMDES) and methyltriethoxysilane (MTES). They were dried at ambient pressure after solvent exchange with hexane. Several inexpensive lightweight materials were incorporated in the aerogel formulations, such as cotton, polypropylene, urethane foam, or cellulose, which made ambient drying easier. Some of the composites were treated with 2-aminopropyl triethoxysilane (APTES) to increase water repellency. Others were filled with oxide powders such as MgO or phosphoric acid to increase flame retardancy. By combining an aerogel with different filler materials, some flexibility was imparted to the aerogel.

2:30 PM

(GOMD-S1-103-2024) Preparation of Paraffin/Aerogel Composites for PCM Applications

S. Kearney[2]; S. Guttikonda[3]; L. C. Klein*[1]

1. Rutgers University, MS&E, USA
2. UMBC, Chemistry, USA
3. Rutgers University, C&BE, USA

Phase change materials (PCMs) are materials that can be used for energy storage through the process of changing phases, for example, melting and solidifying. The latent heat of transformation needed for the change allows the phase change materials to store and release heat. This cycle of storing and releasing heat can be used to make more effective thermal insulation that reduces the energy used to heat buildings. It is also known that silica aerogels are effective insulators, are highly porous and have very low thermal conductivities. This study combines paraffin waxes that melt around 60°C with aerogels to form composites that are good insulation with the added ability to store heat through a phase change. Using granular aerogel samples made in a previous study, composites were formed in three different ratios by weight, 1:1, 1:2, and 2:1 aerogel to wax. These samples were then immersed in a constant temperature water bath. A thermocouple was imbedded in the sample. The times at which the composites were able to reach temperature, melt, solidify and cool were recorded. The physical properties were observed as well. The opacity or translucency changed with ratio, indicating the degree of compatibility of the aerogel and the wax. Those samples that were better mixed had the ability to retain heat longer than others.

2:50 PM

(GOMD-S1-104-2024) A brief review of the development of MOF glasses

Y. Yue*[1]

1. Aalborg University, Denmark

Metal-organic frameworks (MOFs) are microporous inorganic-organic hybrid materials constructed by metallic nodes and their organic ligands. In 2015, the first MOF glass, i.e., ZIF-4 $[Zn(C_3H_3N_2)_2]$ glass, was reported. At the same year, the first coordination polymer glass was invented. In this talk, I will briefly review the milestones of the development of the MOF glasses. The composition expansion and fabrication techniques of MOF glasses will be presented. The main breakthroughs in understanding of glass formation and structure in MOF glasses will be displayed. The main functionalities and applications of MOF glasses will be outlined. Finally, I point out some major challenges and perspectives concerning future research and development of MOF glasses.

S4 Outreach Glass Technology Manufactury Recycling & Cross-Cutting Topics

Session 2: Challenges in Manufacturing IV

Room: Peeble Beach
Session Chairs: Katelyn Kirchner, The Pennsylvania State University; Irene Peterson, Corning Incorporated

1:20 PM

(GOMD-S4-033-2024) Dynamic and static corrosion of chromium-alumina refractory during waste glass melting

J. Klouzek*[1]; R. Pezl[1]; M. Vernerova[1]; P. Cincibusova[1]; T. Jin[2]; P. Hrma[3]; A. A. Kruger[4]; D. P. Guillen[5]; R. Pokorny[1]

1. University of Chemistry and Technology Prague, Czechia
2. Pacific Northwest National Lab, USA
3. AttainX, USA
4. US Department of Energy, Office of River Protection, USA
5. Idaho National Lab, USA

Despite the excellent chemical and thermal resistance of Monofrax® K-3, an electrofused chromium alumina refractory, the highly corrosive environments present during the vitrification of nuclear waste can lead to significant K-3 refractory wear, affecting melter reliability and lifetime. This study investigates the three main types of refractory wear: subsurface corrosion, melt line corrosion, and thermal spalling. Corrosion tests have been performed using both static and dynamic conditions, simulating the effect of forced melt convection on the corrosion rate. The results agree with theoretical diffusion-controlled corrosion models wherein the subsurface corrosion increases with increasing melt flow velocity, while the melt line corrosion appears to be virtually independent of it. Furthermore, since the driving force for the refractory dissolution is identical for both flux line and subsurface corrosion, we show that based on the Cr_2O_3, Al_2O_3, and alkali content in the glass, the corrosiveness of the used glasses is consistent for both flux line and subsurface corrosion tests. The results of this work will be used in computational fluid dynamics models of vitrification melters to simulate the effect of melter processing conditions (temperature, bubbling rate, number of pouring cycles) and the waste glass composition on the corrosion of Monofrax® K-3 melter refractory.

1:40 PM

(GOMD-S4-034-2024) Accelerated Corrosion Testing of Refractory in Contact with Glass Melts

J. Amoroso*[1]; W. Li[1]; M. Page[1]; N. Rod[1]

1. Savannah River National Laboratory, USA

Accurate and reproducible estimates of glass-contact refractory loss are needed to better understand mechanistic corrosion phenomena and to develop predictive models for refractory component service lifetime. Accelerated laboratory tests that vary temperature, time, and glass composition have been studied to better understand the driving forces affecting the corrosion rates of refractory ceramic materials. These tests are used to estimate the physical refractory loss and to evaluate chemical and microstructural changes from corrosion and wear. In this work, fused cast refractory Monofrax® K3 was tested against several simulated Hanford nuclear waste glasses using a modified ASTM C621 static test method for isothermal corrosion resistance of refractories. Corrosion behavior between the submerged refractory and refractory at the melt-line are compared to understand different corrosion mechanisms. In addition, a new method to rapidly and accurately estimate the refractory total volume loss is presented. Results and observations are discussed in the context of using accelerated testing for long-term prediction of refractory loss.

2:00 PM

(GOMD-S4-035-2024) Integrating Artificial Intelligence for Enhanced Color and Optical Properties of Glass Products

D. Güldiren*[1]

1. Sisecam Science, Technology and Design Center, Turkey

The production of glass with the desired color and optical properties is a process affected by a multitude of parameters in glass manufacturing. Beyond the addition of specific oxides to the glass batch, operational furnace parameters play a crucial role. Understanding, predicting and correlating the effects of all these parameters on the final product are essential for achieving high quality and efficient glass production with minimal losses. This knowledge allows for precise control and optimization of the manufacturing process, ensuring the production of glass with the specified characteristics in a cost effective and resource efficient way. The improvement of computer technology has led glass science towards data analytics-based approaches. A strategy for data-driven modeling involves utilizing datasets and machine learning algorithms, to model the chemical and physical properties of glass. Furthermore, the incorporation of AI in glass production not only enhances the quality of the final product but also significantly reduces the time-consuming tasks traditionally associated with manual adjustments. Within this framework, an extensive investigation focusing on the prediction of color and optical properties of glass will be discussed. The study involves the utilization of machine learning techniques by examining datasets and complemented experimental studies conducted to validate and establish correlations between the model predictions and actual experimental outcomes.

2:20 PM

(GOMD-S4-036-2024) The infinite lives of glass (Invited)

A. Durán*[1]

1. Instituto de Ceramica y Vidrio (CSIC), Glasses, Spain

A key issue in the approval of IYOG2022 was the power of glass as a tool to build a more sustainable and a fairer planet. Glass containers represent the best example of circular economy, where one bottle is produced from other bottle, closing the circle of non-waste process. But glass in every application can also have also infinite lives. In particular, a main aim of flat glass industry is to strongly increase the use of cullet of high quality to arrive to the goal of including more than 80% of recycled glazing. Integrated systems for recycling flat glass products are being designed with some successful models in Europe. Other emerging problems are the end-of-life treatments of PV panels or eolic turbine blades of composite polymeric materials containing up to 80% of reinforcing fibers of high quality and cost. The most efficient methods leading to circular economy are the Close Loop Recycling (CLR), when glass cullet is remelted for regeneration of original articles, with the same quality standards, maintaining the value, saving energy and reducing CO_2 emissions. When it is not possible to use CGR, Open Loop Recycling (OLR) offers solutions in which 'recovered' glass is part of the raw materials to produce new products, of different value methods. Several methods of OLR and are revised in this talk. Foams and geo-polymers play a key role in OLR as well as the crushing machines for producing different glass products as raw materials.

2:50 PM

(GOMD-S4-037-2024) Modeling the Flow of Waste Glass in New York State

D. Saadatpour*[1]; C. Wilkinson[1]

1. Alfred University, Inamori school of engineering, USA

The economics of glass recycling remain a challenge in the United States. The European Union is capable of recycling 80-90% of container glass, in the US the same number is only 30-40%. New York State has an approximate recycling rate of 33%. Here we propose a model to better understand the flow of waste glass in New York State, with the goal of elucidating feasible improvements to the recycling system. The novel model proposed here assumes that glass will get recycled if the cost of recycling is comparable to or less than a landfill. From the model, we're able to derive two recommendations that have the potential to change the recycling rate in NYS. In the presentation, we will discuss the model formation, the insights gained from the model, and the weaknesses thereof. The work presented here is supported by the New York State Department of Environmental Conservation.

S6 Mark Davis Honorary Symposium

Session 6: Mark Davis Honorary Symposium

Room: Turnberry
Session Chair: Ina Mitra, Schott, Germany

1:20 PM

(GOMD-S6-007-2024) Copper in the crystallization process of glasses : coloring and opacification properties (Invited)

L. Cormier*[1]; L. Gardie[1]; C. Noirot[1]; N. Schibille[2]

1. Sorbonne University - CNRS, IMPMC, France
2. CNRS, Iramat, France

Since Antiquity, crystallization has been used by glassmakers to obtain specific coloration or opacification for the manufacture of decoration or glassy objects Copper is known to be a multivalent element that colors glasses in blue (Cu^{2+}), red or orange (nano or micro-crystals of metallic copper Cu^0 or cuprite Cu_2O). It can also be associated with the formation of calcium antimonates crystals that were specifically used to provide opacification. In this study, we will present results on the redox and crystallization of copper in silicate glasses. We show how copper reduction, from Cu^{2+} to Cu^+ and Cu^0, can be controlled, emphasizing correlations between copper and lead contentson the crystallization. Examples cover several red and orange Roman mosaic tesserae (4th century). In the case of turquoise opaque glasses, the color is brought by copper and opacification by antimony. Antimony and copper are multivalent elements that can be present in different oxidation states once present in the glass matrix or in calcium antimonate crystals. The redox coupling can then be a factor influencing the crystallization of calcium antimonates We will discuss the impact of copper in the crystallization process of calcium antimonate crystals.

1:50 PM

(GOMD-S6-008-2024) Recent research on Li_2O-Al_2O_3-SiO_2 glass-ceramics for expansion of applications (Invited)

S. Nakane*[1]

1. Nippon Electric Glass, Japan

Applications of LAS GC have been extended to electronic and optical devices and production process equipment in addition to their conventional use in cookware. For further expansion and application to new markets, we demonstrate three topics of our research on the material and production processes from viewpoint of glass phases. The first topic is spherical LAS GC powder for a filler application. It has been developed successfully, which can be prepared in a single heat treatment where spheroidizing utilizing viscous flow and crystallization are achieved simultaneously by considering the kinetics of the two phenomena. Second, high transparent LAS GC was obtained by composition design of the glass-matrix phase. Third, fan shape of feeder in forming process designed by thermo-fluid analysis has accomplished to prevent devitrification and form the largest sheet of LAS GC.

2:20 PM

(GOMD-S6-009-2024) Sr-Fresnoite based piezoelectric glass-ceramic for high-temperature applications

M. Letz*[1]; M. Letz[1]

1. Schott AG, R&D, Germany

Sr-fresnoite ($Sr_2TiSi_2O_8$) is a highly intersting system for piezoelectric sensors. It has no ferroelectric trasnitions which limits the absolute value of the piezoelectric coefficients but allows high temperature applications up to 600°C and more. In the present work we report on a glass ceramic system with $Sr_2TiSi_2O_8$ as a crystalline phase. Symmetry breaking and in particular crystalline orientation is obtained by making use of directed surface crystallization. The piezoelectric coefficients are in the same range as other high temperture single crystal materials $d_{33} = 10$, $d_{31} = 1.5$, and $d_{15} = 34$ (pC/N). The voltage coefficients are very competitive in this system $g_{33} = 103$, $g_{31} = 15$, and $g_{15} = 233$ ($\times 10^{-3}$ V m/N) due to the -- compared to most ferroelectric materials -- low values of the tensor of the permittivity ($\varepsilon_{33}{}^{T} / \varepsilon_0 = 11.5$; $\varepsilon_{11}{}^{T} / \varepsilon_0 = 16.5$, both at 1 kHz). Especially the low resistivity makes the material system applicable at high temperatures. We report a specific resistivity of $\rho \sim 10^{12}\Omega$-cm at 300 °C and 10^6 at 850 °C which has a potential to be further increased by a tight control of alkali impurities in the raw materials. The lack of a Curie temperture of a ferroelectric transition, which leads to reduced ageing and fatigue under operation, in combination with high resistivity and large volatge coefficients makes the material class highly interesting for high temperature sensor applications.

2:40 PM

(GOMD-S6-010-2024) First principles study on mechanism of anomalous thermal expansion behaviors of cordierite

K. Umemoto*[1]; S. Nakane[1]

1. Nippon Electric Glass, Fundamental Technology Division, Japan

To design heat resistance glasses, it is essential to understand materials with a low thermal expansion coefficient. Cordierite ($Mg_2Al_4Si_5O_{18}$) is one of such materials. Another attractive property of cordierite is an anisotropic thermal expansion behavior, i.e., negative thermal expansion along the c axis between room temperature and about 1,000 degrees. Computationally, these properties have been studied mainly by classical model potentials so far. In this study, we will perform first principles computational studies on cordierite, using quasi-harmonic approximation and molecular dynamics simulations within the framework of the density functional theory. We will find that our first principles study successfully reproduces thermal expansion behaviors of cordierite as for both volume and lattice constants. By making a detailed analysis of thermal vibrations of structural units in atomic scale, the origin of anomalous thermal expansion of cordierite will be identified. In addition, we will discuss which LDA or GGA is more suitable for description of thermal expansion behaviors of cordierite.

3:00 PM

(GOMD-S6-011-2024) Glass Interaction and EMA behavior in Imaging Fiber Optics (Invited)

P. L. Higby*[1]

1. SCHOTT North America, Inc., USA

High-NA Imaging fiber optics are produced with a rod-in-tube process and require glasses which are able to withstand multiple draw steps at softening-point viscosities while in contact with other glasses. The addition of Extra Mural Absorption in the form a high-absorbing black glass increases the complexity of the composite material. Practical application of Glass Science to boundary interactions, including diffusion and crystallization can explain the optical behavior of final components.

<u>S1 Fundamentals of the Glassy State</u>

Session 6: Mechanical Properties of Glasses III: Strengthening

Room: Bel Air I
Session Chair: Cindy Rountree, CEA

3:40 PM

(GOMD-S1-105-2024) Increase in glass laminate stress through heat-treatment below the glass transition temperature (Invited)

E. M. Aaldenberg*[1]; T. M. Gross[1]; S. D. Ianson[1]

1. Corning Incorporated, Science & Technology, USA

In a glass laminate sheet structure consisting of an interior core glass and an exterior clad glass, the layers are fused at high temperature. As the structure cools, a compressive stress develops in the outer clad layer resulting in strengthened glass. This development occurs when the core glass shrinks more than the clad glass, that is, when the thermal expansion coefficient of the core glass is greater than the clad glass. The resulting laminate stress formed by rapid cooling can be further increased through a low temperature heat-treatment when there is a crossover in the thermal expansion curves as a function of temperature in the vicinity of the glass transition range.

4:10 PM

(GOMD-S1-106-2024) Glass with hydration-induced compressive stress profiles

T. M. Gross*[1]; E. M. Aaldenberg[1]; J. Wu[1]; Z. Zheng[2]

1. Corning Incorporated, New Materials and Processes, USA
2. Corning Incorporated, MTE, USA

A potassium phospho-aluminosilicate (KPAS) glass composition is described that can be strengthened by water vapor to achieve deep compressive stress profiles. This material was initially discovered through a series of hydration experiments in which the KPAS specimen achieved a 29 micron compressive depth after being held in a 85°C, 85% relative humidity chamber for 65 days, thus exhibiting diffusivity orders of magnitude greater than comparative glasses. Not only did the KPAS glass have a high Vickers indentation crack resistance of >20 kilograms force (kgf), but it also displayed considerable stored energy at failure. This indication of a residual stress profile was subsequently measured and a compressive stress (CS) of 400 MPa and compressive depth of layer (DOL) of 29 microns was found. It is demonstrated that hydration strengthened glasses are capable of a variety of stress profiles and can provide high retained strength following flaw introduction compared with ion-exchanged soda-lime silicate glass. It is further shown that the process can be optimized by utilizing pressurized steam vessels to achieve stress profiles with surface CS >300 MPa and DOL >30 microns in less than 8 h, making this a practical solution for manufacturing strong glass. The sustainability benefits of steam strengthening include less waste byproduct and lower carbon footprint compared to traditional molten salt ion-exchange strengthening.

4:30 PM

(GOMD-S1-107-2024) Time Dependence of Macrodeformation of Ultra-Thin Glass Induced by Ion Exchange

J. Lee*[1]; S. Ko[1]; J. Lee[1]; S. Park[1]; Y. Choi[1]

1. Korea Aerospace University, Republic of Korea

In an attempt to better understand time dependent evolutions of macrodeformation such as deflection, i.e., warpage or bending, of flat glass during ion exchange, we have performed experiments in which only one face of ultra-thin glass undergoes $Na^+ \leftrightarrow K^+$ ion exchange via a molten-salt-bath-free ion exchange process. Time-dependent changes in radius of curvature of the ultra-thin glass are in-situ monitored for various ion exchange temperatures, and interpreted in a quantitative manner. The related applications are proposed with a special attention to the position selectability of our molten-salt-bath-free 'dry' ion exchange technique.

4:50 PM

(GOMD-S1-108-2024) Development of new composition and surface treatment to improve fracture resistance of UTG for foldable display

S. Kim*[1]; J. Nam[1]

1. Samsung Display Co. Ltd., Republic of Korea

The worldwide foldable device market has been remarkably grown and reached more than 20 million units in 2023 and will be demanded around 100 million units in 2028, as both embedded technologies and performances of foldable devices have been advanced consistently. Ultra-thin glass (UTG) has been typically employed as cover material of flexible devices due to its superior features of surface quality and durability as well as higher reliabilities in harsh environments compared to plastic filems. However, it is essentially required to improve fracture resistance of UTG due to the inherent shortcoming, fragilness. In this presentation, the new glass composition was successfully developed to improve the impact resistance of UTG for the cover window of foldable display devices for the world's first, as high as 2.7 times. The developed new composition has equivalent folding capabilities of commercial UTG products with chemical strengthening. We also suggested new figure of merits (FOM) that can explain impact resistances of both laboratory melted and directly formed glass samples. In addition, we developed a new surface treatment technology of UTG that can induce the expansion of the glass structure and form compressive residual stresses on the surface of cracks, which can eventually delay the crack propagation. We confirmed that both dynanic and static fracture characteristics were succesfully improved compared to results from convenional glass composition and finishing processes.

5:10 PM

(GOMD-S1-109-2024) Structural Analysis of Sodium Alumino-Silicate Glasses for Ultra-Thin Glass via Molecular Dynamics and Solid-State NMR

K. Park*[1]; J. Nam[2]; S. Kim[2]; W. Chung[1]

1. Kongju National University, Division of Advanced Materials Engineering, Republic of Korea
2. Samsung Display Co., Ltd, Republic of Korea

Sodium aluminosilicate (SAS) glass, excelling in chemical strengthening, is ideal for ultra-thin, lightweight applications, notably Ultra-Thin Glass (UTG) in foldable devices. UTG's rising demand for flexible electronics necessitates enhanced impact resistance for device longevity. To resist stresses like pen drops, UTG must dissipate impact energy effectively, especially when under 50 μm thick. Considering that impact energy can be mitigated through densification, coordination change, and shear flow before crack generation within the glass structure, in addition to chemical strengthening, a well-designed glass can significantly enhance impact resistance. After a compositional study, we recently manufactured a new sodium alumino-silicate-based UTG that exhibited substantially improved impact resistance compared to conventional commercial UTG. However, the structural origin of this enhanced impact resistance has not been thoroughly elucidated. In this study, we employed molecular dynamics (MD) simulations and solid-state NMR analysis to investigate the structural origin of the improved impact resistance, comparing it with the commercial SAS glass composition. we also examined a B_2O_3-included SAS glass, less resistant than commercial UTG, for contrast. To understand their impact resistance contributions, we analyzed various structural factors of UTG compositions - bond lengths, angles, coordination numbers, accessible volume, etc.

Session 9: Metallic Glasses

Room: Shoal Creek

Session Chairs: Ralf Busch; Paul Voyles, University of Wisconsin

3:40 PM

(GOMD-S1-110-2024) Are metallic glasses brittle or ductile? (Invited) ***WITHDRAWN***

J. Schroers*[1]

1. Yale, USA

Crystalline metals generally exhibit ductility which is enabled by dislocation sliding. We show here that metallic glasses, which carry ductility through shear banding as opposed to dislocation sliding, exhibit ductility only in certain stress fields and such ability is an intrinsic property. Such ability, only depending on chemistry and fictive temperature of the metallic glass, manifests in the ability to form stable shear bands that carry plasticity. We measured this quantity, for a range of metallic glasses to represent the material class of metallic glasses. If a metallic glass behaves ductile or brittle in a given application is determined by the comparison between and the applied stress field, ; if > the metallic glass will behaves brittle, if < the metallic glass will behaves ductile, and indicates how ductile. Measured, which are different for compression or tension, and the concept of comparing it with can explain the mechanical properties of metallic glasses and their apparent contradicting brittle and ductile characteristics. Proposed concept allows to determine the behavior of a metallic glass in an application and lays the foundation of using metallic glasses as structural materials.

4:05 PM

(GOMD-S1-111-2024) Size dependent vitrification in metallic glasses (Invited) ***MOVED to 1:50 PM***

I. Gallino*[1]; D. Cangialosi[2]

1. Technical University Berlin, Materials Science and Engineering, Germany
2. Donostia International Physics Center, Spain

By means of fast scanning calorimetry (FSC) we have observed up to 40 K reduction in the glass transition temperature of bulk metallic glasses in samples with sizes below 10 μm. We have investigated different compositions in a wide range of time scales in terms of vitrification kinetics via the cooling rate-dependence of the fictive temperature. We have observed a pronounced size dependent vitrification kinetics, which is more evident at low cooling rates. The important implication of this outcome is that mild reductions of the sample size in metallic glasses allow exploring thermodynamic states, in terms of fictive temperature, deep down in the energy landscape.

4:30 PM *WITHDRAWN*

(GOMD-S1-112-2024) Temperature dependence of pressure sensitive flow in bulk metallic glass composites (Invited)

P. Saini*[1]; Y. Zhao[4]; B. Li[3]; Z. Long[3]; U. Ramamurty[2]; L. Ramasubramanian[1]

1. Indian Institute of Technology, Delhi, Materials Science and Engineering, India
2. Nanyang Technological University, Singapore
3. Shi-changxu Innovation Center for Advanced Materials, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China
4. Institute of Materials Research and Engineering, Agency for Science, Technology and Research, Singapore

The constraint factor, C, defined as hardness, H, to the yield strength, σ_y, ratio, is an indirect measure of the pressure sensitivity in materials. Previous investigations determined that C is is greater than 3 for bulk metallic glasses (BMGs) and increases with increasing temperature, below their glass transition temperature, T_g. In this study, the variations in C for two BMG composites (BMGCs), which have an amorphous matrix and in situ precipitated crystalline β-Ti dendrites, which in one case transforms under stress to α″-Ti and deforms by slip in the other, as a function of temperature are examined and compared with that of a BMG. For this purpose, instrumented indentation tests and uniaxial compression tests were performed to measure the H and σ_y, respectively, on all alloys and their constituents at temperatures in the range of $0.48T_g$ and $0.75T_g$. σ_y and H of the BMGC with transforming dendrites (BMGC-T) increase and remain invariant with increasing temperature, respectively. Alternately, in BMG and the BMGC with non-transforming dendrites (BMGCNT), the same properties decrease with increasing temperature. BMGC-T has the highest C of ~4.93 whereas that of BMGCNT and BMG are ~3.72 and ~3.28, respectively, at $0.48T_g$. With increasing temperature, C of the BMG and BMGCNT increases with temperature, but that of the BMGC-T decreases. The values of C and their variations as a function of temperature will be explained in detail in this talk.

4:55 PM

(GOMD-S1-113-2024) Size-effects in tensile fracture of rejuvenated and annealed metallic glass *MOVED TO 2:20 PM*

G. Kumar*[1]

1. University of Texas, Dallas, USA

Metallic glass samples with diameters ranging from sub-100 nm to 100 μm were subjected to cryogenic rejuvenation and annealing above glass transition temperature before tensile loading at room temperature. Shear-localized failure with no ductility is observed in large samples whereas the smaller diameter specimens show ductile necking irrespective of the structural state of metallic glass. With decreasing sample diameter, the fracture surface changes from vein pattern to featureless in the shear-localized samples and the ductility increases in the necked samples. Despite similar size-dependent trends, the changes in deformation mode and fracture morphology occur at different diameters in as-cast, rejuvenated, and annealed samples. The critical diameters for transitions from shear localization to necking and from vein pattern to smooth fracture surface shift to larger values in cryogenically rejuvenated samples whereas annealing has the opposite effect. Structural rejuvenation suppresses shear localization and catastrophic tensile failure in nanoscale metallic glasses.

5:15 PM

(GOMD-S1-114-2024) Recent development in the application of bulk metallic glasses *WITHDRAWN*

Y. Li*[1]; K. Gao[1]

1. Insitute of Metal Research, Chinese Academy of Sciences, China

Over the past decades, considerable efforts have been made in the commercial application of bulk metallic glasses (BMGs). Despite great challenges faced by the industrial players, significant progress has been achieved, and millions of commercial products for various kinds of applications have been shipped around the world. Here in this presentation, we shall show the alloys suitable for the actual products in the application and discuss the merits of the processing technique of BMGs over the existing processing techniques and materials. Most importantly we demonstrate the typical examples of products over the past few years. Finally, future directions of the industrialization of BMGs are also discussed.

Session 4: Atomistic simulations and predictive modelling of Glasses

Room: Bel Air II
Session Chair: Hiroyuki Inoue, The University of Tokyo

3:50 PM

(GOMD-S1-115-2024) Deformation and Cracking Behavior of Glass under Sharp Contact Loading Studied in Classical Molecular Dynamics Simulation (Invited)

L. Huang*[1]; H. Liu[1]; Y. Shi[1]

1. Rensselaer Polytechnic Institute, Materials Science and Engineering, 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. Our studies show that the indenter sharpness controls the shear band formation, and the interaction between shear bands dictates the crack initiation. Shear bands and residual stress fields in a model metallic glass from our simulated nanoindentation tests are consistent with observations in soda-lime silicate (SLS) glass from the instrumented indentation in experiments, as both of them favor shear deformation under sharp contact loading. We further investigated the role of densification in the deformation behavior of glass under sharp contact loading. Our simulations indicate that glass with a higher densification ability under indentation has less stress build-up and less localized shear deformation during loading, as well as smaller residual stress build-up after unloading. However, our studies show that both instantaneous and permanent densification need to be tuned for designing damage-resistant glasses.

4:20 PM

(GOMD-S1-116-2024) Densification and plastic flow in alkaline-earth aluminoborosilicate glasses: insights from atomic scale simulations

H. Ikeda*[1]; G. A. Rosales-Sosa[1]; Y. Kato[1]; S. Nakane[1]; G. Molnár[3]; E. Barthel[2]; H. Yamazaki[1]

1. Nippon Electric Glass Co., Ltd., Fundamental Technology, Japan
2. ESPCI Paris, Soft Matter Sciences and Engineering, France
3. Contacts and Structures Mechanics Laboratory (LaMCoS), France

Alkaline-earth aluminoborosilicate glasses (ABS) are important in various technological applications such as display panels. For these applications, fracture resistance is a key parameter. It is considered that the susceptibility for fracture results from a balance between the capacity of glass to undergo densification and localized plastic deformation (shear bands). To obtain insights into the role of compositions on densification and localized plastic deformation, we build MD structural models of alkaline-earth aluminoborosilicate glasses with different SiO_2/B_2O_3 ratios and different alkaline-earth cations (Ca, Mg). Their physical and mechanical properties were investigated using the SHIK potential. The calculations were able to reproduce well our experimental trends of density and elasticity. Moreover, an investigation of densification by MD calculations revealed that boron oxide has an important influence on the onset pressure for densification while having less influence on the maximum densification ability. These results agree with our recent experimental results showing that the onset pressure has an impact on the intensity of residual stresses under indentation. Finally, it was also found that the number of local plastic events under pure shear increased with boron content providing insights of composition dependence on strain localization behavior. The effect of plastic deformation on the atomic structure of the glass will be discussed.

4:40 PM

(GOMD-S1-117-2024) Impact of Atomic Defects on Ceria Surfaces on Chemical Mechanical Polishing of Silica Glass Surfaces

A. Pedone*[1]

1. University of Modena and Reggio Emilia, Italy

The process of polishing and planarization of silica-based glasses is of fundamental importance in the glass industry because it allows the production of defect-free ultra-smooth glass surfaces essential for a wide range of applications, including display panels, flat glass for window panes, optical glasses, precision glass lenses, glass magnetic memory disks, silicon wafers, etc.[1] We will present how atomic defects, such as oxygen vacancies and Ce^{3+} ions, on cerium oxide (ceria) surfaces impact the Chemical Mechanical Polishing (CMP) for silica glass finishing. Using Density Functional Theory (DFT) and Reactive Molecular Dynamics simulations, the interaction of orthosilicic molecules and silica glass with dry and wet ceria surfaces is explored. Reactive MD simulations demonstrate that ceria surfaces with 30% Ce^{3+} ions on (111) planes exhibit higher polishing efficiency, attributed to increased Si-O-Ce bond formation. The simultaneous presence of oxygen vacancies and various acidic and basic sites on ceria surfaces enhances polishing efficiency, involving acid-base reactions with silica. Defective surfaces show superior efficiency by removing silicate chains, contrasting with non-defective surfaces removing isolated orthosilicate units. References [1] L. Wang, P. Zhou, Y. Yan, D. Guo, Investigation on nanoscale material removal process of BK7 and fused silica glass during chemical-mechanical polishing, International Journal of Applied Glass Science. 12 (2021) 198–207.

5:00 PM

(GOMD-S1-118-2024) Nano-Scale Indentation Studies on Aluminosilicate Glasses: Unraveling Structural Alterations and Mechanical Properties

A. Pallini*[1]; A. Pedone[1]

1. University of Modena and Reggio Emilia, Chemical and Geological Sciences (DSCG), Italy

Hardness is a crucial property governing the mechanical response of solid materials to applied stress. This study employs Molecular Dynamics simulations to investigate nano-scale indentation tests, providing valuable insights. Our focus is about on understanding structural alterations occurring during the interaction of a diamond cone-shaped indenter with oxide glass surfaces. To comprehend the influence of Al and the role of Na ions, we compare two glasses: one with albite composition (12.5%Na_2O, 12.5%Al_2O_3, 75%SiO_2) where sodium compensates AlO4- tetrahedra charges, and its sodium silicate glass (12.5%Na_2O, 87.5%SiO_2) where sodium acts as a network modifier. We delve into the intricate mechanics of nano-indentation, scrutinizing changes in the structure during and post-indentation, providing essential insights into the underlying mechanisms that correlate structural modifications with the resultant properties. Our study explores the impact of densification on bulk and surface structure, elastic moduli and hardness. By conducting a comprehensive examination, we contribute valuable insights into the behavior of aluminosilicate glasses at the nano-scale, enhancing our understanding of the intricate relationship between composition, structure, and mechanical properties in these materials. This research significantly advances our knowledge of the nano-scale mechanical behavior of aluminosilicate glasses, paving the way for tailored material design and engineering applications.

S3 Optical and Electronic Materials and Devices Fundamentals and Applications

Session 2: Charge and Energy Transport in Disordered Materials

Room: Peeble Beach
Session Chairs: Gabriel Agnello, Corning Incorporated;
Caio Bragatto, Coe College

3:40 PM

(GOMD-S3-013-2024) Behavior of Protons in Water and at the Water/Silica Interface (Invited)

S. H. Garofalini*[1]

1. Rutgers Univ, USA

Because of their important role in fundamental processes in materials chemistry, the behavior of protons in water and at the water/silica interface has been studied in molecular dynamics simulations using a robust reactive interatomic potential. With respect to water, most studies have focused on the transfer processes of the excess proton from the H_3O^+ ion, allowing for eventual proton conduction. However, there has been far less attention given to the initial auto-dissociation process of a water molecule with a neighbor molecule to form the H_3O^+ ion and its associated OH^- ion. The current simulations evaluate the auto-dissociation of water molecules in bulk water and at the water/silica interface. Significant short-lived auto-dissociation events seen in the simulations of bulk water are consistent with advanced ab-initio calculations that include nuclear quantum effects. The role of the local electric fields from neighboring water molecules on proton transfer is evaluated in bulk water and shown to be consistent with ab-initio calculations. Proton transfer events are significantly enhanced at the water silica interface, consistent with the increased acidity of water and acids at this interface.

4:10 PM

(GOMD-S3-014-2024) An Electrostatic Charging Mechanism of Contacted Glass Surfaces (Invited)

D. Thelen*[1]; J. M. Mis[2]; A. Antony[2]; R. G. Manley[1]

1. Corning Research and Development Corporation, USA
2. Corning Incorporated, USA

Electrostatic charging of contacted glass surfaces can lead to manufacturing issues that include particle contamination on glass product surfaces, and electrostatic discharge in electronic devices built on glass substrates. Manufacturing these glass products and glass-substrate-built devices commonly require glass contact to temporarily hold the glass in place during transport and/or stationary processing steps. The presence of humidity leads to adsorbed water on the glass surface, limiting the direct contact between contacting material and glass surfaces, and enabling a surface conduction mechanism on the glass. In this talk, we will describe a contact charging mechanism that predicts charging levels that are consistent with the magnitude and polarity of the measured glass charging. The driver for this mechanism is the Volta Potential between the contacting material and glass surfaces. Glass surface conduction mechanisms subsequently lead to charging of non-contacted glass surfaces for the duration of contact between contacting material and glass surfaces. After separation, the total surface charge on the non-contacted surfaces remains conserved, and only the electrostatic field and potential (i.e., voltage) are increased. Numerous corresponding measurements of this contact-separation procedure were performed by lift-tester experimental hardware, including electrical characterization using charge electrometers and electrostatic field meters.

4:40 PM

(GOMD-S3-015-2024) Ion-Dynamics of Sodium Alumino Phospho Silicate glasses: Composition-Structure-Property correlation

S. R. Keshri*[1]; I. Mandal[2]; A. Gaddam[5]; A. R. Allu[4]; N. Krishnan[3]; N. Gosvami[1]

1. Indian Institute of Technology Delhi, Materials Science & Engineering, India
2. Indian Institute of Technology Delhi, School of Interdisciplinary Research, India
3. Indian Institute of Technology Delhi, Civil Engineering, India
4. CSIR-Central Glass & Ceramic Research Institute, Energy Materials & Devices, India
5. CICECO – Aveiro Institute of Materials, University of Aveiro, Chemistry, Portugal

Absence of a unified ion-conduction model and composition-structure-conductivity correlation in glass materials hinders the development of novel glass electrolytes possessing essential RT ionic conductivity (~10^{-3} S/cm) for solid-state batteries. In that respect, SiO_2 was substituted for P_2O_5 in the sodium aluminophosphate glass up to 20 mol% and its properties were evaluated using XRD, DSC, Raman Spectroscopy, and Impedance Spectroscopy. MD simulations were performed to study the structure of the glasses by evaluating the coordination number of ions, Q^n and TOT bond distributions. The substitution of SiO_2 leads to Si competing with P to form Si-O-Al over P-O-Al bonds, thereby increasing the concentration of Na^+ acting as charge compensators. The glass with 15 mol% SiO_2 exhibits highest DC ionic conductivity of ~9×10^{-6} S/cm at 473K. The diffusion coefficient derived from MD simulations further confirms that 15 mol% SiO_2 glass has the highest DC ionic conductivity. The ion-dynamics was further assessed by evaluating the characteristic microscopic lengths for ion-movement with AC conductivity analysis, while also incorporating the scaling procedures of conductivity spectra. It confirms 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.

Session 4: Glass Devices I

Room: St. Andrews
Session Chair: Juejun Hu, Massachusetts Institute of Technology

3:40 PM

(GOMD-S3-016-2024) Advanced Patterning of Second-Order Optical Nonlinearity in Niobate Amorphous Thin Films through Imprinting Thermo-Electrical Poling Process (Invited)

L. D. Karam[1]; F. Adamietz[1]; S. Boonsit[2]; G. S. Murugan[2]; N. Courjal[3]; M. Dussauze*[1]

1. CNRS / Université de Bordeaux, Institut des Sciences Moléculaire, France
2. Optoelectronic Research Centre, United Kingdom
3. FEMTO-ST Institute, France

The fabrication of new amorphous thin films in the Nb_2O_5-Na_2O system, prepared by radio frequency sputtering, and the induced second-order optical nonlinearity (SONL) by thermo-electrical poling are reported. XRD confirmed the amorphous character of the films, and Raman and EDS spectroscopies have confirmed the successful introduction of sodium in the niobate matrix. The resulting films were of good optical quality, with optical loss less than 1 dB/cm, high refractive index (2.2 at λ=1 µm) and a wide transparency window spanning from the visible to mid-infrared (exceeding λ=5 µm). A thermo-electrical imprinting process has been employed to induce SONL response in the niobate thin films. By characterizing the geometry and the magnitude of the SONL response, a key aspect of thin film's poling mechanisms compared with bulk glasses was established. This lies in the appearance of a charge accumulation at the film/substrate interface, described by the Maxwell–Wagner effect. A way to minimize this effect was then proven by promoting an induced built-in static field in the plane of the film using a microstructured electrode. A SONL susceptibility as high as 29 pm/V was measured, and its geometry and location were controlled at the micrometer scale. This work paves the way for the future design of integrated nonlinear photonic circuits based on amorphous inorganic materials, enabled by the spatially selective and high SONL susceptibility of these promising and novel optical materials.

4:10 PM

(GOMD-S3-017-2024) Deep etching technique and machine learning based design for high performance glass-based optical devices (Invited)

A. Ueno*[1]; Y. Ono[1]; K. Sano[1]; A. Kiyama[1]; A. Suguro[1]; Y. Hayashi[1]

1. AGC Inc., Innovative Technology Laboratories, Japan

Glasses are expected to see increasing applications in integrated photonics with superior optical properties and thermal durability. On the other hand, designing and fabricating high-performance glass optical devices requires not only knowledge of glass materials but also complex optical design and advanced fabrication technologies. To address this issue, we have successfully developed a rapid and high aspect ratio etching technique for glass using catalysts. Additionally, we have established a device design technology that balances manufacturability and optical performance through machine learning. This presentation will introduce demonstrations of each technology with prototyping metasurfaces and waveguide devices.

4:40 PM

(GOMD-S3-018-2024) Fast ionic exchange in chalcogenide glasses for infrared optics with gradient refractive index

X. Zhang*[1]; C. Fourmentin[1]; G. Druart[2]; F. De La Barrière[2]; L. Calvez[1]

1. University of Rennes/CNRS, Institute of Chemistry, France
2. ONERA, DOTA, France

This presentation will be on the development of infrared transmitting chalcogenide glass optics with gradient refractive index, obtained by using an innovative ionic exchange method. One of the techniques used often by optical designer for simplifying optronic systems is to integrate more complex components. One of the options is, for example, to use gradient index (GRIN) optic for imaging applications. Concerning infrared optics for thermal imaging, chalcogenide glasses appear as the only choice for obtaining reproducible gradient index with useful size. Different research groups have proposed different methods including inter-diffusion, controlled crystallization. In this work, we will use ionic exchange for creating highly reproducible refractive index gradient in chalcogenide glasses. Specific glass compositions, containing mobile ions have been optmized and an innovative fast-ionic exchange process has been developed. Large diffusion distance can be obtained quickly and radial GRINs with sample diameters around 13 mm and a refractive index difference greater than 0.1 have been demonstrated. In addition, a negative constringency has been measured, which is highly desired for simplifying the optical system. The obtained GRIN profile is a polynomial profile of order two.

5:00 PM

(GOMD-S3-019-2024) Solution Processing of $Ge_2Sb_2Se_4Te_1$ Phase Change Material for Optical Applications

D. Wiedeman*[1]; R. Sharma[1]; E. Bissel[1]; P. Banerjee[1]; B. Mills[2]; J. Hu[2]; M. Sykes[3]; J. Stackawitz[3]; J. Klucinec[3]; C. Schwarz[3]; K. Richardson[1]

1. University of Central Florida, USA
2. Massachusetts Institute of Technology, USA
3. Ursinus College, USA

Chalcogenide based phase change materials are important for creating novel optical and photonic devices, improving on current devices for future applications. Solution processing, via dip coating, spin coating, or drop-casting, is a low-cost, high-throughput alternative method of depositing thin films, which allows for greater composition diversity. In this work, we performed a detailed systematic study of the solution derived drop-casted film of Ge2Sb2Se4Te1 alloy in an ethylenediamine and ethanedithiol mixture. The composition, morphology and structural properties of the films were analyzed by employing scanning electron microscopy, energy dispersive X-ray spectroscopy, Raman spectroscopy, and X-ray diffraction. Our findings provide insight into a potential route for scalable $Ge_2Sb_2Se_4Te_1$ films.

5:20 PM

(GOMD-S3-020-2024) Solution Deposition of Optical Phase Change Materials

B. Mills*[1]; R. Sharma[2]; D. Wiedeman[4]; C. Schwarz[3]; E. Bissell[5]; C. Constantin Popescu[1]; D. Callahan[6]; P. Banerjee[5]; K. Richardson[2]; J. Hu[1]

1. Massachusetts Institute of Technology, Materials Science and Engineering, USA
2. University of Central Florida, CREOL, College of Optics and Photonics, USA
3. Ursinus College, Physics and Astronomy, USA
4. University of Central Florida, Chemistry, USA
5. University of Central Florida, Materials Science and Engineering, USA
6. Charles Stark Draper Laboratory, Inc, USA

Characterized by repeatable, non-volatile control of material properties, chalcogenide phase change materials (PCMs) have been adopted as the functional material in a variety of electronic and photonic devices. While there is a large variety of elemental compositions that may exhibit desired properties for optical phase change materials, slow iteration time associated with traditional thin film deposition techniques, such as evaporation and sputtering, inhibits efficient materials exploration. Solution processing has been demonstrated as a viable option for creating high quality chalcogenide thin films via spin-coating or drop-casting, with the versatility and speed necessary for high throughput testing of material compositions. We present a platform for synthesis, integration and on-chip cycling characterization of solution-deposited optical phase change materials.

5:40 PM

(GOMD-S3-031-2024) Advances in Optical Fibers (Invited)

W. Kim*[1]; C. Baker[1]; S. Bayya[1]; T. Zhou[2]; D. Rhonehouse[1]; F. Kung[2]; G. Chin[2]; D. Boyd[1]; R. Nicol[3]; V. Nguyen[1]; K. Ewing[1]; D. Gibson[1]; J. Frantz[1]; R. Gattass[1]; J. Sanghera[1]

We report our recent progress in Erbium doped fibers (EDF) devel- oped for space applications such as in satellite communications. These fibers are typically sensitive to the high radiation and the fiber performance deteriorates due to cosmic rays. Various efforts have been made to improve the radiation stability of these fibers. Here we present our recent study on the effect of various dopants with varying concentrations incorporated into the fiber core to further reduce the radiation induced gain degradation and improve the performance of the fibers. We also report our recent progress in the development of IR transmitting organic/inorganic hybrid materials composed of chalcogenide elements, such as sulfur and selenium, along with organic and/or inorganic crosslinking moieties. This class of materials is referred to as organically-modified chalcogenides (ORMOCHALC) and is being developed for IR optics and fibers to provide size, weight, and performance advantages at low cost (SWaP-C). Multiple chalcogenide cladding layers with varying refractive indices can coat chalcogenide core fiber materials to form optical waveguides. Here, we report a successful demonstration of waveguiding & transmission of infrared light in a ORMOCHALC fiber.

S6 Mark Davis Honorary Symposium

Session 6: Mark Davis Honorary Symposium

Room: Turnberry
Session Chair: Bill James, Schott Germany

3:50 PM

(GOMD-S6-012-2024) Proccesing of rare-earth-doped nanostructured glass-ceramics for enhanced photoluminiscence (Invited)

M. Sedano[1]; A. Durán[1]; J. Fernández[3]; R. Balda[2]; M. Pascual*[1]

1. Institute of Ceramics and Glass, CSIC, Glass, Spain
2. University of Basque Country, Spain
3. Donostia International Physics Center DIPC, Spain

The field of photonics demands the design of new rare-earth (RE)-based optical materials for their use in efficient optical devices. Oxyfluoride glass-ceramics (GCs) combine the transparency and both mechanical and chemical resistance of aluminosilicate glasses with the low phonon energy and facile incorporation of RE ions in the fluoride crystals. The incorporation of RE ions in the crystalline phases enhances the optical emission intensity, a major property of these materials. Moreover, the additional presence of metallic nanoparticles can further enhance the luminescent response. These materials are suitable for the preparation of preforms as precursors for the drawing of optical fibers and as substrates for waveguides written using laser radiation and some examples of the materials preparation and its possible applications will be provided in this presentation. By the other hand, transparent GC materials have also been obtained by spark plasma sintering (SPS). This approach combines thermal action with simultaneous compression of the material to reach full densification and high homogeneity in a short time. The structural, mechanical, and optical properties have been characterized and compared with GCs of the same composition prepared by conventional heat treatment. The results confirm the suitability of the SPS processing for the preparation of highly dense and transparent oxyfluoride glass-ceramics containing nanocrystals.

4:20 PM

(GOMD-S6-013-2024) Dispersion of elasto-optic tensor elements in glass using acousto-optic diffraction

A. Jenkins[2]; C. Sutherland[2]; U. Werner-Zwanziger[1]; J. Zwanziger*[1]

1. Dalhousie University, Chemistry, Canada
2. Dalhousie University, Physics and Atmospheric Sciences, Canada

I had the pleasure of knowing Mark Davis as a scientific colleague, and over the years had many informative and inspiring discussions with him on optical properties of glass, and especially the interplay between stress, strain, and optical response. He was a wonderful scientist and individual, and it's an honor to participate in a symposium in his memory. In this talk I would like to outline our recent progress in measuring the dispersion of the full elasto-optic tensor in glass. We adapted the method due to Dixon and Cohen, to measurements at various wavelengths. In this method, an acoustic pulse is transmitted through both the sample and a reference, and the intensity of Bragg diffraction from the induced density grating is related to the elasto-optic tensor element for the chosen polarization, determined as a ratio to the response of the reference sample (fused quartz in the present case). We will show how the method can be used at different wavelengths in order to determine the dispersion of the response, which we then fit to a model due to Wemple and DiDomenico in order to interpret it microscopically.

4:50 PM

(GOMD-S6-014-2024) Laser Glass Development at SCHOTT (Invited)

L. Bradley*[1]; E. Feverston[1]; J. S. Hayden[1]; J. Ivy[1]; M. Kocher[1]; B. Morgan[1]; A. Rawlings[1]; J. Whetstone[1]

1. SCHOTT North America, Inc., USA

Laser glass is a cornerstone of SCHOTT's portfolio serving the energy, defense, and materials manufacturing industries. The North American Research & Development team is co-located with the Advanced Optics business unit enabling rapid transfer from development to production. SCHOTT's current developments supporting technology innovations leverage key material development and metrology contributions made by Mark Davis. This talk will highlight SCHOTT's capabilities and innovation initiatives advancing the development of next-generation laser glasses.

Thursday, May 23, 2024

S1 Fundamentals of the Glassy State

Session 4: Atomistic simulations and predictive modelling of Glasses

Room: Bel Air II
Session Chair: Hiroyuki Inoue, The University of Tokyo

9:20 AM

(GOMD-S1-119-2024) Understanding diffraction peaks of P_2O_5 glass

Y. Onodera[1]; H. Masai[2]; S. Kohara*[1]

1. National Institute for Materials Science (NIMS), Japan
2. National Institute of Advanced Industrial Science and Technology (AIST), Japan

P_2O_5 is a typical network forming oxide with Q^3 tetrahedral motifs, in which three bridging oxygens (BOs) and one non-bridging oxygen (NBO) are bonded to a phosphorus atom. To understand diffraction peaks of P_2O_5 glass, a three-dimensional structure model that is consistent with neutron and X-ray diffraction data is constructed by a combined reverse Monte Carlo (RMC) and classical molecular dynamics (MD) simulations. Partial structure factors obtained from the RMC–MD model indicate that a doublet first sharp diffraction peak (FSDP) of P_2O_5 glass is originated from the Q^3 network, which is composed of two different length scales formed by P–O bonds, i.e., P–BO and P=NBO bonds. We discuss origins of the diffraction peaks deduced from the three-dimensional glass structure model via topological analyses.

9:40 AM

(GOMD-S1-122-2024) Structure-property relationships of CaO-MgO-Al_2O_3-SiO_2 fiber glasses from molecular dynamics simulations and QSPR analysis

W. Xie*[1]; H. Li[2]; D. R. Neuville[3]; J. Du[1]

1. University of North Texas, Materials Science and Engineering, USA
2. Nippon Electric Glass, USA
3. Université de Paris, France

Glass fiber-reinforced plastic (GFRP) composites have been widely used in automobiles, wind turbine blades, and chemical storage for lightweight and high-strength. In this work, CaO-MgO-Al_2O_3-SiO_2 (MCAS) glass fibers with low boron and lithium are obtained by the molecular dynamics simulation with recently developed effective partial charge composition-dependent boron potentials. The addition of Li_2O was found to improve the elastic moduli while surprisingly decreasing the liquid temperature of glass fibers. The weakened network connectivity has positively lowered liquid temperature for the transformation to more boron Q^2 and silicon/aluminon Q^3. Higher oxygen packing density and coordination numbers of [AlO_5] and [BO_4], larger-membered oxide rings, and intensified polyhedral connections can be used to explain the improved mechanical properties. More computational characterizations are rendered to obtain atomic mobility, vibration density of states, neutron/X-ray diffractions, and MD-based quantitative structure-property relationship (QSPR).

Session 6: Mechanical Properties of Glasses IV: Outstanding mechanical properties

Room: Bel Air I
Session Chair: Satoshi Yoshida, AGC Inc.

9:20 AM

(GOMD-S1-123-2024) Toughening of glasses via metal nanoparticle incorporation at a small volume fraction (Invited)

K. Shinozaki*[1]

1. Osaka University, Graduate School of Engineering, Japan

Imparting ductility to glasses effectively counters brittleness caused by stress concentration. Recently, we focused on the impact of ductile metal nanoparticles such as Ag and Ni in glass. We found even trace amounts of metal additives can significantly improve fracture toughness. Ni nanoparticles of different sizes were dispersed in SiO_2 glass to investigate the effect of the particle size. Ni nanoparticles (0.5 vol. %) of two sizes (average particle sizes: 119 and 30 nm) were precipitated in the SiO_2 glass by sintering on Ni nanoparticle-dispersed SiO_2 glass powder. The fracture toughness obtained by microcantilever beam tests was significantly enhanced from 0.71 $MPam^{1/2}$ for non-doped silica glass to 1.02 and 2.03 $MPa\ m^{1/2}$, respectively, for the glass samples incorporated with small (30 nm) and larger Ni nanoparticles (119 nm). This indicates the significant enhancement of fracture surface energy with the dispersion of the metal nanoparticles in the glass matrix, despite their small volume fraction (0.5 vol. %). Moreover, the fracture surface exhibited a cup–cone structure, indicating ductile fracture. In conclusion, we propose the cost effective method to apply ductility on glass by means of metal nanoparticles dispersion.

9:50 AM

(GOMD-S1-124-2024) Indenting glasses with indenters of varying stiffness and sharpness

J. Christensen*[1]; N. Krishnan[2]; M. Bauchy[3]; M. M. Smedskjaer[1]

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. Indian Institute of Technology Delhi, Department of Civil Engineering, India
3. University of California, Department of Civil and Environmental Engineering, USA

Instrumented indentation is a versatile technique that is commonly used for the evaluation of mechanical properties of glasses, typically following some standardized practices for the experimental procedure and setup. In this study, we systematically investigate the effects of both indenter sharpness and stiffness on the indentation response (deformation mechanism, cracking behavior, hardness, etc.) of three glasses, specifically, a sodium silicate, a sodium borate, and a sodium borosilicate. Compared with the common Vickers indenter, we find that increased indenter sharpness reduces both the magnitude of the indentation size effect and the crack initiation resistance, the latter being correlated to less densification of the glass under the indenter. For indenters of the Vickers geometry, we observe no effect of the indenter material when the indenter is much stiffer than the glass sample. However, using an indenter material of similar stiffness to that of the sample entails deformation of the indenter, reducing the effective sharpness of the indenter and changing the indentation response accordingly. These findings can guide the design of laboratory indentation experiments, potentially bringing them closer to mimicking real-life damage events.

10:10 AM

(GOMD-S1-125-2024) Raman spectroscopy investigation of plastically-deformed alkaline-earth aluminoborosilicate glasses

G. A. Rosales-Sosa*[1]; Y. Kato[1]; S. Nakane[1]; M. Bourguignon[2]; E. Barthel[2]; H. Yamazaki[1]

1. Nippon Electric Glass, Fundamental Technology Division, Japan
2. ESPCI-Paris, SIMM, France

Strain localization (shear-banding) has been proposed in the past to influence strongly the resistance to crack initiation in oxide glasses (initiation sites) in addition to the effects of non-conservative volumetric strain. However, due to the difficulty of direct evaluation of the indentation plastic zone, it has been difficult to obtain progress in the field of strain localization. Recently, it has been shown that the resistance to crack-initiation in alkaline earth aluminoborosilicate glasses is correlated with the morphology of strain localization as observed directly from the plastic zone. Moreover, it seems that the relative ratio of glass formers $[SiO_2]/[B_2O_3]$ plays a key role in both strain localization and crack initiation. In this study, we investigate the structural changes of alkaline-earth (Ca, Mg) aluminoborosilicate glasses under hydrostatic pressure (Multi Anvil Cell - MAC) and under indentation. The results suggest that structural changes under both types of mechanical tests lead to similar structural changes as seen from the Raman spectra. Using the results from MAC experiments, calibration curves were proposed to evaluate the relative density changes as a function of gravity center shifts in Raman spectra for a wide range of compositions. Finally, Raman maps were built on the cross-section of indents providing a clear view of the relative density changes, strain localization, and structural changes in these plastically deformed glasses.

10:30 AM

(GOMD-S1-126-2024) Composition dependence on shear localization under indentation in alkaline earth aluminoborosilicate glasses

M. Bourguignon*[1]; G. A. Rosales-Sosa[2]; Y. Kato[2]; S. Nakane[2]; H. Yamazaki[2]; E. Barthel[1]

1. Soft Matter Sciences and Engineering, ESPCI Paris, PSL University, CNRS, Sorbonne University, France
2. Nippon Electric Glass Co., Ltd., Fundamental Technology Division, Japan

Silicate glasses exhibit a unique blend of properties, including mechanical rigidity and transparency, however, their application is frequently limited by their low resistance to fracture. It has been proposed the resistance of oxide glasses to crack initiation under mechanical indentation could be explained by the ability of the material to undergo densification and localized plasticity. To gain insights into the plasticity of oxide glass, we employ a technique involving the creation of cross-sections passing through indentation imprints that allows direct examination of the deformation zone. Several aluminoborosilicate glasses with different B_2O_3/SiO_2 ratios and two types of alkaline-earth cations were prepared. Their physical and mechanical properties were measured, and their indentation cross-sections, with three different indenters, were examined. It was found that the relative amount of boron and the type of alkaline-earth cation have a strong impact on the presence of shear bands but also on the surface roughness within the plastic zone. Multiple shear bands and high roughness seem to correlate well with low resistance to crack initiation under indentation. Our results point to shear localization as a major determinant of crack initiation.

10:50 AM

(GOMD-S1-127-2024) Mechanical properties and local structure of rare-earth-rich borate glasses

S. Sasaki*[1]; A. Masuno[2]; H. Inoue[3]; Y. Yanaba[3]

1. Hirosaki University, Science and Technology, Japan
2. Kyoto University, Graduate School of Engineering, Japan
3. University of Tokyo, Institute of Industrial Science, Japan

The R_2O_3–B_2O_3 glasses (R = rare earth element and Y) were synthesized using an aerodynamic levitation technique. The dependence of mechanical properties on the amount and the kind of R_2O_3 was investigated. The density increased with increasing the atomic weight of R. The packing density decreased with an increase of ionic radius of R^{3+}. The Vickers hardness H_V and Young's modulus E increased with decreasing of ionic radius of R^{3+} and they were greater than 10 GPa and 130 GPa, respectively. The experimental values of Young's modulus were approximately twice the values that were calculated using the Makishima-Mackenzie equation. The discrepancy between the experimental and calculated values was assumed to be caused by the use of inappropriate dissociation energies of B-O bonds. All B atoms in R_2O_3-rich R_2O_3–B_2O_3 glasses form isolated BO_3 without any B-O-B networks, which is significantly different from the structure of conventional borate glasses. Optimizing the dissociation energies to reflect the characteristic local structure around B atoms successfully resolved the discrepancy.

Session 7: Glass Under Extreme Conditions

Room: Turnberry
Session Chairs: Madoka Ono, Hokkaido University;
Jingshi Wu, Corning Incorporated

9:20 AM

(GOMD-S1-128-2024) Glasses under Multi-Megabar Pressures (Invited)

S. Lee*[1]

1. Seoul National University, Republic of Korea

Recent advances in element-specific spectroscopic probes, including solid-state nuclear magnetic resonance (NMR) and inelastic x-ray Raman scattering (IXRS) have provided a rare opportunity to precisely measure the structural changes in glasses under extreme pressure conditions. Here, we provide an overview of the latest experimental breakthroughs achieved through NMR and IXRS into structures of glasses under several hundred GPa (i.e., multi-megabars). Correlation NMR techniques involving quadrupolar nuclides identify pressure-induced changes in short-to-intermediate range structures of oxide glasses at high pressure. The first high-resolution NMR spectra of oxide glass compressed using diamond anvil cells extends the pressure record of such studies from 24 to 65 GPa. We also quantify how structural changes in glasses affect the nature of nuclear spin interactions at high pressure beyond megabars, accounting for an increase in configurational entropy during densification. Finally, IXRS allows us to quantify the detailed electronic bonding characteristics of low-Z amorphous oxides beyond several megabars, uncovering the electronic origins behind the incompressibility of amorphous oxides .

9:50 AM

(GOMD-S1-129-2024) In Situ High-Pressure Neutron Diffraction Study of Calcium Aluminosilicate Glass (Invited)

L. V. Gammond*[1]; A. Zeidler[2]; R. Youngman[1]; H. Mohammadi[2]; H. E. Fischer[3]; P. S. Salmon[2]

1. Corning Incorporated, USA
2. University of Bath, Physics, United Kingdom
3. Institut Laue Langevin, France

Knowledge of the pressure-induced structural transformations in oxide glasses can be used to design new materials and inform models of natural magmatic fluids, but obtaining information on the structure of these disordered materials during compression remains a challenge. In this study, in situ high-pressure neutron diffraction was used to measure the structure of $(CaO)_{19}$ $(Al_2O_3)_{20}$ $(SiO_2)_{61}$ glass at room temperature and pressures up to 17.5(5) GPa. ^{27}Al magic angle spinning nuclear magnetic resonance spectroscopy was used to characterize the Al speciation in the as-prepared glass and samples recovered to ambient conditions from high pressure. The structural changes during compression include an increase in the average Al-O coordination number from 4.02(5) at ambient conditions to 5.9(1) at 17.5(5) GPa, which is accompanied by an increase in the average Al-O distance from 1.76(1) to 1.89(1) Å over the same pressure range. Glasses recovered to ambient conditions from 8.2(5) and 17.5(5) GPa have average Al-O coordination numbers of 4.34(5) and 4.42(5), respectively. These results show that the structural reorganization of $(CaO)_{19}$ $(Al_2O_3)_{20}$ $(SiO_2)_{61}$ glass during compression to 17.5(5) GPa results in a collapse of the network marked by the conversion of Al-centered units from tetrahedral to octahedral coordination. The changes lead to permanent densification and the retention of five- and six-coordinated Al in the glass recovered to ambient conditions from high pressure.

10:20 AM

(GOMD-S1-130-2024) Structure of densified SiO_2 glass synthesized under extreme condition

S. Sato*[1]; M. Miyakawa[2]; T. Taniguchi[2]; Y. Onodera[2]; K. Ohara[3]; k. Ikeda[4]; N. Kitamura[1]; S. Kohara[2]

1. Tokyo University of Science, Japan
2. National Institute for Materials Science (NIMS), Japan
3. Shimane University, Japan
4. Neutron Industrial Application Promotion Center, Japan

Glassy SiO_2 is applied to various optical devices, such as optical fibers. In particular, the physical properties of high refractive index and low dispersion are necessary to achieve its high performance. These properties can be improved by increasing the density and structural ordering. Thus, the synthesis of densified SiO_2 glass has been recognized as an important issue in glass science and technology. We recently found the evolution of the first sharp diffraction peak (FSDP), which is a distinct feature of the intermediate range order, in the X-ray diffraction data of SiO_2 glass recovered after hot compression at a pressure of 7.7 GPa and temperatures up to 1200 °C. However, the samples compacted at the pressure of 8 GPa or more were crystallized by heterogeneous nucleation, which may occur at impurities of the surface of pristine SiO_2 glass. In this study, we succeeded in recovering densified SiO_2 glasses after hot compression at a pressure of 9.4 GPa by using a surface treated SiO_2 glass as a starting material. We report the structure of the densified SiO_2 glasses revealed by high-energy X-ray diffraction and neutron diffraction.

10:40 AM

(GOMD-S1-131-2024) Comprehensive Insights into Hot-Compressed Silica Glass: Exploring its Characteristic Properties

M. Ono*[1]; H. Tokunaga[2]; S. Hiiro[1]; K. Kizaki[1]; M. Watanabe[2]; K. Hayashi[2]

1. Tohoku University, Engineering, Japan
2. AGC Inc., Japan

Hot-compressed silica glass is garnering significant attention due to its high transparency and elevated refractive index resulting from its homogeneously densified structure. In a previous study, we unveiled that such densification induces lower thermal conductivity, a result not immediately intuitive. Our research delves into the intricate details of the amorphous structure modifications induced by the hot-compression process at the melting temperature. This investigation may illuminate the mechanisms behind the suppression of thermal conductivity and expansion, as well as their relationships with the boson peak. The implications of our findings provide a comprehensive understanding of hot-compressed silica glass through a synergy of experimental analyses encompassing thermal conductivity, expansion, and optical properties. Theoretical modeling delineates the attributes of the intermediate ordering of the silica glass structure concerning macroscopic properties.

11:00 AM

(GOMD-S1-132-2024) Controlling the atomic structure and thermal conductivity of disordered SiO_x thin films

K. A. Kirchner*[1]; M. Ono[2]; J. C. Mauro[1]

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

Understanding and controlling the mechanisms for structure-property-performance relationships in disordered systems is a constant challenge. For bulk silica glass, the importance of topological fluctuations has been realized, and through pressure-quenching these topological fluctuations can be manipulated to induce advantageous property responses. Instead of pressurizing, this work explores how topological fluctuations can be manipulated by changing film thickness and the substrate crystal surface of thin films. One such property of interest is thermal conductivity, where we experimentally and computationally show that thermal conductivity behavior is dependent on the substrate onto which the SiO_x film was deposited. Discussions will center around modeling results that examine how structural features change as SiO_x film thickness decreases from 3-dimensions to near 2-dimensions.

11:20 AM

(GOMD-S1-133-2024) Temperature and thermal stress analysis of ultrashort-pulsed laser processed glass

J. Wu*[1]

1. Corning Incorporated, Science & Technology Devision, USA

When glass absorbs high energy from ultrashort-pulsed lasers, a very rapid melting-cooling event occurs. Images taken by a Scanning Electron Microscope (SEM) reveal a surface feature which elucidates the glass is heated to above 2000 °C. A series of voids along the laser path is also observed and analyzed by SEM and High-angle Annular Dark-filed Scanning Transmission Electron Microscopy (HAADF-STEM). Molecular Dynamic simulation predicting observable voids in fused silica glass requires the temperature to be above 10,000 Kelvin. This suggests that the thermal effect from nonlinear absorption along cannot explain the void generation. Thermal stress analysis based on three different types of glasses revealed that stress generated by laser heating is highly correlated to thermal expansion coefficient. Such thermal stress may be a key factor for laser cutting.

11:40 AM

(GOMD-S1-134-2024) Mechanisms behind the Structural Evolution of Ge-Sb-S Chalcogenide Glasses upon Gamma Irradiation

M. Kang*[1]; B. Sohn[2]; Q. Du[3]; D. Ma[3]; R. Pujari[3]; L. Sisken[4]; C. Blanco[4]; C. Goncalves[4]; C. Arias[4]; A. Zachariou[4]; A. Yadav[4]; S. Novak[5]; C. Schwarz[6]; I. Luzinov[5]; J. Hu[3]; A. M. Agarwal[3]; D. T. Tan[2]; K. Richardson[4]

1. Alfred University, New York State College of Ceramics, USA
2. Singapore University of Technology and Design, Engineering Product Development, Singapore
3. Massachusetts Institute of Technology, Department of Materials Science and Engineering, USA
4. University of Central Florida, CREOL, College of Optics and Photonics, USA
5. Clemson University, Department of Materials Science and Engineering, USA
6. Ursinus College, Department of Physics and Astronomy, USA

We present a combined theoretical-experimental approach to the quantitative processing-structure-property relationship correlating the time-dependent structural and optical responses of chalcogenide Ge-Sb-S bulk glasses to their metastable topological coordination defects. These defects are created upon gamma-ray exposure and subsequently undergo relaxation at room temperature. Multi-faceted aspects of such a key infrared chalcogenide glass, including optical, electronic, morphological, chemical, and microstructural properties, were monitored and cross-correlated as a function of time following gamma irradiation in order to identify origins behind the material system's behavior with such exposure as compared to base unirradiated material. Our findings may shed light on the lingering question on the microscopic origin behind the self-healing process in chalcogenide glasses. The behavior in metastable bulk chalcogenide glasses serves as a key cornerstone that will enable the material system to be deployed as robust, reversible radiation sensors in extreme environments such as space and ground-based radioactive facilities where gamma ray is characteristically abundant.

S3 Optical and Electronic Materials and Devices Fundamentals and Applications

Session 1: Laser Interactions with Glasses

Room: Shoal Creek
Session Chair: Keith Veenhuizen, Lebanon Valley College

9:20 AM

(GOMD-S3-021-2024) Lattice engineering of laser-fabricated crystals in glass: parent glass to macroperiodic structures (Invited)

E. J. Musterman*[1]; A. M. Kiss[2]; V. Dierolf[3]; H. Jain[1]

1. Lehigh University, Materials Science and Engineering, USA
2. Brookhaven National Laboratory, National Synchrotron Light Source II, USA
3. Lehigh University, Physics, USA

Localized laser heating offers the ability to micro-fabricate single crystal architectures of unlimited length in glass. The lattice of these crystals can be further engineered by intrinsic stresses leading to novel lattice deformations caused by the steep temperature gradients around the laser focus. This ability to locally functionalize the glass with a crystal lattice engineered across several length scales makes this process particularly desirable for optical, photonic, and quantum applications. In this presentation, we follow the evolution of the lattice of model Sb_2S_3 crystal formed congruently in glass throughout the laser-fabrication process. We monitor the evolution of the initial parent glass structure under static laser irradiation through the earliest stages of crystal formation. We show the crystal seed not only grows, but also rotates during the earliest stages of growth. The laser is then scanned to grow extended crystal lines, which tend to form edge dislocations of the same sign in the lattice leading to an overall lattice rotation. This rotation is initially complex, but anisotropy in the model systems settles the rotation about a single axis that is parallel to the glass surface and normal to the laser scanning direction, forming macroperiodic structures of lattice orientation tens to hundreds of microns long. The overall evolution of lattice is offered as a timeline of how the lattice may develop for laser-fabricated crystals in glass.

9:50 AM

(GOMD-S3-022-2024) Formation of tin-iron-soda-silicate glass anode and solid electrolyte interface by laser irradiation

F. Sato*[1]; T. Honma[1]

1. Nagaoka University of Technology, Japan

Oxide-based all-solid-state batteries (ASSBs) are expected to be the next-generation batteries. The high interface resistance between the electrode and solid electrolyte is a challenge in the practical use of ASSBs. The focus in this study was the laser irradiation process. Through this process, the glassy active material can be adhered to the solid electrolyte which is expected to reduce the resistance of ASSBs. In this research work, the interface formation between in-iron-soda-silicate anode glass 55SnO-15Na2O-yFe2O3-(30-y) SiO2 (yFe-SNS) and solid electrolyte ceramics was conducted. The anode slurry prepared was prepared by mixing 6.75 Fe-SNS and polyimide binder and then applied onto the solid electrolyte through the screen-printing method. The sample was laser irradiated at the power of 3 W and the scanning speed was above 100 mm/s. This resulted into the densification of the anode layer and the interface formation with the solid electrolyte. The laser-irradiated sample exhibited conductivity on the order of 10-5 Scm-1 at room temperature. Compared to the sintering process, a significant reduction in resistance was observed. These results indicate that this material achieved thickness control of the anode layer, densification and interface formation which can reduce the interface resistance challenge faced by the ASSBs and has the potential to be used as an anode for ASSBs.

10:10 AM

(GOMD-S3-023-2024) Nonlinear Optical study of ITO nanocrystals embedded within aluminoborosilicate glass using Z-scan

A. Ashjari*[1]; B. Topper[2]; D. Möncke[1]

1. Alfred University, Inamori school of engineering, USA
2. University of New Mexico, Center for High Technology Materials, USA

Glasses incorporating tin-doped indium oxide nanocrystals can be regarded as materials characterized by remarkable nonlinear optical response. The current study aimed to investigate the nonlinear optical responses of ITO nanocrystals embedded in the aluminoborosilicate glass matrix using the Z-scan technique utilizing a 550 picosecond 532 nm laser. Inhomogeneity in the host glass prior to crystallization prevented accurate measurement of the nonlinear response in the experimental setup used, which exploited the beam radius measurement method. However, the glass after 10 hours subsequent heat treatment at 650, resulting in precipitation of tin-doped indium oxide nanocrystals with 5-10 nm crystallite size determined by electron microscopy images, demonstrates strong effective nonlinear optical responses. Both the nonlinear absorption coefficient and nonlinear refractive index are measured for this nano-phase glass ceramic. The possible nonlinear mechanisms in the sample are discussed, including two-photon absorption, saturable absorption, free carrier refraction, and self-focusing/defocusing. Interestingly, glass ceramic shows both positive and negative nonlinear refraction and absorption, depending on the location measured. Furthermore, the effect of incident light intensity on the optical response of the material is investigated, in which permanent changes in the response magnitude are observed after initial irradiation.

10:30 AM

(GOMD-S3-024-2024) Characterization of Ge Nanoparticles Formed in Glass by Femtosecond Laser Irradiation by Raman Spectroscopy

A. Tsekrekas*[1]; H. Jain[1]; V. Dierolf[1]

1. Lehigh University, Institute for Functional Materials and Devices, USA

Irradiation of oxide glasses by femtosecond laser has been shown to produce metallic and semiconducting nanoparticles in the vicinity of beam focus inside the sample. Characterization of the size and distribution of such nanoparticles in glass by conventional transmission electron microscopy (TEM) can be an arduous task due to the sample preparation that is required for their observation. Raman spectroscopy can be an alternate approach to determine the size of metallic nanoparticles based on the phonon confinement model. Streaks of germanium (Ge) nanoparticles have been created in La_2O_3-B_2O_3-GeO_2 glass via femtosecond laser irradiation before it starts crystallizing. Raman spectroscopy area scans were collected of the transverse cross sections of formed streaks of Ge nanoparticles to indicate their relative locations within the laser modified region. The phonon confinement model has been applied to these area scans to obtain quantitative information about the size of the nanoparticles which can be used to determine the size distribution relative to the laser beam focus within the modified region. With this relatively fast and more efficient technique than TEM, dependence of the characteristics of Ge nanoparticle formation has been determined relative to laser parameters (intensity, depth of focal point, exposure time, etc.).

10:50 AM

(GOMD-S3-025-2024) Crystal-phase selective crystallization of glass using a spatial light modulated laser beam

K. J. Veenhuizen*[1]; O. Magneson[1]; V. Dierolf[2]; H. Jain[3]

1. Lebanon Valley College, Physics, USA
2. Lehigh University, Physics, USA
3. Lehigh University, Materials Science and Engineering, USA

Spatially-selective devitrification of glass can be achieved via focused laser irradiation, enabling the creation of crystal lines which can serve as interconnects within integrated optics. It should be possible to create multiple-crystal-phase structures within the inhomogeneous temperature profile, where the position of each phase can be controlled by the laser intensity distribution, improving flexibility in designing multifunctional optical elements. We have tested this hypothesis in the model glass 50PbO–40Bi2O3–10Ga2O3. Differential scanning calorimetry demonstrates this glass crystallizes into multiple phases. This was verified by X-ray diffraction of crystal powders prepared via conventional heat treatment at each respective peak crystallization temperature, showing the formation of a cubic phase at lower temperatures and triclinic phase at higher temperatures. Laser fabricated crystals in glass were studied using confocal Raman microscopy, within which the presence of multiple phases was observed. For crystal lines created by a Gaussian beam, the triclinic structure formed in the center of the laser modification and cubic structure in the periphery, consistent with DSC and XRD measurements. By controlling the temperature profile within the glass by spatial light modulation of the input laser beam, spatially-selective control of the crystal phases was achieved.

Session 2: Charge and Energy Transport in Disordered Materials

Room: Peeble Beach
Session Chairs: Gabriel Agnello, Corning Incorporated;
Caio Bragatto, Coe College

9:20 AM

(GOMD-S3-026-2024) Effective charge carrier density in lithium disilicate glasses (Invited)

V. M. Zallocco[1]; J. Campos[1]; A. Rodrigues*[1]

1. Federal University of Sao Carlos, Materials Engineering, Brazil

The ionic conductivity of alkali glasses increases orders of magnitude for a small variation (say, doubling) of the alkali concentration. Thus, calculating the effective charge carrier's density is a crucial matter that has not yet been solved. The weak electrolyte theory proposed by Souquet in the 70s predicts that only part of the available alkali ions participate in the glass ionic conductivity. In the present work, we calculate the effective charge carrier's density by measuring the electrode capacitance of a lithium disilicate glass in contact with gold electrodes. We had previously investigated the factors that affect its electrode capacitance. Our finding shows that an input voltage of 60 mV proved suitable for minimizing potential electrochemical processes. Electrode polarization data were reproducible from the second impedance cycle onward. Additionally, our results indicated that smoother surfaces closely approximate ideal electrode spike behavior. Our results show that the effective number of charge carriers, calculated by the space charge theory, is 5 to 12% between 130 to 280 °C and approximately 1% at 25 °C for lithium disilicate glass. The number of total alkali ions extrapolated from our results notably matches that calculated through density measurements, which validates both the model and the applied methodology.

9:50 AM

(GOMD-S3-027-2024) Progress Towards New Sodium Mixed Oxy-Sulfide Glassy Solid Electrolytes (Invited)

S. W. Martin*[1]; M. P. Olson[1]; A. G. Wakefield[1]; N. Riley[1]

1. Iowa State University, Materials Science & Engineering, USA

While Lithium batteries are currently the most popular battery for grid scale energy storage, the rapidly increasing demands for Lithium to electrify transportation will soon outpace available geological reserves. For this reason, sodium batteries, with their comparable volumetric energy storage density, yet orders of magnitude lower cost, have been of interest for more than 50 years. The lack of a high conductivity, low cost, and electrochemically stable solid electrolyte has been a central reason for the current lack of a commercially available Na battery. In this talk, I will describe our more recent progress in developing new chemistries of Na-based glassy solid electrolytes that can be formed as thin films and in characterizing the many thermal, chemical, electrochemical, and mechanical properties needed of them.

10:20 AM

(GOMD-S3-028-2024) Characterization of Li-Si-P-S-O-N Glassy Solid Electrolytes

V. M. Torres*[1]; P. Philipp[1]; C. Lyle[1]; A. R. Carr[1]; S. W. Martin[1]

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

The development of a glassy solid electrolyte (GSE) that is easily synthesized and promises electrochemical stability in contact with lithium metal is still to be seen. However, new mixed oxy-sulfide-nitride (MOSN) GSEs have been investigated as a means to easily synthesize and improve properties of the materials, Here the MOSN GSEs $0.58Li_2S + 0.378SiS_2 + 0.042[(1\text{-}x)LiPO_3 + (x)LiPON]$ (y = 0.0 to 1.0) were prepared by a melt quench-synthesis using LiPON as the source of N in these glasses. Differential scanning calorimetry (DSC) was used to asscertainf the glass transition and crystallization temperatures along with the working range for these materials. Electrochemical impedance spectroscopy (EIS) measured the Li$^+$ ion conductivity of these glasses. Raman and Infrared spectroscopies were employed to identify key structural species in these glasses. Additionally, XPS was used as well to validate the presence of nitrogen species in these glasses and further elucidate the structure-property relationship nitrogen's role. From the investigation it was found that the addition of nitrogen decreases the crystallization temperature and working range.

10:40 AM

(GOMD-S3-029-2024) Structure-property relations in the $60Li_2S + 30SiS_2 + xLiSbO_3 + (10\text{-}x)LiPO_3$ glass system

W. Fettkether*[1]; C. Lyle[1]; S. W. Martin[1]

1. Iowa State University, Materials Science & Engineering, USA

The electrochemical and mechanical properties of glassy solid electrolytes (GSE) in the [$Li_2S - SiS_2 - LiPO_3$] system make them promising candidates for inclusion in solid-state batteries. However, a significant challenge facing these sulfide-rich compositions is their reactivity towards oxygen and H_2O. One strategy to address this issue is to substitute the P-S bond present in the glass structure with a less reactive alternative. The theory of hard and soft acids and bases (HSAB) predicts that the "softer" antimony cation will form a stronger bond with sulfur than the phosphorus cation, reducing the reactivity of the GSE. To test this hypothesis, $LiSbO_3$ was synthesized and utilized to create samples in the $60Li_2S + 30SiS_2 + xLiSbO_3 + (10\text{-}x)LiPO_3$ glass series. Thermal, chemical, electrochemical, and spectroscopic techniques were employed to characterize the effects increasing antimony content produces in these GSEs.

11:00 AM

(GOMD-S3-030-2024) Using LAMMPS to Shed Light on Haven's Ratio: Calculation of Haven's Ratio in Alkali-Silicate Glasses using Molecular Dynamics

T. Salrin[1]; L. Johnson[1]; C. B. Bragatto*[1]

1. Coe College, Physics Department, USA

Haven and Verkerk studied the diffusion of ions in ionic conductive glasses with and without an external electric field to better understand the mechanisms behind ionic conductivity. In their work, they introduced the concept now known as Haven's Ratio (H_R), given by the ratio of the tracer diffusion coefficient (D_{self}) of ions to the diffusion coefficient from steady-state ionic conductivity (D_σ), calculated by the Nernst-Einstein equation. D_σ can be challenging to obtain experimentally since the number of charge carriers has to be implied, a subject still under discussion in the literature. Molecular dynamics (MD) allows for the direct measurement of the mean squared displacement (r^2) of diffusing cations, which can be used to calculate D, avoiding the definition of a charge carrier. Using MD, the authors have calculated r^2 of three alkali ions (Li, Na, K) at different temperatures and concentrations in silicate glass, with and without the influence of an electric field. Results found for H_R generally fall close to 0.6 at lower concentrations ($x = 0.1$) and close to 0.3 at higher concentrations ($x = 0.2$ and 0.3), comparable to the literature, implying that the electric field introduces new mechanisms for the diffusion of ions.

Session 4: Glass Devices II

Room: St. Andrews
Session Chair: Xianghua Zhang, University of Rennes/CNRS

MOVED TO WEDNESDAY AT 5:40

(GOMD-S3-031-2024) Advances in Optical Fibers (Invited)

W. Kim*[1]; C. Baker[1]; S. Bayya[1]; T. Zhou[2]; D. Rhonehouse[1]; F. Kung[2]; G. Chin[2]; D. Boyd[1]; R. Nicol[3]; V. Nguyen[1]; K. Ewing[1]; D. Gibson[1]; J. Frantz[1]; R. Gattass[1]; J. Sanghera[1]

1. Naval Research Laboratory, Optical Science Division, USA
2. URF, USA
3. Jacobs, USA

We report our recent progress in Erbium doped fibers (EDF) developed for space applications such as in satellite communications. These fibers are typically sensitive to the high radiation and the fiber performance deteriorates due to cosmic rays. Various efforts have been made to improve the radiation stability of these fibers. Here we present our recent study on the effect of various dopants with varying concentrations incorporated into the fiber core to further reduce the radiation induced gain degradation and improve the performance of the fibers. We also report our recent progress in the development of IR transmitting organic/inorganic hybrid materials composed of chalcogenide elements, such as sulfur and selenium, along with organic and/or inorganic crosslinking moieties. This class of materials is referred to as organically-modified chalcogenides (ORMOCHALC) and is being developed for IR optics and fibers to provide size, weight and performance advantages at low cost (SWaP-C). Multiple chalcogenide cladding layers with varying refractive indices can coat chalcogenide core fiber materials to form optical waveguides. Here, we report a successful demonstration of waveguiding & transmission of infrared light in a ORMOCHALC fiber. We will also briefly report our progress in 3-D printing of various polymer fibers in various sizes and shapes.

9:20 AM

(GOMD-S3-032-2024) Dispersion-engineered, lithography-free, chalcogenide and oxide metacoatings for telecommunication and computing (Invited)

B. Gholipour*[1]

1. University of Alberta, Edmonton, Electrical and Computer Engineering, Canada

Chalcogenide phase-change materials (PCMs) are high refractive index, reconfigurable material platforms across the visible/telecom band, exhibiting reversible, volatile, and non-volatile transitions facilitated by their inherently large/switchable thermo-optic coefficients and reversible phase transitions between glassy and crystalline states with starkly different optoelectronic properties. However, the mitigation of high insertion losses when introducing many of these alloys to the vicinity of waveguide platforms due to their inherent absorption across this band has resulted in devices with large lateral footprints and/or poor modulation contrasts and an incessant search for low-loss/high switching contrast alloys. Here, we show non-resonant, subwavelength patterning that enables dispersion engineering (metacoating) of chalcogenide glasses through lithography-free, bottom-up growth and patterning techniques, paves the way to the realization of alloys with tunable optical and electronic properties. We show that tunability may be achieved without the need for stoichiometric changes to chemical composition through glancing angle deposition and oxidation techniques. We also go on to demonstrate how interlayer nanostructuring enables ultra-compact phase/intensity modulators with tunable insertion losses.

9:50 AM

(GOMD-S3-033-2024) Firing characteristics of glass systems in silver pastes at Ag/Si interface in Si solar cells

J. Tong[1]; Y. Lai*[1]

1. National United University, Materials Science and Engineering, Taiwan

Different glass systems were used to investigate the role of glass frits in the Ag paste on metallization of front contact in solar cells. Four glass systems primarily composed of V_2O_5, Bi_2O_3, and TeO_2 were prepared and subjected to high-temperature sintering to form an ohmic contact with Si emitter. The sample printed with silver paste containing Bi_2O_3 glass frits was immersed in an etching solution to observe the distribution of inverted pyramidal patterns. After a firing temperature of 750°C, the inverted pyramidal patterns are clearly observed in Bi_2O_3 based glass. On the other hand, V_2O_5, and TeO_2 based glass frits required a firing temperature of 800°C to observe the inverted pyramidal patterns.

10:10 AM

(GOMD-S3-034-2024) Local dielectric and electromechanical responses of antimony sulfide crystals embedded in glass by surface probe techniques

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Antimony sulfide (Sb_2S_3) is an emerging semiconductor for photovoltaics, infrared optoelectronics, energy storage, and phase change applications. It has much lower optical losses at telecom wavelengths than the current optical and electronic phase change material, $Ge_2Sb_2Te_5$ (GST). Sb_2S_3 can be crystallized or amorphized with a low-power optical laser. In addition, it has been reported as a piezoelectric and ferroelectric. Controlled heating of Sb_2S_3 glass with CW laser can result in rotating lattice single (RLS) crystals embedded within the substrate. The lattice of RLS crystals rotates in orientation along the scanning direction, which can be controlled by changing laser parameters. These metamaterials with engineered lattice orientation and curvature offer new functionalities for integrated photonics. We have investigated their local dielectric and electromechanical behaviors by piezoresponse force microscopy (PFM). A hysteretic electromechanical response is observed in Sb_2S_3 RLS as well as cerammed crystals, which is absent in surrounding glassy Sb_2S_3. Parallel characterization with complementary scanning probe techniques shows the difference between the two types of crystals, but reveals that neither is due to ferroelectricity. These results demonstrate the care that must be taken to interpret PFM data. Possible origins of this behavior are discussed as well as their implications for Sb_2S_3 as a functional material.

10:30 AM

(GOMD-S3-035-2024) Real-time and label-free detection of strepatividin-biotin interaction by bio-functionalized chalcogenide glass fiber sensors for the mid-infrared

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Biofunctionalized infrared optical chalcogenide glass fibers have been designed for evanescent wave mid-infrared spectroscopy. Surface functionalization of the fiber tapered sensing zone have been achieved by reactivity of a maleimide function on sulfhydryl moieties of the glassy surface. Biotin-streptavidin interaction were studied by fiber evanescent wave spectroscopy. Kinetic measurements comparisons of functionalized and non-functionalized fiber surfaces for various concentration has demonstrated the bio-selectivity of the functionalized glass fiber. The protein enrichment of the functionalized glassy surface allows for a significant increase of the protein detection limit, greater than two order of magnitude as compared to reference non-functionalized fibers. A detection of minute quantities at concentrations as low as 10 parts-per-billion protein is also demonstrated.

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