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ABSTRACT BOOK

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Introduction

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How to Use the Abstract Book

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

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Monday, May 21, 2018

Award Lectures

Stookey Lecture of Discovery

Room: El Mirador (22nd Fl)

8:00 AM

(GOMD-AW-001-2018) Combinations of different nucleation and crystallization mechanisms to develop tailor-made glass-ceramics

W. Hoeland*[1]

1. Ivoclar Vivadent AG, Liechtenstein

Glass-ceramics possess the specialty of enabling the combination of different properties within one material. The development of glass-ceramics with high strength and high toughness combined with translucency and different colors lead to the discovery and subsequent commercialization of biomaterials for dental restoration. Other types of multicomponent glass-ceramics allow the combination of high mechanical parameters and preferred thermal properties or radiopacity. Thus, the development of bioactive glass-ceramics which are machinable as well as other technical products, e.g. machinable glass-ceramics with magnetic properties, was possible. The development of all these products is based on the selection of specific multicomponent chemical systems and the discovery of controlled nucleation and crystallization processes of the base glasses. The main focus of the lecture is the presentation of twofold or even multifold nucleation and crystallization mechanisms. Combinations of different internal (volume) mechanisms, e.g. the precipitation of mica and apatite, or surface + internal mechanisms, e.g. the crystallization of leucite and apatite, are demonstrated. Furthermore, the use of these reactions to develop products as biomaterials with preferred forming technologies, e.g. molding or machining is discussed.

S1: Fundamentals of the Glassy State

Session 5: Computer Simulations and Modeling I

Room: La Vista A/B (22nd Fl)

Session Chairs: Walter Kob, Laboratoire Charles Coulomb; Jessica Rimsza, The University of North Texas

9:20 AM

(GOMD-S1-001-2018) Machine learning force fields: Extension from metals to amorphous materials (Invited)

V. Botu*[1]; A. Tandia[1]; K. Vargheese[1]

1. Corning Incorporated, USA

The topic of machine learning based force fields has gained significant interest in the past few years. The ability to describe forces on atoms without apriori defining a functional form, that explicitly maps atomic positions to the force, provides for a more generalized framework that extends beyond a particular class of material. The protocol for constructing such force fields includes: (i) generating the data, often done so using ab initio simulations, (ii) identifying suitable descriptors for an atom and its environment, (iii) leveraging machine learning algorithms to build models, and (iv) validating the models. In this presentation a demonstration of constructing such force fields is discussed, using the examples of metallic Al and extending it to amorphous SiO2. To validate such models, both thermodynamic and kinetic properties of materials, e.g., phonon density of states, activation barriers, etc., are estimated. By automating the construction of such force fields, the research community can quickly leverage such approaches for their application of interest. Further, a discussion on the challenges, and opportunities as a result, that the community faces in leveraging such machine learning based force field approaches to push the envelope of materials modeling are put forth.

9:50 AM

(GOMD-S1-002-2018) Atomistic origin of enhanced durability in solvated bulk alkali-silicate glasses (Invited)

W. Ching*[1]; K. Baral[1]; A. Li[2]

1. University of Missouri-Kansas City, USA
2. Corning Incorporated, USA

In-depth understanding of silica-water interaction is vital to the mechanical strength of silicate glasses and in enhancing their chemical durability. We report the results of ab initio calculation of the electronic structure, mechanical and optical properties of single (Li_2O, Na_2O, K_2O) and mixed (Li_2O-Na_2O, Na_2O-K_2O, Li_2O-K_2O) alkali silicate glasses at 30% molar percent of alkali oxides. The results are compared with the corresponding anhydrate models. Complex patterns of molecular water (H_2O), dissociated water (OH) with the accompanying formation of new bonds with alkali ions, and in breaking the silicate network are revealed. The atomistic origin of the enhanced properties due to hydration is explained in terms the distribution and strength of various bond pairs including the hydrogen bonding. A single quantum mechanical metric, the total bond order density (TBOD), is used to characterize the internal cohesion as a function of chemical composition and the observed mix-alkali effect in these models.

10:20 AM

(GOMD-S1-003-2018) Predicting the glass transition temperature of multicomponent oxide glasses using artificial neural networks

D. R. Cassar*[1]; E. Dutra Zanotto[1]

1. Vitreous Materials Laboratory, Department of Materials Engineering, Brazil

The glass transition temperature (T_g) is a kinetic property of major importance for both fundamental and applied glass science. The objective of this work was to design and implement a machine learning algorithm to predict T_g for multicomponent oxide glasses containing up to 35 different chemical elements. We used an artificial neural network computational model with a supervised learning algorithm. For this task, we collected almost 45,000 reported values of T_g and fed our algorithm. Initially, with the raw data, we were able to predict T_g for 99% of our data with an error below 13%. However, a fraction of the data was poorly described by the various network topologies tested. We believe that this may be due erroneous data or the dependence of T_g on measurement parameters, such different heating/cooling rates for example. We identified these "outliers"—which were less than 6% of the initial dataset—using a ranking method. We then proceeded to train a new neural network without these outliers. In the end, our best network was able to predict 99% of the data with no more than 6% of error. This level of uncertainty is not far from the typical experimental uncertainty and allows one to predict the T_g reliably, significantly aiding in the development of new glass compositions.

10:40 AM

(GOMD-S1-004-2018) Developing ReaxFF potential for modeling amorphous silicon oxycarbide

I. Ponomarev*[1]; P. Kroll[1]

1. University of Texas, Arlington, Chemistry and Biochemistry, USA

Amorphous silicon oxycarbide (a-SiCO) ceramic materials provide a wide range of applications. They are used as membranes for gas separation, radiation-tolerant materials, thermal barrier coatings, and anode materials in Li-ion batteries. To enable accurate large-scale atomistic simulations of SiCO, we develop a new reactive force field – ReaxFF – that promises DFT-accuracy at significantly

lower computational costs. Unfortunately, current parameterizations of ReaxFF for interaction between the elements Si, C, and O have significant flaws. Compared with ab-initio MD simulations, they neither match enthalpy differences nor kinetic stability at high temperature. Most importantly, however, none of the current ReaxFF parameter sets replicates an amorphous SiCO glass phase, which has been subject of many experimental studies. We develop new ReaxFF parameters using a library of DFT-computed data. The library includes not only observed SiO_2 and SiC structures, but also more than 10,000 hypothetical crystalline SiCO structures. Moreover, it comprises over 1,000 models of amorphous SiCO with a manifold of geometries and bonds. Based on this "Big Data" exploration, new Reax-Force Fields for SiCO show agreement between ReaxFF and DFT energies. Moreover, the amorphous SiCO glass phase is reproduced and remains kinetically stable up to temperatures observed in experiment.

11:00 AM

(GOMD-S1-005-2018) A Bayesian Optimization Framework for Glass Viscosity Modeling

A. Tandia*[1]; C. Erickson[2]; Y. Shu[1]

1. Corning Incorporated, Modeling & Simulation, USA
2. Northeastern University, USA

Machine learning models using artificial neural networks and Gaussian processes have become an important and efficient tool in Corning for glass property predictions. Different architectures in neural network or different covariance functions in Gaussian processes will output different predictions. We propose a practical Bayesian Optimization framework for automatically generating the best models in the black box manner, based on the choice of the number of layers/nodes, the number of neurons in each layer, the activation function for the neurons, and the best learning rate in a neural network, or the choice of the covariance and the mean functions for the Gaussian Process modeling framework. In addition, we compare black box and gray box models using the VFT and MYEGA equations that predict the viscosity of a glass composition at a given temperature. The method is more robust and efficient than manually defining architectures or selecting covariance and mean functions from random or grid searches.

11:20 AM

(GOMD-S1-006-2018) First-principles molecular dynamics studies of telluride glassy materials: $Ge_2Sb_2Te_5$ and $Ge_{15}Ga_{10}Te_{75}$ as prototypical cases

C. Massobrio*[1]

1. CNRS-IPCMS-UNR 7504, France

Telluride glasses are known to be much more difficult to synthesize than their lighter chalcogen counterparts. As such, telluride glasses can be classified as unstable, being prone to crystallization. This feature is one of the reason of the success of tellurium-based phase-change materials, such as the prototypical $Ge_2Sb_2Te_5$ composition, for data optical data storage and computer memories. The amorphous structure of $Ge_2Sb_2Te_5$ (GST) has been the object of controversial structural models. By employing first-principles molecular dynamics within density functional theory, we are able to obtain quantitative agreement with experimental structural findings for the topology of glassy GST. To this end, we take full advantage of the exchange-correlation (XC) functional (Becke-Lee-Yang-Parr, BLYP), combined with appropriate options for the non-local part in the pseudopotential construction for Ge. The atomic structure of glassy GST is characterized by Ge atoms lying in a predominant tetrahedral network, albeit a non-negligible fraction of Ge atoms are also found in defective octahedra. As an alternative glass, more intended for far-infrared application, the structural properties of $Ge_{15}Ga_{10}Te_{75}$ will be also presented. At variance with results published recently for a close composition, we have taken into account the role of the van der Waals dispersion forces.

11:40 AM

(GOMD-S1-007-2018) Ab initio molecular dynamics simulation of alkali-doped aluminosilicate glass

K. Baral*[1]; W. Ching[1]

1. University of Missouri-Kansas City, Department of Physics and Astronomy, USA

Ab initio molecular dynamics simulation of alkali-doped aluminosilicate glass Alkali-doped aluminosilicate glasses find wide application in a chemically strengthened glass. The structures and properties of alkali aluminosilicate glasses with different alkali to aluminum ratio containing around 600 atoms have been simulated using ab initio molecular dynamics (AIMD) within the VASP package. The electronic structure, mechanical and optical properties of these glasses are calculated from first-principle OLCAO method. The local atomic environment of alkali ions in the silica and alumina matrix is probed in details including the short- and medium-range order properties. The internal cohesion and strength of these models are quantified calculating the interatomic bonding in terms of the quantum mechanical metric, the total bond order density (TBOD). The properties are critically analyzed comparing with the experimental and other simulated results.

Session 6: Mechanical Properties of Glass I

Room: El Mirador West (22nd Fl)
Session Chairs: Lothar Wondraczek, University of Jena; Shigeki Sawamura, Friedrich-Schiller-University Jena

9:20 AM

(GOMD-S1-008-2018) Static Fatigue Limit of Silica Glass

J. H. Seaman*[1]; P. J. Lezzi[1]

1. Corning Incorporated, USA

In this research, the static fatigue limit, or the threshold stress intensity factor, K_o, for first sub-critical crack growth, has been measured directly in silica glass for T ≥ 700°C using the double cantilever beam (DCB) crack growth technique. Values measured were 0.48, 0.52, and 0.61 $MPa \bullet m^{1/2,}$ at 700°C, 725°C, 800°C respectively. Slow crack growth curves (K-v) have been measured from room temperature up to 850°C with slow crack growth essentially not occurring for T > 900°C. For a constant applied stress intensity factor, K_P, increasing temperature was found to decrease crack velocity and the slope of Region I was found to decrease. Cracks growing near the static fatigue limit had a time-dependence, where crack growth decreased and appeared to stop at $K_P \approx K_o$. A simple fracture mechanics model predicts a measurable static fatigue limit in silica glass for T ≥ 700°C by assuming a water-assisted stress relaxation mechanism at the crack tip.

9:40 AM

(GOMD-S1-009-2018) Silica Glass Fiber Strength and Water Entry into the Glass Surface

M. Tomozawa*[1]; E. Aaldenberg[1]; P. Miller[1]; X. Ding[1]

1. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA

A new glass fiber strengthening method was developed. A fiber was subjected to a high tensile stress at a temperature far below the glass transition temperature for a short time in air. The observed strengthening was attributed to a fast relaxation of mechanical stress at the surface which is promoted by a trace amount of water and the resulting surface compressive layer. Subsequently, an alternative explanation involving a surface swelling due to the entry of a large quantity of hydroxyl water promoted by tensile stress was proposed. In order to test the swelling mechanism, a large quantity of hydroxyl water was introduced into the glass surface by diffusion at 500°C, far below T_g. The mechanical strength decrease of the fibers with hydroxyl water diffused into the surface was measured by two-point bending. Results of these studies indicate that the strengthening

mechanism of swelling stress formation by hydroxyl water entry into silica glass fibers could not account for the observed strengthening of silica glass fibers.

10:00 AM

(GOMD-S1-010-2018) Strength of Silica Glass: Chemical Swelling versus Stress Relaxation

S. Wiederhorn*[1]; T. Fett[2]; G. Schell[2]; M. J. Hoffmann[2]

1. National Institute of Standards and Technology, USA
2. Karlsruhe Institute of Technology, Germany

Two theories have been suggested for the increased strength of silica glass that comes in contact with water at high temparatures and applied tensile stresses. In one, the water causes a stress relaxation of the glass at the surface, which converts into a compressive stress when the applied stress is released; in the second a chemical reaction between water and the silica glass causes a volume expansion that accounts for the compressive stress at the glass surface. This talk shows that in either case, the compressive stress level required for strengthening can be achieved, but that the chemical reaction theory requires fewer ad hoc assumptions.

10:20 AM

(GOMD-S1-011-2018) Static Fatigue and Compressive Stress Generation in an Aged Crack

P. J. Lezzi*[1]; J. H. Seaman[1]

1. Corning Incorporated, USA

In classic experiments by Michalske and others, it was found that cracks aged statically below the fatigue limit acquired a temporary strength increase compared to the non-aged crack. In our previous work we have observed that cracks growing near the fatigue limit exhibited a time dependent slowing down of crack growth. Both of these phenomena are related to a toughening of the crack tip that we attribute to a water-assisted surface stress relaxation mechanism. To test this hypothesis, the K-v crack growth curves have been measured using the double cantilever beam (DCB) experimental technique for two commercial glasses, a sodium aluminosilicate, and a potassium aluminosilicate, both of which exhibit clear fatigue limits in air. Using polarimetry, it is shown that the stress state near an unloaded but previously aged crack tip is opposite in sign to the stress state near the tip of a crack held in Mode I loading. These results clearly indicate that a stress relaxation mechanism is occurring at the crack tip.

10:40 AM

(GOMD-S1-012-2018) Effects of surface hydration on the mechanical response of silicate glasses

N. Sheth*[1]; C. G. Pantano[1]; S. H. Kim[1]

1. Pennsylvania State University, Material Science and Engineering, USA

The chemical reactions between water and silicate glass can nucleate and expand strength-controlling defects on the glass surface, ultimately reducing the usable strength of glass. Surface treatments, specifically acid leaching, result in controlled alteration of the surface structures (BO, NBO, OH) and incorporation of molecular water into the glass structure. One may expect that water in the acid leached surface facilitates mechanochemically-induced bond dissociation events, compromising desirable mechanical properties such as fracture resistance. However, the opposite is observed. This talk will focus on the effects of acid leaching and subsequent heat treatments on the mechanical and mechanochemical properties of silicate glasses. Differences in the mechanical behavior including hardness, modulus, indentation fracture resistance, crack initiation, and wear resistance in different environments will be discussed.

11:00 AM

(GOMD-S1-013-2018) Fracture toughness of silicates in aqueous electrolyte solutions

J. M. Rimsza*[1]; R. Jones[2]; L. Criscenti[1]

1. Sandia National Laboratories, Geochemistry, USA
2. Sandia National Laboratories, Mechanics of Materials, USA

Crack propagation in silicates is enhanced in aqueous solutions and in the presence of dissolved electrolytes due to deprotonation of the silicate surfaces and chemical reactions between water and strained siloxane bonds at the crack tip. To identify the coupled chemical-mechanical mechanisms which govern silicate fracture in water, molecular dynamics simulations of sub-critical fracture in amorphous silica were performed with a reactive force field. Slit cracks were introduced into bulk silica models and propagated as mode I fractures. Slit cracks were filled with reactive water molecules and NaCl as the model electrolyte. The average fracture toughness of silica decreased in pure aqueous and aqueous electrolyte environments. The role of defect concentrations, crack tip radii, and solution composition on fracture toughness, surface structure, stress distributions, and crack depth are discussed. Infiltration of the silica slit crack with reactive water molecules and electrolyte ions allowed for hydroxylation and an atomistic investigation of decreasing fracture toughness of silicates in aqueous conditions. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

11:20 AM

(GOMD-S1-014-2018) Spectral unmixing of Raman profiles relate structural heterogeneities to plastic flow in silicate glasses (Invited)

V. Pukhkaya[1]; M. Christine[2]; V. Martinez[2]; B. Champagnon[2]; E. Burov[4]; J. Teisseire[4]; B. Ruffle[3]; E. Barthel*[1]

1. CNRS/ESPCI, SIMM, France
2. ILM, France
3. LCC, France
4. SVI, France

Although plasticity plays a central role in the damage mechanics of silicate glasses, we still have a poor understanding of the nature of plasticity and especially its relation to formulation and structure. The major stumbling block is our poor knowledge of structural heterogeneity in silicate glasses due to a paucity of relevant investigation tools. In this respect, one of the most useful techniques is Raman spectroscopy, which provides insightful data of bond vibrations hence atomic configurations. However, reconstruction of local structure from Raman data is difficult due to the wide distribution of modes resulting in somewhat nondescript spectroscopic features. To extract sharper signatures of local heterogeneities in silicate glasses, we have prepared composition gradients through interdiffusion at glass-glass interfaces and acquired large series of Raman spectra along the direction of the gradients (profiles). The resulting collection of spectra is analyzed with non negative matrix factorization with sparsity constraint, evidencing a reduced set of elementary Raman spectra, each of which reflects a local environment. Correlation with microprobe composition measurements reveals the local environment type and correlation with nanoindentation measurements performed across the same interface provides for interpretation of plastic yield as a function of local structure.

Session 7: Non-Oxide Glasses I

Room: La Vista D/E (22nd Fl)
Session Chairs: Pierre Lucas, Univ of Arizona; David Le Coq, University of Rennes 1

9:20 AM

(GOMD-S1-015-2018) Chalcogenide glass: Enabling monolithic photonic integration on 2-D materials (Invited)

H. Lin[1]; S. Yi[1]; Y. Huang[1]; D. Kita[1]; S. Deckoff-Jones[1]; K. Wang[1]; L. Li[1]; J. Li[1]; Z. Luo[1]; H. Wang[1]; S. Novak[2]; A. Yadav[2]; C. Huang[3]; D. Hewak[3]; T. Gu[1]; K. Richardson[2]; J. Hu*[1]

1. Massachusetts Institute of Technology, USA
2. University of Central Florida, USA
3. University of Southampton, United Kingdom

Two-dimensional (2-D) materials are of tremendous interest to integrated photonics given their singular optical characteristics spanning light emission, modulation, saturable absorption, and nonlinear optics. To harness their optical properties, these atomically thin materials are usually attached onto prefabricated devices via a transfer process. Here we present a new route for 2-D material integration with planar photonics. Central to this approach is the use of chalcogenide glass, a multifunctional material which can be directly deposited and patterned on a wide variety of 2-D materials and can simultaneously function as the light guiding medium, a gate dielectric, and a passivation layer for 2-D materials. Besides claiming improved fabrication yield and throughput compared to the traditional transfer process, our technique also enables unconventional multilayer device geometries optimally designed for enhancing light-matter interactions in the 2- D layers. Capitalizing on this facile integration method, we demonstrate a series of highperformance photonic devices including ultra-broadband on-chip polarizers, energyefficient thermo-optic switches, as well as graphene and black phosphorus-based mid-IR waveguideintegrated photodetectors and modulators.

9:50 AM

(GOMD-S1-016-2018) Solution processing and properties of dip-coated chalcogenide alloy (Ge-Sb-Se-Te) films

Q. Altemose*[1]; M. Kang[2]; C. Blanco[2]; C. Schwarz[1]; K. Richardson[2]; J. Hu[3]

1. Ursinus College, Physics & Astronomy, USA
2. University of Central Florida, CREOL, USA
3. Massachusetts Institute of Technology, Materials Science & Engineering, USA

This work reports our investigation of the solution processing of targeted chalcogenide (ChG) alloys and the resulting structural, chemical, and optical properties of the dip-coated films. ChGs are known for their excellent infrared (IR) transparency, large index of refraction, low coefficient of thermal expansion, low change in refractive index with temperature, and ability to be compositionally tuned. The process of dissolving ChGs in solution and dip-coating substrates to create thin films of ChG materials can enable conformal coating and provide additional functionalities over that of thermally evaporated ChG films. The goal in this work is to maintain the targeted alloy composition and optical film quality compared to that of thermally evaporated thin films of similar composition. A targeted ratio of ethanethiol and ethylenediamine is used to dissolve bulk chalcogenide glasses (Ge_2-Sb_2-Se_4-Te_1) and to avoid compositional segregation. Glass substrates are then dip-coated into the solution for varying durations and then annealed. Long term solution evaporation rates were studied and correlated to elemental dissolution, changes in solution viscosity (η), remaining residual solution composition, and resulting film properties. Optimal evaporation durations, solution viscosity, solution chemistry, and dip-coated film properties are reported.

10:10 AM

(GOMD-S1-017-2018) Characterization of nanostructures created by multiphoton lithography in germanium-doped arsenic selenide chalcogenide glass as a route to functional optical devices

C. Schwarz*[1]; C. Grabill[2]; G. Richardson[2]; S. Labh[2]; A. Young[2]; A. Vyas[2]; M. Truman[1]; B. Gleason[3]; K. Richardson[4]; A. Pogrebnyakov[5]; T. Mayer[6]; S. Kuebler[2]

1. Ursinus College, Physics & Astronomy, USA
2. University of Central Florida, Chemistry, USA
3. Clemson University, USA
4. University of Central Florida, CREOL, USA
5. Pennsylvania State University, Materials Science & Engineering, USA
6. Pennsylvania State University, USA

This work reports a detailed study of the processing and multiphoton lithography (MPL) of the chalcogenide glass (ChGs) germanium-doped arsenic triselenide $Ge_5(As_2Se_3)_{95}$ and $Ge_5(As_3Se_7)_{95}$ and how the chemical networking, nano-structure morphology, and appearance of the resulting features are affected by the deposition rate, chemical composition, and etch processing. ChGs have excellent infrared (IR) transparency, low coefficient of thermal expansion, large index of refraction, and low change in refractive index with temperature. ChG based devices are promising for a wide range of industrial and commercial applications including waveguides, periodic plasmonic structures, and optical sensors & detectors. Through compositional variation their properties can be tuned for additional functionalities. Photo-sensitive thin films of $Ge_5(As_2Se_3)_{95}$ were created by thermally deposition of bulk ChGs onto silicon substrates. These films were photo-patterned and cross-linked by MPL and then chemically etched to dissolve the unexposed material, leaving free-standing structures. The nano-structure chemical composition and morphology were characterized and correlated with the film composition, thermal deposition, laser irradiation dose, and chemical etch processing.

10:30 AM

(GOMD-S1-018-2018) Highly Nonlinear Soft Glass Optical Fibers for MIR Applications (Invited)

Y. Ohishi*[1]

1. Toyota Technolological Institute, Japan

Highly nonlinear fibers have attracted much attention in recent years because they paved the way for the development of compact nonlinear devices for applications such as supercontinuum (SC) generation, wavelength conversion, pulse compression, parametric amplification, etc. Currently, highly nonlinear fibers are mainly made of silica glass. Because of the maturity in fabrication technology, their chromatic dispersion can be tailored almost freely by changing the microstructure in the cladding. However, the nonlinear refractive index n_2 of silica glass is only 2.2×10^{-20} m^2/W, which is low and restricts further improvement of fiber nonlinearity. Additionally, silica fiber is not transparent at wavelengths longer than 3 μm, which makes applications beyond this wavelength difficult. Highly nonlinear microstructured optical fibers (MOFs) made of soft glasses, such as tellurite glass, and chalcogenide glass, have been demonstrated for nonlinear applications. Soft glasses, such as tellurite glass and chalcogenide glass, have the nonlinear refractive index higher than that of silica glass by at least one order of magnitude. Moreover, these glasses have broad transparency ranges in the mid-infrared (MIR). Highly nonlinear MOFs made of those soft glasses have been demonstrated for nonlinear applications. Here, we present a new prospect of highly nonlinear soft glass optical fibers for MIR applications.

11:00 AM

(GOMD-S1-019-2018) Laser-induced dewetting of silver-doped chalcogenide glasses (Invited)

A. Douaud[1]; S. H. Messaddeq[1]; O. Boily[1]; Y. Messaddeq*[1]

1. Université Laval, Centre d'Optique, Photonique et laser, Canada

The spontaneous formation of self-assembled and/or self-organized patterns in Chalcogenide glasses is well-known and is produced with the interaction of light in the UV or visible region depending on the glass composition. Recently, we have reported the observation of laser-induced dewetting responsible for the formation of periodic relief structures in silver-based chalcogenide thin-films. By varying the concentration of silver in the system Ag_x $(As_{20}S_{80})_{100-x}$ with (x= 0,4,9 and 36), different surface reliefs are formed. Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) images of the irradiated spots show the presence of a periodic structure of ripples aligned perpendicularly to the electric field of incident light. The evolution of the surface changes as a function of laser parameters (power density, duration of exposure, and polarization) as well as film thickness and silver concentration will be presented. We will also compare the laser-induced dewetting to thermal dewetting in the same matrix.

S3: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 1: Dynamics, Nanograting

Room: La Vista F (22nd Fl)

Session Chair: Jianrong Qiu, South China University of Technology

9:20 AM

(GOMD-S3-001-2018) Time-resolved Measurements of Ultrafast Laser-material Interactions in Transparent Materials (Invited)

M. R. Ross*[1]

1. Corning Incorporated, Laser Processing, USA

The use of ultrafast lasers in transparent material processing is experiencing large growth and being applied to an expanding number of applications. A cascade of physical processes, on timescales ranging from femtoseconds to microseconds or longer, follows laser irradiation of transparent materials by ultrafast pulses. While the processes involved are generally agreed upon, a detailed description accounting for the many possible combinations of laser and material parameters is lacking. Moreover, most studies of ultrafast laser-material interactions focus on surface processes, leaving limited descriptions of bulk processes. To gain a full understanding of these processes it is required to take measurements on several relevant timescales. Measurements ranging from time-resolved imaging, spectroscopy and polarimetry to variation of laser and material parameters all help inform our understanding of these many processes. We will present on several example measurements and results that help inform our knowledge of laser-glass interactions. In one example, time-resolve pump-probe imaging allows estimates of cooling timescales for very hot material by capturing fluorescent and blackbody light emitted in the nanoseconds following laser-material interaction.

9:50 AM

(GOMD-S3-002-2018) Polarization-dependent periodic phase separation in glass induced by femtosecond laser pulses (Invited)

Y. Shimotsuma*[1]; Y. Tsuji[1]; K. Tomura[1]; M. Shimizu[1]; K. Miura[1]

1. Kyoto University, Department of Material Chemistry, Japan

The polarization-dependent periodic nanostructure is one of the interesting photoinduced structure by the femtosecond laser pulses. Even now detailed formation mechanism is under debate. In the case of simple glass composed of network former oxides (SiO_2, GeO_2, etc.) the subwavelength nanoplanes consisting of oxygen defects and nanopores were aligned in the direction perpendicular to the laser polarization. While, we have recently observed that the periodic phase separation in nanoscale also occurred in Al_2O_3-Dy_2O_3 binary glass with a low glass formation ability. In this case, we confirmed that the crystallization were periodically photoinduced in the subwavelength nanoplanes. Particularly, we have also observed that the garnet ($Dy_3Al_5O_{12}$) and the perovskite phase ($DyAlO_3$) can be selectively precipitated according to the laser condition. We believe that the electrostriction effect leading to the nonlinear optical response effects on this phenomenon.

10:20 AM

(GOMD-S3-003-2018) Femtosecond laser-induced 3D nanograting in fused silica with a dynamic regulating excitation process (Invited)

Y. Dai*[1]

1. Shanghai University, Physics, China

Femtosecond laser pulses direct writing 3D micro/nano-structure is one of the leading edge topics in the fundamental research field of laser interaction with transparent materials. The induced nanograting demonstrates unique advantages in the applications of high-density 5D optical storage and integrated polarizing elements. We control spatial-temporal characteristics of femtosecond pulse to study the physical origin of 3D nanograting. The method for active control of front tilt of a femtosecond pulse is demonstrated for quantification with transformation of a spatial chirp pulse, which results from the spectrum separation in space when the incident pulse passes through angular dispersion elements, further makes a difference on the density distribution of induced plasma by an asymmetric excitation at focus. That leads to an anisotropic expansion and deformation of the induced plasma driven by a pondermotive force for formation of 3D nanograting. Also, a temporally delayed femtosecond double-pulse laser irradiation is used to study the plasma excitation process during the formation of nanograting. Present results provide further insights into the understanding of formation of 3D nanograting, explore the potential on the spatial-temporal characteristics of pulse as a new freedom to speed up its formation, and improve the efficiency in fabrication of integrated optics.

10:50 AM

(GOMD-S3-004-2018) Temperature dependence of intense laser-induced damage threshold of fused silica at different laser pulse widths (Invited)

H. Deng[1]; X. Dong[1]; X. Yuan[2]; W. Liao[2]; L. Liu[1]; W. Zheng[2]; X. Zu*[1]

1. University of Electronic Science and Technology of China, School of Physical Electronics, China
2. Research Center of Laser Fusion, China Academy of Engineering Physics, China

Intense laser has been widely used for the investigations of laser-matter interaction, such as laser micro-machining, laser-driven accelerators, high harmonic generation in solids and terahertz generation in solids. However, the output energy of laser system is limited by the damage of optical elements. Fused silica is usually employed for optical elements in high energy laser system. In this report, the temperature dependence of laser-induced damage threshold on fused silica was studied from 80K-296K at different pulse widths. We found that the damage threshold has similar law for both nanosecond and femtosecond pulse widths as pulse duration large than 260fs. That is, damage threshold increases first and then decreases with decreasing of temperature. The maximum damage threshold is about 170K for different pulse widths and do not effect by pretreatment processes of fused silica. We also found that the damage threshold of fused silica is independent with temperature as pulse duration less than 100fs (this result provides a direct judgement for the long-existing debate about the dominant channel in generation of conduction band electrons). Physics models are discussed for these discovered experiment scaling laws.

11:20 AM

(GOMD-S3-005-2018) Crystal Lattice Engineering during Single Crystal Growth by Laser-induced Solid-Solid Conversion (Invited)

V. Dierolf*[1]; K. J. Veenhuizen[2]; C. Au-Yeung[1]; S. McAnany[3]; B. Aitken[4]; D. Nolan[4]; H. Jain[3]

1. Lehigh University, Physics, USA
2. Lebonan Valley College, Physics, USA
3. Lehigh University, Materials Science and Enginnering, USA
4. Corning Incorporated, USA

Spatially selective heating of a glass using lasers allows to precisely control the conversion of a glass into a single crystal. In particular, we have shown that it is possible to perform this conversion without ever melting the glass. In such a solid-solid conversion, the growth conditions are highly constrained, which produce unusual crystallization characteristics. In this presentation, we will give an overview of the most unique features which include preferred orientation of seed crystals, controlled rotation of the crystal lattice orientation both along and perpendicular to the growth axis. These concepts will be introduced for crystallization on the surface of a chalcogenide glass using a cw-laser as well as for 3D-crystallization inside a lithium niobosilicate glass. The dependence of these phenomena on the properties of the laser irradiation (polarization, beam profile, and intensity) will be discussed. This novel capability enables several potential applications. We will highlight potential applications of these new capabilities for quasi phase matching in non-linear applications, index-graded crystals for improved waveguiding, and chiral crystals for non-reciprocal optical devices.

S4: Glass Technology and Cross-Cutting Topics

Session 1: Glass Surface Characterization and Corrosion

Room: La Vista C (22nd Fl)
Session Chairs: Nicholas Smith, Corning Incorporated; Robert Schaut, Corning Incorporated

9:20 AM

(GOMD-S4-001-2018) X-ray absorption near-edge structure (XANES) spectroscopy of glasses (Invited)

G. Henderson*[1]

1. University of Toronto, Earth Sciences, Canada

X-ray absorption near-edge structure (XANES) spectroscopy is an element-selective technique used to probe the electronic, structural and magnetic properties of materials, including glasses. The XANES itself results from excitation of a core electron to an unoccupied state. It can provide information on the coordination, oxidation state and electronic structure of elements within non-crystalline materials, both from the bulk of the material and from the surface and near-surface. Experiments may measure the transmission of X-rays through the sample (for hard X-rays) but this is not suitable for soft X-rays due to attenuation issues. For light elements and surface studies, two main detection methods are usually used: Total Electron Yield (TEY) and Fluorescence Yield (FY). TEY probes a sample depth of approximately 1-10 nm while the FY detection sample depth is somewhat deeper (on the order of 7-10x the TEY sample depth) but nevertheless remains surface sensitive. In addition there are now a number of additional partial fluorescence detection methods including Inverse Partial Fluorescence Yield (IPFY) and High Energy Fluorescence detection (HERFD). I will give an overview of the application of XANES to glass studies with emphasis on recent results from light elements such as O, Li, Na, Ca and Mg K-edges of alkali and alkaline-earth containing silicate glasses.

9:50 AM

(GOMD-S4-002-2018) Precise analysis of glass surface using C_{60} ion beam (Invited)

Y. Yamamoto*[1]

1. Asahi Glass, Japan

X-ray photoelectron spectroscopy (XPS) analysis using Ar ion sputtering is one of the most accepted techniques for depth profiling in practical analysis, while this technique is known to be inadequate for quantitative analysis of glass including mobile ions such as soda-lime-silica glass. A cluster ion sputtering such as buckminsterfullerene (C_{60}) and Ar cluster has been recently recognized to suppress the degradation of organic materials, while the application has been limited for inorganic materials yet. Here, for the precise depth profiling on glass surface, C_{60} ion sputtering was applied to suppress the migration of mobile ions in glass. In our best knowledge, it has been the first time to succeed the precise XPS depth analysis of soda-lime-silica glass (70.4SiO_2, 0.9Al_2O_3, 7.3MgO, 7.8CaO, 13.6Na_2O in mol%) without compositional change by using C_{60} ion sputtering. The precise analysis revealed various phenomena, such as the compositional change during Ar ion sputtering and various properties related to float glass surface. Furthermore, I will show recent topics related to the precise analysis of glass surface.

10:20 AM

(GOMD-S4-003-2018) LEIS Analysis of Display Glass Surfaces

C. V. Cushman[1]; P. Bruener[2]; J. Zakel[2]; T. Grehl[2]; C. T. Dahlquist[1]; B. M. Lunt[3]; J. Banerjee[4]; N. J. Smith[4]; M. R. Linford*[1]

1. Brigham Young University, Chemistry and Biochemistry, USA
2. ION-TOF GmbH, Germany
3. Brigham Young University, Information Technology, USA
4. Corning Incorporated, Science and Technology Division, USA

Multicomponent glasses are the dominant substrate for manufacturing flat panel displays (FPDs). As FPD critical dimensions decrease, substrate surface composition has an increasingly important impact on the FPD manufacturing process. Glass surface composition affects thin film adhesion, charge buildup, rate of surface contamination, etc. The outermost atomic layer is likely to have the strongest influence on these surface-mediated processes. We use high-sensitivity low energy ion scattering spectroscopy (HS-LEIS) to evaluate a series of alkali-free display glass samples exposed to production line chemistries including HCl, TMAH, industrial detergents, and atmospheric plasma. These are compared to as-formed glass surfaces, fracture surfaces, and the surfaces of glass fibers. Using LEIS, we quantify the concentrations of Ca, Sr, Sn, Mg, Al, and Si on these surfaces. Resolving the strongly overlapping Al and Si peaks is challenging in LEIS. Accordingly, we discuss data acquisition and fitting approaches for resolving these signals. Our analysis reveals stark compositional differences in the glass surface compositions as a function of forming process, where fracture and glass fiber surfaces have higher modifier concentration than the as-formed glass surface. The acidic treatments rapidly deplete the glass surface of alkaline earth modifier species, while one detergent dramatically increases the Al concentration at the glass surface.

10:40 AM

(GOMD-S4-004-2018) Temperature-Resolved ToF-SIMS of Display Glass Surfaces

C. V. Cushman*[1]; C. T. Dahlquist[1]; S. S. Parker[1]; J. B. Clawson[1]; B. M. Lunt[2]; J. Banerjee[3]; N. J. Smith[3]; M. R. Linford[1]

1. Brigham Young University, Chemistry and Biochemistry, USA
2. Brigham Young University, Information Technology, USA
3. Corning Incorporated, Science and Technology Division, USA

Multicomponent glasses are preferred substrates for manufacturing flat panel displays, and their surface properties can influence the display manufacturing process. The hydroxylation state of the surface is thought to be important in mediating properties like

adhesion and charging. Few studies address the surface hydroxyl concentration of planar substrates, and fewer still attempt to quantify them on multi-component glass surfaces. This is a challenging analytical task because (i) planar substrates have low surface areas and relatively low hydroxyl densities, (ii) glass surface composition typically varies from its bulk composition, (iii) multicomponent glasses can have hydroxyl groups of different identity, and (iv) analyses are complicated by the presence of mobile modifier ions. Here, we use temperature-resolved time-of-flight secondary ion mass spectrometry (ToF-SIMS) to evaluate the surface-hydroxyl concentration on glass substrates representative of display glass materials. These samples were exposed to various surface treatments, including aqueous solutions of acids, bases. We have previously reported how similar treatments alter the inorganic surface compositions of such glasses (Cushman, et al., J. Am. Ceram. Soc. 2017, 100, 4770-4784.). Accordingly, in this study, we aim to link the complex interactions that relate surface composition and hydroxylation.

11:00 AM

(GOMD-S4-005-2018) Corrosion of aluminoborosilicate glasses in the acidic regime

N. Stone-Weiss*[1]; N. J. Smith[2]; R. Youngman[2]; E. M. Pierce[3]; H. Eckert[4]; A. Goel[1]

1. Rutgers University, Materials Science and Engineering, USA
2. Corning Incorporated, Science and Technology Division, USA
3. Oak Ridge National Lab, Environmental Sciences Division, USA
4. University of Sao Paulo, Sao Carlos Institute of Physics, Brazil

Aluminoborosilicate glasses comprise the vast majority of essential glasses used in both everyday life and for cutting edge-technological applications. These glasses show a wide range of composition-dependent properties which are exploited for applications spanning from ultra-strong cell phone touch displays and thermal resistant glasses to glasses for nuclear waste immobilization. Understanding the mechanisms of glass corrosion in many aqueous environments is of crucial importance for the development of functional industrial glasses in this composition regime. While chemical durability of aluminoborosilicates has been widely studied in neutral to alkaline pH for nuclear waste containment applications, developing a fundamental understanding of their corrosion in acidic solutions can facilitate the development of (i) methods for using chemical treatments to create glasses with altered properties and (ii) specifically-designed solutions to provide uniform isochemical etching. We aim to develop non-empirical models relating structure-composition-chemical dissolution to predict acidic corrosion behavior in this system and in other mixed network former systems. By correlating structural changes taking place in the glass network via NMR spectroscopy with elemental release profiles in acidic solutions (pH 0 – 4), we expect to gain a complete picture of the factors governing glass corrosion across a broad composition space.

11:20 AM

(GOMD-S4-006-2018) A structural approach to understand the aqueous corrosion of aluminoborate glasses

S. Kapoor*[1]; P. Dabas[1]; R. Youngman[2]; N. J. Smith[2]; A. Goel[1]

1. Rutgers University, Materials Science and Engineering, USA
2. Corning Incorporated, USA

Understanding the structural drivers governing the chemical durability of borate based glasses is becoming increasingly relevant with the advent of multicomponent borate glasses for functional applications in human biomedicine, waste management and electronic packaging. The present study is focused on understanding the composition-structure-chemical durability relationship in Na2O-Al2O3-B2O3 based ternary system. The changes in chemical durability of glasses in relation to the structural changes have been investigated through 11B and 27Al MAS-NMR spectroscopy. Addition of Al2O3 changes the dissolution behavior of the binary alkali-borate from congruent to incongruent with aluminum showing minimal tendency to leach out of the glass structure into the aqueous solution. Interaction of glass with water leads to an increase in Al-coordination from AlIV to AlVI with simultaneous formation of Boehmite (γ-AlO(OH)) crystalline phase in the glasses post dissolution. Furthermore, with increase in dissolution time, there is an increase in the fraction of tetrahedral boron and decrease in the fraction of BIII non-ring structures in the glass after immersion.

S5: Dawn of the Glass Age: New Horizons in Glass Science, Engineering and Applications

S5 Keynote Session

Room: El Mirador East (22nd Fl)
Session Chair: Kathleen Richardson, University of Central Florida

9:25 AM

(GOMD-S5-001-2018) The "road and less traveled by", with David Pye, has made all the difference (Invited)

C. Quackenbush*[1]

1. Halcyon Associates, USA

The problem orientation of an engineering education is excellent training for the myriad issues encountered in industry: technical problems, business problems or people problems. Many I did not face alone; Dave Pye was there to help, long after I left Alfred. Selected vignettes show how his advice, and teaching helped with industry problems, some I am proud to have solved, some I did not solve (and still drive me crazy), and some that may never be solved.

9:55 AM

(GOMD-S5-002-2018) Anomolous Color Vision Correction: Learning to Believe the Colorblind (Invited)

D. McPherson*[1]

1. EnChroma, Inc., USA

In honor of my mentor and doctoral advisor David Pye I am presenting some recent, and hopefully interesting work that demonstrates just how far afield one can wander when curiosity is the guide. Since 2010 EnChroma has been manufacturing and selling lenses that help the anomalous trichromatic color deficient to discriminate confusing colors (red versus green). This is made possible by selective filtering incoming light to re-balance the photo-pigment quantal cache. In spite of tens of thousands of testimonials and user-uploaded reveals totaling billions of views, there are skeptics saying there is no way to prove that they are actually seeing these colors. I will present the results of dichotomous cap arrangement, color naming, "pop out", afterimage and memory color tests, to show that colors categorically named correctly by the color deficient are indeed correctly perceived.

Science and Education I

Room: El Mirador East (22nd Fl)
Session Chair: Arun Varshneya, Saxon Glass Technologies, Inc.

10:30 AM

(GOMD-S5-003-2018) Glass Formulation Development for Nuclear Waste Vitrification (Invited)

I. Joseph*[1]; B. W. Bowan[1]; I. L. Pegg[2]

1. SNC Lavalin, Nuclear, USA
2. Catholic University of America, Vitreous State Laboratory, USA

Vitrification is the preferred method for treatment of high-level nuclear waste in the United States, and many other countries, due to the superior chemical durability of the glass waste form. In the United States, nuclear waste is generally vitrified into a borosilicate glass waste form in joule heated ceramic melters (JHCMs). The glass compositions selected for waste vitrification must meet certain

product quality (chemical durability) and processing (viscosity, electrical conductivity) requirements. Crystallization of the glass is also an important factor that could affect both melt processing and product glass durability. Glass compositions to treat a high-alkali, high-sulfate wastes have to be tested to ensure high sulfate solubility and low levels of corrosion of melter materials of construction, such as glass contact metal alloys and refractories. In addition to these requirements, to be economical, the glass compositions should allow high waste loadings and show good processing characteristics. This presentation will discuss the development of optimized glass compositions for nuclear waste treatment that involves glass formulation design aided by property-composition models, crucible-scale glass preparation and characterization, and bench-scale testing to assess processing rate, followed by testing in JHCMs of various scales to determine processing characteristics and potential for secondary phase formation.

10:45 AM

(GOMD-S5-004-2018) Technology Advancements in Radioactive Waste Vitrification Programs (Invited)

B. W. Bowan*[1]

1. SNC Lavalin/Atkins, USA

In the United States, and throughout the world, vitrification has been adopted as the reference approach for stabilizing high level radioactive wastes (HLW) generated from defense or civilian fuel reprocessing programs. Joule-heated ceramic melter (JHCM) technology, is one of two widely adopted, global approaches for converting HLW into durable, borosilicate glass suitable for long term, geologic disposal. Each HLW storage or production site, presents unique challenges to the vitrification process, from chemistry complexities, to physical scale of the treatment process. Accordingly, technology modifications have been required over the past five decades, to assure economic and reliable application of the JHCM technology. This paper, will review the evolution of JHCM technology since its initial deployments in the 1980's, to its adoption at the world's largest radioactive waste vitrification plant, the Hanford Waste Treatment and Immoblizaton Plant (WTP) in Washington state. JHCM technology enhancements at the Rokkasho (Japan) nuclear complex and the Defense Waste Processing Facility at the Savannah River Site (South Carolina) will be presented along with a review of the JHCM development program for the Hanford WTP.

11:00 AM

(GOMD-S5-005-2018) Underappreciated Contributions to The "Non-Equilibrium, Non-Crystalline State of Matter That Appears Solid on a Short Time Scale but Continuously Relaxes Toward the Liquid State" Age (Invited)

W. LaCourse*[1]; A. Clare[1]

1. Alfred University, Inamori School of Engineering, USA

The terms "fiber optic", "photonic", "chemically strengthened", "low e" etc., are often used to emphasize the tremendous impact of glass on the lives of nearly everyone, and therefore as justification for declaring that the world has entered "The Glass Age". While recognizing the importance of the above, the present paper emphasizes the impact of many less-well-known glass developements such as the "armonica", Pyescraper, marble, and LDP Non-Stainable Glass. Any single one of these developments might be labled as nano-influential. None-the-less, if integrated over the 60 year period from May 1959 to May 2019, they speak with a singular, loud accoustic emission: We have indeed entered the Age of Non-Equiliburium, Non-Crystalline (but not Amorphous) State of Matter that Appears Solid on a Short Time Scale but Continuously Relaxes Toward the Liquid State. Amen.

11:15 AM

(GOMD-S5-006-2018) Oxide Glass Structure: Towards a Working Hypothesis for the 21st Century (Invited)

A. Wright*[1]

1. University of Reading, United Kingdom

During the 20th Century there were three major theories of the structure of oxide glasses, viz. the Early Crystallite Theory (discrete crystallites separated by some form of "grain boundary"), the Random Network Theory (continuous statistically-disordered network) and the Cybotactic Theory (continuous network with spatial fluctuations in the degree of order). The problem is that NOT ONE of these theories can be eliminated, as a result of X-ray or neutron diffraction studies, nor on the basis of small-Q scattering (SAXS or SANS) data. Thus an alternative (thermodynamic) approach is required, and it will be demonstrated that two of these three theories have problems in explaining the chemical nanoheterogeneity of glasses having more than one component, the process of devitrification/crystallisation (especially that of nucleation), and/or cationic conduction in glasses containing network-modifiers, thus leading to a possible working hypothesis for the 21st Century.

11:30 AM

(GOMD-S5-007-2018) Sub-Micron Fracture Mechanism in Silicate Glasses Activated by Permanent Densification (Invited)

A. Wereszczak*[1]; S. B. Waters[1]; R. J. Parten[1]; L. D. Pye[2]

1. Oak Ridge National Lab, USA
2. Emeritus, Alfred University, USA

Several silica-based glasses were fractured at high strain energy via drop-weight testing. A cylindrical specimen was used to promote initially simple, axisymmetric, and uniform compression. The uniaxial compressive impact strain was sufficiently high to qualitatively cause permanent densification. Produced fragments were collected for postmortem and a fraction of them, for all the silica-based glasses, consistently had distinct sub-micron-sized fractures (~ 300-1000 nm), designated as "microkernels", on their surfaces. They would most often appear as a sub-micron pore on the fragment - an event that suggested the microkernel had popped out as a consequence of the local crack plane running through it, tensile-strain release, and the associated formation of the fragment it was on. No fractographic evidence showed the microkernels were associated with local failure initiation. However, their positioning and habit often suggested they were associated with localized crack branching and that they could have influenced secondary fracturing that occurred during overall crushing and comminution and associated fragment size and shape creation.

S1: Fundamentals of the Glassy State

Session 5: Computer Simulations and Modeling II

Room: La Vista A/B (22nd Fl)
Session Chairs: Carlo Massobrio, CNRS-IPCMS-UNR 7504; Hiroyuki Inoue, The University of Tokyo

1:20 PM

(GOMD-S1-020-2018) Local structure orders in metallic liquids and their influences on the dynamics of glass and phase selection (Invited)

C. Wang*[1]

1. Iowa State University, Ames Laboratory and Department of Physics, USA

Accurate description of atomic structures of undercooled metallic liquids and glasses is vital to understanding the dynamics the glasses and the mechanisms that influence phase selection during the crystallization process. By combining adaptive genetic algorithm, cluster alignment, molecular dynamics simulation and experimental

synthesis and characterization, we have developed an integrated approach to identify and quantify the short- and medium-range orders in metallic liquids and glasses. Using this approach, we can identify not only local structure order well beyond the first atomic shell (e.g., $Cu_{64.5}Zr_{35.5}$), but also dominate non-icosahedral motifs in the disordered metallic alloys (e.g., $Al_{90}Sm_{10}$). We showed that the short- and medium-range orders in undercooled metallic liquids are strongly dependent on the cooling rate. We also demonstrated that the dynamics in the glassy phase and the phase selection/transformation pathways are strongly influenced by the structure motifs in the undercooled liquids. Supported by US-DOE under Contract No. DE-AC02-07CH11358 and in collaboration with Y. Zhang, F. Zhang, Y. Sun, Z. Ye, K. M. Ho, M. I. Mendelev, R. N. Napolitano, R. Ott, and M. J. Kramer.

1:50 PM

(GOMD-S1-021-2018) A New Transferable Inter-Atomic Potential for Borosilicate Glasses

M. Wang[1]; M. M. Smedskjaer[2]; J. C. Mauro[3]; M. Bauchy*[1]

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA
2. Aalborg University, Denmark
3. Pennsylvania State University, USA

Molecular dynamics simulations of borosilicate glasses are notoriously challenging due to various coordination states exhibited by boron atoms, which can be 3- or 4-fold coordinated. Here, we present a new empirical force-field for modified borosilicate glasses. Although the potential retains a simple formulation (2-body interactions, fixed partial charges, constant parameters), it is found to offer an excellent transferability to a wide range of compositions, from silicate to borate glasses. The evolution of the coordination number of boron atoms upon varying glass compositions is well reproduced.

2:10 PM

(GOMD-S1-022-2018) Yield Surface for Oxide Glasses

S. Sundararaman*[1]; W. Kob[2]; S. Ispas[2]; L. Huang[1]

1. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA
2. University of Montpellier, France

The plastic response of oxide glasses is a complex phenomenon that has not been well understood. Elucidating the contribution of shear deformation and densification under sharp contact loading using continuum scale modeling would require an accurate constitutive law valid for a wider range of stress states. Given reliable force fields, molecular dynamics simulations of glasses under pure shear, pure hydrostatic and various combination of stress states can be carried out to calculate the yield surface and the permanent densification in glass recovered from different stress states, which will provide critical inputs for developing constitutive laws. In this work, we have developed improved potentials for oxide glasses, which can not only predict reliably density and elastic moduli at ambient conditions, but also their response to external stimuli like high pressure. Such force fields were used to study the effects of pre-densification and composition on the yield surface for various glasses to better understand the plastic deformation of amorphous materials.

2:30 PM

(GOMD-S1-023-2018) Predicting Q-Speciation in Binary Silicate and Phosphate Glasses using Statistical Mechanics

M. S. Bødker[1]; J. C. Mauro[2]; S. Goyal[3]; X. Guo[3]; R. Youngman[3]; M. M. Smedskjaer*[1]

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. Pennsylvania State University, USA
3. Corning Incorporated, USA

Predicting the compositional evolution of the atomic-scale structure of oxide glasses is important for developing quantitative composition-property models. In binary silicate and phosphate glasses, addition of network modifiers generally lead to depolymerization of the networks as described by the Q-speciation. Upon the initial creation of non-bridging oxygens and thus partly depolymerized Q species, a variety of network former/modifier interactions exists. Here, based on ^{29}Si and ^{31}P magic angle spinning nuclear magnetic resonance spectroscopy data from literature, we present a statistical description of the compositional evolution of Q-speciation in these glasses by accounting for the relative enthalpic and entropic contributions to the bonding preferences. We show that the entire glass structure evolution can be predicted based on experimental structural information for only a few glass compositions in each series. The model also captures the differences in bonding preferences in glasses with different field strengths of the modifier cations.

2:50 PM

(GOMD-S1-024-2018) Machine learning based prediction of dissolution kinetics in silicate glasses

N. Krishnan[1]; S. Mangalathu*[2]; M. M. Smedskjaer[3]; A. Tandia[4]; M. Bauchy[2]

1. Indian Institute of Technology, Civil Engineering, India
2. University of California, Los Angeles, USA
3. Aalborg University, Denmark
4. Corning Incorporated, USA

Silicate glasses, due to the exposure to water during service life, undergo corrosion and dissolution. Accurate predictions of dissolution kinetics in these glasses are hindered by the lack of fundamental understanding and the large number of intrinsic and extrinsic factors controlling the process. To address this issue, we use a data-driven approach to predict the dissolution kinetics of glasses. To this extent, we use high fidelity experimental measurements on the dissolution rates of aluminosilicate glasses. Glasses with varying compositions exposed to a wide range of pH values, ranging from acidic to basic, are considered. We investigate the efficiency of four classes of machine learning methods namely, linear regression, support vector regression, random forest and artificial neural network. We observe that, while linear methods fail in predicting the dissolution rates, artificial neural network provides accurate predictions exhibiting an excellent match with the experimental results. Through a detailed study, we show that the machine learning techniques can be used to identify the input-output relationship of the data, that is, linear vs. non-linear and ultimately, to predict accurately the dissolution kinetics of glasses. Overall, such data-driven approaches can be useful in glass science to understand the governing mechanisms, and to accelerate the design of commercial glasses.

3:10 PM

(GOMD-S1-025-2018) Structural modelling of SiO_2 crystals and glass

A. Takada*[1]

1. Asahi Glass Company, Japan

Glass structures have been investigated by computer simulation. The Short-range order can be analysed by using distribution of bond lengths, bond angles and Qn species. On the other hand, In the case of the intermediate-range order, analysing the radial distribution functions, structure factor and distribution of ring size are popular methods, however, they are still insufficient to understand the order. SiO_2 system has several polymorphs and it shows diverse intermediate-range order. In this study, the author investigated the structural features of SiO_2 appearing either in crystals and glasses in terms of dynamical structure changes, ring distortion and Voronoi tessellation. These indices characterized the structural features of SiO_2 system.

Session 5: Computer Simulations and Modeling III

Room: La Vista A/B (22nd Fl)

Session Chairs: Adama Tandia, Corning Incorporated; Carlo Massobrio, CNRS-IPCMS-UNR 7504

3:40 PM

(GOMD-S1-026-2018) MD Simulations of the Melting of Sodium and Lithium Metasilicates

A. Cormack*[1]; J. Horwath[1]; B. Hadden[1]

1. Alfred University, USA

Melting has been described as the single most important phase change in fundamental (materials) science. However, none of the theories put forward come close to explaining experimental observations, and this particularly true of silicate materials. In this presentation, we describe the application of molecular dynamics to probe the structural changes that occur on heating crystalline sodium and lithium metasilicates to above their melting temperatures. The behavior of these two silicates is different; sodium silicate shows a pronounced pre-melting regime, associated with an excess heat capacity, whereas the lithium metasilicate does not. In melting, however, both show a change from a single distribution of Q_2 units in the crystal to a distribution of multiple Q_n units in the melt (and subsequent glass). The simulations allow us to shed light on the role played by the alkali ions in the pre-melting regime, as well as identifying the initial mechanisms that lead to the reduction in the number of Q_2 species. Our results may be expected to provide some insight into the structural stability of silicate glasses.

4:00 PM

(GOMD-S1-027-2018) Insight of structure-property relationships of boroaluminosilicate glasses from molecular dynamics simulation

D. Lu*[1]; J. Du[1]

1. University of North Texas, Materials Science and Engineering, USA

Boroaluminosilicate glasses find wide technological applications such as display, chemically strengthened glasses, laboratory glassware, and nuclear waste vitrification. As one of the earliest commercial applications of boroaluminosilicate glass compositions, studies on structure-properties relationship of Pyrex® and related compositions are therefore important to provide a better understanding of general boroaluminosilicate glasses. Recent experimental studies provided detailed characterizations of these glasses (e.g. Smedskjaer et al., Appl. Phys. A 116 (2014) 491). In this paper, we applied molecular dynamics simulations with two different sets of empirical potential parameters to investigate the structure features of the Pyrex® glass family by systematic variations of the Si/Al ratio. The short and medium range structures as well as properties such as elastic moduli of these glasses were analyzed and compared with available experimental data. A strong correlation of boron coordination and mechanical properties was observed.

4:20 PM

(GOMD-S1-028-2018) Structure of the glass by intermediate oxides

H. Inoue*[1]

1. The University of Tokyo, Institute of Industrial Science, Japan

The addition of other oxides is essential for the glass containing intermediate oxides as a main component. The glass forming ability depends on the kinds of the intermediate oxides and the additives. The relation between the glass forming region and its atomic arrangement has been discussed. Some glasses based on the intermediate oxide exhibit different features from glasses based on network forming oxides, such as silicate, borate and phosphate. Our group has developed a gas levitation furnace and has prepared several binary intermediate oxide glasses in a region with much lower glass forming ability. We have analyzed their atomic arrangement by x-ray diffraction measurements using synchrotron radiation facility and structural models using molecular dynamics technique. The coordination numbers of Ti and Al atoms were larger than 4 and the packing densities were as extremely high as about 60%. As the basic structure of these glasses, the close packed structure of oxygen atoms could be adopted, Ti, Al and Ta atoms were put on octahedral sites, a part of oxygen atoms was replaced with Ba or La atoms and oxygen deficiencies were introduced. For this model, total correlation function after structural relaxation at 293 K using molecular dynamics method was agreed with the experimental one. We have found that atomic arrangement based on close packed structure can be adopted to the glasses based on the intermediate oxide.

4:40 PM

(GOMD-S1-029-2018) Effect of cooling rate and system size on MD simulations of sodium borosilicate glasses

J. Du*[1]; L. Deng[1]

1. University of North Texas, Materials Science and Engineering, USA

Molecular dynamics simulations have been widely used to understand silicate glass structure and properties. With the recent development of boron potentials, MD simulations of borosilicate glasses become possible. Due to the nature of coordination change of boron as a function of thermal history and composition, how simulation can handle the cooling rate effect in borosilicate glasses becomes critical. In this talk, we systematically studied the simulation system size and cooling rate effect on structure features such as boron coordination, Qn speciation and non-bridging oxygen distributions, ring size distributions, and properties such as glass transition temperature, elastic moduli and vibration density of states. The results provide insight on the cooling rate effect on these glasses and challenges posed in simulation borosilicate glasses. Finally, we make suggestions of protocols of MD simulations of these glasses.

5:00 PM

(GOMD-S1-030-2018) On the Limitations of Thermodynamic Approach to Glass Property Prediction

A. Priven*[1]

1. Corning Korea, Republic of Korea

One of the most popular approaches to prediction of glass properties as functions of chemical composition and temperature, the thermodynamic approach, is based on the assumption that glass is structurally similar to the equilibrium mixture of the stable crystalline phases; accordingly, the physical properties of a glass can be predicted from the equilibrium concentrations of solid species calculated from a thermodynamic model. In this presentation, the reasons of this situation are discussed. First, the practical application is limited to the chemical systems for which all required thermodynamic parameters are already determined, which is only a very little part of the variety of known glass-forming systems; however, for these well-studied systems, much simpler empirical models give accurate enough predictions. Another reason of limited applicability of mentioned approach is the uncertainly of the temperature at which the structure of glass is assumed to match equilibrium state, especially for the multi-component glasses. Finally, nobody has proven that the structure of any amorphous material can be presented as a superposition of available crystalline structures; in general case, this assumption looks very weak, and, most probably, it can be applied only in some limited compositional space. Some recommendations on the improvement of this situation will be given.

Session 6: Mechanical Properties of Glass II

Room: El Mirador West (22nd Fl)
Session Chairs: Lothar Wondraczek, University of Jena; Shigeki Sawamura, Friedrich-Schiller-University Jena

1:20 PM

(GOMD-S1-031-2018) Scratch-hardness of glass (Invited)

S. Sawamura*[1]; L. Wondraczek[1]

1. Friedrich-Schiller-University Jena, Germany

Modern applications of glass, in particular, covers and substrates in handheld electronic devices, rely on the material's mechanical performance and visual appearance. In this context, scratching is of fundamental importance, both in reducing optical appeal and initiating surface defects. In an effort to provide quantitative descriptors for the scratch resistance of glasses, here, we consider the associated energetics of deformation. We focus on the scratch hardness which is defined by the projected area and the lateral force of scratching. We evaluated the scratch hardness of silicate, borate, phosphate, chalcogenide, and metallic glasses, searching for trends with variuos structural parameters. Interestingly, the scratch hardness doesn't show alinear relationship with the normal indentation hardness, reflecting inherent differences in the underlying deformation mechanism.

1:50 PM

(GOMD-S1-032-2018) Indentation Deformation Mechanisms in Ternary Alkali Aluminosilicate Glasses

T. M. Gross*[1]

1. Corning Incorporated, Physical Properties, USA

The role of alkali field strength on indentation deformation mechanisms was analyzed for $20R_2O$-$10Al_2O_3$-$70SiO_2$ glasses. Glasses containing higher field strength alkali ions have higher packing density and deform with more subsurface shear faulting. Median/radial crack formation in glasses that deform with shear cracking damage is highly dependent on the testing environment. The indentation residual stress coupled with shear cracks present in the deformation zone set up a condition ideal for subcritical crack growth. If water is removed from the system such as by indenting and holding the glass under dry nitrogen, this fatigue mechanism is prevented. For glasses that do not contain damage in the deformation zone, i.e. no flaws are present, this fatigue mechanism also does not occur.

2:10 PM

(GOMD-S1-033-2018) Ex-situ Raman Investigation of Indentations in Vitreous Silica

N. T. Wiles*[1]; G. G. Moore[2]; S. P. Baker[1]

1. Cornell University, Materials Science, USA
2. Corning Incorporated, Characterization Sciences, USA

Densification and shear have been identified as the primary modes of plastic deformation under indentation in silicate glasses. Densification has been observed in many compositions, and methods have been developed to quantify densification. However experimental confirmation of the atomic mechanisms that enable densification is incomplete. Some authors have suggested that a change in bond angle between tetrahedra accommodate densification, and others argue that the rings of tetrahedra become smaller accommodate densification. In order to provide experimental evidence to test these hypotheses, we have combined Raman spectroscopy with indentation techniques to probe local structural changes in silica glass induced by densification. We began by collecting spectra of pristine silica which we compared to spectra from inside indentations. We observed large structural changes in the silica which vary continuously with increasing indentation load. We show clearly that the "defect" bands around 600 cm^{-1} and 500 cm^{-1} associated with 3 and 4 member rings increase in size and become broader. We correlate that to an increase smaller rings and a decrease in larger rings. We support the hypothesis that the rings of tetrahedra deform during densification which leads us to the conclusion that densification requires the cleavage and reformation of bonds.

2:30 PM

(GOMD-S1-034-2018) Constitutive Modelling of Indentation Cracking in Fused Silica (Invited)

S. Bruns*[1]; K. Durst[1]

1. Technical University Darmstadt, Physical Metallurgy, Germany

During nanoindentation two distinct regimes are found for fused silica: plastic deformation and cracking. Plastic deformation occurs either by volume conservative shear flow or inelastic densification. Cracking appears for pyramidal Indenters aligned along the indenter edges. In this work cohesive zone FEM is used to study this behavior. In a 3D model, median/radial cracking is considered by introducing cohesive element planes aligned along the indenter edges perpendicular to the indented surface. The approach by Lawn, Evans and Marshall (LEM) is used to relate crack length and loading to fracture toughness. The role of densification on indentation crack growth is critically examined using a pressure independent von Mises and a pressure dependent Drucker-Prager Cap constitutive model. The constitutive models were calibrated fitting experimental load-displacement curves. The results show that Drucker-Prager Cap model delivers an accurate description of the elastic-plastic material response. Moreover it is found that densification leads to shorter crack lengths, thus smaller K values. Evaluating K based on LEM, the fracture toughness of fused silica is overestimated by 10-25 %. This is found for both constitutive laws. It is therefore concluded that LEM is not applicable for fused silica using common calibrations. This is however not caused by densification but by the materials low E/H ratio.

3:00 PM

(GOMD-S1-035-2018) Sharp Indentation of Silicate Glasses: A Conical Indenter Sensitivity Study

B. C. Davis*[1]; I. Reimanis[1]

1. Colorado School of Mines, Metallurgical and Materials Engineering, USA

The mechanics associated with sharp indentation of silicate glasses continues to garner considerable attention; however, there is still a significant need for understanding fundamental mechanical responses over several length scales. Most studies employ Vicker's indenters to supply the damage and supplement this experimental work with 3D FEA models with 45deg or 90deg symmetry. The solve times of these models preclude extensive sensitivity studies involving indenter shape, force and material properties. In this research, a conical indenter and 2D axisymmetric FEA model are used to perform a sensitivity study with 10^2-10^3 unique model solutions. The FEA model is validated by experimental data generated with the conical indenter in select cases. The intention of this study is to indicate variable sensitivities and guide a more intelligent forward path for investigating and defining the mechanical response of glass to mechanical contact.

Session 6: Mechanical Properties of Glass III

Room: El Mirador West (22nd Fl)
Session Chairs: Lothar Wondraczek, University of Jena; Shigeki Sawamura, Friedrich-Schiller-University Jena

3:40 PM

(GOMD-S1-036-2018) Adaptive and Crack Resistant Aluminoborate Glasses (Invited)

M. M. Smedskjaer*[1]; K. Januchta[1]; K. F. Frederiksen[1]; N. Mascaraque Alvarez[1]; R. Youngman[2]; M. Bauchy[3]

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. Corning Incorporated, USA
3. University of California, Los Angeles, USA

The inherent brittleness and poor crack resistance of oxide glasses are among their main limitations for enabling future applications. Impact or scratch events can lead to formation of cracks that amplify local tensile stresses, resulting in catastrophic failures. Therefore, increasing the hardness and crack resistance of glasses is critical for the development of damage resistant and mechanically durable glasses. We have recently discovered that alkali aluminoborate glasses exhibit a superior resistance to sharp contact-induced cracking compared to most oxide glasses. The high crack resistance is associated with the ability of the glasses to self-adapt the connectivity of their network under compressive stress, which facilitates densification and thus aids in dissipation of the energy supplied during impact. Here, based on series of aluminoborate glasses comprising various alkali and alkaline earth oxide modifiers, we discuss the dependence of the glasses' structural and mechanical properties on the field strength (ratio of charge to size) of the modifiers. We show that the stiffness, hardness, deformation mechanism, and toughness depend on a fine balance between the atomic bonding energy, the packing efficiency of the atoms, and the ability of the network to densify reversibly or irreversibly, with each of these features showing a different dependence on the modifier field strength.

4:10 PM

(GOMD-S1-037-2018) A structural approach towards the design of a hard and crack-resistant Al_2O_3–rich glass

A. Rebecca*[1]; S. Kapoor[1]; K. Januchta[2]; R. Youngman[3]; L. Huang[4]; M. M. Smedskjaer[2]; A. Goel[1]

1. Rutgers University, Materials Science and Engineering, USA
2. Aalborg University, Department of Chemistry and Bioscience, Denmark
3. Corning Incorporated, Science and Technology Division, USA
4. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA

Designing new glasses with excellent ability to resist stress-induced crack initiation and growth is of utmost importance for advanced glass applications. Al_2O_3-rich glasses have been shown to possess both high hardness (H_V) and crack resistance (CR). However, their limited glass forming ability and extremely high processing temperatures (>1800°C) constrains them to the realms of academic research. In this study, we report on the structural design of a hard (H_V > 7 GPa at 200 gf Vickers load), crack-resistant glass with Al_2O_3 > 30 mol.%. The as-designed glass can be synthesized by conventional melt-quench technique at temperature ≤ 1675°C and can be produced in any desired shape and size. The Vickers' hardness of the annealed glass was measured to be ≥7 GPa at 200 gf, while no cracks were observed up to 2 kgf load under ambient conditions. The MAS-NMR spectroscopy adjoined with atomic force microscopy (AFM) and simulated nano-indentation studies have been employed to understand the structural origin of the elastic and mechanical properties of this glass.

4:30 PM

(GOMD-S1-038-2018) Loading Rate Sensitivity of Silicate Glass Plasticity Mechanisms

Z. Rouse*[1]; S. Baker[1]

1. Cornell University, Materials Science & Engineering, USA

It is known that silicate glasses can undergo one of two distinct modes of plasticity: shear or densification. Shear deformation can manifest either through homogeneous shear or through the formation of shear bands, a type of inhomogeneous flow during which strains are highly localized into thin sheets of material. Since shear band intersections can act as crack nuclei, shear bands can dramatically impact the bulk properties of silicate glasses. Remarkably, a mechanistic understanding of silicate glass shear banding is largely absent. To help address this problem, we probed the different loading rate dependencies of these different plasticity modes. We performed an indentation study of calcium aluminosilicate (CAS) glasses along the tectosilicate line in a range from 40-100% SiO_2. Previous work has shown that there is a plasticity mode shift between shear and densification across this compositional range. Through indentation across the full CAS compositional range at loading rates spanning several orders of magnitude (10^2 to 10^6μN/sec), the rate dependencies of both shear and densification plasticity modes have been explored. SEM imaging of the residual indents offers further evidence of how silicate glass shear band prominence is affected by loading rate. We draw conclusions on how loading rate is an important variable in our fundamental understanding of silicate glass plasticity.

4:50 PM

(GOMD-S1-039-2018) Nature of Rigid-Resilient Transition in Calcium Borosilicate Sealing Glass–Ceramics: Effect of Preferred Orientation

J. Yan*[1]; T. Zhang[1]

1. Fuzhou University, China

At present, the insufficient thermo-mechanical stability of sealing glass presents a challenge for solid oxide fuel cells (SOFCs). In this work, we report for the first time that a rigid-resilient transition occurs in a calcium borosilicate sealing glass upon heating at 700°C for different durations. The elastic modulus increases from 28–40 GPa for 24 h to 92–105 GPa for 100 h, while the corresponding hardness increases from 2.5–3 GPa to 8–9 GPa. In addition, a possible mechanism for the rigid-resilient transition has been proposed. The reported results provide a new approach to solve the sealing problem of SOFCs.

5:10 PM

(GOMD-S1-040-2018) Strength Testing of Glass Sectored Flexural Specimens

A. Wereszczak*[1]; B. A. Oistad[1]; B. Chen[1]; O. Jadaan[2]

1. Oak Ridge National Lab, USA
2. University of Mount Union, USA

The sectored flexural specimen is harvestable out of glass tubes and cylinders, and its geometry and test method are under consideration for potential standardization. The specimen was developed over a decade ago for strength-measurement studies in which flaws located on a tube's or cylinder's outer surface are limiters of axial tensile failure stress. With its versatile geometry, the associated axial tensile failure stress can be analytically calculated from the failure force measured from simple uniaxial bending, and multiple specimens (and test data) can be generated from a single tube or cylinder. An example of a sectored flexural specimen geometry, and its harvesting out of borosilicate tubes, test fixturing, flexure testing, and failure stress analysis are described. This manuscript has been authored by UT-Battelle, LLC, under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy.

5:30 PM

(GOMD-S1-041-2018) Electric field-assisted ion-exchange of silicate glass

V. M. Sglavo*[1]; G. Pintori[1]

1. University of Trento, Dept. of Industrial Engineering, Italy

In this work, electric field – assisted ion exchange was carried out on silicate glass to enhance sodium-potassium interdiffusion and improve the mechanical resistance. Electric fields with variable intensity were applied cyclically in both direct and inverted polarization. Energy Dispersion X-ray Spectroscopy was carried out to determine the potassium concentration in the surface layers of the samples. Flexural tests and Vickers indentation were used to characterize the mechanical performances of the strengthened material. It is shown that the application of the electrical field allows to enhance Na-K interdiffusion to a large extent, thus reducing the treatment time well below the hour. The analysis of the effect of electrical field frequency and intensity pointed out irreversible phenomena in the ion-exchange process which allows to reinforce both surfaces thus allowing to reach very high mechanical performances.

Session 7: Non-Oxide Glasses II

Room: La Vista D/E (22nd Fl)

Session Chairs: Pierre Lucas, Univ of Arizona; David Le Coq, University of Rennes 1

1:20 PM

(GOMD-S1-042-2018) Expanding the Abbe Diagram of Long-Wavelength Infrared Region (Invited)

Y. Choi*[1]; J. Lee[1]; W. Lee[1]; J. Choi[2]; W. Chung[3]

1. Korea Aerospace University, Republic of Korea
2. Korea Photonics Technology Institute, Republic of Korea
3. Kongju National University, Republic of Korea

Spurred by the recently emerging interests in miniaturized long-wavelength infrared (LWIR) camera module for use in mobile devices like smartphones, for example, chalcogenide glasses are gathering much attention as LWIR lenses due to their inherent compositional flexibility as well as moldability. Together with the rapid advancement of uncooled micro-bolometer as a LWIR image sensor, performance of the corresponding LWIR lens assembly needs to be further enhanced in terms of size and optical aberrations. In order to configure a better LWIR lens assembly, chalcogenide glass compositions exhibiting a wide variation of not only refractive index but also dispersion are required, which means the LWIR Abbe diagram needs to be further expanded. However, all of the commercially available chalcogenide glasses capable of transmitting LWIR region, i.e., 8~12 μm, fall into a low-dispersion category. In this regard, we have attempted to develop highly dispersive chalcogenide glasses in the LWIR region. In this talk, we discuss parameters affecting the refractive index dispersion of chalcogenide glass over the LWIR region, and then introduce some new chalcogenide glasses with a high-dispersion property. In addition, it is described that an experimental demonstration concerning all-chalcogenide-glass-based lens doublet consisting of high- and low-dispersion glasses, which minimizes chromatic and spherical aberrations.

1:50 PM

(GOMD-S1-043-2018) Athermal Glass for Infrared Optics

M. J. Davis*[1]

1. SCHOTT North America, Inc., R&D, USA

The ability of an optical component or system to preserve its performance while undergoing temperature changes is an important consideration to the optical designer (Jamieson, 1981). Materials that are athermal, i.e. the relevant optical figure-of-merit (FOM) is temperature independent, are beneficial to a wide variety of applications, including: a solid etalon used as a wavelength reference filter; a fiber strain sensor based on Bragg reflection as well as other specific fiber types; and as a lens within an optical system. Infrared-transmitting, chalcogenide glass compositions have been identified that attain athermality for one or more of these FOM's, each of which depend on refractive index, its change with temperature, and thermal expansion. Such data, including the temperature-dependent shift of Fabry-Perot etalon interference fringes, will be presented in light of these various potential applications.

2:10 PM

(GOMD-S1-045-2018) Transparent oxyfluoride nano-glass ceramics with optical and photonic applications (Invited)

A. Durán*[1]

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

Transparent oxyfluoride glass-ceramics (OxFGCs) have attracted great interest in the field of photonics since the pioneering work of Wang and Ohwaki. Alumina-silicate glass matrices are particularly suitable for their excellent mechanical, thermal and chemical properties compared to phosphate or fluoride glasses. On the other hand, fluoride crystals, especially those containing Ln^{3+} ions, are especially good hosts for their low phonon energy and offer high solubility of Rare-Earth (RE) ions. The classical processing route to obtain transparent OxGFCs consists in a controlled crystallization of the precursor glass made by melt-quenching. However, this processing method faces the problem of the high melting temperatures that cause a fluorine loss, limiting the final crystal content to less than 10 wt%. On the other hand, the sol-gel process is a suitable alternative to prepare such materials due to the low synthesis and sintering temperatures involved, thus allowing the preparation of novel compositions, especially as thin films, with higher crystal content up to 20 wt%. In this work we will show the results, obtained in the last five years, for bulk, optical fibers and thin films. In particular, the relation between processing, structure and improved optical properties will be discussed focusing on the superior optical properties of these materials as compared to the precursor glasses

2:40 PM

(GOMD-S1-046-2018) Ti-N Containing Silicate Oxynitride Glasses

G. Scannell*[1]; L. Wondraczek[1]

1. Friedrich-Schiller-University Jena, Otto-Schott Institute for Materials Research, Germany

Titanium nitride has been incorporated into a lithium, aluminum, titanium silicate glass. These glasses were produced in a nitrogen atmosphere at 1400 °C using a centrifugal induction furnace with a nominal nitrogen content of 5 equivalent mol%. Ti content (both TiN and TiO_2) was varied from 5 to 20 mol% and Al_2O_3 content from 5 to 10 mol%. Glasses were checked for crystallization using x-ray diffraction and the structure was characterized using Raman spectroscopy. Stability of the nitride during melting decreased with increasing TiO_2 and/or Al_2O_3 contents. The solubility of the nitride in the glass was also observed to decrease with TiO_2 and Al_2O_3 content, causing the formation of a titanium nitride rich layer forming on the surface of the glass. Electrical properties were investigated using impedance spectroscopy and mechanical behavior using Vickers indentation.

S3: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 1: Laser Crystallization and Modification

Room: La Vista F (22nd Fl)
Session Chair: Shifeng Zhou, South China University of Technology

1:20 PM

(GOMD-S3-006-2018) Femtosecond laser induced crystallization in transparent oxide glasses (Invited)

B. Poumellec*[1]; J. Cao[2]; M. Lancry[1]

1. CNRS-UnivParisSud, ICMMO/SP2M, France
2. Beijing Institute of Technology, Laser Micro/Nano-Fabrication Laboratory, School of Mechanical Engineering, China

One way for addressing the requirements of achieving frequency converters is to precipitate optical non-linear crystals along waveguides that can be elaborated in the same time. The technique of Direct Laser Writing with femtosecond laser is proposed in this direction. During the presentation, I will make a short review on published results. From that and our own results in silica based glasses, I will suggest a mechanism for the thermal control of the crystallization with such a powerful laser according to the glass physico-chemical properties. Another important aspect for integrated optics, is the control of the direction of the crystals. We will show, alike other authors, that there is a laser parameter domain where a classical mechanism based on thermal gradient is suggested for driving the crystal orientation. But in that case it is difficult to have the polar axes of the crystals in the direction of the waveguide light polarization. However, in Li_2O-Nb_2O_5-SiO_2 glass, there exists another laser parameter domain where the crystal orientation is tunable with the writing light polarization. The constraint here is that crystal size has to be nanoscopic. Therefore, the pulse energy and speed of writing should be adjusted accordingly. This is the first time that the motive action of light in crystal growth has been clearly demonstrated. Associated mechanism of action of light on crystals will be presented.

1:50 PM

(GOMD-S3-007-2018) Fabrication of rotating lattice lithium niobate single crystal lines within lithium niobosilicate glass via femtosecond laser irradiation

K. J. Veenhuizen*[1]; I. Crawley[2]; S. McAnany[3]; D. Nolan[4]; B. Aitken[4]; 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
4. Corning Incorporated, USA

Femtosecond laser irradiation enables a spatially selective growth of lithium niobate ($LiNbO_3$) crystals deep within lithium niobosilicate (LNS) glass ((100-x) $LiNbO_3$ – x SiO_2) making these crystals potentially useful as passive and active optical interconnects in a 3D integrated optical assembly. This work explores the different achievable growth modes of $LiNbO_3$ in LNS glass by systematically varying laser scanning speed, laser power, and glass composition. Two growth modes are observed: (1) a polycrystalline growth mode, which emerges above a critical laser scanning speed depending on the amount of glass former, and (2) a single crystal growth mode exhibiting intriguing lattice orientation behavior. In the case of the latter mode, the lattice gradually rotates until the c-axis at the center of the crystal cross-section becomes parallel with the laser scanning direction. In addition, there is a symmetric lattice misorientation with respect to c-axis orientation in the center of the crystal cross-section that increases radially outward to the crystal-glass interface. Lattice rotation rates as a function of laser processing parameters are determined. The effect of different laser intensity distributions on the lattice orientation is also investigated.

2:10 PM

(GOMD-S3-008-2018) Space-Selective Modification of Glass by Using Femtosecond Laser (Invited)

S. Zhou*[1]; J. Qiu[2]

1. South China University of Technology, School of Materials Science and Engineering, China
2. Zhejiang University, College of Optical Science and Engineering, China

Laser induced modification and damage in transparent materials (e.g., glass) has attracted considerable interest and been studied since the advent of high power pulsed lasers. Especially while using a femtosecond laser as the irradiation source, the tight focusing and nonlinear nature of the absorption make it possible to confine the absorption to the focal volume inside the bulk of the material, allowing for micromaching in extremely small region. In this talk, we introduce the progress in space-selective modification of glass by using femtosecond laser. We show that some fundamental processes, including valence state change of dopant, decomposition of cluster, element redistribution, phase transition and nanocrystallization, can occur in the femtosecond laser irradiation region inside glass. As a result, the optical response of the modified glass can be controlled. For examples, the luminescence properties of main group ions doped glass can be tuned and tunable luminescence can be achieved. The microstructures with multicolor luminescence can be induced. The results suggest that space-selective modification of glass by using femtosecond laser can be applied to fabricate various types of 3D active microstructures.

2:40 PM

(GOMD-S3-009-2018) In situ observation of Sb_2S_3 crystal formation in Sb-S-I glass by micro x-ray diffraction

C. Au-Yeung*[1]; C. Stan[2]; H. Jain[1]; V. Dierolf[1]

1. Lehigh University, USA
2. Lawrence Berkeley National Laboratory, USA

Fabricating single crystals in glass via laser-heating provides a new class of metamaterials that can introduce multiple novel functionalities for micro/nano-opto-electro-mechanical systems. Single crystal growth has been successfully achieved via continuous wave laser heating to create crystal dots and 2D architectures in Sb-S-I chalcogenide glasses. In these crystal architectures formed by a solid-solid transformation under steep temperature gradient, a rotating lattice is identified. Recent ex-situ micro scanning x-ray diffraction experiments, μSXRD, and electron back scattered diffraction, EBSD, analysis have characterized the nature of the observed lattice rotation. However, these do not provide information on the detailed process of lattice formation that proceeds via crystal nucleation and growth. Here we present in situ observation during Sb_2S_3 crystal formation under laser/X-irradiation, which provides insight of the origin of the rotating lattice within these single crystals. We observe that a single crystal diffraction pattern first forms gradually and then begins to rotate i.e. the entire seed crystal rotates while maintaining a clear diffraction pattern. As the crystal continues to grow, the diffraction pattern stabilizes, and the seed crystal rotation stops. The implications of these observations for lattice rotation and crystal growth in a confined medium will be discussed.

3:00 PM

(GOMD-S3-010-2018) Femtosecond Laser Modifications of Lanthanum-Rich Optical Glasses

D. K. Dobesh*[1]; S. K. Sundaram[1]

1. Alfred University, Glass Science, USA

Femtosecond laser allows for precise modifications of glasses spatially as well as temporally. The irradiation will alter structural connectivity, which can be tailored by selection of the base glass composition. Our investigation was focused on the optical refractive index modification from a high repetition rate femtosecond laser on lanthanum-rich aluminosilicates enabling high contrast refractive

index changes. The linear and non-linear refractive indices were measured using an optical prism coupler, including measurements in the terahertz (THz) spectrum. The ion distribution and network polymerization were investigated using Raman, Nuclear magnetic resonance (NMR) and Fourier-Transform Infrared (FTIR) spectroscopy to correlate the high contrast refractive index zones modified by the laser source to glass structure. Optical breakdown and structural relations with rare-earth element content within the glass was the basis for the effects due to the coupling of the laser source. Ion polarizability and the network structure connectivity were investigated for modifying optical properties. We will present our results on the structure-optical properties correlation in these glasses.

Session 1: Laser Crystallization

Room: La Vista F (22nd Fl)
Session Chair: Bertrand Poumellec, UPSud

3:40 PM

(GOMD-S3-011-2018) Ultrafast laser processing of glass and sapphire using nondiffracting beams (Invited)

F. Courvoisier*[1]; R. Meyer[1]; J. DelHoyo[1]; C. Xie[1]; L. Rapp[1]; L. Furfaro[1]; P. Lacourt[1]; M. Jacquot[1]; L. Froehly[1]; R. Giust[1]; J. Dudley[1]

1. CNRS, FEMTO-ST Institute, France

Ultrafast lasers used for micro and nano machining now offer the reliability and performance for mass production. In the particular field of transparent materials processing, a key capability of ultrashort pulses is that they can drill and modify matter from inside the material itself. We demonstrate that using appropriate beam shaping, it is possible to produce voids or nano-channels using a single pulse in even the hardest materials, and this has recently led to major advances in the field of stealth dicing, which is a non-ablative technique used to cleave and separate transparent materials at extremely high processing speeds. We report novel recent developments where Bessel beam have been used to create cracks and cleave sapphire, but also where symmetry has been broken to enhance cleaveability of laser-processed glass. The research leading to these results has received funding from the European Union Seventh Framework Programme [ICT 2013.3.2 Photonics] under grant agreement No 619177 TiSa-TD and from the European Research Council (ERC-CoG-682032-PULSAR).

4:10 PM

(GOMD-S3-012-2018) Challenges of fabrication of single crystal architecture in glass: Transition from dot to line

D. Savytskyy[1]; V. Dierolf[2]; N. Tamura[3]; H. Jain*[1]

1. Lehigh University, International Materials Institute for New Functionality in Glass, USA
2. Lehigh University, Physics Department, USA
3. Lawrence Berkeley National Laboratory, USA

Laser-induced crystallization of glass has become a viable method for fabricating single-crystal architecture in glass (SCAG), where a CW laser may be used to heat the glass locally to initiate nucleation and form a seed crystal, which is then grown into a single crystal line. In this region of transition from dot to line, sometimes we observe unwanted grain boundaries during the growth of Sb_2S_3 SCAG in Sb-S-I glass as a model system. In particular, such grain boundaries are observed during the growth of Sb_2S_3 crystals in $16SbI_3$–$84Sb_2S_3$ glass, whereas they are absent in Sb_2S_3 glass. We correlate this difference in tendency to form multiple grains with the relative glass forming ability i.e. the dynamics of nucleation and crystal growth as determined by differential scanning calorimetry (DSC). On the basis of this understanding, methods to minimize the appearance of grain boundaries in the transition region are suggested.

4:30 PM

(GOMD-S3-013-2018) Compositional dependence of nucleation and growth of single crystal $LaBGeO_5$ in La_2O_3-B_2O_3-$2GeO_2$ glass by femtosecond laser irradiation

S. McAnany*[1]; K. J. Veenhuizen[2]; D. Nolan[3]; B. Aitken[3]; V. Dierolf[4]; H. Jain[1]

1. Lehigh University, Materials Science & Engineering, USA
2. Lebanon Valley College, Physics, USA
3. Corning Incorporated, USA
4. Lehigh University, Physics, USA

Selective heating of glass using a femtosecond laser offers a unique processing technique for creating optically active 3D single-crystal architecture in glass, which can be used to create photonic integrated circuits for optical telecommunication. It has been shown that under certain processing conditions, single crystal $LaBGeO_5$ architectures can be formed in glass of the same stoichiometric composition. Notwithstanding, fabrication of single crystal from incongruent glass composition can broaden the applicability of this technique, as the composition can be tailored to manipulate the nucleation and growth stages of the crystallization process. Accordingly, in this work, the effect of glass composition i.e. x in xLa_2O_3-B_2O_3-$2GeO_2$ (x = 0.8 - 1.2) on the formation of $LaBGeO_5$ single crystal architectures by femtosecond laser irradiation is investigated. In particular, the laser processing parameters necessary to create the single crystal for each composition are correlated with the nucleation and growth characteristics as determined by differential scanning calorimetry.

4:50 PM

(GOMD-S3-014-2018) Non-perturbative quantum method for the interaction between intense laser and fused silica

H. Deng[1]; X. Dong[1]; X. Yuan[2]; W. Liao[2]; L. Liu[1]; W. Zheng[2]; X. Zu*[1]

1. University of Electronic Science and Technology of China, School of Physical Electronics, China
2. Research Center of Laser Fusion, China Academy of Engineering Physics, China

The study of interaction between intense laser and solids is one of the most active research frontiers. Two different methods, classical approximation and a quantum perturbation approach, have been usually adopted to describe the interaction between solid state electron and laser. However, they all have limitations. In the classical approximation, laser field is treated as an alternating electric field and the quantum nature is neglected. In the case of the quantum perturbation approach, the time dependent perturbation theory is employed to calculate the laser-electron interaction. This perturbation treatment of laser-electron interaction has limitation in the high intensity laser, especially at laser intensities as high as the order of terawatt, which can now be easily reached by femtosecond laser. Non-perturbative quantum method overcomes limitations of tradition approaches and its application is no longer limited by laser parameters. In this report, a general theoretical scheme of non-perturbative quantum method for the interaction between intense laser and solids is introduced, and two examples of the application of this method in the interaction between fused silica and femtosecond laser are presented. One example is the calculation of energy absorption rate of conduction band electron in fused silica, the other is the phenomena of cold impact ionization in fused silica.

S4: Glass Technology and Cross-Cutting Topics

Session 1: Glass Surface Modification and Electric Field Effects

Room: La Vista C (22nd Fl)
Session Chairs: Nicholas Smith, Corning Incorporated; Robert Schaut, Corning Incorporated

1:20 PM

(GOMD-S4-007-2018) Optical and chemical functionalities controlled at the micrometer scale in glassy materials by an imprinting thermo-electrical process (Invited)

M. Dussauze*[1]; A. Lepicard[1]; F. Bondu[1]; V. Rodriguez[1]; L. Karam[1]; F. Adamietz[1]; K. Richardson[2]; T. Cardinal[3]; E. Fargin[3]

1. ISM University of Bordeaux, France
2. University of Central Florida, CREOL, USA
3. ICMCB-CNRS, France

Merging functionalities of integrated photonic and surface science engineering in a single device has the potential to become a ubiquitous technology, allowing individuals to assess their health or environment and impacting a wide range of economic and industrial domains. In this context, we report on the ability of a thermal poling treatment to be considered as an imprinting process modifying optical properties as well as surface chemistry of glasses. Concerning optical properties, the formation of gradient of refractive index (GRIN) with large variations (up to 5.10^{-2}) have been optimized. such an imprinting process of GRIN has been demonstrated by forming matrices of micro-lenses (sizes 5-100μm) on large area (tens of centimeters square). Using this process, second order optical properties have been implemented in isotropic materials at the micrometer scale. A geometry control of the electro-optical anisotropy induced has been controlled in periodic structure as shown by the fabrication of SHG gratings. Such patterning of optical responses can be obtained successfully on both oxide and chalcogenide glasses. Finally, by combing specific structural rearrangements and charge implementations, we have demonstrated very strong and localized influence of the μ-poling treatment on surface reactivity, surface potential, and surface durability.

1:50 PM

(GOMD-S4-008-2018) Chemical structure and mechanical properties of soda lime silica glass surfaces treated by thermal poling in inert and reactive ambient gases

J. Luo[1]; M. Lanagan[2]; C. G. Pantano[3]; S. H. Kim*[1]

1. Pennsylvania State University, Chemical Engineering, USA
2. Pennsylvania State University, Engineering Science and Mechanics, USA
3. Pennsylvania State University, Materials Science and Engineering, USA

This talk addresses the effects of anodic thermal poling at 200°C in various gas environments (Ar, N_2, O_2, H_2O) as a means to modify the surface mechanical properties of soda lime silica float glass. Systematic analyses of the chemical composition, thickness, silicate network, trapped molecular species and hydrous species in the sodium-depleted layers revealed correlations between subsurface structural changes and mechanical properties such as hardness, elastic modulus and fracture toughness. A silica-like structure was created in the inert gas environment through restructuring of Si-O-Si bonds at 200°C in the Na-depleted zone. This silica-like surface also showed enhancement of hardness comparable to that of pure silica glass. The anodic thermal poling condition was found so reactive that O_2 and N_2 species can be incorporated into the glass, which also alters the glass structure and mechanical properties. In the case of the anodic surfaces prepared in a humid environment, the glass showed an improved resistance against crack formation, which implies that abundant hydrous species incorporated during thermal poling could be beneficial to improve the toughness.

2:10 PM

(GOMD-S4-009-2018) Texturizing Approaches for the Controllable Alteration of Contact interactions between Glass and Metal Surfaces

G. Agnello*[1]; H. Jing[1]; T. Brown[1]; N. Z. Zhelev[1]; R. Manley[1]; J. Banerjee[1]

1. Corning Incorporated, USA

As flat panel glass functional thicknesses continue to decrease and product attribute requirements for high end consumer electronics applications become more stringent, contact events (whether frictive or normal in nature) between glass and other surfaces become increasingly problematic. These types of events can directly lead to glass surface Electrostatic Charging (ESC) as well as related stiction phenomena, which can, in turn, contribute to critical yield losses in the manufacture of flat panel displays. Glass surface texturing methods can be effective in minimizing tribo-charging as well as in altering the sticking behavior between such surfaces and other contacting materials. Here we report the effects of various texturizing approaches on stiction and ESC. The data suggest that the processes used for texturing, composition of the glass, and the conditions through which contacts are made play significant roles in how surfaces accumulate and/or dissipate ESC and whether or not said charge is directly correlated with adhesion behavior. In an attempt to explain some of the observed trends, ionic, dispersive and/or liquid mediated inter-surface forces are discussed with reference to the data.

2:30 PM

(GOMD-S4-010-2018) Electrostatic charging and retraction force measurements upon contact separation of glass and various roughness controlled surfaces

N. Z. Zhelev*[1]; G. Agnello[2]; T. Brown[2]; I. Bhattacharyya[1]; R. Manley[1]

1. Corning Incorporated, Thin Films and Surfaces, USA
2. Corning Incorporated, Display Technology Development, USA

Electrostatic charging and glass stiction are two common problems that flat panel display manufacturers experience during production. Here, we present experimental results based on a custom designed measurement system, which allows us to explore the interaction between thin glass sheets and special micro-machined flat silicon vacuum plates. By coating the plates with a range of metallic and dielectric coatings, and through controlling for nanoscale roughness and conditions of contact (contact load/time, vacuum force, retraction speed, as well as relative humidity and temperature), we can create an accurate tribo-electric series for various glass types. Simultaneously, we can study how the force required to separate the glass from the vacuum plate depends on the contacting surface material. Further, we investigate the relationship between electrostatic charging and the force of separation. We also explore the role of roughness, relative humidity and glass chemistry.

2:50 PM

(GOMD-S4-011-2018) Effect of Different Factors on Conveyance mode Tribo-charging of Display Glasses

I. Bhattacharyya*[1]; N. Z. Zhelev[1]; G. Agnello[2]; C. Cole[2]; R. Manley[1]

1. Corning Incorporated, Thin Films and Surfaces, USA
2. Corning Incorporated, USA

Electrostatic charging of insulator materials is poorly understood since there is no mobile charge carrier present in perfect insulators. In general, there have been a number of mechanisms proposed to explain tribocharging in insulator materials, which included electron transfer, mobile ion transfer from adsorbed water layer on insulator surface or even material transfer. Display glasses which have fairly complex surface composition pose sufficient challenge to study

electrostatic charging due to tribology. However, it is necessary to understand interactions of different materials with commercial glasses in order to address yield/cost issue related to electrostatic charging in processing lines. Here, we present tribocharging study of different materials that can potentially interact with sheet glass in a manufacturing line. With the use of customized equipment, we mimic the rolling and planar friction/rubbing motions of a conveyance belt in a production line and study the effect of contacting material, glass type, contact force and relative humidity. By utilizing this study, we could eventually choose appropriate material for conveyance along with the right contact force and ambient conditions to mitigate any electrostatic charging related failures.

Session 1: Coatings, Adhesion, and Reactivity of Glass Surfaces

Room: La Vista C (22nd Fl)

Session Chairs: Robert Schaut, Corning Incorporated; Nicholas Smith, Corning Incorporated

3:40 PM

(GOMD-S4-012-2018) Reactivity of Water on CAS Glasses Surfaces using Molecular Dynamic Methods

L. Wang*[1]; G. Agnello[2]; R. Manley[2]; N. J. Smith[2]; A. Cormack[1]

1. Alfred University, USA
2. Corning Incorporated, USA

Glasses based on ternary calcium aluminosilicate (CAS) compositions play important roles in display glasses. The difficulty in experiments is to understand the surface structures and to track the corresponding surface reactivities. In this presentation, we explore the surface structures and reactivities of four different CAS compositions, using molecular dynamics methods. Our simulations track the evolution of various structural species that form from the initial reactions of water molecules with the glass surfaces, over a 5 ns period at room temperature. These include species such as Al-OH_2, Al-OH, Si-OH, and Si-OH_2. Where dissociation of the water molecules is involved, we also investigate the behavior of both of the dissociation products. From these results, it is possible to comment on the role of surface chemistry in the surface reactivity.

4:00 PM

(GOMD-S4-013-2018) Roughness effect on adhesion between glassy silica and polyimides

S. Lee*[1]; R. J. Stewart[2]; A. R. Rammohan[2]

1. Corning Technology Center Korea, Modeling, Republic of Korea
2. Corning Incorporated, USA

The adhesion between rough glassy silica and polyimide is investigated by molecular dynamics simulation. A pulling force is applied to mimic the experimental detachment process, and the potential of mean force is measured to calculate the adhesion energy of the interface. Various rough silica surfaces are generated varying roughness amplitude, spacing, and surface hydroxylation densities in an attempt to investigate the influence of surface characteristics on adhesion. The calculated results reveal that R_a is the most effective parameter within the considered conditions. Adhesion can increase when roughness spacing decreases due to the surface area expansion, but if vacant volume exists at the interface, adhesion decreases. Competition of these two factors leads to the maximum adhesion energy at a specific spacing of roughness, and hence spacing of roughness is another key parameter for the adhesion between glassy silica and polyimides.

4:20 PM

(GOMD-S4-014-2018) Crystallization mechanism of BaO-CaO-Al_2O_3-SiO_2 glass thin films

F. O. Mear*[1]; T. Carlier[1]; S. Saitzek[1]; J. Blach[1]; R. Podor[2]; L. Montagne[1]

1. Lille University, France
2. Marcoule Institute for Separation Chemistry, France

Glasses and glass-ceramics are a technological solution to achieve efficient materials able to operate at high temperatures, such as for enamel protective coatings applications. To overcome cracking when subjected to thermal cycles, self-healing is a promising solution. The self-healing property is defined as the capacity of a material to recover its mechanical integrity and initial properties after destructive actions of external environment or under internal stresses. We have developed an innovative approach based on self-healing glassy thin films. They are based on a heterostructure made of alternating layers of glass-ceramics and active particles, deposited by PLD or EB-PVD. The characterization of the films has been carried out with ellipsometry, ToF-SIMS, AFM, electron microprobe and XPS. The self-healing effect has been observed in-situ at high-temperature by environmental SEM (HT-SEM). Since glass-ceramics have superior mechanical properties than glasses, we investigated the glass to glass-ceramic transformation of our glass thin films. The composition of the glass is 28BaO-14CaO-10Al_2O_3-48SiO_2. Glass thin films of 150 nm thickness were elaborated by PLD and their crystallization was studied in-situ by HT-XRD and HT-SEM. The crystallization behavior of the thin glass layer was compared to the bulk one, and some difference was observed.

Session 4: Waste Immobilization - Corrosion I

Room: La Vista D/E (22nd Fl)

Session Chair: Karine Ferrand, SCK-CEN

3:40 PM

(GOMD-S4-015-2018) Comparisons of Volcanic Glass Dissolution Microstructures in Roman Marine Concrete and Surtsey Basalt (Invited)

M. D. Jackson*[1]

1. University of Utah, Geology and Geophysics, USA

Dissolution of volcanic glass has occurred over the past 50 years in tephra deposits at Surtsey volcano, a young oceanic island in Iceland, and over the past 2000 years in Roman marine harbor concretes. The glass, gel, and authigenic mineral microstructures of these systems provide guideposts for evaluating long term performance of nuclear waste glass and cementitious waste forms. In Roman concretes with Campi Flegrei pumice aggregate, early Stage I dissolution at 60–95°C produced pozzolanic calcium-aluminum-silicate-hydrate binder (C-A-S-H). Slower Stage III dissolution at ambient temperatures above and below sea level then produced zeolite and Al-tobermorite cements that enhance chemical and mechanical resilience. By contrast, partial Stage III basaltic glass dissolution at Surtsey above sea level at 25–100°C has produced nanocrystalline clay mineral (nontronite), zeolite and Al-tobermorite in time-lapse 1979 and 2017 drill cores. Stage III dissolution in the submarine hydrothermal system at 100–141°C is nearing completion. Nanocrystalline clay mineral (nontronite) is abundant, and zeolite and Al-tobermorite mineral cycling is occurring in chemically dynamic microenvironments. Lower temperatures, higher Si/Al activity, alkalinity, and pH in ancient Roman marine concrete produced reduced dissolution rates and negligible clay mineral, relative to young Surtsey basalt.

4:10 PM

(GOMD-S4-016-2018) Measured Parameters for ANL Glass Dissolution Model

W. Ebert*[1]; C. Snyder[1]; J. Jerden[1]

1. Argonne National Lab, USA

Modified Product Consistency Tests were conducted with AFCI and LRM glasses at 70 and 90 °C to measure the effects of glass composition and various imposed solution pH, Al and Si concentrations on the residual and Stage 3 glass dissolution rates and the initiation of Stage 3 behavior. Various amounts of K_4SiO_4 glass and reagent $Al(OH)_3$ were mixed with the crushed glass (-200+325 mesh size fraction) and demineralized water (glass S/V ratio about 2000 m^{-1}) in Teflon vessels; the pH was adjusted with dil. NaOH when the test was assembled. Solutions were analyzed bi-weekly to track the solution composition and indicate the initiation of Stage 3. Stage 3 was triggered in all tests with AFCI glass at 90 °C and pH 12.5 after about 60 days, but was not triggered in tests at pH 11.5, 10,5, or 9.5 or in tests at 70 °C. Solids examined after the tests were completed indicate phillipsite had formed in tests showing Stage 3 behavior, but not in other tests. An aluminosilicate similar to chabazite formed in the tests conducted with LRM glass at 90 °C showing Stage 3 behavior. The measured B concentrations were used to quantify the residual and Stage 3 glass dissolution rates. Both rates depended on temperature, but were independent of the Al and Si concentrations and pH. Combination with results of previous tests at 125, 150, and 200 °C provided activation energies for the two glasses and simple rate laws were derived for use in modeling.

4:30 PM

(GOMD-S4-017-2018) Induced Stage III Glass Dissolution Behavior

J. V. Crum*[1]; B. Parruzot[1]; J. Ryan[1]; l. Seymour[1]; J. F. Bonnett[1]

1. Pacific Northwest National Lab, USA

Aluminoborosilicate glasses are utilized to immobilize nuclear waste in many countries. During glass dissolution studies, three distinct stages of corrosion behavior have been observed over time in static conditions: fast dissolution in dilute conditions (Stage I), very slow dissolution as reaction proceeds (Stage II), and an occasionally observed dramatic acceleration in corrosion (Stage III). High release rates during Stage III relative to Stage II are a concern when predicting the performance of glasses over geologic time scales. Stage III is often accompanied by the formation of zeolite phases, but forecasting the initiation of Stage III behavior is highly unpredictable in a laboratory setting likely due to the variability of zeolite nucleation time. In an effort to gather Stage III dissolution data in a more systematic way, several zeolite phases (i.e., P1, P2, analcime, and clinoptilolite) were seeded into static glass dissolution tests at various temperatures during Stage II to induce Stage III behavior sooner and in a more predicable time frame. The responses of several simulated waste glasses to the different zeolite seeds are presented along with solids analysis of the corroded glasses and secondary phases precipitated during testing. The Stage II and Stage III dissolution rates were determined at multiple temperatures and an activation energy was calculated.

4:50 PM

(GOMD-S4-018-2018) Glass alteration monitored by Raman spectrometry: From boron to other species

B. Parruzot*[1]; A. M. Lines[1]; S. A. Bryan[1]; J. Ryan[1]

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

An in-situ Raman system was custom-built to monitor up to 10 experiments simultaneously via in-situ probes immersed in the leachate. Utilizing in-situ measurement allows for the continuous collection of data while also limiting perturbations brought to the experiment during samplings (e.g. changes in temperature, contamination). The technique was shown to be useful when the glass was exhibiting Stage III behavior. To date, we have focused on relating the amount and speciation of boron in solution. Boron speciation remains simple, with resolvable Raman signals indicating the transition of two species between pH 8 to 11. Glass corrosion introduces many other species into solution, however. Many of these either have a measurable impact on the extent of corrosion or can provide insight into corrosion mechanisms. Detailed speciation in solution is valuable to characterize the geochemical interaction between the different components in the system, including both solids and solutes. Further, the impact of these species can be evaluated independently of whether they are released during glass alteration (e.g. silicates) or already present in the groundwater contacting the glass (e.g. nitrates). This study will propose a survey of relevant species and discuss the applicability of Raman monitoring to their quantification and speciation in conditions relevant to glass alteration in a repository environment.

S5: Dawn of the Glass Age: New Horizons in Glass Science, Engineering and Applications

Glass: Yesterday, Today and Tomorrow

Room: El Mirador East (22nd Fl)

Session Chair: Mark Mecklenborg, The American Ceramic Society

12:20 PM

(GOMD-S5-008-2018) A Mentor and a Gentleman: L. David Pye and IJAGS (Invited)

M. Affatigato*[1]

1. Coe College, Physics, USA

This short presentation will focus on the work Prof. L. David Pye carried out after his formal retirement, focusing on his founding of the International Journal of Applied Glass Science (IJAGS). Using his diplomatic and scientific skills, Prof. Pye was able to initiate an international journal that has quickly attained a high impact in the field. On the personal side, the presenter will speak to the great advice and mentoring he received as he worked with Dr. Pye over the last few years, and to his observations on the kind and wise manner in which he carried out his work. From his constant analysis of the field to his unending interest in students and young researchers, Dr. Pye is a model of professional courtesy and mentorship. Finally, the presentation will cover the scientific impact that Prof. Pye has had through the foundation of IJAGS, affecting the global glass community as well as academic organizations.

12:40 PM

(GOMD-S5-009-2018) Glass Through the Ages (Invited)

M. K. Choudhary[1]; J. C. Mauro[2]; L. D. Pye[3]; K. Richardson[4]; A. K. Varshneya*[5]; E. Dutra Zanotto[6]

1. Owens Corning, USA
2. Pennsylvania State University, USA
3. Alfred University, USA
4. University of Central Florida, USA
5. Saxon Glass Technologies, Inc., USA
6. Federal University of Sao Carlos, Brazil

The development of glass through the ages is chronicled. Attention is paid to its ageless beauty and its near-lossless light transmission. More properties that distinguish glass from other materials are highlighted. The audience is polled to list the ten glass applications and/or processes that changed the world. (Results will be presented at the banquet.)

1:00 PM

(GOMD-S5-010-2018) Welcome to the Glass Age (Invited)

J. C. Mauro*[1]

1. Pennsylvania State University, Materials Science & Engineering, USA

In this tribute to David Pye, I welcome the audience to the Glass Age, discussing the numerous transformative technological and societal advancements made possible by glass. Thanks to advances in our fundamental understanding of glass physics and chemistry, the pace of innovation in glass science and technology is only accelerating. I will offer some perspective on the unique capabilities offered by glass to solve some of our world's most urgent challenges in the areas of healthcare, information technology, energy, and the environment. Realizing the potential of the Glass Age will require collaboration, resources, and support, but it is an opportunity we cannot afford to waste.

Science and Education II

Room: El Mirador East (22nd Fl)
Session Chair: Edgar Dutra Zanotto, Federal University of Sao Carlos

1:25 PM

(GOMD-S5-011-2018) Thinking at Different Wavelengths- Glass Art, Science, and Education (Invited)

R. Brow[1]; M. Reidmeyer*[1]; P. Freudenberger[1]

1. Missouri S&T, Materials Sci & Engrg, USA

Prof. David Pye has long recognized that the aesthetic qualities, scientific mysteries, and technological applications of glass inspire students with different interests and perspectives to work with and study our favorite material. At Missouri S&T, we find that students discover glass by following similar paths. Some students are attracted to study glass because of familiar or exciting applications, from cell phones to wound-healing glass fibers. Some enter through our Hot Glass Shop and Gaffer's Guild, where they learn to control the flow and form of molten glass and where their creative talents spark their technical interests. Others discover glass in their sophomore lectures and labs, where students learn to apply principles of physics and chemistry to understand composition-structure-property relationships, and where their creativities are sparked by assignments to design their own glass compositions. In this talk, we will review how we try to weave art and science and technology into the classroom, laboratory, and studio experiences of our students, to provide them with the broad, glassy perspective championed by Prof. Pye.

1:40 PM

(GOMD-S5-012-2018) Things I Wish I Learned in School: What 20 Years of Glass Innovation has Taught (Invited)

M. Dejneka*[1]

1. Corning Incorporated, USA

Universities do a great job of preparing students for the work force. However, they cannot teach us everything, nor can we retain all that is taught or appreciate the importance of seemingly mundane properties like liquidus or viscosity until we need to get a glass article into production. This talk will show how the optimization of minor secondary properties can make the difference between an invention and a billion dollar success. We will also explore how remarkable technologies like transparent nano-composites for 3-D displays or fluorescent microbarcodes can be relegated to the shelf for non-technical reasons. It will conclude with lessons learned and some tips for success.

1:55 PM

(GOMD-S5-013-2018) The functional glass movement (Invited)

H. Jain*[1]

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

Glass has served the society with various functions over centuries. Thus wrote David Pye 47 years ago, "Glass is a versatile and sometimes enigmatic substance. It functions equally well as a carrier of light, a protector of man and his inventions,…". Notwithstanding these age old attributes of glass, there appears to have started a renaissance, indeed a functional glass movement of research activity worldwide, as evidenced by the formation of 'International Materials Institute for New Functionality in Glass (IMI-NFG)' and 'Functional Glass Manufacturing Innovation Consortium (FGMIC)' in USA, 'Center for Research, Technology and Education in Vitreous Materials (CeRTEV)' in Brazil, and very recently EUs 'Centre for Functional and Surface Functionalized Glass (FunGlass)' in Slovakia. This talk will present a synopsis of scientific and engineering advancements, and education of glass through this global movement that led to Corning's declaration of present times as the 'Glass Age', or Pye's recognition as 'A special moment in time representing the arrival of the Glass Age'. Selected examples of the speaker's favorites will be included to make the point.

2:10 PM

(GOMD-S5-014-2018) Dave Pye's Borate Conference of 1977 (Invited)

S. Feller*[1]

1. Coe College, Physics, USA

The Ninth International Conference on Borate Glasses, Crystals, and Melts was held in Oxford in July 2017. However, The first borate conference, meant to be stand alone, and entitled Borate Glasses: Structure, Properties, Applications, was organized by Dave Pye, Norbert Kreidl, and others forty years earlier in June 1977. This meeting was held in Alfred, NY. Many luminaries in the field gave papers including Norbert Kreidl, Dave Griscom, Phil Bray, Al Cooper, Evgenny Porai-Koshits, Chuck Kurkjian, Bill LaCourse, and Dave Pye, of course. A wonderful book of proceedings came out as well. In this talk, in honor of Dave Pye, I will review the conference highlights, many of which remain important today. This conference especially resonates with me since it was my first professional meeting. Besides the science I will relate a few stories concerning the conference. The NSF is thanked under grant DMR 1407404 for support.

2:25 PM

(GOMD-S5-015-2018) THE GLASS OF WINE: A Toast to L. David Pye (Invited)

J. F. Shackelford*[1]

1. University of California, Davis, Materials Science and Engineering, USA

A career spent focusing on glass science at the University of California, Davis that is also home to the premier wine science program in America has led to a simple observation: wine is a rare beverage that is still predominantly stored, shipped, and consumed in glass. The intersection of two multi-billion dollar industries (glass and wine) is the subject of a new book, The Glass of Wine, by J.F. and P.L. Shackelford published by Wiley in conjunction with the American Ceramic Society. The book reviews the historical intertwining of glass and wine along with discussions of the culture and tradition of glass bottle and stemware designs. Not surprisingly, our research on the historical origins of glass was dependent on none other than Professor David Pye. When William Ellis wrote the cover article on "Glass" in the National Geographic 25 years ago, he turned to David Pye to recreate the historical origins of glassmaking. So, we raise the glass of wine in a toast to David, an indispensible scholar and leader in the glass community for this past half-century (and beyond) – salute!

2:40 PM

(GOMD-S5-016-2018) The Italian Connection (Invited)

A. Montenero*[1]

1. University of Parma (Italy) - Italian Association of Glass Technologists, Italy

Long time ago, at beginning of eighties, I switched from the UV Spectroscopy to a more applied field, the Glass. That time in Parma, Italy, there were three Glass Companies with about 3000 of workers. Then I was looking for an Institution where I could learn the best approach to my new research field. My choice was the SUNY College of Ceramics at Alfred. My application as visiting Professor had been accepted and I arrived to Alfred. The first person I met was Prof. David Pye. He was very kind with me and soon we became good friends and my skills in Glass Science improved a lot and we started with a fruitful cooperation. After that, I went many times in Alfred and Prof. David Pye came to Italy, mainly in Parma, attending many Conferences organized by the Italian Glass Association, ATIV and by the University of Parma. Cooperation and friendness never stopped.

2:55 PM

(GOMD-S5-017-2018) Dave Pye - Outer Space Visionary (Invited)

H. J. Stevens*[1]

1. Alfred University, Glass Engineering and Science, USA

Lunar Glass, as many know, was discovered during the Apollo Mission XII in the fall of 1969. The existance of glass on the moon puzzeled many geologists, especially as they pondered how such glass could have been created. To address this creation question, Dave Pye offered to apply Glass Science to obtain substaintial information of the Lunar Glass's formation history. Dave drafted a proposal to NASA, which was promptly funded and Alfred's Lunar Glass Project was launched in the Summer of 1970. This visionary work will be reviewed including the results of the study on ten NASA provided Lunar Glass samples, as well as additional visionary contributions Dave has made to the Glass Science community.

3:10 PM

(GOMD-S5-018-2018) Outlandish Ideas for a Better Glass World (Invited)

M. Rasmussen*[1]

1. Alfred University, retired, USA

As a scientist, artist and humanitarian, David Pye makes his life matter in the world of glass. Reading voraciously, reaching out to friends and colleagues, he takes action to solve a problem, despite the nay sayers who warn him that his outlandish idea will cost too much, will fail, has been tried before. So how did he persuade the National Science Foundation to fund a small glass program at the New York State College of Ceramics at Alfred University? Aware of technical and economic challenges to the US glass industry, confident this his glass scientist and engineer colleagues could help meet those challenges, he entered a National Science Foundation (NSF) competition and won the first national competition in the history of Alfred University. The Center for Glass Research became one of the premier NSF's industry-university-government centers in the United States. He put his formula for success into practice again when he created an educational study center to combine artistic creativity with scientific research. The Paul Vickers Gardner Glass Center at Alfred University holds the promise that future glass artists and scientists will discover the secrets imbedded in historic glass art for application in technical glass research. During his half-century career, David Pye has applied his formula for reading, research, reaching out, "ruminating" and acting to bring his seemingly outlandish ideas to fruition for a better world of glass.

S5 President's Session

Room: El Mirador East (22nd Fl)
Session Chair: Manoj Choudhary, International Commission on Glass, MKC Innovations LLC

3:45 PM

(GOMD-S5-019-2018) Standing on the shoulders of giants: The role of David Pye at ICG (Invited)

A. Durán*[1]

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

David Pye was professor of glass science at the School of Ceramic Engineering and Materials Science at Alfred University along with different positions in this university. His research on the behaviour of glass-forming melts including nucleation, crystallisation, redox effects, and nuclear waste vitrification have greatly contributed to the base of scientific knowledge continuing as research topics of many of today's young research scientists. His series on "Advances in the Melting and Processing of Glasses, Natural Glasses and Borate Glasses", stands out among the extensive literature on glass and ceramics. From this large and intense activity David Pye won international recognition and arrived to be President of the American Ceramic Society in 2008-2009 and President of the International Commission on Glass during 1997-2000. From this position, David guided the ICG in the transition to the new century establishing a Strategic Planning Committee that presented the new perspectives and challenges of ICG in the "Glass in the New Millennium: Challenges and Breakthrough Technologies" in Amsterdam in 2000. For this huge work he received in 2010 the President Award of the International Commission on Glass. This talk intends to highlight some of the ideas and results of the work of David Pye at ICG, from his role in the Technical Committes to that of President of the association.

4:00 PM

(GOMD-S5-020-2018) Prof. L. D. Pye: The brilliant glow of a multifaceted person in the journey of a multifaced material: Glass (Invited)

A. Yaraman*[1]

1. Advisory Board of Sisecam Academy Sisecam, Turkey

Glass, a passion of humanity in one form or another for 5000 years, has served us admirably and nobly. As one of the most widely used manufactured materials and certainly the most versatile, it is our heritage from the past and yet remains a challenge for the future. It is a privilege to honor Prof. L.D. Pye in this Symposium to celebrate his decades of dedicated contribution and service to the glass science and technology, his devotion to the educational enterprise, his endless energy for promoting cooperative and collaborative work at every possible platform, which also embraces a wide international scope. And most importantly, his innovativeness and accomplishments have lit up the path for the advancement of this unique material glass. His remarkable insight and his distiguished leadership have ensured our ambitions for continuous improvement of this fascinating material. His visionary approach and fantastic ability to build networks with the objective of expanding the scientific developments worldwide will always be highly regarded. His strong support of, and exceptional work in International Commission on Glass, as well as his commitment and invaluable efforts in broadening the involvement in glass research activities within the spirit of camaraderie and friendship will always be acknowledged, admired and greatly appreciated within the world of glass and beyond.

4:15 PM

(GOMD-S5-021-2018) L. David Pye and the Vitrification of High Level Waste (HLW) (Invited)

C. M. Jantzen*[1]

1. Savannah River National Laboratory, USA

I met Dr. Pye in 1982 and we were both new to the field of vitrifcation of High Level Waste (HLW) but not new to the field of glass chemistry. The Savannah River National Laboratory (SRNL), then known as Savannah River Laboratory (SRL) had numerous subcontracts with Dr. Pye and Alfred University over the next two decades that supported many graduate student studies. Dr. Pye and Alfred University also worked with our sister site, the West Valley Nuclear Fuel Services (WVNFS) who were also building and starting up a HLW melter in the same time frame. Dr. Pye hosted many symposiums at Alfred that brought the HLW glass communities and the non-nuclear glass communities together. The one that stands out as the most memorable in my mind was the Symposium (summer 1983) that melded together researchers studying natural glasses, manufactured glasses, and nulcear waste glasses. The diversity of the speakers and audience made it a huge success. David Pye and I have remained colleagues and friends for 35 years.

4:30 PM

(GOMD-S5-022-2018) Some Reflections on David Pye and a Short Review of Recent Progress in Multiscale Modeling and Dynamic Experiments on Various Glasses (Invited)

J. W. McCauley*[1]

1. Johns Hopkins University, HEMI, USA

My close friendship with David Pye began when I became the Dean of the New York State College of Ceramics at Alfred University in 1990, working with him on The NSF Industry- University Center for Glass Research. Working with Patel, ARL, and Strassburger, Ernst Mach Institute (EMI), high-speed cameras were used in Edge-on Impact (EoI) and ballistic arrangement impact tests to quantify damage and fragment formation on Starphire®, Borofloat® and fused silica glass plates. At ARL in 2011, Gazonas and I, with a large team, initiated an in-house multi-year program to lay the groundwork for Multiscale Modelling of non-crystalline ceramics (glass) in extreme environments. The premise of the work assumed that the properties resulted from multi-scale structures due to chemical nano-heterogeneities that control Short Range Order-SRO (bond lengths and angles), Intermediate Range Order-IRO (ring structure, nano/micro "crystallites") and macro-defects and free volume. A Materials by Design approach was used to try to establish generic, physics based methodology to compositionally design optimum glasses for specific applications. A dual theoretical and experimental approach using concurrent multi-scale modeling at the atomic (quantum mechanics), molecular dynamics and continuum (finite element analysis) scales was employed.

4:45 PM

(GOMD-S5-023-2018) Global glass education and training: Relevant skill sets for next-generation glass scientists and engineers (Invited)

K. Richardson*[1]

1. University of Central Florida, CREOL, USA

Education of 'next-generation glass scientists and engineers' goes beyond being 'book smart' or having meaningful hands-on experience in the laboratory. Future glass experts, the products we academics aim to produce, will need a combination of fundamental skill sets with real-world awareness of the global aspects of their future employer's business. That business could be in the commercial sector or in an academic or government research laboratory. David Pye pioneered this thinking in his efforts to expose all levels of students to the global nature of our discipline, through his efforts to bring world recognized 'glass legends' to the Alfred University classroom. Additionally, through his leadership in ACerS, ICG and most recently, the Ceramic and Glass Industry Foundation, David has extended this thinking in his approach to 'learning from our past to make a stronger future'. This talk highlights some of these contributions and the impact they have had on past Alfred graduates. The new face of global experiences in glass is presented and we postulate how future training may shape the expectations employers have, in their quest to identify and hire, the next generation work-force in our discipline.

5:00 PM

(GOMD-S5-024-2018) Alfred University and David Pye: Force for the Future (Invited)

M. Zupan*[1]

1. Alfred University, USA

Since the founding of the NYS College of Ceramics on its campus in 1900, Alfred University has been a force for the future of glass. It was the first to start a glass science program in 1936, and the first to offer a Ph.D. in glass science in 1991. Its graduates' contributions to glass science are legendary, but for more than five decades one alumnus, L. David Pye, class of '59, drove many of the advancements at Alfred. He was one of the founding directors of the National Science Foundation's Industry-University Center for Glass Research at Alfred, and the primary author of the proposal for the Ph.D. in glass science. He was a prolific researcher, and perhaps most importantly, a mentor to generations of Alfred University students who have gone on to make significant contributions to the field.

Poster Session and Student Poster Competition

Room: Salon del Rey (Mezzanine Level)

6:30 PM

(GOMD-GSP-P001-2018) Influence of vanadium oxide doping on the structure, properties and dissolution behaviors of ISG nuclear waste glasses

X. Lu*[1]; J. Neeway[2]; J. Ryan[2]; J. Du[1]

1. University of North Texas, Material Science and Engineering, USA
2. Pacific Northwest National Laboratory, USA

Transition metal oxides are commonly present in nuclear waste and they can alter the structure, properties, and dissolution behavior of the glasses used to immobilize these wastes. V_2O_5 has been proven to improve sulfur solubility in borosilicate glasses, which is essential for immobilization of sulfate containing wastes. However, high V_2O_5 addition decreases melt processing rates due to the increase of melt foaming. In this study, we systematically investigated vanadium oxide addition (up to 8.0 mol%) in the International Simple Glass (ISG), a model nuclear waste glass system, with a composition (mol%) of $60.2SiO_2$-$16.0B_2O_3$-$12.6Na_2O$-$3.8Al_2O_3$-$5.7CaO$-$1.7ZrO_2$. Physical properties and optical properties of ISG altered by vanadium oxide were studied. It was found that both glass transition temperature and density decreased with increasing V_2O_5 addition. Interestingly, hardness and brittleness of the glasses decreased with higher V_2O_5 addition, while fracture toughness increased. From UV-Vis spectroscopy test, vanadium ions were found to be mostly 5+ at low V_2O_5 addition, while V^{4+} and V^{3+} appear in the glasses with high V_2O_5 addition. Additionally, static chemical durability tests were performed at 90 °C with a starting pH value of 7 and a surface-area-to-solution-volume of 200 m^{-1} for 112 days in order to test the effect of V_2O_5 on chemical durability.

(GOMD-GSP-P002-2018) DFT calculations of ^{29}Si and ^{31}P NMR in silicophosphates

I. Ponomarev*[1]; P. Kroll[1]

1. University of Texas, Arlington, Chemistry and Biochemistry, USA

We investigate ^{29}Si and ^{31}P NMR in silicophosphate glasses by density functional theory (DFT) calculations within the gauge-including projector augmented wave (GIPAW) method. Glass models are generated via melt-quench simulations using either ab-initio molecular dynamics (MD) throughout or classical potential MD combined with DFT optimization. Our target is to quantify the impact of neighbors and local structure on the chemical shift of ^{29}Si and ^{31}P and to provide means to extract that information from experimental data. Considering 4-coordinated Si atoms we establish correlations between ^{29}Si chemical shift and the Si-O-(Si,P) angles on neighboring O sites. Differences in slopes of angular correlations need to be taken into account when extracting bond angle data. For 6-coordinated Si atoms the Si-O bond lengths add to impact of Si-O-(Si,P) angles. In both cases, each P atom as second nearest neighbor to Si causes a 5-6 ppm decrease of the ^{29}Si chemical shift. We further establish angular correlation functions between ^{31}P chemical shifts and neighboring P-O-(Si,P) angles for both $[PO_{3/2}O]$ and $[PO_{4/2}]^+$ sites. The presence of Si in second coordination to P causes a decrease of the ^{31}P signal by 4-5 ppm for every Si atom. Finally, we apply our correlation functions to analyze ^{29}Si and ^{31}P NMR spectra of sol-gel derived silicophosphates to extract structural information: second neighbors, bond angles, $Si^{[6]}$-O bond distances.

(GOMD-GSP-P003-2018) Time and Humidity Dependence of Indentation Cracking in Aluminosilicate Glasses

T. K. Bechgaard*[1]; J. C. Mauro[2]; M. M. Smedskjaer[1]

1. Aalborg University, Denmark
2. Pennsylvania State University, Department of Materials Science and Engineering, USA

The inherent brittleness and poor crack resistance of oxide glasses have always been among their main limitations for advanced applications. As the formation of cracks leads to amplification of applied tensile stresses and ultimately catastrophic failure, there is an interest in understanding the composition and structure dependence of crack initiation and growth. The resistance to cracking can conventionally be measured using instrumented indentation that mimics the real-life damage for certain applications. Wada introduced a method to evaluate the crack resistance by counting the number of initiated cracks as a function of the applied load. Experiments have shown that the environmental humidity and the time period between indentation and crack counting affect the crack resistance value, but unfortunately these parameters are not always reported in literature studies. Here we study the time and humidity dependence of crack initiation in calcium aluminosilicate glasses. Depending on the experimental conditions (time and humidity), the crack resistance of an aluminosilicate glass can vary more than 100%. Furthermore, the observed radial/median cracks can initiate several hours after indentation. These results therefore indicate the need of a standardized procedure for determination of crack resistance to allow comparison of data from different research groups.

(GOMD-GSP-P004-2018) Initial-dissolution rate of the International Simple Glass in dilute and saturated conditions

A. J. Fisher*[1]; J. Neeway[2]; J. Ryan[2]; M. Asmussen[2]; R. J. Hand[1]; N. C. Hyatt[1]; C. L. Corkhill[1]

1. University of Sheffield, Material Science and Engineering, United Kingdom
2. Pacific Northwest National Lab, USA

The initial dissolution rate of the International Simple Glass (ISG), a reference high-level-waste simulant base glass, was determined under a range of dilute, saturated, acidic and alkali conditions (pH[RT] 4.5 − 12) and over the temperature range 23 – 90 °C. This work was conducted as part of an intra-laboratory study using the single-pass-flow-through methodology, which produced results that were in excellent agreement, but disagree with results previously published in the literature. Through application of the transition state theory, we obtained the fundamental parameters necessary to model the dissolution kinetics; activation energy (E_a), pH power law coefficient (η) and the intrinsic rate constant (k_0). To develop knowledge in the field of glass dissolution at the fundamental level and to build a robust safety case for the geological disposal of vitrified nuclear waste, it is imperative that the kinetics governing glass dissolution are well understood, with data reported as accurately as possible. This is especially evident in the case of a widely studied international reference sample such as the ISG.

(GOMD-GSP-P005-2018) Phase Separation in SiO_2-Al_2O_3-BaO-BaF_2 Oxyfluoride Glasses from Molecular Dynamics Simulations

J. Zhao*[1]; X. Chen[1]; J. Du[2]; Q. Xu[1]; Z. Luo[1]; X. Qiao[1]; X. Fan[1]

1. Zhejiang University, Materials Science and Technology, USA
2. University of North Texas, USA

Oxyfluoride glass ceramics are good host for rare earth ions and transition metal element due to the low photon energy and good mechanical properties. For some of the oxyfluoride glass ceramics, phase separation can be considered as the precursor of crystallization. Therefore, knowing the phase separation mechanism is critical for the preparation of oxyfluoride glass ceramics in optical application. However, there are two questions not completely resolved yet: with how much fluoride, phase separation will take place in a certain system and how to define the occurrence of phase separation. With the help of Molecular Dynamics (MD) simulations, a series of aluminosilicate oxyfluoride glass in SiO_2-Al_2O_3-BaO-BaF_2 system was studied. Results shows that phase separation with immiscible fluoride rich phase and oxide rich phase will take place with more than 15 mol% fluoride in the system. This study prove the feasibility of the potential we used and can help to guide the preparation of aluminosilicate oxyfluoride glass ceramics with MD simulations.

(GOMD-GSP-P006-2018) Structure of Glassy Silica: Assessing the Role of the Synthesis Method

T. Du*[1]; M. M. Smedskjaer[2]; H. Li[1]; M. Bauchy[3]

1. Harbin Institute of Technology, School of Civil Engineering, China
2. Aalborg University, Department of Chemistry and Bioscience, Denmark
3. University of California, Los Angeles, Department of Civil and Environmental Engineering, USA

Glassy materials can be synthesized through several techniques, including melt-quenching, sol-gel, and vapor deposition. Although all these techniques yield a disordered atomic network, it remains unclear to what extent the final structure of the glass depends on the synthesis method. This problem is significant as, for a given glass composition, different structures can yield different engineering properties. Here, based on reactive molecular dynamics simulations, we investigate the structure of three silica glass models generated by melt-quenching, sol-gel, and vapor deposition. The structural properties (e.g., density, bond distances, bond angles, and ring size distributions) of the three glass models are thoroughly analyzed and compared. Based on these results, we reveal how the synthesis method controls the stability of glasses.

(GOMD-GSP-P007-2018) Structure of deeply supercooled liquid and amorphous alumina

C. Shi*[1]; D. Berman[2]; J. Du[2]; R. Weber[3]; O. L. Alderman[3]; C. J. Benmore[1]

1. Argonne National Lab, X-ray Science Division, USA
2. University of North Texas, Materials Science and Engineering, USA
3. Materials Development, Inc., USA

The structure of liquid alumina has recently been determined using a combination of high-energy x-ray diffraction, aerodynamic levitation with laser-heating and reverse Monte Carlo simulations (Skinner et al. PRB 2013, 024201). Our best model consistent with

diffraction data shows that the melt is composed predominantly of AlO4 and AlO5 units, in the approximate ratio of 2:1, with only minor fractions of AlO3 and AlO6 units. The majority of Al-O-Al connections in the liquid involve corner-sharing polyhedra, although a significant minority involve edge-sharing polyhedra. Triply shared oxygen atoms in the melt prevent Al2O3 from forming a glass, however the fabrication of amorphous thin films is possible. Previous NMR experiments suggest the amorphous structure is similar to that of the liquid, rather than crystalline corundum that comprises of only AlO6 octahedra. Here we present high energy x-ray experiments on liquid alumina supercooled to 500 degrees below the melting point. Temperature dependence of the liquid structure are studied and compared to the structure of amorphous thin films.

(GOMD-GSP-P008-2018) Molecular Dynamic Simulation of Ultrafast Laser Effects on Oxide Glasses

S. T. Locker*[1]; S. K. Sundaram[1]

1. Alfred University, Glass Science, USA

Preliminary experimental results have shown low energy (500 nJ) femtosecond irradiation of multiple oxide glasses can cause measureable increase in surface hardness and index of refraction without influencing surface chemistry, elemental concentration or inducing stress fields. We have modelled the effects of high and low pulse energies on optical and mechanical properties, specifically, observing changes to refractive index (RI) during laser irradiation and after allowing the glass structure to equilibrate. Two and three body potentials have been used for modeling structures ranging from 100 to 5000 atoms, analyzing both bulk and surface effects. This study was focused on modeling the variation to RI with respect to laser-irradiated region to determine if RI changes locally concentrated or observable outside of the laser focal point. Ab initio and classical molecular dynamic (MD) simulation tools were utilized in understanding internal effects at play in the glass structure and interaction mechanisms between the pulse-laser and glass.

(GOMD-GSP-P009-2018) Structure of SnO-P_2O_5 Glasses: Results from High-resolution ^{119}Sn and ^{31}P NMR

Y. Xia*[1]; M. A. Marple[1]; I. Hung[2]; Z. Gan[2]; S. Sen[1]

1. University of California, Davis, Materials Science and Engineering, USA
2. National High Magnetic Field Laboratory, Center of Interdisciplinary Magnetic Resonance, USA

The compositional evolution of the phosphate network in binary SnO-P_2O_5 glasses with 35≤ mol% SnO ≤60 is studied using two-dimensional ^{119}Sn and ^{31}P nuclear magnetic resonance (NMR) spectroscopy. The ^{119}Sn NMR results suggest that the Sn-O coordination environment in these glasses is close to a trigonal pyramid and is independent of chemical composition. Moreover, these ^{119}Sn NMR spectral line shapes do not display any signature corresponding to the presence of a significant concentration of tin as Sn^{4+} in these glasses. On the other hand, the phosphate Q^n species concentrations, as obtained from the analyses of the ^{31}P NMR spectral line shapes, indicate that the Q-speciation largely follows a binary model of network modification. The density and the glass transition temperature T_g of these glasses are measured and these properties show distinct compositional trends consistent with the corresponding structural evolution of the glass network. We hypothesize that the unusually low T_g of these glasses (235-265 °C) corresponding to that of the analogous alkali or alkaline-earth phosphate glasses is related to the low coordination number of Sn which leads to a lesser degree of connectivity of the phosphate chains in the Sn-phosphate glasses.

(GOMD-GSP-P010-2018) XPS analysis of nuclear waste glass corrosion in determining the elements, oxygen speciation and alteration layer thickness

H. Liu*[1]; D. Ngo[1]; J. Du[2]; S. H. Kim[1]

1. Pennsylvania State University, Chemical Engineering, USA
2. University of North Texas, USA

Compositional changes in uncorroded and corroded International Simple Glass (ISG) surfaces were tracked with X-ray Photoelectron Spectroscopy(XPS). To reveal the initial glass surface state effect on corrosion result, we compare corrosion results of polished only sample and polished and annealed sample. The polished and annealed ISG shows remaining Na and B ions after leaching in saturated SiO_2 solution at 30°C for 21 days, in contrast of which the polished only ISG glass, treated with the same corrosion condition, didn't show any. Additionally, surface oxygen speciation is of great importance in determining corroded surface state and understanding the corrosion process. A stoichiometry-based algorithm via elemental composition has been developed to quantify oxygen speciation more accurately, compared to the typical O 1s peak-fitting approach. It presents the changing of bridging oxygen, non-bridging oxygen and hydroxyl species before and after corrosion. Meanwhile, depth profiling with XPS is able to acquire the alteration layer thickness and it demonstrated good consistence with spectroscopy ellipsometry's measurement.

(GOMD-GSP-P011-2018) On the speciation of mixed sodium-potassium silicate glasses by NMR spectroscopy

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1. University of Southern Denmark, Department of Chemical Engineering, Biotechnology and Environmental Technology, Denmark
2. Bollerup Jensen A/S, Denmark
3. University of Southern Denmark, Department of Physics, Chemistry and Pharmacy, Denmark

Water-glasses are a subset of alkali-silicate glasses which are water soluble, in contrast to most other silicate glasses. Highly concentrated aqueous solutions of water-glasses are used as surface sealants on concrete, fire-retardant, as flocculants in water remediation and as a green alternative in wood preservation and formaldehyde free adhesives. The concentration and choice of alkali metal greatly affect the properties of the final material. However, only binary sodium silicate and potassium silicates are available commercially. Thus a series of mixed sodium-potassium silicate glasses with compositions $nSiO_2 \bullet xNa_2O \bullet (1-x)K_2O$ (where: n=2 or 3.3; and $0 \le x \le 1$) were prepared to investigate the composition/structure of the glass and whether this affects the composition of the aqueous water-glass solutions with a view to potential applications as a flux in welding rods and surface sealants on concrete. Solid state ^{23}Na, ^{29}Si, and ^{39}K MAS NMR was used to gain information regarding the Q speciation, and the local environment of sodium and potassium, whereas liquid state ^{29}Si NMR yielded information on the Q speciation of the water-glass solutions at different concentrations. Viscosity measurements where obtained for aqueous solutions of the glasses. Initial results and conclusions based on and viscosity measurements will be presented.

(GOMD-GSP-P012-2018) Femtosecond Laser Modification of Mn – Doped Zinc Borosilicate Glasses

G. J. Vander Stouw*[1]; S. K. Sundaram[1]

1. Alfred University, The Inamori School of Engineering, USA

Glasses of composition 55 ZnO * $20B_2O_3$ * $25SiO_2$ by molar ratio were prepared via melting and solidification. These glasses were doped with Mn via $MnCO_3$ at Mn:Zn ratios of 0, 0.005, 0.01, and 0.015 respectively. The glasses were irradiated using ultrashort femtosecond laser pulses at 13 μJ (~6.5 fs, 800 nm central wavelength) applied longitudinally on the samples. The glasses, prior and post irradiation, were examined using x-ray photoelectron spectroscopy (XPS), x-ray diffraction (XRD), micro-hardness

indentation test, terahertz time-domain spectroscopy, differential scanning profilometry, and Raman spectroscopy to study the structural and chemical changes occurring due to the irradiation in relation to the Mn:Zn ratio. In addition, spectrofluorometry was used to measure the emission, excitation, phosphorescence spectra, and phosphorescence decay curve of the samples. Our major results and interpretations will be presented.

(GOMD-GSP-P013-2018) Crystallization Control in Doped Glass-Ceramics for Tuning Luminescence

J. Chen*[1]; S. Zhou[1]; J. Qiu[2]

1. School of Materials Science and Engineering, South China University of Technology, State Key Laboratory of Luminescent Materials and Devices, China
2. College of Optical Science and Engineering, Zhejiang University, China

The manipulation of light in bulk optical glasses have recently attracted much attention in diverse fields, not only for the fundamental scientific significance but also because of the practical applications, ranging from photovoltaics and photocatalytic reactions to optical sensing and smart lighting. Here, we report on the spectroscopic regulation in ion-doped optical glass-ceramics fabricated through crystallization control. By rational control of the relaxation of glass, the chemical state and local chemical environment of the incorporated active dopant can be deliberately tuned. We successfully employ self-limited nanocrystallization to extend near-infrared emission in Cr-doped germanate glass-ceramic through simultaneous control of the chemical state and local environment of Cr dopant. In another example, multiscale structured glass with rich microstructures spanning the nano- (down to ~ 50 nm) and micrometer scales (up to ~ 70 μm) is demonstrated. Importantly, the unique multiscale configuration enables simultaneous control of the chemical state and local chemical environment of the Eu dopant. This allows us to generate color-switchable emission (blue, red to white) with high brightness and build a colorimetric temperature sensor. Our results highlight the design strategy that the crystallization control of glass may provide opportunities for the development of a new generation of photonic glass.

(GOMD-USP-P014-2018) Solution-based Coating of Chalcogenide Alloy (ChA) GeSbSeTe Films

C. Blanco*[1]; M. Kang[1]; Q. Altemose[2]; C. Schwarz[2]; K. Richardson[1]; J. Hu[3]

1. University of Central Florida, USA
2. Ursinus College, USA
3. MIT, USA

Phase change materials (PCMs) are of interest for integrated photonic applications where alloys are typically formed into films enabling switching via optical or electrical stimulus. This effort discusses the processing and characterization tools used to prepare Ge2-Sb2-Se4-Te1 bulk chalcogenide alloys (ChA) into solutions that can be deposited onto conformal (shaped) surfaces as films. ChA's have been dissolved into a mixture of Ethylenediamine and Ethanethiol and later deposited onto substrates to create films that were spatially homogeneous with the goal of target 1mm thickness with good spatial uniformity, compositional integrity and low optical loss. By changing the solvent ratio and the glass loading level we were able to achieve films that maintain the parent glass stoichiometry. Other variables such as dipping time, heat treatment, and solution viscosity were varied to allow tuning of thickness and roughness of the film. The viscosity of the solution was also studied to see at what viscosity the best films were formed. Using instruments such as SEM, FTIR, and white light interferometer, we were able to determine the thickness of the films, composition, surface roughness, and amount of solvent in the film. By changing parameters and studying the changes with the instruments above we were able to design a film that contains the correct ratio of elements and we are able to tune the thickness of the film.

(GOMD-USP-P015-2018) An anomaly in the glass transition widths of mixed alkali lithium cesium borate glasses

T. Mehmen*[1]; H. Rea[1]; A. DeCeanne[1]; S. Feller[1]

1. Coe College, Physics, USA

Using differential scanning calorimetry, glass transition widths (ΔTg), were measured based on the glass transition onset temperature (Tg), and the glass transition end temperature (Te). Previous studies on binary alkali borates by Anthony DeCeanne et al[1]. show an anomaly in the ΔTg around an R value of 0.05, where R is the molar ratio of modifier to boron oxide. This same anomaly is shown when using the mixed alkalis, lithium and cesium, as modifiers with varying abundances at R values ranging from 0.03-0.07. Density measurements were also taken to help further understanding of this anomaly. Acknowledgements: The National Science Foundation under grant DMR 1407404, Coe College Physics Department for ongoing support

(GOMD-USP-P016-2018) Residual Stress Field around Sharp Indent

Y. Zhai*[1]; L. Huang[1]; T. M. Gross[2]

1. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA
2. Corning Incorporated, USA

Although residual stress around sharp indent in transparent materials like oxide glass can be easily visualized by using a polarized microscope, it is very difficult to quantify its spatial distribution. By using a double indentation method, we measured the radial and tangential residual stress components around Vickers indents. This method is to use a small indent as a microprobe to measure the residual stress at a specific point near a large indent. By measuring the lengths of cracks from the small indent, and comparing them with those developed at the same load in a stress free region, the residual stress field around the big indent can be calculated from fracture mechanics analysis. In this work, this method was used to study residual stress in Na_2O-Al_2O_3-SiO_2 and CaO-Al_2O_3-SiO_2 glasses with equal amount of modifier and Al_2O_3 content over the composition range where the indentation behavior changes from normal to anomalous. The residual stress field is correlated with the fracture toughness, crack initiation load and indentation deformation modes to better understand the response of glass to sharp contact loading.

(GOMD-USP-P017-2018) Multicomponent Glass Surface Hydroxyl Groups by Temperature-Resolved ToF-SIMS: Viability and Challenges

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1. Brigham Young University, Chemistry and Biochemistry, USA
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Surface hydroxyls are thought to be among the most important moieties in governing surface-mediated processes on glass surfaces. These surface mediated processes, which include wetting, adhesion, contamination, static charge buildup, and static discharge, have an important influence on the performance of silicate glasses in many applications, including their use as substrates for flat panel displays. Few techniques have the requisite sensitivity and surface specificity to quantify surface hydroxyls on planar glass substrates. Here, we use temperature-resolved time-of-flight secondary ion mass spectrometry (TR ToF-SIMS) to quantify this important functional group on a range of silicate glass compositions hydroxylated by exposure to a range of wet chemical treatments including acids, bases, etchants, and industrial detergents. This poster focuses on the viability and challenges of TR ToF-SIMS for this application, including a discussion of sample preparation, data acquisition, spectral interferences, and data processing.

(GOMD-USP-P018-2018) Raman Spectroscopy Study of Bioactive Glass Doped with Cerium Oxide

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2. Kennesaw State University, Chemistry and Biochemistry, USA
3. Missouri University of Science & Technology, Materials Science & Engineering, USA

In this project, a bioactive glass with mixed-valence-state (Ce+3 and Ce+4) cerium oxide nanoparticles is being investigated as a carrier and delivery system for therapeutic nanoparticles. The therapeutic potential of nanoceria depends on an appropriate Ce+3/Ce+4 ratio and different starting concentrations of cerium oxide can lead to different oxidation states of cerium. Therapeutic cerium can be released from the glass when the glass dissolves in distilled water or simulated body fluids. In the first phase of this study, bioactive glass has been prepared using varying cerium oxide concentrations. In the second phase, the prepared glasses will be dissolved in either water or simulated body fluid and the nanoparticles present in soluble and insoluble fractions will be analyzed by Raman spectroscopy.

(GOMD-P020-2018) Structure of amorphous hafnia nanoparticles

C. J. Benmore*[1]; L. Gallington[1]; L. Skinner[1]; R. Weber[2]; S. Ushakov[3]; A. Navrotsky[3]; A. Vazquez-Mayagoitia[4]; J. Neuefeind[5]; M. Stan[4]; J. J. Low[4]

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2. MDI, USA
3. University of California, Davis, USA
4. Argonne National Lab, USA
5. Oak Ridge National Lab, USA

Understanding the atomic structure of amorphous solids is important in predicting and tuning their macroscopic behavior. The agglomeration of amorphous nanoparticles condensed from the gas phase has been studied using a combination of high-energy x-ray diffraction, neutron diffraction, and molecular dynamics simulations. The diffraction results reveal an average Hf-O coordination number of approximately seven exists in both the amorphous nanoparticle form as well as the high temperature liquid phase. Our ab initio and classical molecular dynamics simulations show that density has a strong effect on the polyhedral connectivity. Although edge sharing $HfO_{6.7}$ polyhedra dominate models of the bulk liquid and amorphous nanoparticle clusters, the formation of distinct edge- and corner-sharing units leads to a splitting and sharpening of the Hf-Hf peaks in the amorphous pair distribution function. The Hf-O-Hf bond angle distribution in amorphous HfO_2 is found to resemble that observed in the monoclinic crystalline phase rather than the higher temperature tetragonal or cubic phases.

(GOMD-P021-2018) Molecular Dynamic Simulation studies of Vanadium Lithium Borate-Based Glasses

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1. School of Physics, Institute of Science, Suranaree University of Technology, Thailand
2. Synchrotron Light Research Institute, Thailand

Vanadium lithium borate-based glass is a possible candidate as cathode of lithium-ion batteries. In this work, a glass system of $0.5(V_2O_5)$-$0.5(Li_2O$-$B_2O_3)$ is introduced. In order to clearly understand this glass structure, molecular dynamics (MD) simulation using DL_POLY MD package with the Buckingham potential is employed. The ten pair radial distribution functions of this glass were obtained from the MD simulation. To address a local structure around V atoms in its glass structure, the MD-EXAFS is subsequently simulated by extracting the individual clusters around each vanadium atom from the final MD configuration, calculating the EXAFS signal for each cluster using FEFF8.2 and then averaging the EXAFS signal for all clusters in the simulation. By comparison with the measured EXAFS spectrum at V K-edge of this glass, a good agreement between calculated and measured EXAFS data was obtained leading to a fully address of local structures of this glassy materials with a mean V-O coordination network of 3.82(1).

(GOMD-P022-2018) Silica content effects on the elastic and structural properties of calcium aluminate glass: Insights from molecular dynamics

H. Jabraoui*[1]; M. Badawi[1]; A. Atila[2]; S. Ouaskit[2]; S. Lebègue[1]; Y. P. Vaills[3]

1. University de Lorraine, France
2. Université Hassan II de Casablanca, Morocco
3. Université d'Orléans, France

We have investigated the elastic constants of low silica calcium aluminosilicate glasses with a low content of silica (5–20 mol%) and [CaO]/[SiO2] =2 by mean of simulation and modeling using molecular dynamics. we have used two methods; the minimization energy at zero temperature (Zero-T) and a second one that allows to calculate the elastic constants at finite temperature (FT). The reliability of the two methods to calculate elastic constants has been evaluated comparing our results with those measured already using Brillouin light scattering (BLS) spectroscopy. At the same time, we show that the elastic constants decrease as the amount of silica increases in the glass network. Then, we provided new insights related to the elastic constant behaviors when silica content decreases using some structural features such as pair distribution functions, oxygen kinds, and parameter of short range order. These properties are not easily accessible from experiment; therefore, our simulations nicely complement the current knowledge on how the low silica contents influence the physicochemical properties of the calcium aluminate glasses.

(GOMD-P023-2018) Characterization of Ion Exchange Stress Profiles with Induced Mechanical Stress

J. Finkeldey*[1]; C. Smith[1]; T. M. Gross[1]

1. Corning Incorporated, USA

The principle of superposition is well known in the field of fracture mechanics. It states that for linear elastic materials, individual components of stress are additive. When applied to tempered glass, it allows us to understand how internal stresses from chemical tempering respond to external stresses such as bending. We will demonstrate experimentally the effect of bending on a range of ion-exchange induced stress profiles. Fixtures with known bend radii were fabricated and stress profiles of tempered and non-tempered glasses were measured in both flat and bent configurations. The experimental results compare favorably to those calculated using the superposition principle. The effect of imposed bending on the mechanical response of glasses will also be presented.

(GOMD-P024-2018) Synthesis and Characterization of Modified Vanadium Glass Cathodes

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

The desire for scalable energy storage technologies with higher specific energy densities is critical for electric vehicles and grid energy storage. Glass cathodes can have a capacity up to 500 mAh/g and typically can be created in facile melt quench procedures making them scalable. Glasses have been shown to have improved performance, both in capacity and rate capability, compared to their crystalline counterparts for several systems containing vanadium. The increased performance in the glass system is linked to the lack of irreversible loss that occurs from crystalline phase changes. However, the difference in performance between various glass systems still needs investigation. An analysis of the effect of alkali borates and how they alter the glass system has not been performed, and this study is investigating the effects of altering the content of lithium borate to modify the boron coordination, and thus the boron superstructures and non-bridging oxygen (NBO) sites that form.

The $Li_xB_yO_{(x+3y)/2}$:V_2O_5 system is under study for a possible cathode material. From literature, the $LiBO_2$-V_2O_5 glass system showed promising performance. Charge transport, both electrical and ionic, must be optimized for glass cathodes to be viable. Impedance data, FTIR, Raman, and battery cycling data will be related to ionic conductivity, electrochemical performance, and glass structure as the lithium borate content changes.

(GOMD-P025-2018) ZnS: Ag scintillating membrane for rapid isotopic analyses of waterborne special nuclear materials

Y. Wu*[1]; A. Trofimov[1]; C. Li[1]; A. Darge[1]; K. Brinkman[1]; T. DeVol[1]; S. Husson[1]; L. G. Jacobsohn[1]

1. Clemson University, USA

This work aims at developing the technology for rapid activity determination and isotopic quantification of waterborne special nuclear materials (SNM) through the development of reactive scintillating membranes based on ZnS: Ag. Reactive membranes with U and Pu selective ligands will enable the rapid isolation and concentration of samples from solution and, after addition of ZnS: Ag, will enable quantitative elemental analyses using advanced radiometric spectroscopy and luminosity measurements. The ultimate outcome will be a fast and reliable method to conduct forensics of debris from a nuclear event for activity and isotope quantification. This approach is based on the detection and measurement of the alpha radiation emitted from U and Pu. ZnS: Ag is the most efficient scintillator for alpha particle radiation. Its high luminosity of 60,000 photons/MeV, light emission centered at 450 nm matching peak response of photomultiplier tubes and Si-PM photodetectors, the fast decay time of ~0.2 ms, and non-hygroscopic nature make this scintillator the ideal choice for this application. In this work, ZnS: Ag nanoparticles were prepared and characterized on their microstructure, luminescence, and scintillation. Proof-of-concept tests of the reactive scintillating membranes for the detection of U were successfully carried out.

(GOMD-P026-2018) Strong thermally stimulated luminescence quenching effect of Nd^{3+} in borate glasses

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1. Universidad de la República, Centro Universitario Regional del Este, Uruguay

Rare earth (RE) ion doped borate glasses present high optical transparency, mechanical, chemical and thermal stability. For these reasons, they are largely studied for solid-state lighting and thermoluminescent dosimetry applications. Here, we report the preparation of oxyfluoroborate glasses belonging to the system (31-x) % NaF 22.77 % BaO 46.23 % B_2O_3 with x=0 to 1 % Nd^{3+}. Glasses were prepared by the melt/quenching technique. Glass crystallization was studied using thermal analysis and X-ray diffraction techniques. Optical absorption spectra were studied on undoped and on doped samples showing typical RE transitions. Thermally stimulated luminescence (TL) was studied on undoped and doped glass samples and glass ceramics. The analysis of the glow curve was done using the general model fitting approach. Results indicate the existence of a single TL band near 335 K. The intensity of the TL signal diminishes as the concentration of dopant increases, showing the typical quenching effect observed for other similar samples. On the other hand, it was observed that the tendency of crystallization increases with increasing dopant concentration. TL analsysis of glass ceramics were done in the same way. From our results, we observed that Nd^{3+} presents a strong quenching effect that should be in small amount for glasses to be used these materials as TL detectors.

(GOMD-P027-2018) Laser trimmed hybrid chalcogenide metasurface

T. Gu*[1]; M. Chen[1]; Z. Wang[1]; D. Mao[1]

1. University of Delaware, USA

Chalcogenide glass is a special class of 'soft' materials possessing unique optical properties. Its low activation energy allows tunability of those materials at low intensity. As the incident light excites local material, the lossy atomic network can be re-arranged and thus exhibit distinguished optical and thermal behavior. In this work, we study near-bandgap laser-induced arsenic sulfide microstructure under silicon meta-surface. The localized laser irritation modifies chalcogenide's electronic bandtail stations, which exhibits a periodic ripple nanostructure in transmission electron microscopy experiments and polarization-dependent photoluminescence. A layer of subwavelength nanostructured silicon membrane cladding adds a level of spectral and spatial tunability of those light emitting chalcogenide materials. The new device design of metasurface heterostructures can be an low cost alternative for critical components in advanced imaging systems.

(GOMD-P028-2018) Structural and optical analysis of calcium and lithium borate glasses doped with Dy^{3+} for thermoluminescent dosimetry

S. R. de Souza*[1]; E. S. Bannwart[2]; N. B. Pimentel[2]; J. E. de Souza[1]

1. Iowa State University, MSE, USA
2. Universidade Federal da Grande Dourados, Physics, Brazil

Presently, calcium and lithium borate glasses, particularly in the composition of tetraborates, CaB_4O_7 and $Li_2B_4O_7$, are being extensively studied due to their interesting thermoluminescence (TL) response with possible environmental and/or medical applications as radiation dosimeters. Moreover, this borate glasses present low melting temperature, high thermal and chemical stability and high transparency in the UV region. The addition of lithium oxide to the CaO-B_2O_3 binary system changes its thermal properties by decreasing the glass transition and melting temperatures. Furthermore, a liquid-liquid phase separation in this binary system is avoided after lithium oxide addition. In the present work, the influences of Dy^{3+} and the substitution of calcium oxide by lithium oxide on optical and structural characteristics of the glasses were evaluated by Raman and IR spectroscopies, UV-Vis absorption, fluorescence, density and thermoluminescence measurements. Different glass compositions were obtained with the effective atomic number (Z_{eff}) changing from that of human tissue (Z_{eff} = 7.42) up to that of human bone (Z_{eff} = 13.17). Nevertheless, thermoluminescence may be greatly affected by Li^+ in concentrations below 10 mol%, while Dy^{3+} can form substitutional complex defect with borates promoting significant changes in the TL emission.

(GOMD-P029-2018) Structural and Electrical Characterization of Borate Glasses in the B_2O_3 – CaO – Li_2O System

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2. Universidade Federal da Grande Dourados, Laboratório de Materiais Cerâmicos Avançados - LMCA, Faculdade de Ciências Exatas e Tecnologia - FACET, Brazil

Glass samples were prepared in the compositions $67B_2O_3$ - (33-x) CaO - xLi_2O in mol% (with x = 0, 5, 10, 15, 20, 25, 30, 33), referred to as CaBO (x = 0), CaLiBO (x = 5, 10, 15, 20, 25 and 30) and LiBO (x = 33), to assess their structural, thermal and electrical properties. We used the conventional melting and casting process, by using appropriate amounts of the reagents. Homogeneous and transparent samples were obtained, with no evidence of devitrification, which was confirmed by X-Ray Diffraction (XRD). Changes in the physicochemical properties due to the increased concentration of Li_2O in the vitreous samples were evaluated by Differential Thermal

Analysis (DTA), Fourier Transform Infrared Spectroscopy (FTIR) and Impedance Spectroscopy (IS). From the thermal analysis typical curves of vitreous materials were observed and it was observed that the increase of Li_2O turned the glass transition temperature (T_g) lessened as the Li_2O is incorporated into the glass structure acting as a modifier of the network glass. Also with respect to the addition of Li_2O, the results obtained by IS we observed a decrease in electrical resistivity, reaching variations greater than 10 orders of magnitude, when this property is assessed at 300 °C. This decrease is mainly due to the smaller ionic radius of Li^+ ion compared to the ionic radius of ion Ca^{2+}.

(GOMD-P030-2018) Evaluation of novel leaching assessment for nuclear waste glasses

C. L. Thorpe[1]; C. Mann[1]; A. J. Fisher[1]; R. J. Hand[1]; N. C. Hyatt[1]; C. L. Corkhill*[1]; M. J. Schweiger[2]; J. Mayer[2]; C. Arendt[2]; A. A. Kruger[3]; D. Kosson[4]

1. University of Sheffield, Materials Science and Engineering, United Kingdom
2. Pacific Northwest National Lab, USA
3. US Department of Energy, USA
4. Vanderbilt University, USA

Project GLAD (Glass Leaching Assessment for Disposability), funded by the Department of Energy Office of River Protection Waste Treatment & Immobilization Plant Project through the EM International Program, investigates a new leaching approach for assessing the durability of ILAW glasses at relevant temperatures and conditions of disposal, using two established U.S. Environmental Protection Agency (EPA) leaching protocols. We critically appraise the application of these methodologies, through investigation of the dissolution of three ILAW glasses (LAW-A44, ORP-LB2 and LAW-A23) as a function of temperature, pH, leaching duration and groundwater composition. Results are compared with those from established leaching methodologies currently accepted in Europe for evaluation of high level waste glasses, including PCT, MCC-1 and SPFT protocols. The advantages and limitations of the EPA methods are discussed and their reproducibility is assessed by comparing results across multiple laboratories.

(GOMD-P031-2018) Corrosion of ISG Glass Studied Using Spectroscopic Ellipsometry, X-ray Photoelectron Spectroscopy and Specular Reflection Infrared Spectroscopy

D. Ngo*[1]; H. Liu[1]; S. H. Kim[1]

1. Pennsylvania State University, Chemical Engineering, USA

Corrosion of ISG glass, a 6-oxide borosilicate glass, in aqueous solutions with or without the presence of electrolyte has been studied using different spectroscopic techniques. Specular reflection infrared (SR-IR) spectroscopy was used to study the silicate network structure in the corrosion experiments. The SR-IR results reveal a significant change of the network structure within 3 days of experiments and the surface layer is rich in silica when the glass samples were further corroded in the solutions. A chemometric analysis of SR-IR spectra shows the contribution of 4 significant components to the SR-IR data set. The alteration layer thickness increased with leaching time as revealed by spectroscopic ellipsometry (SE) that also shows the variations in the optical constants and porosity of the leached layers. The SE results also show that, after 7 days in leaching solution, the corrosion rate of ISG glass in solution of 13 mM KCl decreased significantly in comparison to that of ISG glass in pure water or 13 mM LiCl solutions. It is from X-ray photoelectron spectroscopy (XPS) measurements that mobile elements in the surface layer were completely dissolved after 7 days of experiments. The combination of these techniques provides a better understanding of ISG glass corrosion under different experimental conditions.

(GOMD-P032-2018) Impacts of Uncertainties on Hanford LAW Glass Estimates

V. Gervasio*[1]; J. Vienna[1]; D. Kim[1]; A. A. Kruger[2]

1. Pacific Northwest National Lab, Energy and Environment Directorate, USA
2. US Department of Energy, Office of River Protection, USA

Current estimates suggest that one of the rate limiting processes for Hanford tank waste cleanup is the rate of low-activity waste (LAW) treatment. Maximizing LAW loading in glass can reduce mission duration and cost. A set of models and constraints less conservative than those intended for plant commissioning was produced. These models and constraints allow for significant increase in waste loading, but may be more impacted by process and prediction uncertainties. The objective of this study was to quantify the impacts of expected uncertainties on glass amount for the Hanford mission. The anticipated prediction and process/composition uncertainties impact on estimated LAW glass amount at Hanford are shown. Applying the current set of advanced glass models and constraints generated 282,350 MT of LAW with effectively no impact of uncertainties. Relaxing ad-hoc compositional constraints while maintaining adequate glass properties has the potential to decrease glass amount by 10.6 relative percent (252,490 MT) for the case with no uncertainties. Addition of uncertainties increases glass mass 9.1 relative percent. The glass mass estimate without ad-hoc composition constraints but applying full uncertainties (275,359 MT) was 2.6 relative percent lower than that with the ad-hoc constraints (282,562 MT). The calculations, in which uncertainties are most influential, and the estimated glass masses are presented.

(GOMD-P033-2018) Flexible thin film ceramics for high temperature thermal sensing applications

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1. University of Memphis, Dept. of Physics and Materials Science, USA
2. Emerging Measurements, USA
3. ENrG Inc., USA

Thermographic phosphors have the ability to detect changes in temperatures as small as 0.01 °C over a wide range of temperatures, remotely and instantaneously. Direct deposition of phosphor powders onto the substrate of interest is on occasions viable for temperature measurement. Nevertheless, such coatings may be difficult to remove, if required, so other possibilities for expanding functionalities are being explored. The authors have previously experimented with encapsulating thermographic phosphors successfully in inert encapsulants such as silicones and aerogels successfully. They are deployed as removeable and reattachable sheets of controlled thickness. However, the maximum temperature of operation has been limited by the flash point of the encapsulating material. In this work the authors report for the first time the use of flexible ceramic films capable of tolerating temperatures up to 1200 °C coated with a thin film of thermographic phosphors as a temperature sensor for high temperature applications. Results will demonstrate the feasibility of the tested layer structure as a thermal sensors for high temperature application.

Tuesday, May 22, 2018

Award Lectures

George W. Morey Award Lecture

Room: El Mirador (22nd Fl)

8:00 AM

(GOMD-AW-002-2018) Chemically strengthened glass: Science, technology and its future

A. K. Varshneya*[1]

1. Saxon Glass Technologies, Inc., USA

Glass can be chemically strengthened by immersion in a bath of molten alkali salt at temperatures lower than the glass transition temperature. An ion exchange between a small host ion, such as Na^+, with a larger invading ion, such as K^+, results in the development of high magnitude surface compression which strengthens the glass product. Except for some minor details, the science of stress development is now largely understood. Technology, on the other hand, is saddled with several nasty issues particularly relating to the degradation of the salt by increasing contamination and its periodic disposal. The consumer market is also somewhat difficult, particularly because of the perception that, upon strengthening, glass should be near-unbreakable. Despite these issues, many glass products are being, or could be, chemically strengthened. Examples are the high strength laminated windshields for aircraft cockpit, display windows in personal mobile electronic devices, packaging for parenteral drugs, vehicular transparencies, hurricane-resistant architectural windows, armor, large curved television, and thinner glass substrates for solar energy harvesting. This presentation reviews the science, the technology and the future outlook for chemically strengthened glass.

S1: Fundamentals of the Glassy State

Joint Session: Symp 1, Sessions 2 and 5: Modelling and Simulation of Glass Crystallization

Room: La Vista A/B (22nd Fl)

Session Chairs: Jincheng Du, University of North Texas; Carlo Massobrio, CNRS-IPCMS-UNR 7504

9:20 AM

(GOMD-S1-047-2018) Rapid crystallization of phase change materials: Density functional simulations (Invited)

J. Akola*[1]; J. Kalikka[3]; M. Ropo[3]; R. O. Jones[2]

1. Norwegian University of Science and Technology, Department of Physics, Norway
2. Forschungszentrum Juelich, PGI-1, Germany
3. Tampere University of Technology, Laboratory of Physics, Finland

Crystallization of phase change materials has been studied by extensive density functional/molecular dynamics simulations. Four crystallization simulations of amorphous $Ge_2Sb_2Te_5$ (460 atoms) have been completed at 600 K with simulation times up to 8.2 ns. A sample with a history of order crystallizes completely in 1.2 ns, but ordering in others takes more time and is less complete. The amorphous starting structures without memory display phases (<1 ns) with subcritical nuclei (10–50 atoms) ranging from nearly cubical blocks to stringlike configurations of ABAB squares and AB bonds extending across the cell. Percolation initiates the rapid phase of crystallization and is coupled to the directional p-type bonding. The results emphasize the stochastic nature of crystallization and the importance of sufficiently large samples. This is particularly evident in describing the role of crystallites that can merge to form larger units or hinder complete crystallization by the formation of grain boundaries. Amorphous Sb is known to crystallize extremely rapidly. Crystallization of Sb has been studied at 600 K using six simulations with up to 882 atoms. Crystallization proceeded layer-by-layer in most cases and was rapid (~36 m/s). Diffusion plays a minor role in the process, and the evolution of bond lengths and ring statistics supports the bond-interchange model of Sb-rich phase change materials.

9:50 AM

(GOMD-S1-048-2018) Ab Initio Simulations of Crystallization of Phase-Change Materials (Invited)

R. Mazzarello*[1]; W. Zhang[2]; I. Ronneberger[1]

1. RWTH Aachen University, Germany
2. Xi'an Jiaotong University, China

Phase-change materials (PCMs) can switch rapidly and reversibly between the amorphous and crystalline phase at high temperature. Yet, the two phases are stable at room temperature and exhibit pronounced optical and electrical contrast. These unique properties are exploited in electronic non-volatile random access memories (PC-RAM), where heating is induced by the Joule effect. Recently, nanosecond-fast crystallization of phase-change memory cells of size of less than 10 nanometers has been reported. These time and length scales are almost within reach of first-principles methods based on density functional theory. Here we present our ab initio molecular dynamics simulations of crystallization of two technologically important PCMs, namely $Ge_2Sb_2Te_5$ and Ag,In-doped Sb_2Te. We consider models of the two compounds containing up to 900 atoms. We first discuss the links between the fragility of the supercooled liquid phase of these materials and the ability of the glass to crystallize rapidly at high temperature and yet to be extremely stable at room temperature. We then show that our high-temperatures simulations yield crystal growth velocities in good agreement with experimental data. These simulations indicate that fast crystal growth stems from the large diffusion constants and sticking coefficients and the presence of a sharp crystalline-liquid interface.

10:20 AM

(GOMD-S1-049-2018) Atomistic Simulation of Crystallization Kinetics and Aging of Amorphous GeTe Nanowires (Invited)

S. Gabardi[1]; E. Baldi[1]; E. Bosoni[1]; D. Campi[1]; S. Caravati[1]; G. C. Sosso[3]; J. Behler[2]; M. Bernasconi*[1]

1. University of Milano-Bicocca, Materials Science, Italy
2. University of Goettingen, Germany
3. University of Warwick, United Kingdom

Tellurium-based glasses such as GeTe and GeSbTe alloys are of interest for application in nonvolatile phase change memories owing to their ability to undergo a fast and reversible transformation between the crystalline and amorphous phases upon Joule heating. A very attractive option for the development of these memories involves the use of nanowires (NWs). For this application, insights into the thermal properties of such NWs and, in particular, into the crystallization kinetics of the amorphous and supercooled liquid phases at the atomic level are crucial. Toward this end, we have performed atomistic simulations of ultrathin NWs (9 nm in diameter) of GeTe by making use of an interatomic potential generated by the neural network fitting of a large ab initio database. By melting a portion of the NW, we investigated the velocity of recrystallization as a function of temperature. The simulations show that the melting temperature of the NW is about 100 K below the melting temperature of the bulk, which yields a reduction by about a factor of 2 of the maximum crystallization speed. Further, a study of the structural properties of the amorphous phase of the NW suggests a possible origin of the reduction of the resistance drift observed experimentally in NWs with respect to the bulk. The analysis is based on the results of our previous study of this phenomenon in the bulk.

10:50 AM

(GOMD-S1-050-2018) A new way to study glass ceramic nucleation: Combining grand canonical monte carlo with enhanced sampling techniques and implicit solvents

M. E. McKenzie*[1]; J. C. Mauro[2]

1. Corning Incorporated, Science & Technology, USA
2. Pennsylvania State University, Materials Science and Engineering, USA

This presentation will cover the thermodynamic work of crystal nucleation where it is decomposed into three parts: 1) formation of cluster, 2) solvation of the cluster, and 3) the transition into a crystalline solid. Using the Grand Canonical Monte Carlo (GCMC) method coupled with umbrella sampling, we create an ensemble of different clusters and compositions. From this ensemble of relative formation energies, the solvation energies are calculated and added into the overall thermodynamic barrier. These solvation energies are needed to study the preference of the meta-stable cluster precursors. Using an enhanced sampling technique (Steinhardt Q4 bias), we can monitor the energy required to shift the cluster into its crystalline lattice. This combined approach using three different well studied systems (lithium disilicate, barium silicate, and soda lime silicate), we find the thermodynamic work was within 20% of experimental measurements. We are also able to find the correct meta-stable precursors for the nucleation event. Fundamentally understanding each separate factor allows us to better understand their influences upon nucleation.

11:10 AM

(GOMD-S1-051-2018) Molecular dynamics study of spontaneous nucleation and crystallization in barium sulfide (Invited)

J. P. Rino*[1]

1. Center for Research, Technology and Education in Vitreous Materials, Brazil

We proposed and tested an effective pair potential to model semiconductor barium sulfide, BaS. We have previously shown that our model correctly describes several dynamic and thermodynamic properties for this system (J.P. Rino, Comput. Mat. Sci. 92 (2014) 334-342). More importantly, the current simulations were able to capture the the spontaneous crystal nucleation and grain growth process in its supercooled region. The nucleation and crystallization kinetics of BaS, at a fixed supercoling, were then studied. We were able to observe the emergence of the nuclei and their crystal growth through one- and two-body correlations functions, such as the mean square displacement, incoherent intermediate-scattering function, pair distribution function, and coordination number. Statistics of the first nucleation event, as a function of temperature were also performed.

11:40 AM

(GOMD-S1-052-2018) Avalanche-mediated crystallisation of an aged hard-sphere glass (Invited)

C. Valeriani*[1]; P. Montero[1]; P. Rosales[1]; P. N. Pusey[2]; E. Sanz[1]

1. Universidad Complutense de Madrid, Spain
2. University of Edinburgh, United Kingdom

Glasses are formed from the super-cooled liquid state when motion is arrested on the scale of the particle diameter. Such states are thermodynamically unstable and may crystallize shortly after the initial quench (poor glass formers). Crystallization can also arise in mature, well-formed glasses after a long period of apparent stability. The microscopic mechanism of this process (devitrification) remains elusive. In recent numerical studies, it has been shown that devitrification of aged hard-sphere glasses happen via cooperative, stochastic particle rearrangements called avalanches. Quiescent periods, with particles rattling in their nearest-neighbors cages, are interrupted by avalanches, with a subset of particles undergoing large rearrangements. The amount of crystal in the system increases during an avalanche, even though crystallizing particles differ from avalanche-like ones. The appearance of avalanches is independent both on particles' dynamics (whether Newtonian or Brownian) and on the employed simulation ensemble (constant volume versus constant pressure). When increasing density, the avalanche mechanism becomes more evident and crystallization is retarded due to a decrease of the avalanche emergence likelihood. Work is ongoing aiming at unraveling the structural features of avalanchepropense regions in a glass.

12:10 PM

(GOMD-S1-053-2018) Interface structure of nuclear waste glasses and spinel/inverse-spinel $NiFe_2O_4$ from Molecular dynamics simulations

W. Sun*[1]; J. Du[1]

1. University of North Texas, Material Science and Engineering, USA

Understanding spinel crystal growth in glass melts is critical for efficient processing of nuclear waste glasses. The interface structures between boroaluminosilicate nuclear waste glasses and $NiFe_2O_4$ spinel/inverse-spinel structures were investigated by using molecular dynamics simulation with recently developed empirical potentials. The bulk and surface behaviors of spinel and inverse-spinel $NiFe_2O_4$ crystals were first studied by using the energy minimization method and the results show good agreement with experimental results in terms of structure, energetics and mechanical properties. International simple glass (ISG) chosen as a model system for the nuclear waste glasses were then generated using MD simulations. The glass/spinel interfaces were then investigated using MD. The z-density profiles showed the preferential adsorption of specific ions from glass to nearby crystal surfaces, which suggested ordering of atoms on the glass side in close proximity to $NiFe_2O_4$ crystals. In addition, it was found that there exist exchange of B^{3+} ions from glass and Fe^{3+} ions from crystal at the interface area between the glass and $NiFe_2O_4$ crystals with different surface orientations.

Session 6: Mechanical Properties of Glass IV

Room: El Mirador West (22nd Fl)

Session Chairs: Lothar Wondraczek, University of Jena; Shigeki Sawamura, Friedrich-Schiller-University Jena

9:20 AM

(GOMD-S1-054-2018) Ion Exchange Strengthening of Silicate Glasses (Invited)

C. Kayaalp[1]; B. Kayacan[1]; N. Özben[1]; S. Atilgan[1]; B. Ogut[1]; L. Simurka[1]; D. Güldiren[1]; B. Okan[1]; M. Çelikbilek Ersundu[2]; I. Sokmen*[1]

1. Türkiye Sise ve Cam Fabrikalari A.S., Science and Technology Center, Turkey
2. Yildiz Technical University Department of Metallurgical and Materials Engineering, Turkey

Ion exchange is a chemical strengthening technique that improves the mechanical strength of glasses by modification of the surface chemical structure via immersion of the glass into a molten KNO_3 salt bath, wherein small sodium ions in the glass structure are replaced by potassium ions, thereby inducing the formation of a compressive stress layer. Present study compares the ion exchange behaviors of sodium alumina silicate glass composition, lead free crystalline glass composition and two different soda lime silicate glass compositions with different alumina contents by applying KNO_3 salt bath at varying temperatures and time intervals. Mechanical properties of ion exchanged glasses in terms of strength, hardness, scratch and indentation crack formation behaviors were studied by different techniques. The magnitude of residual stress and depth of stress layer of the glass samples after ion exchange were measured by surface stress meter which is based on the theory of photoelasticity.

9:50 AM

(GOMD-S1-055-2018) Chemical strengthening of silicate glasses: Dangerous and beneficial impurities

V. M. Sglavo*[1]

1. University of Trento, Dpt. Industrial Engineering, Italy

Ion-exchange process has gained remarkable interest during past fewthe last years for chemical strengthening silicate glasses because of its suitability and flexibility in the applying reinforcement of to different components with different geometriyes and thickness. higher strength than thermal tempering. In this technique, glass is in direct contact with molten salt at a temperature below its transition temperature. Several variables like glass composition, molten bath composition, temperature, and time can affect the efficiency of the ion-exchange process. In this researchDuring a typical industrial process, sodium atoms contained in the glass are substituted by potassium ions diffusing from the molten salt. An interesting aspect regards the presence of impurities in the bath, introduced with the raw salt or accumulated during the process. In the present work, the effect of variable sodium, magnesium and calcium concentration in the, effect of molten bath on the efficiency of the ion exchange process was analyzed. The addition of limited quantities of silica was also studied as remedial action for non-efficient salts.

10:10 AM

(GOMD-S1-056-2018) Thermal tempering ability of Soda-Borosilicate glasses and their frangibility

M. Ono*[1]; Y. Kato[1]

1. Asahi Glass Company, Research Center, Japan

Fracture pattern in tempered glass determines the safety of the glass. For example, window glass for automobile has a regulation of least fragment density so as not to provide large glass debris. In order to satisfy the regulation, glass is usually thermally tempered by rapid quenching at around softening temperature. By the tempering, glass obtains large inner tensile stress which triggers large number of small fragments when it is broken. Some soda-borosilicate glasses have large thermal expansion coefficients (α_{HT}) above T_g while those below T_g (α_{LT}) are similar to sodalime glass. We have done thermal tempering tests onto these soda-borosilicate glasses. The amount of the residual stress was significantly enhanced by the increase of α_{HT}. However, the fragment density of the tempered soda-borosilicate glasses with larger tensile stress was much smaller than that expected from sodalime glass. The difference of the frangibility of soda-borosilicate glasses are also discussed.

10:30 AM

(GOMD-S1-057-2018) Surface Shear Stress Relaxation

E. Aaldenberg*[1]; J. H. Seaman[3]; T. Blanchet[2]; P. J. Lezzi[3]; M. Tomozawa[1]

1. Rensselaer Polytechnic Institute, Materials Engineering, USA
2. Rensselaer Polytechnic Institute, Mechanical, Aerospace, and Nuclear Engineering, USA
3. Corning Inc., USA

Glass optical fibers have been strengthened by a short heat-treatment at a temperature much less than the glass transition temperature while a tensile stress is applied. The strength increase relative to the strength of a fiber heat-treated under no applied stress was approximately equal to the amount of applied stress during the treatment. This strengthening was explained by a relaxation of the applied tensile stress from the surface of the glass such that when the applied stress is released, the surface layer of the glass springs back into compression. Subsequently, Wiederhorn et al. proposed an alternative model to describe the strengthening which involved a volumetric swelling of the glass due to water diffusion and reaction with the glass. They suggested that the reaction was promoted by tensile stress and that a volume change would lead to a surface compressive layer. In this study, an experiment to distinguish between the two models was conducted: shear strain was applied to a silica glass rod through a constant angle of twist and the decrease in torque was measured over a heat-treatment period.

10:50 AM

(GOMD-S1-058-2018) Glass Compression Strength

J. Swab*[1]; C. Meredith[1]

1. Army Research Laboratory, USA

The intrinsic compression strength of ceramics and glasses can be very difficult to determine. The specimen geometry and fixture used to apply the load, if not properly designed, can result in the generation of tensile stresses that lead to premature fracture and misleadingly low strength values. Often the compression strength is inferred from hardness values but this is not appropriate for ceramics and glasses. The compression strength is an input parameter in numerous modeling and simulation packages used to predict performance in some applications. As a result it is imperative that the compressive strength of the candidate material be properly and accurately measured. A borosilicate and soda-lime-silicate float glasses were machined into dumbbell-shaped specimens that were designed to induce fracture from within the gage section while minimizing the stress concentrations that can lead to the undesirable tensile stresses. Quasi-static experiments were performed using a screw-driven load frame and the fracture process was recorded with a high speed camera. Dynamic experiments were performed using a split-Hopkinson pressure bar setup with bars having the same diameter as the specimen and an ultra-high speed camera to record the fracture process. This presentation will summarize the results to date and determines if the compression strength of these glasses is strain rate dependent.

11:10 AM

(GOMD-S1-059-2018) Effect of Case Depth on Abrasion Resistance and Dynamic Fatigue in Chemically Strengthened SLS Glass

W. LaCourse*[1]; N. J[1]; M. Wisniewski[1]; M. O'Connell[2]

1. Alfred University, Inamori School of Engineering, USA
2. GE Aviation, USA

Chemically strengthened (K^+ for Na+) SLS glass with case depths between 15 and 60 microns show varying degrees of strength retention and resistance to dyamic fatigue when exposed to either pre- or post-strengthening abrasion. Minimum case depths on the order of 40 - 50 microns are required for acceptable abrasion resistance. The stressing rate dependence ("n" value) of MOR for determined from log σ_{MOR} vs. log ($d\sigma/dt$) varies with case depth and abrasion. Experimental "n" values can be substantially higher than predicted suggesting both residual stress and chemical effects at the crack tip.

11:30 AM

(GOMD-S1-060-2018) Strength of Aged Soda Lime Silicate Glass and E-glass Fibers

J. Van Sant[1]; I. Reimanis*[1]; D. Diercks[1]

1. Colorado School of Mines, USA

Mechanical strength degradation of fibers via exposure to moisture was studied in soda lime silicate glass and in E-glass. Aging experiments were performed on both atom probe tomography and transmission electron microscopy (TEM) specimens to examine chemical changes in the glasses. A focused ion beam (FIB) was used to impart a crack-like notch which was then sequentially observed by TEM after various aging treatments. Soda lime silicate glass exhibits a higher degree of chemical reactivity than E-glass in humid conditions. The corresponding single fiber tensile tests were performed to correlate the chemical activity during aging with the strength. In addition, the FIB was used to impart a crack-like notch in fibers to examine whether or not the local fracture toughness is influenced from aging.

S2: Glasses in Healthcare - Fundamentals and Application

Fundamentals of Bioactive Glass I: Atomic and Molecular Structure

Room: El Mirador East (22nd Fl)
Session Chairs: Nicholas Smith, Corning Incorporated; Steven Jung, Mo-Sci Corporation

9:20 AM

(GOMD-S2-001-2018) Modeling and characterization of bioglasses: New insight by solid state Nuclear Magnetic resonance (NMR) / Dynamic Nuclear Polarization (DNP) techniques (Invited)

C. Bonhomme*[1]; J. Du[2]; J. M. Rimsza[2]; C. Combes[3]; K. Leyngardigal[3]

1. UPMC, France
2. University of North Texas, USA
3. CIRIMAT, France

Solid state NMR techniques are of paramount importance for in-depth characterization of bioglasses. Indeed, NMR is sensitivite to short- and medium-range order due to the variety of the involved interactions: chelical shift, homo- and heteronuclear dipolar interactions, quuadrupolar and paramagnetic interactions. NMR is unique in the sense that it remains sensitive to structure and dynamics (over orders of magnitude) even in the case of disordered or amorphous derivatives. In this presentation, the latest developements in solid state NMR will be presented including: ultra-fast MAS, methodology for quadrupolar nuclei (I > 1/2), ultra-high fied NMR, instrumentation and DNP for huge sensitivity enhancement, modeling of glasses, first-principles calculation of NMR parameters for NMR/DNP applications. A particular emphasis will be put on Dynamic Nuclear Polarization as it enables the implementation of "impossible NMR experiments". All abovementioned points will be illustrated by recent results otained in our laboratory and related to bioglasses.

9:50 AM

(GOMD-S2-002-2018) Structure and properties of B_2O_3/SiO_2 substituted Na_2O-CaO-SrO-P_2O_5-SiO_2 bioactive glasses from combined study of experiments and molecular dynamics simulations

M. Ren*[1]; X. Lu[1]; L. Deng[1]; P. Kuo[1]; J. Du[1]

1. University of North Texas, USA

The effect of B_2O_3/SiO_2 substitution in SrO containing 55S4.3 bioactive glasses on glass structure and properties such as ionic diffusion and glass transition temperature (Tg) was investigated by combining experiment synthesis, characterization, in vitro bioactivity testing and molecular dynamics simulations with newly developed potentials. Simulation results were used to explain glass properties such as Tg and bioactivity. The fraction of bridging oxygen linearly increased with increasing B_2O_3 content, resulting in an increase of overall glass network connectivity. Ion diffusion behavior was found to be sensitive to glass composition changes and trend of change with the level of substitution is also temperature dependent. The experimental results show a decrease of Tg with increasing B_2O_3 content. This is explained by the increase of ion diffusion coefficient and decrease of diffusion energy barrier (Ea) in glass melts as suggested by high temperature range (above Tg) diffusion calculation as B_2O_3/SiO_2 substitution increases. Below Tg, an increase of Ea for modifier ions was observed with B_2O_3/SiO_2 substitution, which is consistent with the increase of glass network connectivity. The change of bioactivity with B_2O_3/SiO_2 substitution was discussed with the change of pH value and release of boric acid to the solution.

10:10 AM

(GOMD-S2-003-2018) Atomistic Simulations of the Initial Stages of the Sol-Gel Synthesis of Bioactive Glasses (Invited)

A. Cormack*[1]

1. Alfred University, USA

Understanding polycondensation in aqueous solutions is of central importance for the development of more effective biomaterials by sol-gel approaches. In this presentation, the atomic-scale evolutions of a calcium-containing precursor solution corresponding to a typical sol-gel bioactive glass and of a corresponding Ca-free solution were compared using reactive molecular dynamics simulations. The simulations highlight a significantly faster rate of condensation in the presence of calcium, resulting in the formation of large and ramified silica clusters within 5 nanoseconds, which are absent in the Ca-free system. This different behavior is interpreted in terms of a Ca-induced nanosegregation in calcium-rich and silica-rich regions, which promotes the condensation reactions within the latter. By identifying a possible mechanism behind the limited incorporation of calcium in the silica nanoclusters formed in the early stages of the sol-gel process, it is anticipated that further studies will facilitate the engineering of enhanced initial calcium incorporation and thus produce sol-gel biomaterials with improved properties.

10:40 AM

(GOMD-S2-004-2018) Bioactive Glasses Structure determination via Molecular Dynamics Simulations and NMR-DFT calculations (Invited)

A. Pedone*[1]

1. University of Modena and Reggio Emilia, Italy

Molecular dynamics simulations and NMR-DFT calculations have become fundamental techniques to get insights on the structure and properties of glasses. In the last decades, such technique has been extensively used to understand the relationships between the composition, structure and bioactivity of glasses used in healthcare. In our research group we have employed a synergetic experimental and computational approach to better characterize the structure and properties of potential bioactive glasses doped with specific ions to confer to the glass specific properties such as the ability to reduce reactive oxygen species (ROS) or to inhibit the formation of dental caries by maintaining at the same time bioactivity. This approach is based on the direct comparison of the experimental NMR spectra with those computed by using density functional calculations coupled with molecular dynamics and Spin effective Hamiltonians. Emphasis will be given to the decisive role of this approach both as interpretative tool for a deeper understanding of the spectral behavior of complex systems and as predictive instrument to map NMR data into a distribution of structural parameters and backwards.

11:10 AM

(GOMD-S2-005-2018) Solid State NMR Approaches for the Structural Characterization of Bioglasses (Invited)

H. Eckert*[1]

1. University of Sao Paulo, Physics, Brazil

Research and development of bio glass-ceramics over the last 40 years have greatly enhanced the quality of life. Silicate-based glasses and glass-ceramics are being widely used for bone and tissue healing application owing to their ability to bond to and integrate with living bone in the body without forming fibrous tissue around them or promoting inflation or toxicity. Improved glass compositions containing MgO, B_2O_3, and Al_2O_3 have been developed, and the introduction of templated sol-gel synthesis to this field has resulted in new mesoporous bioglasses with improved biological performance. In the search for structure-property relationships, solid-state nuclear magnetic resonance has proven to be a powerful tool for elucidating the short- and medium-range order of these

materials. The present lecture will summarize the state of the art in this field, detailing various recent advanced solid-state NMR approaches involving the use of magnetic-dipole dipole interactions for proving spatial proximity of nuclear species. New results obtained on mechanically stabilized mesoporous biosilicate glasses will be discussed.

11:40 AM

(GOMD-S2-006-2018) Structure of $Na_2O–B_2O_3–P_2O_5–SiO_2$ based model bioactive glasses

N. Stone-Weiss*[1]; N. J. Smith[2]; R. Youngman[2]; E. M. Pierce[3]; H. Eckert[4]; A. Goel[1]

1. Rutgers University, Materials Science and Engineering, USA
2. Corning Incorporated, Science and Technology Division, USA
3. Oak Ridge National Lab, Environmental Sciences Division, USA
4. University of Sao Paulo, Sao Carlos Institute of Physics, Brazil

P_2O_5 plays an important role in enhancing the bioactivity of most commercial bioactive glasses such as 45S5 and 13-93, largely due to its compatibility with mineral phosphate in bone tissue. Likewise, it is an important component in borosilicate-based bioactive glasses. However, its presence in borosilicate glasses leads to several structural changes that can have a significant impact on their glass forming ability, processing, dissolution behavior and ultimately its bioactivity. Therefore, in order to design novel borosilicate-based bioactive glass compositions it is imperative to understand the influence of P_2O_5 on the glass structure – property relationships. In this study, we aim at understanding the influence of P_2O_5 on the structure of glasses designed in the sodium borosilicate system over a wide composition space including per-boric (Na/B <1), sub-boric (Na/B = 1), and per-alkaline (Na/B >1) regimes. The glass structure has been examined using 1D and 2D MAS-NMR spectroscopic techniques. Our future work will focus on correlating these structural trends with observed elemental release behavior for these glasses in neutral – to – alkaline solutions relevant for biological applications.

S3: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 1: Applications

Room: La Vista F (22nd Fl)
Session Chair: Jingshi Wu, Corning Incorporated

9:20 AM

(GOMD-S3-015-2018) Ultrashort pulsed laser induced luminescence in functional glasses (Invited)

Q. Zhao*[1]

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

Ultrashort laser pulses can not only induced upconversion luminescence and long persistent luminescence but also black-body radiation in doped and undoped functional glasses. Firstly, this talk will review the ultrashort laser pulses induced luminescence phenomena. Then, we will present several progresses of ultrashort laser pulses induced luminescence in our group. Finally, the potential applications of ultrashort laser pulses induced luminescence will be demonstrated.

9:50 AM

(GOMD-S3-016-2018) Treatment of a leucite toughened dental glass-ceramic by a CO_2 laser

M. D. Bilandzic*[1]; C. Roos[1]

1. RWTH Aachen University, Department of Materials and Process Technology Glass and Composites, Germany

Laser technology has become even in modern dentistry a very important instrument. The usual application field of a dentist is hard and soft tissue surgery. A CO_2 laser provides the ideal wavelength and energy for modifying dental material such as dental glass-ceramics. This is because of laser beam absorption of about 95% in these aluminosilicate-based glasses which leads to high temperatures. To process a dental glass-ceramics with an optimum temperature profile or an efficient laser parameter setting and to achieve proper material behavior, a variety of material and laser interaction settings need to be investigated. Especially an investigation on how the crystals in the glassy matrix will change after an in situ laser treatment is of prior interest. Our investigations are focusing therefore on the basic processability of a dental glass-ceramic system (SiO_2-Al_2O_3-K_2O-Na_2O-CaO-MgO) by irradiating samples with a CO_2 laser (λ=10.6μm). In terms of surface behavior we investigate thereby especially the crystallinity ratio before and after the laser-processing and relate this to an optimum laser and material combination.

10:10 AM

(GOMD-S3-017-2018) In-Situ Raman Analysis of Laser Modified Oxide Glasses

S. T. Locker*[1]; S. K. Sundaram[1]

1. Alfred University, Glass Science, USA

Low-energy ultrafast laser pulses have been proven to optimize surface hardness in oxide glasses through structural densification. This effect is believed to be a result of decreasing interbonding angles and bonding distances. Raman spectroscopy will allow us to determine the structural effect leading to densification. Using in situ high-temperature Raman, we have investigated whether the laser-induced structural effects are reversible at any temperature beneath the glass transition temperature. Simulation studies have shown low-energy pulse laser effects to be reversible after irradiation, however, the change to optical properties were rescinded after allowing the glass to equilibrate at room temperature. We have used a low-energy femtosecond pulse laser, in-situ Raman spectroscopy, extended X-ray absorption fine structure (EXAFS) and X-ray absorption near edge structure (XANES) to characterize laser irradiated glass structure. We will report a case study on the structural changes in oxide glass after femtosecond pulse irradiation at various temperatures.

10:30 AM

(GOMD-S3-018-2018) Piezoelectric and ferroelectric properties of lithium niobate crystal lines laser-written deep inside glass (Invited)

K. J. Veenhuizen*[1]; L. Li[2]; S. McAnany[3]; I. Crawley[4]; D. Nolan[5]; B. Aitken[5]; S. Jesse[2]; S. Kalinin[2]; V. Dierolf[4]; H. Jain[3]

1. Lebanon Valley College, Physics, USA
2. Oak Ridge National Lab, USA
3. Lehigh University, Materials Science and Engineering, USA
4. Lehigh University, Physics, USA
5. Corning Incorporated, USA

Whereas the piezoresponse of free-standing, bulk single crystals, such as lithium niobate, prepared through conventional methods is well-understood, the effect of spatial confinement on the piezoelectric and ferroelectric properties of femtosecond laser-induced crystals in glass remains unexplored. Accordingly, piezoresponse force microscopy is utilized to map the spatial variation of the piezoresponse within lithium niobate crystals grown deep within lithium niobosilicate glass. Using lattice orientation maps of the crystals in glass acquired through electron backscatter diffraction analysis, the

piezoresponse of the crystals is correlated with their lattice rotation. In addition, the phase of the piezoresponse provides ferroelectric domain orientation information within the confined crystals. This work provides the first report of the native domain structure within laser-written crystals in glass, showing for lithium niobate a non-uniform ferroelectric domain structure within the crystal. Such crystals possess oppositely oriented domains at the nanoscale near the center of the crystal cross section, and large, uniformly oriented domains away from the center.

11:00 AM

(GOMD-S3-019-2018) Long lasting phosphorescence in transition and rare earth metal-doped glasses induced by ultrashort laser pulses

J. Qian*[1]; Q. Zhao[1]

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

Ultrashort laser pulses induced long lasting phosphorescence (LLP) in glasses was first reported at the end of the last century. Since then, contributions to elucidate the dynamics and mechanisms of laser-induced LLP have been made. In this presentation, we talk about a few new properties accompanying the LLP process induced by ultrashort laser pulses in a series of home-made transition and rare earth metal-doped glasses. Careful comparisons are made about the LLP property for various dopants and different glass compositions. Besides, the potential applications of laser induced LLP are discussed.

11:20 AM

(GOMD-S3-020-2018) Crystallization Behavior during Non-isothermal Laser Treatment of Fe-Si-B Metallic Glass

S. S. Joshi*[1]; A. V. Gkriniari[1]; S. Katakam[1]; N. B. Dahotre[1]

1. University of North Texas, Materials Science and Engineering, USA

Fe-Si-B metallic glass foils were crystallized using various input laser fluences. Thermokinetic conditions evolved during non-isothermal laser treatments were predicted using a multiphysics thermal model. Temperature, and corresponding heating and cooling rates generated were also extracted. Crystallite size was measured using x-ray diffraction and transmission electron microscopy. The fraction of crystallization was estimated with a differential scanning calorimetry. There was an initial increase in the crystallite size for lower laser fluence. The crystallite size reached a saturation for higher laser fluence range (0.6–0.9 J mm^{-2}). The fraction of crystallization steadily increased with the laser fluence. Unlike conventional processes, in the present situation the dynamic effects during laser processing dominated the crystallization and growth process. Rapid heating rates during laser processing led to an upward shift in the onset of crystallization temperature. Faster cooling rates upon termination of laser treatment prematurely arrested the crystallite growth yielding much finer crystallite sizes.

Session 3: Optical Fibers and Waveguides

Room: La Vista C (22nd Fl)

Session Chairs: Xianghua Zhang, CNRS - Université Rennes 1; Johann Troles, University of Rennes 1

9:20 AM

(GOMD-S3-021-2018) Novel chalcogenide glass fibers and fiber tapers for Mid-infrared SC generation (Invited)

S. Dai*[1]; X. Wang[1]; P. Zhang[1]

1. Ningbo University, Laboratory of Infrared Materials and Devices, China

Chalcogenide glass (CHG) fibers are excellent candidates for broadband supercontinuum (SC) generation due to their excellent MIR transparency and high third-order nonlinearity. Recently, ultra-broadband MIR SC generations have been achieved in ChG fibers pumped by a OPA laser. However, most ChG fiber media for SC generation, such as As_2S_3 and As_2Se_3, contain the toxic element arsenic. Thus, security issues may occur during glass preparation, fiber drawing, and performance testing. Meanwhile, Te-CHG based glasses have the highest optical nonlinearity and broadest transmission window, therefore, Te-CHG fibers are expected to generate the widest spectrum of SC. In this presentation, we report on the fabrication and characterization of two novel kinds of Ge-Sb-Se and Ge-Te-AgI chalcogenide fibers, and an As-S chalcogenide fiber taper. By pumping a 20-cm-long Ge-Sb-Se fiber with a core diameter of 23 μm using 150 fs pulses at 6.0 μm, supercontinuum spanning from ~1.8 to ~14 μm was generated. The double-cladding Ge-Te-AgI step-index fiber with a length of 14cm generates a MIR SC spanning from 2.0 μm to 16 μm, for a 40-dB spectral flatness. And, an SC generation spanning from 1.4 to 7.2 μm was achieved by pumping a 12-cm-long As-S tapered fiber with femtosecond laser pulses at 3.25 μm.

9:50 AM

(GOMD-S3-022-2018) Novel transparent glass-ceramic fiber obtained by the powder-in-tube technique (Invited)

S. Chenu*[1]; D. Pomarede[2]; J. Auguste[2]; G. Humbert[2]; A. Fernandes Carion[1]; M. Allix[3]; C. Genevois[3]; E. Veron[3]; J. Duclere[1]; P. Roy[2]; P. Thomas[1]; G. Matzen[3]; G. Delaizir[1]

1. SPCTS Laboratory, France
2. Xlim Research Institute, France
3. CEMHTI Laboratory, France

Since several years, optical fibers attract more and more attention in the materials science community thanks to the rising development of optical fibers with glass-ceramic core. Indeed, the introduction of crystals in the core of an optical fiber by means of glass-ceramic confers a crystalline environment to the luminescent ions used as doping elements and this crystalline media significantly increases the spectroscopic efficiency of the system and allows new radiative transitions. In this current work, we present experimental results about the fabrication of glass-ceramic-core optical fibers by the Powder-in-Tube process. The glass-ceramic we used, which derives from the system SiO_2–Na_2O–ZnO–Ga_2O_3 can contain up to 50 $_{wt}$% of $ZnGa_20_4$ spinel crystals and can be efficiently doped with transition metals. Moreover the size of its nanostructure can be tailored depending on the SiO_2 concentration, making this matrix a material of choice for the development of active glass-ceramic optical fibers. SEM-EDS measurements illustrated an evolution of the fiber core composition (compared to the starting bulk material) induced by the diffusion of SiO_2 from the fiber cladding, and TEM imagery demonstrated the formation of nanocrystals in the fiber core. Then, this glass-ceramic will be doped with Ni^{2+} ions in order to generate luminescence emissions in the range 1100 – 1500 nm.

10:20 AM

(GOMD-S3-023-2018) Tellurite optical fibres for 1-5 μm sources: Supercontinuum engineering, spectroscopic applications, hybrid fibres (Invited)

F. Smektala*[1]

1. University of Bourgogne, ICB, Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-UBFC, France

Infrared tunable fibered sources are actually in strong development and commercial sources based on fluoride glasses are today available. However, tellurite fibers present several intrinsic advantages by comparison to fluorides, even if less mature for now. Indeed, the interest of tellurites is their high non linearity, 10 to 50 times higher than fluorides. Several centimeters of fibers are sufficient to generate broadband spectra with tellurites when several meters are necessary with fluorides. Another interest of tellurites is their chromatic dispersion, with a zero dispersion wavelength (ZDW) around 2μm, a wavelength where femtoseconde fibered sources are now available. In the case of fluoride glasses, the ZDW is located at

lower wavelengths, around 1.5μm. Here, we present an overview of the elaboration of various tellurite microstructured or step-index fibers, with engineered dispersion, with regards to numerical aperture and core fiber diameter. The fine control of the optogeometrical parameters of the fibers allows a supercontinuum engineering and a broadband generation covering the whole 1-5μm range. Most of pollutant and greenhouse gases emitted by human activity absorb in the mid-IR and spectroscopic experiments realized on gases between 1 and 5 μm are presented. The possibility of the elaboration of hybrid electrical-optical fibers is also discussed.

10:50 AM

(GOMD-S3-024-2018) Thermally Drawn Electrically Conductive Composite Glass Fibers

F. Tan*[1]; S. Chen[1]; G. Tao[1]; J. Kaufman[1]; R. M. Gaume[1]; A. Abouraddy[1]

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

Electrically conductive amorphous materials exhibit the promising potential of being flexibly and thermally formed on a large scale as specialized electronic components in the form of drawn fibers, such as electrodes. We have found that thermally drawing glass/carbon-nanofiber composites from a consolidated bulk composite is hampered by carbon-reactivity and volatilization. We propose utilizing powder composites in lieu of bulk for thermally drawing a fiber comprising a pure glass cladding and composite core. In this strategy, glass viscous flow serves two goals: powder densification and fiber-forming. Therefore, viscosity matching between core and cladding plays a critical role in the continuity of the fiber. A series of microstructure, electrical, thermal and chemical characterizations were performed to study the thermally drawn glass fiber. By understanding of the basic physical mechanisms underlying the fiber formation process, we have successfully demonstrated cladding and core glass material combinations suitable for potential incorporation of crystalline semiconductor or conductor materials into the glass fiber. Furthermore, we have demonstrated that inserting additional metal cores in the thermally drawn fibers helps enhance the electrical conductivity by a factor of 30.

11:10 AM

(GOMD-S3-025-2018) All-Infrared supercontinuum generation in a step-indexed Se-based chalcohalide glass fiber (Invited)

X. Wang*[1]; R. Wang[1]; Z. Zhao[1]

1. Ningbo University, China

Mid-infrared (MIR) supercontinuum (SC) generation have been studied for decade in many infrared (IR) glass fibers. Chalcogenide (ChG) glasses are well known for their unique and striking characteristics in IR, transparence from visible up to 25 μm and high nonlinearity. Traditional selenide fiber is transparent near up to 12 μm but completely opaque in visible. It has been found that chalcohalide(ChH) glasses, who combined ChG with halogen or metal halide, could increase the optical band-gap and become transparent in visible while maintaining well IR transparence. However, halide is non-resistant to water, that hindering the application of ChH glasses. It is impossible to fabricate ChH fibers by method of conventional crucible or rod-in-tube. Here, a novel ChG fiber, based on $GeSe_2$-Ga_2Se_3-CsI glasses, with a perfect core-cladding structure was fabricated via extrusion-drawing method. This glass has excellent transparent both in red-visible and MIR, from 620 nm up to 19 μm. With lower material zero dispersion wavelength (ZDW) of 3.2 μm (in glass) and 2.5 μm (in fiber). This ChH glass has a higher nonlinear refractive index than that of AsS glass. Although the fiber shows slightly high loss, a broadband all-IR (1.31 μm to 12.6 μm) SC generation was generated in the 14-cm long fiber when pumped at 2.9 μm or 6.3 μm with a 150-fs pulse at a repetition rate of 1 kHz.

11:40 AM

(GOMD-S3-026-2018) Fabrication of tapered chalcogenide microstructured optical fibers for enhancing the non linear properties

J. Troles*[1]; C. Caillaud[2]; M. Meneghetti[1]; Y. Wu[1]; C. R. Petersen[3]; O. Bang[3]; J. Adam[1]; L. Brilland[2]

1. University of Rennes, France
2. SelenOptics, France
3. Technical University of Denmark, Denmark

Chalcogenide glasses are known for their large transparency window and their high nonlinear optical properties. Indeed, they can be transparent from the visible region up to the mid-infrared (mid-IR) until 12 μm. They present also a high nonlinear coefficient (n_2), 100 to 1000 times larger than for silica, depending on the composition. Another great advantage of chalcogenide glasses is the possibility to draw them into optical fibers. In the last 15 years, microstructured optical fibers (MOFs) have been realized with chalcogenide glasses. The recent improvements in the realization of chalcogenide microstructured fibers more particularly the fabrication of tapered fibers permit investigations in numerous fields of applications, such as telecommunication, infrared interferometry, sensors, and generation of mid-IR supercontinuum

S4: Glass Technology and Cross-Cutting Topics

Session 4: Waste Immobilization - Corrosion II

Room: La Vista D/E (22nd Fl)
Session Chairs: Aize Li, Corning Incorporated; Mike Harrison, National Nuclear Laboratory

9:20 AM

(GOMD-S4-019-2018) Glass Corrosion: An Interface-Controlled Process (Invited)

C. Lenting*[2]; L. Dohmen[1]; T. Geisler[2]

1. Schott AG, Germany
2. University of Bonn, Steinmann Institut, Germany

Due to its importance for the management of nuclear waste the borosilicate glass corrosion mechanism is for long and thoroughly investigated and controversially discussed in the science and engineering community. Understanding of the mechanism on a molecular level is essential to predict the release of radionuclides by modelling the corrosion rate, and hence assess the safety of the waste package over time scales that exceed any laboratory experiments. On these time frames, only geological glasses or younger archaeological samples can be used for comparison, which, however, reveal corrosion features like pattern formation not commonly observed with nuclear waste glasses. From experience with replacement reactions in the field of mineralogy, we conducted a variety of experiments, highlighting the importance of the reaction interface as the controlling instance of the corrosion progress, featuring congruent glass dissolution of and local silica saturation at the reaction interface (SPFT,AFM), and the formation of a water-rich interfacial layer (in situ Raman, isotope tracers, TEM). Additionally, recent studies report of a nanometer sharp interface (APT) challenging traditional assumptions as well. In this light, a review of previous work and an open discussion about a coherent corrosion mechanism for all types of glasses is needed.

9:50 AM

(GOMD-S4-020-2018) Dynamics of self-reorganization explains passivation of silicate glasses (Invited)

S. Gin*[1]; M. Collin[1]; P. Jollivet[1]; M. Fournier[1]; M. Thiruvillamalai[2]; J. Du[2]; S. Kerisit[3]

1. CEA, DE2D, France
2. University of North Texas, Department of Materials Science and Engineering, USA
3. Pacific Northwest National Lab, Physical & Computational Sciences Directorate, USA

It is acknowledged that passivating layers formed on glass surface are amorphous, porous and hydrated but little is known about how they form, how they passivate the glass and how they turn into more stable crystalline phases as predicted by thermodynamics. This is however a major request for improving the assessment of long-term behavior of high-level waste glasses. Here we first present experimental results on water dynamics in mature passivating gels formed on the International Simple Glass altered at 90°C and pH 7, in order to derive apparent diffusion coefficients. These are of the order of 10^{-20} $m^2.s^{-1}$. Using molecular dynamic simulations with ReaxFF and a second series of experiments with isotopically tagged water molecules, we then show that the ultra-slow diffusivity of water in this type of material can be explained if one consider that water is confined in closed micropores. Pore closure is a consequence of the self-reorganization of the glassy network after the release of mobile species from the pristine material. It is also shown that self-reorganization proceeds by hydrolysis and condensation reactions with a limited mobility of Si.

10:20 AM

(GOMD-S4-022-2018) Lessons in glass corrosion from the de-alloying of metallic systems

J. Ryan*[1]

1. Pacific Northwest National Lab, USA

For decades, there has been general agreement that corrosion is due to the combined contributions of two broad categories of mechanisms: reaction control (solution affinity, local solution changes due to secondary phase precipitation, and kinetic limitations) and transport control (ion exchange, pore tortuosity, and diffusion of rate-limiting ions). Existing models based on these mechanisms predict the resultant solution concentration of boron with reasonable accuracy, given good parameterization. They do not, however, predict (or attempt to predict) the formation of many of the structures observed at the surface of corroding glasses and often are very poor at predicting the concentrations of other ions in solution. Recently, an Energy Frontier Research Center has been formed to examine the mechanistic commonalities and differences between materials systems. In particular, the behavior of metal alloys with exposure to various fluids can provide insight into the corrosion of glass that has the potential to break this logjam. In this talk, we show how the mechanism of morphological evolution seen in corroding metal alloys can account for the dynamic structures and solution responses seen in the study of glass corrosion. Mathematical fits to various long-term corrosion datasets are also presented.

10:40 AM

(GOMD-S4-023-2018) Characterization of simulated silica gels and their interactions with water

T. S. Mahadevan*[1]

1. University of North Texas, Materials Science and Engineering, USA

Exposure of amorphous silica to water results in the formation of silica rich gel layers which provide resistance to further weathering and corrosion. Studying the transport of water and glass components in this gel layer and degradation of the gel structure is important to understand the corrosion mechanisms as well as to predict the durability of the glass especially in the case of nuclear waste glasses. Molecular Dynamics (MD) simulations with reactive potentials that allow for dissociation of water and chemical reactions provides valuable insights into some of the degradation mechanisms. Gel structures can be generated by several ways in MD simulations with the resultant gel structure bearing some of the characteristics of the generation method. In turn, the characteristic pore network and connectivity in the silica gel influence the transport of glass components and the degradation behavior. In this study, we draw a correlation between the nature of silica gel and the reactions that occur on exposure to water. By exposing a gel shielded glass matrix to an aqueous solution of glass components we also investigate the transport of these ions through the gel layer and the dynamics of the glass/gel and gel-water interfaces. Based on these simulations, we attempt to explain experimentally observed corrosion phenomena in multicomponent glasses.

11:00 AM

(GOMD-S4-024-2018) Formation and Structure of Passivation Gels by Reactive Molecular Dynamics Simulations

T. Du*[1]; M. M. Smedskjaer[2]; H. Li[1]; M. Bauchy[3]

1. Harbin Institute of Technology, School of Civil Engineering, China
2. Aalborg University, Department of Chemistry and Bioscience, Denmark
3. University of California, Los Angeles, Department of Civil and Environmental Engineering, USA

The long-term dissolution rate (stage II) of nuclear waste immobilization glasses is thought to be controlled by the hydrated passivation gel that gradually forms on their surface. However, the mechanism of formation of such gel remains debated—i.e., precipitation from the solution or internal reorganization of the glass. Further, the mechanism of stage II dissolution (and its rate-limiting step) remains unclear. Here, based on reactive molecular dynamics simulations, we investigate the kinetics of formation and structure of several gels exhibiting varying compositions (i.e., varying Al/Si ratios) and formation mechanisms (i.e., solution precipitation or in situ glass reorganization). The influence of the composition and structure of the gel on the mobility of hydrated species is studied.

S1: Fundamentals of the Glassy State

Session 2: Crystallization in Glass and Its Applications I

Room: La Vista C (22nd Fl)
Session Chairs: Edgar Dutra Zanotto, Federal University of Sao Carlos; Kenneth Kelton, Washington University

1:20 PM

(GOMD-S1-061-2018) Crystal Nucleation in Metallic and Silicate Liquids and Glasses (Invited)

K. F. Kelton*[1]

1. Washington University, Physics, USA

Glasses and glass ceramics are critically important in modern technology. Crystal nucleation and growth are key for optimizing the production of both materials. This talk will focus on nucleation, which must be suppressed for glass production and subsequent processing, and to ensure long-term stability of the glass. It must be well understood and controlled for the production of glass ceramics and metallic amorphous/crystal composites. Most nucleation data are analyzed within the classical theory of nucleation (CNT), a phenomenological theory developed in the late 1800's. Many of the fundamental assumptions of CNT have been questioned and fits to the data rely on adjustable parameters that cannot be independently checked. Further, many factors not considered within the CNT are now known to play a critical role in nucleation processes. Selected studies in silicate and metallic glasses and liquids will be presented to illustrate these points and to suggest how to move beyond CNT.

1:50 PM

(GOMD-S1-062-2018) Transport mechanism in crystal nucleation in oxide glass-formers (Invited)

D. R. Cassar[1]; E. Dutra Zanotto*[1]

1. Federal University of Sao Carlos, DEMa, Brazil

Some glass forming compositions, such as $Li_2O.2SiO_2$, $BaO.2SiO_2$ and $Li_2O.2B_2O_2$, undergo internal homogeneous nucleation in laboratory timescales when properly heated. The Classical Nucleation Theory (CNT) has been tested for such type of glasses, and the results show a remarkable pattern: i) the temperature of the nucleation rate maximum, T^*, is close to the laboratory glass transition temperature, T_g, and ii) for temperatures above T*, the steady-state nucleation rates, I(T), can be described by fitting with a variable surface energy, $\sigma(T) = a + b.T$ (b>0). With this approach, however, if the $\sigma(T)$ expression obtained for $T > T^*$ is used to predict I(T) data below T^*, the values of I(T) are strongly overestimated. As the diffusing structural units are unknown for complex glass-formers, in this work we test whether the (assumed) diffusion coefficients, D(T), could be the cause of such unexpected failure of CNT at T*. We do so by calculating D(T) in three ways: from viscosity data (the traditional way), from nucleation induction times (used a few times), and from crystal growth rates (rarely or never used). In addition, differently from most previous studies, here we use "clean" datasets in all analyses, that is, for each composition, the I(T) and D(T) data were obtained from samples of the same glass batch. The main results will be thoroughly discussed during the talk.

2:20 PM

(GOMD-S1-063-2018) Nucleation and Crystallization in Binary P_2O_5-SiO_2 Glasses

R. Youngman*[1]; B. Aitken[1]; I. Dutta[1]; B. Wheaton[1]; D. Baker[1]

1. Corning Incorporated, Science & Technology Division, USA

Homogenous glasses can be made via conventional melt quenching in the P_2O_5-SiO_2 binary from 0 to ~30 mol% P_2O_5, and, as P replaces Si, T_g decreases as a consequence of the reduced network connectivity when Q^3 phosphate groups replace Q^4 silicate tetrahedra. ^{29}Si and ^{31}P NMR studies show that mixing between these network structural elements is completely random until reaching a P_2O_5 concentration where phase separation occurs, leading to an increase in T_g and network connectivity, the latter reflecting the stabilization of 5- and 6-fold coordinated silicon groups. Self-nucleating glass-ceramics can be formed from glasses with ~ 30 mol% P_2O_5. These materials contain SiP_2O_7, one of the few crystalline phases stable at atmospheric pressure in which Si is octahedrally coordinated by O. Although stabilization of octahedral Si in the precursor glasses, as well as the onset of phase separation, are observed to correlate with propensity for crystallization of SiP_2O_7 during subsequent heat treatment, the underlying nucleation processes are poorly understood. Here we make use of advanced characterization methods to identify the initial crystal phase formed during nucleation heat treatments, and to follow the evolution of the glass-ceramic microstructure during subsequent heat treatments.

2:40 PM

(GOMD-S1-064-2018) Estimating nucleation temperature range in $BaO•2SiO_2$ and $5BaO•8SiO_2$ glasses by differential thermal analysis

X. Xia*[1]; I. Dutta[2]; J. C. Mauro[3]; B. Aitken[2]; K. F. Kelton[4]

1. Washington University in St. Louis, Institute of Materials Science & Engineering, USA
2. Corning Research and Development Corporation, Corning Incorporated, USA
3. Pennsylvania State University, Department of Materials Science and Engineering, USA
4. Washington University in St. Louis, Department of Physics and the Institute of Materials Science & Engineering, USA

The temperature range for significant crystal nucleation in $BaO•2SiO_2$ and $5BaO•8SiO_2$ glasses is estimated from the crystallization peak height and peak temperature, measured using differential thermal analysis (DTA). For the $BaO•2SiO_2$ glass, the estimated range for significant nucleation is from 660 °C to 770 °C, with a nucleation rate maximum near 712 °C. These results agree with existing nucleation rate data for $BaO•2SiO_2$ glass, obtained using a two-step heat treatment. From DTA studies, the estimated temperature range for significant nucleation in the $5BaO•8SiO_2$ glass is from 675 °C to 790 °C, with a maximum rate near 725 °C. Since direct measurements of the nucleation rate in the $5BaO•8SiO_2$ glass do not exist, we obtained them using the two-step heat treatment method. The results agree well with the DTA estimates. The temperature where growth begins to overlap significantly with nucleation can also be obtained from the DTA method, with the peak height being most sensitive to this. These results are presented and discussed.

3:00 PM

(GOMD-S1-065-2018) Crystallization of sodium molybdato-phosphate and tungstato-phosphate glasses

L. Koudelka*[1]; O. Kupetska[1]; P. Kalenda[1]; P. Mosner[1]; L. Montagne[2]; B. Revel[2]

1. University of Pardubice, General and Inorganic Chemistry, Czechia
2. University of Lille, France

Study of the glass to crystal transformation was realized for two glasses $25Na_2O.50MoO_3.25P_2O_5$ and $25Na_2O.50WO_3.25P_2O_5$ giving the crystalline compounds $NaMoO_2PO_4$ and $NaWO_2PO_4$, respectively. Their XRD patterns were in a good agreement with the Kierkegaards data from 1961. Physico-chemical properties of the corresponding glasses and crystals were compared, as well as their Raman and ^{31}P MAS NMR spectra. Melting points of these two compounds were determined as 695 ±2°C for the molybdenum compound and 875±2°C for the tungsten compound. Crystallization mechanism studied by the method of Day and Ray show on the prevailing surface nucleation. ^{31}P MAS NMR spectra of glasses show the same shape and almost same width, which reflects a similar local environment for P in these glasses. The position of the W resonance at more negative chemical shift is due to the larger electrical field strength of W than Mo. Each crystal have 2 phosphorus sites charge compensated by W (Mo) and Na. This is reflected by the presence of 2 resonances on the 31P NMR spectra. The difference in chemical shifts between the two compounds is again due to electric field effect. Raman spectra show similarity in structural features of Mo and W glasses and Mo and W- isomorphic compounds. Nevertheless, positions of vibrational bands differ due to different masses of both atoms.

Session 2: Crystallization in Glass and Its Applications II

Room: La Vista C (22nd Fl)
Session Chairs: Randall Youngman, Corning Incorporated; Indrajit Dutta, Corning Incorporated

3:40 PM

(GOMD-S1-066-2018) Ge-Ga-S/Se chalcogenide glass-ceramics transparent in the infrared: Multifaceted materials (Invited)

L. Calvez[1]; X. Zhang*[1]

1. University of Rennes 1, France

Chalcogenide glasses (ChG) offer very large potential applications in the IR range. However, the advantages of ChG are largely inhibited by their weak thermo-mechanical properties. Our studies were focused on the enhancement of their thermo-mechanical properties. Fortunately, the nucleation and growth of crystalline particles allow for the increase of hardness and toughness, meanwhile keeping the usual advantage of fabrication versatility. The crystallization behavior and related physicochemical properties of nontoxic $Ge(S/Se)_2$-based ChG were firstly focused on the addition of Ga with or without the addition of alkali halide. Today, such chalcogenide glass-ceramics demonstrate a high potentiel for plethoria applications. In fact, depending on the glass composition, 'a la carte' properties can be obtained. Thus, the possibility to strongly increase the luminescence efficiency by controlled crystallization within ChGC doped with rare-earth will be developped. Moreover, by controlling the generated crystalline species, some ChGC present outstanding properties such as photo-carrier generation for a novel generation of photosolar cells. Also, the possibility to phase change this material from amorphous to crystalline opens the route to new reconfigurable devices such as antennas. Finally, the possibility to accelerate the crystallisation process by using Spark Plasma Sintering will be shown.

4:10 PM

(GOMD-S1-067-2018) Effect of melt size and scale-up protocols on property evolution in $GeSe_2$-As_2Se_3-PbSe (GAP-Se) glass ceramics for infrared GRIN applications

A. Yadav*[1]; A. Buff[1]; M. Kang[1]; L. Sisken[1]; C. Smith[1]; J. M. Lonergan[1]; K. Chamma[1]; C. Blanco[1]; C. Arias[1]; C. R. Baleine[2]; T. Mayer[3]; A. Swisher[4]; A. Pogrebnyakov[4]; A. Hilton[5]; G. Whaley[5]; T. J. Loretz[6]; A. Yee[7]; G. Schmidt[7]; D. Moore[7]; K. Richardson[1]

1. University of Central Florida, CREOL-College of Optics and Photonics, USA
2. Lockheed Martin Corporation, USA
3. Virginia Polytechnic Institute and State University, USA
4. The Pennsylvania State University, Department of Electrical Engineering, USA
5. Amorphous Materials Inc., USA
6. Computer Engineering Services, USA
7. University of Rochester, Institute of Optics, USA

We report on the impact of melt size associated with the scale-up of proto-type lab-scale, multi-component chalcogenide glasses developed for gradient refractive index (GRIN) applications. Such glasses, when subjected to controlled crystallization protocols, result in the formation of mid-IR transparent, nanocomposites. The crystallization behavior and physical property evolution in a $20GeSe_2$-$60As_2Se_3$-20PbSe (20 mol% PbSe) chalcogenide glass has been quantified as melts were scaled from 40g to 1.3kg size. The role of melt size on base glass morphology, starting optical homogeneity and heat treatment induced microstructure from controlled crystallization (post-heat treatment crystalline phases, volume fractions, refractive index change and optical transparency) are presented following a fixed nucleation and growth treatment. Results illustrate the impact of melt size and thermal history on base glass morphology and thermal properties, and resulting microstructural properties of the resulting glass ceramic. The considerations required for transitioning candidate lab-scale optical materials to a commercial scale in light of these findings, are discussed.

4:30 PM

(GOMD-S1-068-2018) Alkaline Earth Aluminosilicate Oxyfluoride Glass Ceramics: From Glass Structure to Crystallization Behaviors

J. Zhao*[1]; X. Chen[1]; J. Du[2]; Q. Xu[1]; Z. Luo[1]; X. Qiao[1]; X. Fan[1]

1. Zhejiang University, Materials Science and Engineering, China
2. University of North Texas, Materials Science and Engineering, USA

Due to various novel features and promising applications of oxyfluoride glass ceramics, understanding of their structure, phase separation and crystallization behavior is critical. This work combines Molecular Dynamics (MD) simulations and experimental method to study the structure feature and evolutions of alkaline earth aluminosilicate oxyfluoride glasses and glass-ceramics. Experimental results show alkaline earth fluoride nanocrystals precipitated from the glass matrix with certain fluoride concentration of CaF2-, SrF2- and BaF2-based aluminosilicate glasses after thermal treatment. MD simulation results reveal that phase separation with fluoride rich regions occurs in certain compositions, and their shape and size are affected by the cation field strength of the alkaline earth ions. Based on the results above, we propose a model to describe the structure and crystallization behavior of such glasses. In this model, the structure of oxyfluoride glass is consist of two immiscible phases: silicate rich phase and fluoride rich phase. And the initial fluoride crystallization would originate from the corresponding fluoride rich glassy phase. With this model, certain type of aluminosilicate oxyfluoride glass ceramics could be designed under the guidance of MD simulation. And it will pave a way to develop new types of rare earth ion doped luminescent glass-ceramics.

4:50 PM

(GOMD-S1-069-2018) Crystal structure of the hexagonal $CaAl_2Si_2O_8$ precipitated in $CaO–Al_2O_3–SiO_2$ glass-ceramics

K. Maeda*[1]; K. Akatsuka[1]; K. Iwasaki[2]; A. Yasumori[2]

1. Asahi Glass Co., Ltd., Innovative Technology Research Center, Japan
2. Toyko University of Science, Japan

Crystallization of glass is one of the practical techniques to make glass tough. We reported that the hexagonal $CaAl_2Si_2O_8$ (dmisteinbergite) precipitated in the $SiO_2–Al_2O_3–CaO$ glass on the metallic molybdenum particle as a nucleating agent. The precipitation of the hexagonal $CaAl_2Si_2O_8$ increased the fracture toughness and decreased the hardness of the glass. As a result, the brittleness defined as toughness-to-hardness ratio decreased 70% from its original glass. In this paper, we report the TEM and XRD analysis results of the glass-ceramics in order to investigate the detail crystal structure of the hexagonal $CaAl_2Si_2O_8$ as well as its crystal orientation together with metallic molybdenum particle. Although the hexagonal image of the precipitated crystal was clearly observed by TEM, the Rietvelt analysis of its XRD pattern suggested the stacking of the hexagonal layers distorted in a few degrees. In terms of the crystal orientation, it was revealed that (001) plane of the hexagonal $CaAl_2Si_2O_8$ and (011) plane of the metallic molybdenum existed in the same plane. The morphology of the crystals and the mechanical properties of the glass-ceramics are also discussed.

5:10 PM

(GOMD-S1-070-2018) Thermodynamic database development of the Li_2O-Al_2O_3-SiO_2(-Na_2O-CaO-MgO) system and its application for the thermodynamic analysis of the glass-ceramics

B. Konar*[1]; I. Jung[2]

1. McGill University, Mining and Materials Engineering, Canada
2. Seoul National University, Department of Materials Science and Engineering, Republic of Korea

A critical evaluation and thermodynamic optimization of the Li_2O-Al_2O_3-SiO_2(-Na_2O-CaO-MgO) system at 1 atm pressure was performed for the first time. In the volatile alkali-rich compositions, where phase equilibrium information was unavailable, new phase diagram experiments were conducted using sealed Pt/Au-Pd/Pt-Rh crucibles. The obtained Gibbs energy functions can reproduce all available and reliable experimental data from 298 K to above liquidus temperatures. The Gibbs energy of liquid oxide solution was described using the Modified Quasichemical Model, where the associate species for charge compensation effect was considered and the liquid-liquid immiscibility and short-range ordering phenomenon were replicated. Several complex solid solutions like β-eucryptite, β-spodumene, were thermodynamically optimized considering their lattice structure and crystal chemistry. With the Gibbs energy description for each phase, any phase diagram and thermodynamic property of this system and its sub-binaries can be calculated. The present thermodynamic database was applied to the thermodynamic analysis of the selective crystallization in glass-ceramics. With the help of the new thermodynamic database, thermodynamic driving forces for glass nucleation in β-eucryptite/β-spodumene (in Li_2O-Al_2O_3-SiO_2 system) compositions were calculated.

5:30 PM

(GOMD-S1-071-2018) Zirconium environment in SiO_2-Na_2O-CaO-Al_2O_3 glass

M. Ficheux*[1]; L. Cormier[2]; E. Burov[1]

1. Saint-Gobain, SVI, France
2. CNRS, IMPMC, France

Zirconium is widely used in glass ceramic as a nucleating agent. It can also enter a few specific glass compositions like nuclear waste insulation tank. We know that in MgO-Al_2O_3-SiO_2-ZnO classical parent glass used in glass ceramic, it can generate some nanoscale phase separations before crystallization. In that case, one phase is highly concentrated in Zr while the main phase is Zr-poor. This phase separated state is a precursor of the crystallization. During classical SiO_2-Na_2O-CaO-Al_2O_3 industrial forming glass, some Zr can leave the Zr-containing wall of the furnace to enter the glass structure. This Zr may generate a macroscopic glassy phase looking like a droplet and inducing defects on the final glass. These droplets can sometime crystalize to create another kind of defect. A structure study of NCAS glassy phases with variable amount of Zr led to understand how Zr environment impacts its crystallization. Various analyses have been realized (XANES,EXAFS,RMN…) to describe Zr environment from its first neighbors to the polymerized glass lattices in order to determine if phase separation also affects crystallization in this system.

Session 3: Structural Characterizations of Glasses I

Room: El Mirador West (22nd Fl)

Session Chairs: Chris Benmore, Argonne National Lab; Sabyasachi Sen, UC Davis

1:20 PM

(GOMD-S1-072-2018) Determining Si-O-Si angle distributions from NMR Spectra (Invited)

P. J. Grandinetti*[1]

1. Ohio State University, Chemistry, USA

It's been 34 years since Dupree and Pettifer first attempted to quantify the Si-O-Si bond angle distribution (BAD) in silica glass from its ^{29}Si NMR spectrum. This approach assumes the 4 linkage angles of a Q4 are uncorrelated, and relies on established correlations between the ^{29}Si chemical shift and the mean Q^4 linkage angle. 2D ^{17}O NMR measurements provide an alternative approach through correlations of the electric field gradient experienced by the oxygen nucleus to the linkage angle and mean Si-O distance. This approach requires few assumptions about the local structure and, in principle, is the most direct probe of the BAD. Additionally, it provides a 2D structural correlation between Si-O-Si linkage angle and mean Si-O distance--revealing an unexpected positive correlation in the case of silica glass. Recently, we have developed a 3rd NMR approach for determining the BAD that exploits correlations of the geminal ^{29}Si J coupling across a Si-O-Si linkage to the linkage angle and the mean linkage angle of the two connected Q^4 tetrahedra. This 2D NMR approach similarly gives a 2D correlated structural distribution. In this talk all three approaches will be explained along with possible systematic biases associated with their underlying assumptions. The resulting distributions from experimental ^{29}Si and ^{17}O NMR results are compared to each other as well as to inversions of diffraction data.

1:50 PM

(GOMD-S1-073-2018) Phase separation in Li- and Na- silicate glasses

J. Wu*[1]

1. Corning Incorporated, Glass Research, USA

It is well known that there are immiscibility boundaries in low alkali binary silicate glasses, and the composition range of the immiscibility boundary becomes smaller from Li to Na. In this study, we obtained clear glasses in the immiscibility region by fast cooling. However, further analysis from transformation range viscosity, dilatometric softening temperature, differential scanning calorimetry (DSC), and scanning electron microscopy (SEM) images showed that the glasses are still phase separated. The topology of the secondary phase changes from discrete droplets to being interconnected as alkali content increases. The size of the secondary phase is in the 50 nm to 500 nm range. Subsequent heat treatments did not have an effect on the topology or mechanical properties. Due to the small size of the secondary phase, and Li^+ and Na^+ migration under the electron beam, it is impossible to perform quantitative analysis of the composition of the two phases. However, using the multiple glass transitions observed in DSC, one can estimate the composition of the two phases.

2:10 PM

(GOMD-S1-074-2018) Study of Lithium borate glass structure

N. Tsuda*[1]; M. Tanida[2]; T. Miyajima[3]; S. Urata[3]; T. Taketoshi[3]

1. Asahi Glass Co., Ltd., Electronic Material General Division, Japan
2. Asahi Glass Co., Ltd., New Product R&D Center, Japan
3. Asahi Glass Co., Ltd., Innovative Technology Research Center, Japan

It is thought that in the alkali borate glass, oxygen coordination type distribution around boron ions has great influence on various properties of glass. However the structure of the lithium borate glass has not been well known. In this study, we researched the glass structure

of the high Li content Li-B-O glass system. Through this research we would like to clarify the relationship between the Li ion diffusion property and the oxygen coordination around boron ions in the glass structure.

2:30 PM

(GOMD-S1-075-2018) New Magnetic Resonance Strategies for the Structural Characterization of Photonic Glasses and Glass Ceramics (Invited)

H. Eckert*[1]

1. University of Sao Paulo, Physics, Brazil

Rare-earth ion (RE) doped glasses and glass-ceramics are luminescent photonic materials with promise for laser applications. To optimize the luminescent properties of these materials, detailed structural information regarding the local environment of the rare-earth species is essential. While solid state nuclear magnetic resonance (NMR) is in general a useful tool for such purposes; unfortunately, the rare-earth ions themselves cannot be studied by NMR due to their paramagnetism. To overcome this difficulty, a three-fold examination strategy has been developed including (1) NMR studies of diamagnetic mimics, (2) NMR studies of framework nuclei affected by paramagnetic interactions, and (3) pulsed-EPR studies sensitive to the magnetic dipolar interactions of the unpaired electrons with nearby nuclear spins, using electron spin echo envelope modulation (ESEEM) and hyperfine sublevel correlation (HYSCORE) spectroscopy. These approaches are complementary in terms of the relevant length scale of the interactions studied and their combination has turned out very successful in elucidating the short- and medium-range order details of the rare-earth ion local environments, allowing a rationalization of the luminescent properties of these glasses on a structural basis. Recent applications of this experimental strategy to fluoride phosphate laser glasses will be discussed.

3:00 PM

(GOMD-S1-076-2018) Photoelasticity and structure of silicate glasses with high polarization ions

A. Saitoh*[1]

1. Ehime University, Materials Science and Engineering, Japan

Glasses with nominal molar compositions of binary xRO–, or xR'_2O_3–(100-x)SiO_2 (R = Sn, Pb, R' = Sb, Bi, x = 40–60 mole%) were prepared and their structures were determined by ^{29}Si MAS-NMR, Raman, and IR spectroscopies. And the effects of composition and structure on stress-induced birefringence were studied. The photoelastic constant (PEC) changes systematically from positive values to negative values when RO or R'_2O_3 increases, and zero compositions (PEC ≈ 0) were experimentally observed. The zero PEC compositions can be predicted from the coordination numbers and bond lengths of the R–O and R'–O, and Si-polyhedra using an empirical model. Compositional dependent changes in the optical property are attributed to changes in the coordination environments of the heavy metal ions and their effects on the silicate anionic network, which leads to an understanding of photoelasticity–structure relationship in silicate glasses.

Session 3: Structural Characterizations of Glasses II

Room: El Mirador West (22nd Fl)

Session Chairs: Chris Benmore, Argonne National Lab; Mario Affatigato, Coe College

3:40 PM

(GOMD-S1-077-2018) Extending the range of Si-29 NMR: Silicate glasses and crystals with abundant paramagnetic transition metal and rare earth cations (Invited)

J. Stebbins*[1]

1. Stanford University, USA

Over 3+ decades, NMR has become an important tool for quantifying the structures of disordered glassy and crystalline silicates, aluminosilicates, and borosilicates. However, because of known (or expected) severe line broadening, almost all of such studies have been on compositions with less than a few % of paramagnetic cations, excluding important families of materials containing abundant transition metals and rare earths with unpaired electron spins. Inspired by recent NMR studies of Li-based transition metal oxide and phosphate battery materials (C. Grey group and others), we have developed methods to observe accurate Si-29 spectra for a variety of Cu2+, Fe2+, Co2+ and Ni2+ silicate crystals and glasses. Spectra can be 100's of times broader than those of diamagnetic glasses, but frequency shifts of 1000's of ppm can potentially provide great sensitivity to local structure and order/disorder. Although the current early states of our data and theoretical understanding do not yet allow detailed interpretations of results, it is clear for glasses such as CoCaSi2O6 and NiCaSi2O6 that spectra and structure are very different from those of the corresponding crystals, probably at least in part to changes in cation coordination. Prospects for greatly expanded applications of this powerful experimental tool to wider composition ranges will be discussed.

4:10 PM

(GOMD-S1-078-2018) Tellurite Glass Structure from Te-125, O-17, and K-39 NMR

M. Garaga[1]; U. Werner-Zwanziger[1]; J. Zwanziger*[1]

1. Dalhousie University, Chemistry, Canada

The complex solid-state chemistry of tellurites, involving multiple coordination environments and the presence of lone pairs, makes the short-range structure of tellurite-based glasses challenging to unravel. Recent work by neutron diffraction and modeling showed convincingly that even in TeO_2 glass, the coordination number is less than four, the value in the thermodynamically stable crystal. We describe work based on Te-125, O-17 and K-39 NMR aimed at determining the short-range structure of TeO_2 and potassium tellurite glasses. We used echo-based, static-sample wide-line methods for Te-125 and K-39, and a variety of one and two-dimensional methods for O-17. By studying a variety of crystals, we were able to establish strong structural correlations between the Te-125 shift tensor elements and the local Te bonding. Furthermore, based on O-17 results we can rule out simple non-bridging oxygen structures as the source of the low coordination number in TeO_2 glass. We found that glassy TeO_2 is best described in terms of the γ TeO_2 polymorph, and could show how the addition of potassium modifies this structure.

4:30 PM

(GOMD-S1-079-2018) Structure of binary alkali and alkaline-earth tellurite glasses: Results from two-dimensional ^{125}Te NMR spectroscopy

M. A. Marple*[1]; Z. Whittles[1]; I. Hung[2]; Z. Gan[2]; S. Sen[1]

1. University of California Davis, Chemical Engineering and Materials Science, USA
2. NHMFL, USA

The structure of tellurite glasses has been studied in the past using a variety of spectroscopic and diffraction techniques. However the complexity of the Te-O coordination environments in these glasses has made unequivocal interpretation of the structural data extremely challenging. For example, distinction between the various co-existing Te-O coordination environments in tellurite glasses is obscured in the typical one-dimensional ^{125}Te NMR spectra as the latter are broadened by a combination of chemical shift distribution and large chemical shift anisotropy. In the present study, we have utilized two-dimensional ^{125}Te isotropic-anisotropic correlation NMR spectroscopy to investigate the compositional evolution of the structural network in binary BaO-TeO_2 and Na_2O-TeO_2 glasses. The results demonstrate that a consideration of the full ^{125}Te chemical shift tensor in combination with the composition dependent evolution of isotropic ^{125}Te NMR line shape yields a consistent structural model of these glasses in terms of the complex tellurium speciation. Progressive addition of the modifier oxide is found to result in a depolymerization of the network of corner- and edge- shared $TeO_{4/2}$ trigonal bipyramids in TeO_2 via their replacement with negatively charged $TeO_{3/2}O$ trigonal bipyramids and $TeO_{1/2}O_2$ trigonal pyramids with one and two non-bridging oxygen, respectively.

4:50 PM

(GOMD-S1-080-2018) Cation Migration Mechanisms in Mixed-Network Former Glasses

W. Wu[1]; W. Wang[1]; S. W. Martin[2]; J. Kieffer*[1]

1. University of Michigan, USA
2. Iowa State University, Materials Science and Engineering, USA

We systematically investigated the modifier cation migration mechanisms in two series of mixed network former glasses, sodium borosilicates (NBS) and sodium borogermanates (NBG), correlating the adiabatic elastic moduli, measured using Brillouin scattering, and the activation energy for ion conduction. We developed a reaction equilibrium model that, in combination with NMR data and elastic properties allows us to determine the the number density of charged oxygen species that can form stable modifier cation sites in the network structure. These sites can involve exclusively non-bridging oxygen (NBO), charged bridging oxygen (CBO) associated with over-coordinated network species, or mixtures of the two. Furthermore, cation jumps can occur between any combination of sites. In NBS glasses cation migration pathways involve mostly sites formed by NBO at high silica concentrations and transition to pathways established by predominantly CBO at high borate concentrations, whereas in NBG glasses, jumps between CBO rich sites dominate across the entire composition range. Allowing for a composition dependence of the activation energy for each jump type, expressed by a low-degree polynomial in number density, we applied a ridge regression technique to identify these type-specific activation energies. Accordingly, all jump pairings have unique character with their activation energies largely independent of glass composition.

5:10 PM

(GOMD-S1-081-2018) Synthesis, structural and magnetic properties of vanadium-lithium-borate glasses

P. Kidkhunthod*[1]

1. Synchrotron Light Research Institute (Public Organization), Research Facility Department, Thailand

In this work, vanadium-lithium-borate glasses, $0.5V_2O_5$-$0.5(Li_2O$-$xB_2O_3)$ with x = 1.0, 2.0 and 3.0, respectively, were prepared by conventional melt-quench technique. The glass samples were characterized by X-ray diffraction, scanning electron microscopy, X-ray absorption spectroscopy, X-ray photoelectron spectroscopy, UV-Visible Spectroscopy and vibrating sample magnetrometry. X-ray absorption near-edge spectra at the V K-edge confirmed the presence of the mixing of V^{4+} and V^{5+} oxidation states and X-ray photoelectron spectroscopy were used to quantify and reveal the amount of V^{4+} and V^{5+} in the glass samples with approximately a ratio of 1:4 for V^{4+}:V^{5+}. The paramagnetic behavior were found for the glass samples with x = 1.0 and 2.0 due to the presence of V^{4+}. However, an influence of B_2O_3 content clearly affected to the glass sample with x = 3.0 resulting to a diamagnetic nature of this glass composition. The local structural information around V atoms in all glass samples were addressed using extended X-ray absorption fine structure technique with a mean oxygen coordinated network of 3.50(1). The notable properties of these glasses suggests a possibility in the energy storage applications eg. cathodes of Li-ion batteries.

Session 5: Computer Simulations and Modeling V

Room: La Vista A/B (22nd Fl)

Session Chairs: Jessica Rimsza, The University of North Texas; Jincheng Du, University of North Texas

1:20 PM

(GOMD-S1-082-2018) Bridging the gap between atomistic and continuum simulations for amorphous solids (Invited)

S. Urata*[1]

1. Asahi Glass Co., Ltd., Innovative Technology Research Center, Japan

Atomistic simulations, such as Molecular dynamics and Monte Carlo methods, are useful to get insightful information on the mechanism of glass toughening. This is because, for example, plasticity originated from atomistic rearrangement in angstrom scale is a key factor to control glass brittleness. In addition, nanoscale phenomena can be visually and theoretically examined by using the simulation techniques. On the other hands, since fracture and crack propagation of glass substrates are macroscale phenomena, continuum simulation technologies are promising approaches to design glass products. It is however they require empirical constitutive law and definition on crack propagation. To bridge the atomistic and continuum methods, we may have three possible multiscale modeling; (1) concurrent coupling, (2) hierarchical coupling and (3) indirect coupling. In this talk, recent development on the three approaches for amorphous glassy materials would be reviewed.

1:50 PM

(GOMD-S1-083-2018) Structural Mechanisms of Plastic Deformation in Hydrostatically Compressed Calcium Aluminosilicates

N. T. Wiles*[1]; S. Goyal[2]; L. M. Morehouse[1]; S. P. Baker[1]

1. Cornell University, Materials Science, USA
2. Corning Incorporated, USA

Decades of research have shed light on plastic deformation in silicate glasses particularly through the use of indentation experiments. Two plastic deformation mechanisms have been identified: densification and shear. Densification has been associated with "anomalous" glasses containing low amounts of modifiers, whereas

shear has been associated with "normal" glasses rich in modifiers. Despite our definitions of plastic deformation mechanisms, we still understand little about the atomic motions which constitute each mechanism and how imposed stresses correlate with each mechanism. We completed a series of molecular dynamics simulations of calcium aluminosilicate glasses along the tectosilicate line in a range from 50-100% SiO_2. This range of compositions spans the spectrum from "normal" to "anomalous" and according to simple models contain no NBOs. We compressed these samples hydrostatically up to 15 GPa and observed structural changes upon the application and release of pressure. We show that throughout the composition range there are variations in the deviatoric strain heterogeneity and degree of densification which can be correlated to structural changes such as coordination number, bond angle distribution, ring size distribution, and the degree of ring puckering.

2:10 PM

(GOMD-S1-084-2018) High-frequency dynamics of liquids: Direct links between dynamical, thermodynamic and structural properties from MD modelling results

L. Wang*[1]

1. Queen Mary University of London, School of Physics and Astronomy, United Kingdom

We develop an approach to liquid thermodynamics based on collective modes including high-frequency transverse modes. We perform extensive molecular dynamics simulations of noble, molecular and metallic liquids and provide the direct evidence that liquid energy and specific heat are well-described by the evolution of high-frequency transverse modes propagating above the Frenkel (hopping) frequency. The agreement between predicted and calculated thermodynamic properties is seen in the notably wide range of temperature spanning tens of thousands of Kelvin. The range includes both subcritical liquids and supercritical liquids. We discuss interrelationships between structure, dynamics and thermodynamics of liquids and supercritical fluids and the structural crossover at the Frenkel line.

2:30 PM

(GOMD-S1-085-2018) Densification of glass under spherical indentation: Comparison between Raman spectroscopy and FEM calculations

G. A. Rosales-Sosa*[1]; Y. Kato[1]; S. Isawa[1]; S. Yoshida[2]; A. Yamada[2]; J. Matsuoka[2]; H. Yamazaki[1]

1. Nippon Electric Glass, Corporate Technology Division, Japan
2. The University of Shiga Prefecture, Center for Glass Science and Technology, Japan

The evolution of plastic deformation during mechanical indentation of oxide glasses is of great importance for understanding their crack initiation behavior and its relation with stress. Recently, Finite-Element-Modeling (FEM) has been successfully used as a tool for predicting the deformation of glass (densification and plastic flow) in a-SiO_2 under sharp-indentation (e.g. Vickers and Berkovich). In this work, the deformation of a-SiO_2 glass subjected to spherical-indentation has been simulated by means of FEM, and compared with experimental data: Raman spectroscopy (densification distribution) and white-light interferometry (indentation-depth profiles). Two different yield functions: 1) a linear type, and 2) elliptical type, were tested in FEM calculations. By using a linear-type yield function, it was possible to reproduce the spherical indentation of silica glass: densification distribution and maximum penetration depth when indented at different mechanical loads from 1 N up to 7 N. This model is promising for investigation the densification phenomena under spherical indentation in other oxide glass systems. The effect of the yield function type on the density distribution will also be discussed.

2:50 PM

(GOMD-S1-086-2018) Investigating the structure and properties of per-alkaline aluminosilicate glasses using molecular dynamics simulations

M. Ren*[1]; J. Du[1]; A. Goel[2]

1. University of North Texas, USA
2. Rutgers University, USA

Classic Molecular Dynamics (MD) Simulations were used to study various peralkaline (Na/Al>1) aluminosilicate glasses to obtain better understanding of the composition–structure–property relationships in this glass system. More than 99% of Al were 4-coordinated in these glasses, validating that Na^+ tend to charge balance $[AlO_4]^-$ network forming units first and then, excess Na^+ was used to create non-bridging oxygen (NBO) on Si. As the drop of Na/Al ratio, the percentage of NBO also decrease, indicating an increase of the glass network connectivity. Oxygen coordination analysis shown that there are a small amount of three-bridging oxygen (TBO) (0.2%--2.6%) in most simulated glasses, playing a role for the charge balance of $[AlO_4]^-$. There tend to be a liner dependence between the formation of TBO and the growth of excess NBO in sodium aluminosilicate glass. Subsequent analysis of the TBO environment shown that OAl_3 and OAl_2Si are dominant tricluster types. In addition, the degree of aluminum avoidance was determined through polyhedral connection probability calculation. The results shown that Al tend to random distributed in the glass structure, suggesting a violation of Lowenstein's rule. These structural properties were used to explain macroscopic properties of glass, such as change of glass transition temperature (T_g) and hardness (H_v) with glass composition.

Session 8: Glass Under Extreme Conditions - Relaxation and Structure, Experiment and Modelization

Room: La Vista A/B (22nd Fl)
Session Chair: Yann Vailles, CNRS-CEMHTI

3:40 PM

(GOMD-S1-087-2018) Relaxation of permanently densified glasses (Invited)

D. de Ligny*[1]; A. Cornet[2]; A. Veber[1]; M. Christine[2]; V. Martinez[2]; K. Januchta[3]; M. M. Smedskjaer[3]

1. University Erlangen-Nürnberg, Materials Sciences and Engineering, Germany
2. University Lyon1, Institut Lumière Matière, France
3. Aalborg University, Department of Chemistry and Bioscience, Denmark

Despite the considerable amount of studies and data on in-situ and ex-situ compression of glasses, very low interest was shown for the reverse transformation, i.e. the relaxation during high temperature annealing, from high density to low density. Densified SiO_2, soda silicate and aluminoborate glasses, obtained from different pressure and temperature routes have been annealed over a wide range of temperatures. In the case of pure silica glass, hot and cold compressions were used to separate the effects of pressure and compression temperature. For soda silicates glasses, the sodium concentration was varied to study the effect of modifiers. And aluminoborate glass will allow us to discuss the effect of the network former elements. In situ micro-Raman / Brillouin spectroscopy, Small Angle X-Ray scattering or Differential Scanning Calorimetry were used to follow the structural and energetic evolution. For pure silica and soda silicate glasses, while density decreases monotonically during ambient pressure annealing, the relaxation takes place through a transitory state, consisting in an increase of the network inhomogeneity seen by both Raman and SAXS. The kinetic is overall faster for cold compressed silica samples as well as for soda silicate glasses. In the case of aluminoborate glasses, a very different dynamic was observed. The

relaxations are very fast and their overall dynamics are closer to the relaxation of the glass transition.

4:10 PM

(GOMD-S1-088-2018) Design and testing of a large sub-hemispherical glass port for a deep-sea camera housing

F. Cazenave[1]; E. H. Baker[2]; N. D. Card[3]; G. D. Quinn[4]; P. Remijan[5]; J. Salem[6]; A. K. Varshneya*[3]

1. Monterey Bay Aquarium Research Institute, USA
2. Connecticut Reserve Technologies, USA
3. Saxon Glass Technologies, USA
4. Private consultant, USA
5. Fathom Imaging Inc., USA
6. NASA Glenn Research Center, USA

A dome-shaped glass port was developed for a sub-sea camera for use on an autonomous underwater vehicle at water depth to 2500m. The unusually large (250mm diameter) and flattened shape of the dome was dictated by optical requirements in order to achieve the highest possible image quality. A first iteration of the dome failed during pressure testing at 2750 psi. Using finite element analysis and fractography to guide, a new design was developed where a titanium ring bonded to the base reduced tensile stress development. Weibull parameters, fracture toughness and slow crack growth parameters of N-BK7 and H-K9L glasses were measured using ring-on-ring and 4-point bend testing. Again, using FEA and the Ceramics Analysis and Reliability Evaluation of Structures (CARES) program, the dome reliability was predicted, and a proof test protocol was established. To further improve the reliability, the glass was chemically strengthened to an optimized surface compression and case-depth. Strengthening was measured on witness specimens subjected to biaxial stresses via ring-on-ring testing. Three domes were successfully proof tested at pressures up to 5000 psi. This presentation shows that, with this systematic approach, deep-water camera domes need not be limited to the usual small diameter hemisphere; the door is open to new shapes having better optical quality with predictable reliability.

4:30 PM

(GOMD-S1-089-2018) Glasses for taming the extreme conditions (Invited)

M. Naji*[1]; G. Guimbretiere[2]; P. Simon[2]; D. De Sousa Meneses[2]; L. Martel[3]; D. Manara[3]; Y. P. Vaills[2]

1. University Sidi Mohamed Ben Abdellah, Physics Department, Morocco
2. Universite d'Orleans, CNRS CEMHTI, France
3. European Commission, Joint Research Centre (JRC), Directorate of Nuclear Safety and Security, Germany

We think of Sahara Desert, volcanic mountains and deep oceans as the most extreme environments. However, the man-made world has its own harsh conditions, such as high temperature and nuclear radiation. Therefore, we need materials that can endure these conditions and simultaneously maintain their performance. Oxide glasses when designed with high precision have the ability to work under extreme conditions of high temperature and radiation, such as glasses for fireplaces, cooktops, nuclear waste immobilization, etc. However, these promising applications depend on the thermodynamic and structural stability of the glass during operation. For example, upon a temperature perturbation the glass undergoes a relaxation - crystallization process, which strongly affects its short and long-term performance. In this presentation, I will cover some applications of glasses under high temperature and radiation, then I will present the instrumental challenges and the methods developed to study glasses in such environments. I will give an insight into the microscopic mechanisms governing glass relaxation – crystallization at high temperature. Lastly, I will give example of encapsulation of plutonium in borosilicate glasses designed for nuclear waste immobilization.

5:00 PM

(GOMD-S1-090-2018) Molecular dynamics (MD) simulations and non-equilibrium modeling to interpret some behaviors through glass transition and in glassy state (Invited)

H. Jabraoui*[1]

1. University de Lorraine, Laboratoire de Physique et Chimie Théoriques (LPCT, UMR CNRS), France

MD simulations are used to elucidate the effect of adding alkali or alkaline oxides on the structural, thermodynamic and elastic properties silicate and aluminosilicate glasses. The space correlation functions are determined to provide the detailed structural analysis. We have extracted the fictive temperature from the volume vs temperature to determine the glass transition using different cooling rates and modifier amounts. These results allow us to draw some general conclusions about the crucial role of the modifier and cooling rate of silicate system properties. On the other hand, we used a simple model of thermally activated hopping in a two-level system associating a master equation approach to investigate some non-equilibrium aspects of the glass transition. With this approach the calculated caloric curves and the fictive temperature of the glass transition are simulated. The frozen-in of the configurational entropy during cooling, as well as the negative overshoot during unfreezing of the system, which are typical features of the glass transition, can be enlightened. Moreover, it is also possible to simulate the so-called entropy production term and to highlight the difference between configurational entropy and entropy production. It is also interesting to clearly show the validity of the Clausius theorem.

S2: Glasses in Healthcare - Fundamentals and Application

Fundamentals of Bioactive Glasses II: Dissolution Behavior and Bioactivity

Room: El Mirador East (22nd Fl)
Session Chairs: Alastair Cormack, Alfred University; Alfonso Pedone, University of Modena and Reggio Emilia

1:20 PM

(GOMD-S2-007-2018) Structural basis for controlled elemental release from multicomponent glasses (Invited)

N. J. Smith*[1]; E. Bakowska[1]; N. Stone-Weiss[2]; A. Goel[2]; J. Klotz[1]; R. Youngman[1]; R. Schaut[1]

1. Corning Incorporated, USA
2. Rutgers University, Material Science, USA

Third-generation biomaterials are predicated on the concept that materials such as multicomponent bioglasses can stimulate specific responses from the body based on tailored ion release in desired mixtures and dose rates. Prospective design of such glasses therefore requires detailed knowledge of aqueous release kinetics from multicomponent compositions, which has its fundamental basis in glass structure. Here, we review results from a host of kinetic studies on simplified glasses in aqueous media, considering the extraction response under conditions far from saturation, in order to offer important insights about the structural drivers for release rates and corresponding congruency across a variety of glassforming systems. These principles pave the way toward modeling and predicting multi-element release from glasses of arbitrary composition, and can be extended into the design of novel bioglasses to provide a custom suite of ions at desired dosage.

1:50 PM

(GOMD-S2-008-2018) Dissolution behavior of Li_2O-ZnO-P_2O_5 glasses in water

H. Zhang*[1]; R. Brow[1]; A. Kumar[1]

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

The dissolution behavior of two series of glasses from the Li_2O-ZnO-P_2O_5 (LZP) system were investigated using calorimetric techniques. The first series of glasses with the molar compositions xLi_2O-(60-x) ZnO-40P_2O_5, 0≤x≤60, have a constant O/P ratio, and the second series glasses, yLi_2O-yZnO-(100-2y)P_2O_5, 25≤y≤35, have a constant nominal Li_2O-to-ZnO ratio, and an O/P ratio between 3.0 and 3.67. Heat released from the dissolution and precipitation reactions were determined using a calorimeter under both dilute and saturated conditions. Changes in solution chemistry were monitored using ICP-OES and phosphate anion distributions were characterized using High Pressure Liquid Chromatography (HPLC). These results will be compared with those predicted from thermodynamic calculations (Factsage). This work was supported by the National Science Foundation (CMMI-1661609).

2:10 PM

(GOMD-S2-009-2018) Mixed Glass Former Effects on the Dissolution Behavior of Na-Ca-Borophosphate Glasses

P. Freudenberger*[1]; Q. Myers[1]; B. Curtis[2]; R. Brow[1]

1. Missouri University of Science & Technology, USA
2. Iowa State University, USA

Na-Ca-phosphate glasses are being used for a variety of biomedical applications due to their biocompatibility and their wide range of compositionally-dependent dissolution rates. Adding borate to a Na-Ca-phosphate glass is one way to tailor dissolution rate, as well as to control the local pH change during dissolution. In the present study, High Pressure Liquid Chromatography (HPLC) was used to characterize the effects of composition on phosphate anion distributions, and ^{31}P and ^{11}B magic angle spinning (MAS) Nuclear Magnetic Resonance (NMR) and Raman Spectroscopies were performed to characterize the development of the resulting borophosphate networks. Static and "semi-dynamic" dissolution studies in water and in phosphate buffer solutions provide information about dissolution kinetics, and thermodynamic models of solution chemistry explain the changes in solution pH as the glasses dissolve.

2:30 PM

(GOMD-S2-010-2018) Impact of rare earth ions on dissolution behavior and cellular proliferation of alkali-free bioactive glasses

S. Gupta*[1]; S. Kapoor[1]; M. Bhamidipati[1]; L. Fabris[1]; A. Goel[1]

1. Rutgers University, Material Science & Engineering, USA

Rare-earth has an increasingly important role in the field of biomaterials. For example, ceria nanoparticles have been shown to act as neuroprotective agents by preventing reactive oxygen species from inducing apoptosis in tissue culture cells, while lanthanum ions have been shown to enhance the ERK phosphorylation and osteoblast differentiation via Gi protein signaling. Therefore, incorporating these ions in the bioactive glass chemistries can allow us to design new-generation of gene activating bioactive glasses with controlled release of functional ions tailored for specific patients and disease states. With this aim, our work is focused on understanding the impact of rare-earth cations (La^{3+}, Ce^{4+}, Nd^{3+}, Sm^{3+}) on the dissolution and in vitro cellular proliferation of alkali-free bioactive glasses designed in the glass forming region of $CaMgSi_2O_6$ – 3CaO-P_2O_5 based pseudo-binary system. The dissolution behavior of melt-quenched glasses has been studied in deionized water and neutral – to – alkaline pH followed by chemical analysis of post-dissolution aliquots by ICP-OES, while the pre- and post-dissolution glass samples were characterized by XRD and FTIR. The effect of rare-earth ions on cell viability and proliferation in bone marrow mesenchymal stem cells (BMSCs) was observed via MTT assay and alkaline phosphatase activity.

2:50 PM

(GOMD-S2-011-2018) Bioactive glasses modified by oxides with potential enzymatic-like activities

G. Malavasi*[1]; L. Menabue[1]; G. Lusvardi[1]

1. University of Modena and Reggio Emilia, Dept. of Chemical and Geological Sciences, Italy

We investigate the ability of bioactive glasses modified with oxides to act as catalase and superoxide dismutase (SOD) mimic materials. In past years, several nano-oxides (i.e. CeO2, CuO, Co3O4, Fe2O3) were investigated because they showed enzymatic-like activities. The ability of these materials to act as enzymes is strictly related to the fast and easy interconversion between their two oxidation states (i.e. Ce3+/Ce4+, Cu+/Cu2+, Fe2+/Fe3+). Therefore, we thought to synthesize glasses with oxides that induce the presence of a double oxidation state. Starting from this state of the art, we have decided to study a) Ce-mesoporous glasses with different compositions and b) molten bioactive glasses based on 45S5 system modified by Mn, Cu, Fe, Co, V, Ti and Zr oxides in order to verify how the glass composition affects the enzymatic-like activity and the bioactivity (ability to form hydroxyapatite). We have tested the SOD and the catalase mimic activities on glasses with different Ce3+/Ce4+ ratio and different oxides. The catalase and SOD mimic activity tests have revealed that the Ce-mesoporous glasses and molten glasses modified by Mn, Cu, Fe, Co and V oxides are able to mimic the activity of the two enzymes. In addition, the FT-IR and XRD analysis have confirmed the material bioactivity. These results highlight that it is possible to obtain a glass with both enzymatic-like activity and bioactivity.

Fundamentals of Bioactive Glasses III: Novel Applications of Bioactive Glasses

Room: El Mirador East (22nd Fl)

Session Chairs: Christian Bonhomme, UPMC; Hellmut Eckert, University of Muenster

3:30 PM

(GOMD-S2-012-2018) Transforming materials science into a finished commercial medical device (Invited)

S. Jung*[1]

1. Mo-Sci Corporation, USA

Commercializing a medical device is far from trivial and much more complex than the initial innovations in materials such as composition or form factor that most material scientists are familiar. Composition or form factor may be critical to the biological properties and functionality of a material, but there are many other stages to the design and testing process that must be considered during the commercialization process for a finished medical device. In fact, additional innovations may be required in areas such as packaging, sterilization, logistics, or storage that are relatively unknown during the material design phase. Additionally, academic research can be augmented with a battery of biocompatibility and toxicity analysis that are well defined by specific ISO standards and can add significant value to the research as a whole, or play a deciding role in filing for intellectual property. This talk will focus on the different stages of medical device commercialization that should be considered for a successful regulatory submission along with estimated timelines for each.

4:00 PM

(GOMD-S2-013-2018) Manufacturing Calcium Phosphate Porous Microspheres for Orthobiologics Applications

I. Ahmed*[1]; Z. Hossain[1]; U. Patel[1]; D. Grant[1]; V. Sottile[1]; B. Scammell[1]

1. University of Nottingham, Faculty of Engineering, United Kingdom

Manufacturing porous microspheres from calcium phosphate materials with nano to micron-range porosity has huge potential in bone repair and regeneration applications where larger external pores within the microspheres could accommodate cells and the smaller pores could be utilised to encapsulate many other types of biological components such as drugs including small molecules, nucleic acids, proteins etc. Our group has successfully managed to manufacture solid (non-porous) and (for the first time) highly porous microspheres from calcium phosphate-based glasses and their scale-up potential (between 1 – 3 kg/h) has also been confirmed. Solid CaP glass microspheres of varying size ranges were successfully manufactured with over 95% efficacy in yield of spherical morphologies. Follow-on studies showed that microspheres with surface and interconnected porosity could also be manufactured, and at similar scale-up yields to the solid microspheres. Further studies also confirmed that human mesenchymal stem cells (hMSC) not only attached to the microspheres, but also migrated to reside within their pores. Recent work has also confirmed that these materials could be delivered down 1mm and 2mm internal diameter needles. These newly developed novel biomaterials are currently being investigated towards delivering the next generation of orthobiologic applications.

4:20 PM

(GOMD-S2-014-2018) Feasibility of 3D macroporous phosphate glass-ceramic scaffolds using the foam replication technique

J. Rocherullé*[1]; F. Cheviré[1]; P. Bénard-Rocherullé[1]; R. Lebullenger[1]; J. Massera[2]

1. University of Rennes, Chemical Sciences Institute - Glass and Ceramic Group, France
2. Tampere University of Technology, BioMediTech and Faculty of Biomedical Sciences and Engineering, Finland

There is great interest in the development of phosphate glasses which are considered as promising biomaterials, particularly in the form of glass fibers. However, there are only a few studies regarding phosphate glass 3D scaffolds as compared to silicate glasses, probably because of the limited chemical durability of phosphate glasses. The aim of this work was to study the feasibility to build a 3D macroporous glass ceramic scaffold using a glass in the Na2O-CaO-P2O5 composition diagram with Tg and Tp values of about 450°C and 590°C, respectively. An aqueous glass slurry containing 40 wt% of glass powder with 4 wt% of PVA as a binder was thick coated in a polyurethane sponge as a template. After infiltration, the sponge has been heat treated up to 650°C according to preliminary TGA-DTA experiments. The 3D structure presents a pore size range from 200 to 500 μm and a porosity of about 80%, values which are considered as optimal for bone regeneration and vascularization. Nevertheless, such a typical 3D scaffold manufacturing involving a firing and sintering step leads, in most cases, to crystallization of the glass which can induce a decrease of the bioactivity. As a consequence and complementary to an analysis of the devitrification kinetics, we have investigated the crystallization pathway by means of in situ High Temperature XRD experiments.

4:40 PM

(GOMD-S2-015-2018) Strength, Toughness and Reliability of Porous Glass (13-93) Scaffold: Influence of a Biopolymer Polycaprolactone (PCL) Coating

Q. Fu*[1]

1. Corning Incorporated, USA

Development of bioactive glass and ceramic scaffolds intended for the reconstruction of large segmental bone defects remains a challenge for materials science due to the complexities involved in clinical implantation, bone-implant reaction, implant degradation and the multiple loading modes the implants subjected to. A comprehensive evaluation of the mechanical properties of inorganic scaffolds and exploration of new ways to toughen brittle constructs are critical prior to their successful application in loaded sites. A simple and widely adopted approach involves the coating of an inorganic scaffold with a polymeric material. In this work, a systematic evaluation of the influence of a biopolymer, polycaprolactone (PCL), coating on the mechanical performance of bioactive glass scaffolds was carried out. Results from this work indicate that a biopolymer PCL coating was more effective in increasing the compressive strength and reliability of the glass scaffold under compression, but less effective in improving its flexural strength and fracture toughness. This is the first report that reveals the limited successfulness of a polymer coating in improving the toughness of strong scaffolds, suggesting that new and novel ways of toughening inorganic scaffolds should be future research directions for scaffolds applied in loaded sites.

5:00 PM

(GOMD-S2-016-2018) Laser based coating of bioactive glasses on titanium alloys for biomedical applications

P. Kuo*[1]; X. Lu[1]; S. S. Joshi[1]; Y. Ho[1]; Y. Xiang[1]; N. B. Dahotre[1]; J. Du[1]

1. University of North Texas, Material Science and Engineering, USA

Laser coating is a new materials processing technique that find wide applications in materials processing. In this paper, we explored the feasibility of using laser as a processing tool for synthesizing the bioactive glass coatings on metal bio-implant material. Bioglass® 45S5 was synthesized and laser coated on Ti-4Al-6V alloy using various laser processing conditions. Microstructure and elemental distribution of the coating were investigated by scanning electron microscope (SEM) and embedded energy dispersive spectroscopy (EDS). Bio-mineralization study were conducted in simulated body fluid (SBF) solution to estimate the biocompatibility. The thermokinetic effects during laser process were simulated using a multi-physics finite element (FE) model. The results indicated successful coating of bioactive glass on the metal substrate with local segregation of Na, P, and Si elements. Considerable dilutions of Al and Ti were discovered in the coating layer and the result corresponds to the computational simulation. The dilution of metal and segregation of Na and P can impact the bioactivity of the coating. The results suggest laser processing is a promising method in applying bioactive glasses coatings and yet further efforts required to optimize laser processing conditions for achieving high adherent coating and retain the bioactivity of Bioglass® 45S5.

5:20 PM

(GOMD-S2-017-2018) Enhanced Bioactivity and Processing of Borophosphate Bioglasses for Soft Tissue Repair

B. Gorin*[1]; J. C. Mauro[1]

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

Bioactive glass is a new alternative for wound therapy. Bioactive glasses have traditionally been used in bone repair, in which silica has been the primary glass former. Silica provides the mechanical strength to take on the structural load of hard tissue. A new borate bioactive glass (1393B) has demonstrated that soft tissue can heal up to five times faster with borate glass than with silicate glass. This is likely due to the tendency of borate glasses to dissolve more quickly

in the body, thereby releasing the cations that promote cell growth more rapidly. 1393B glass was made by a trivial substitution of SiO_2 with B_2O_3, without changing any other constituent in the glass; it was not optimized for bioactivity, nor was it optimized for large-scale manufacturing. In fact, it is very prone to crystallization. A new family of calcium-rich borophosphate bioactive glasses is being pursued. The introduction of higher amounts of phosphorous and calcium, which are used in large amounts in the natural healing process, should promote more rapid growth. By adjusting the composition and balancing the network formers with the network modifiers, the liquidus temperature will be suppressed and the viscosity at that temperature will be increased, slowing the kinetics of crystallization and resulting in more stable glass for manufacturing and storage.

S4: Glass Technology and Cross-Cutting Topics

Session 4: Waste Immobilization - Corrosion III

Room: La Vista D/E (22nd Fl)

Session Chair: Joseph Ryan, Pacific Northwest National Lab

1:20 PM

(GOMD-S4-025-2018) Glass dissolution as a function of pH

D. Strachan*[1]

1. Pacific Northwest National Laboratory, USA

Various rate equations for the dissolution of silicate glasses have been discussed in the literature. In this talk, the published results from studies are discussed in which the dissolution rate data are collected under high flow conditions such that saturation with respect to alteration products is avoided. Additionally, the studies also covered broad ranges of temperature and pH. Starting with nuclear waste glass studies, a two-term rate expression is used to fit data with the result that the data point toward a three-term expression offered by Köhler et al. (2003). These rate expressions contain two or three pre-exponential or rate constants. However, it appears that a single rate constant, an intrinsic rate constant, is consistent with the data. Thus, a rate expression consisting of H^+ and OH^- activities and activation energies for H^+, H_2O, and OH^-. To distinguish between the possible rate laws, more experiments are needed that are more carefully constrained. These may include experiments at pH values that differ by as little as 0.25. Lastly, experiments with glasses of different compositions are needed to determine the dependence of the intrinsic rate constant on the glass composition and structure, i.e. non-bridging oxygens, Si-more carefully constrained O-Si and Si-O-X (X = a matrix-forming element, e.g. Al or Fe), and other glass structural properties, e.g. binding energies.

1:40 PM

(GOMD-S4-026-2018) Impacts of Glass Composition, pH, and T on Glass Corrosion Forward Rate

J. Vienna*[1]; J. Neeway[1]; J. Ryan[1]

1. Pacific Northwest National Lab, USA

Glasses dissolve at the forward rate (r_f) when exposed to very dilute aqueous solutions. It has long been known that pH and T strongly impact r_f, while the impacts of glass composition have remained uncertain. Typically, r_f is modeled as: $r_f = k_0 a_{H+}^{-\eta} \exp(-E_a/RT)$. Correlating the model parameters (k_0, η, and E_a) with composition of the glass has long been challenging. We recently reported a strong positive correlation between the $\log[k_0]$ and E_a parameters fitted to r_f data. This strong correlation (>85%) suggests that neither parameter can be uniquely defined given the scale of uncertainties in measure r_f data. In the present paper, a model was fitted to r_f data generated as part of this study and those found in literature. It was determined that only a relatively small composition effect was seen when fitting the combined data (e.g., 90% of the variation in data was described only by T and pH effects). Relatively weak composition effects where found associated with the $\log[k_0]$ term and not associated with either pH or T. The r_f differences between test glasses, after normalizing for differences in pH and T, were found with variation in the fraction of glass forming tetrahedra contributed by four coordinated boron. The results of experimental work and modeling will be reported.

2:00 PM

(GOMD-S4-027-2018) Use of Monolithic Samples for Corrosion Testing in a Dilute Reactor

M. Asmussen*[1]; J. Neeway[1]; B. Parruzot[1]; E. Brown[2]; D. Swanberg[2]; G. L. Smith[1]; J. Ryan[1]

1. Pacific Northwest National Lab, Energy and Environment Directorate, USA
2. Washington River Protection Solutions, USA

At the Hanford Site the modelling of the long term dissolution of glass waste forms for immobilized low activity waste (ILAW) is in part using based on transition state theory. The rate model is parameterized by measuring the dissolution rate of glass over a range of temperatures, pH values, and solution composition using single pass flow through (SPFT) testing of powdered samples. While the SPFT is a fully capable test method, the long induction times to achieve steady state in the tests, the potential for uncertainty in establishment of a forward dissolution rate during the test, and the limitation of testing a single glass composition in a test can present challenges. The expansion of the composition range of ILAW glass to be produced at Hanford presents a need for more rapid acquisition of dissolution rates. In this presentation, the development of an experimental approach using monolithic glass samples in corrosion testing in a large volume reactor will be given. Through this approach dilute conditions are easily attained in the reactor and steady state dissolution rates can be measured. The dissolution rate is determined by a height change between a protected area of the glass monolith sample and the receded corroded surface. The presentation will encompass technique development, surface protection, height measurement methods and results from testing a series of waste glass compositions.

2:20 PM

(GOMD-S4-028-2018) Deconvolution of Early-Stage Corrosion Reactions that Impact Solution pH and Conductivity

R. Schaut*[1]; S. A. Tietje[1]; N. J. Smith[2]

1. Corning Incorporated, S&T, Glass Research, USA
2. Corning Incorporated, S&T, Surfaces & Interfaces, USA

The corrosion of glass surfaces by unbuffered water involves several steps and changes in reaction mechanism over time. First, leachable modifier cations (i.e. Na, K, or Ca) undergo ion-exchange with charged water species. The release of these cations causes an increase in the solution pH from neutral to basic. The increased solution pH causes hydrolysis of the silicon-oxygen bonds and increases the release of network species to solution. As this shift in mechanism occurs (from ion-exchange to hydrolysis), the corrosion process shifts from incongruent (leaching) to more congruent (dissolution). In this talk, we review findings from in-situ measurements of solution pH and conductivity during glass corrosion that reveal these mechanisms, with new data evaluating the role of carbon dioxide uptake by high pH solutions that are open to ambient air. This has the effect of further buffering the solution back toward neutral pH, and thus slowing reaction rates after high initial release. Results will be shared from well-controlled experiments to deconvolute in-situ measurements of solution pH and conductivity during glass corrosion. We also compare these responses to periodic measurements of solution chemistry by ICP-MS and ion-chromatography and surface chemistry by XPS or D-SIMS. Results will be discussed for a few simple silicate and borosilicate glasses.

2:40 PM

(GOMD-S4-029-2018) Effect of Chemical Strengthening on Glass Water Durability

A. Li*[1]

1. Corning Incorporated, Characterization Science, USA

Chemical strengthening is a well-adopted process throughout industry that is employed to improve mechanical strength in glass and related products. However, currently there is a lack of fundamental understanding related to the effect of ion exchange processes upon the water durability of glass. In this talk, we will focus on the effect of ion exchange on glass water durability and aim to answer three specific questions: 1. Does ion exchange increase or decrease glass chemical durability in water? 2. What are dominating factors (glass composition, compressive stress, free volume change) that increase/decrease glass chemical durability? 3. Is there a mixed-alkaline effect for chemical durability in response to the tuned alkaline identity of the glass surface? The water durability of alkaline aluminate glasses with fixed alkaline content and tuned alkaline identities (Li-Na, Li-K and Na-K) will be compared with ion exchanged glasses and tempered glasses with the same surface compositions. Conclusions will be driven by both experimental and high level computational modeling research approaches.

3:00 PM

(GOMD-S4-030-2018) Mechanisms controlling the short-term dissolution of glasses SON68 and ISG in hyperalkaline conditions at 30°C

K. Ferrand*[1]; S. Liu[1]; K. Lemmens[1]

1. Belgian Nuclear Research Centre, Waste and Disposal, Belgium

Previous work showed that alteration of glasses SON68 and ISG at pH 13.5 at 30 °C was diffusion controlled, evidenced by square root of time dependent increase of elemental concentrations of glass network formers and modifiers in the solution. However, some discrepancies with the diffusion theories were observed: the apparent diffusion coefficients were similar for all leached glass components and the diffusive flux was independent from the elemental concentrations in the solution. To better understand the diffusion process, new static short-term tests were carried out at 30 °C in simulated cement water and KOH at $pH_{(25\,°C)}$ = 13.7 ± 0.2. The results show in some cases a clear drop of the boron dissolution rate, while Si concentrations in the solution increased nearly linearly. Therefore, the rate drop cannot be due to a silicon saturation effect. Additionally, the results show that in general a higher surface area-to-volume ratio (S/V) corresponds to a lower normalized boron release, and that, while in KOH solution stirring speeded up the normalized boron release, in simulated cement water the effect of stirring depended on S/V: at low S/V stirring speeded up dissolution, but at high S/V stirring slowed down the dissolution. This might be due to the presence of calcium in the cement water, which was reported to have antagonist effects on glass dissolution.

3:40 PM

(GOMD-S4-031-2018) Chemical Durability of New Glass Formulations for the Vitrification of UK High Level Waste

M. T. Harrison*[1]

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

In the UK, the Waste Vitrification Plant (WVP) at Sellafield converts the highly active liquid (HAL) waste from the reprocessing of spent nuclear fuel into a glass wasteform suitable for long term storage and disposal. After the completion of reprocessing operations, the high level liquid waste (HLLW) storage tanks will be emptied and washed out to remove any accumulated solids. These solids are expected to contain high concentrations of molybdenum. Hence, new glass formulations are being developed specifically for immobilisation of these waste streams. CaZn glass, which allows for significantly higher MoO_3 by the in situ formation of $CaMoO_4$ crystals, has now been deployed on WVP for standard reprocessing waste with a view to future wash-out waste processing. As a result of this deployment, further improvements to its composition are being investigated with regards to underpinning the chemical durability over a wider range of Li-contents. Recent investigations have also included leach tests at low- and high-temperatures (40 and 90 °C) as well as the effect of Si-saturation in the leachate solutions in order to probe the long-term dissolution rate. In addition to leachate analysis, SEM of the altered CaZn glass surfaces has been performed.

4:00 PM

(GOMD-S4-032-2018) Influence of P_2O_5 on the crystallization and chemical durability of nepheline based glasses

S. Kapoor*[1]; S. Lakshmikantha[1]; J. Marcial[2]; R. Youngman[3]; N. J. Smith[3]; J. McCloy[2]; A. Goel[1]

1. Rutgers University, Materials Science and Engineering, USA
2. Washington State University, School of Mechanical and Materials Engineering and Materials Science and Engineering Program, USA
3. Corning Incorporated, USA

Crystallization of nepheline and other aluminosilicate phases during centerline canister cooling (CCC) of high-level waste (HLW) melt is mainly a function of the composition of the glass-forming melt. Because nepheline crystallization in a HLW glass removes three moles of glass-forming oxides (Al_2O_3 and $2SiO_2$) for each mole of Na_2O, it can result in a severe deterioration of the chemical durability of the final waste form. Therefore, a better understanding of the compositional and structural dependence of nepheline formation in simplified HLW glasses is required in order to design advanced glass formulations with enhanced waste loading. In this pursuit, the present study aims to investigate the influence of P_2O_5 on structure, crystallization and chemical durability of nepheline based glasses. The structural and microstructural characterization of glasses and resultant glass-ceramics have been performed by ^{31}P, ^{23}Na and ^{27}Al MAS-NMR spectroscopy adjoined with XRD and SEM, while their chemical durability has been studied in neutral – to – alkaline pH solutions. The presentation will focus on discussing the results pertaining to chemical durability and crystalline phase evolution in the studied glasses followed by partitioning of phosphorus in resultant glass-ceramics.

4:20 PM

(GOMD-S4-033-2018) Chemical durability of iron phosphate waste forms containing 40 wt% of a high MoO_3 Collins-CLT waste melted in a cold crucible induction melter

J. Hsu*[1]; J. Bai[1]; C. Kim[2]; R. Brow[1]; J. Szabo[2]; A. Zervos[2]

1. Missouri S&T, USA
2. MoSci Corp., USA

The secondary waste stream produced by a uranium extraction process includes high concentrations of MoO_3, ZrO_2, lanthanide oxides, and noble metals that have low solubilities in borosilicate glasses, but greater solubilities in iron phosphate glasses. From the recent studies, a partially crystallized iron phosphate waste form, designated 40wt%-5, containing up to 40 wt% of a high MoO_3 Collins-CLT waste simulant shows good chemical durability. In this work, the 40wt%-5 waste form is melted using a cold crucible induction melter (CCIM). The chemical durability of that 40wt%-5 waste form, evaluated using the product consistency test (PCT), fits the Department of Energy (DOE) high loading waste requirement. Also, the properties, including composition, microstructure and structure, of the 40wt%-5 waste form melted using a CCIM, are consistent to those of the 40wt%-5 waste form melted in a laboratory furnace.

4:40 PM

(GOMD-S4-034-2018) Corrosion Interactions between SS316 and ISG in Nuclear Repository Conditions

X. Guo*[1]; D. Ngo[2]; H. Liu[2]; J. Luo[2]; S. H. Kim[2]; S. Gin[3]; J. Vienna[4]; J. Ryan[4]; J. Du[5]; G. Frankel[1]

1. Ohio State University, Materials Science and Engineering, USA
2. Pennsylvania State University, Chemical Engineering, USA
3. CEA, France
4. Pacific Northwest National Laboratory, USA
5. University of North Texas, Materials Science and Engineering, USA

In the plan for disposal of HLW, radionuclides will be incorporated into molten borosilicate glass, and then cast into stainless steel (SS) canisters. During long time of exposure in the repository, the canisters will corrode and eventually be breached. The groundwater is expected to trigger a severe localized corrosion phenomenon, crevice corrosion, at the metal-glass interface. The goal of this study is to develop a fundamental understanding of the corrosion interactions between SS and nuclear glass. The experiment was carried out by integrating SS with International Simple Glass (ISG) to form a tight crevice, and immersing them in 0.6 M NaCl solution under 90°C. After a certain period of time, the samples were removed from the solutions and subjected to various surface analysis using SEM/EDS, ToF-SIMS, XPS, SR-IR, and Raman spectroscopy. The glass surface that was in contact with SS showed different regimes of corrosion after the exposure, with distinctly different surface morphologies and chemistries. A "band pattern" form of attack that was usually observed on metals during crevice corrosion, was also identified on the glass surface. For ISG samples, depletion of Na, Ca, Zr, and Al elements was identified in this band region, whereas Fe was enriched. The results suggest that SS has a significant effect on the glass corrosion when a confined space forms between these two materials.

Session 5: Optical Fabrication Science & Technology I

Room: La Vista F (22nd Fl)

Session Chairs: Joseph Menapace, Lawrence Livermore National Laboratory; Tayyab Suratwala, Lawrence Livermore National Laboratory

1:20 PM

(GOMD-S4-035-2018) Mechanisms and Strategies for polishing inert materials (Invited)

L. M. Cook*[1]

1. Recursive Systems LLC, USA

An increasing number of key materials in semiconductors are highly inert (e.g., GaN, SiC, and Diamond). For applications such as power ICs and LED substrates, these materials need to be polished to a high degree of smoothness, free from defects which might kill yield, and at a high throughput. This talk reviews common removal mechanisms, and outlines approaches for use in high throughput fabrication processes.

1:50 PM

(GOMD-S4-036-2018) Demystifying classic polishing problems by identifying the underlying phenomena

R. Whitsitt*[1]; B. Myer[1]; M. Brophy[1]; J. DeGroote Nelson[1]

1. Optimax Systems, Inc., Research and Development, USA

A variety of factors among optical materials contribute to specific behaviors that drive the polishing process. The colloquial names of these behaviors have been passed on through the optical fabrication community over generations and in many cases have little to do with, or are somewhat distant from, the underlying phenomena. As optical fabrication technology "migrates from more of an art to a science," familiar obstacles to finishing an optic such as burn, sleek, orange peel, grain decoration, stain, etc., can and should be demystified. In turn, the shared experience of opticians can be better leveraged by the workforce and help illuminate gaps in development. From the perspective of a precision optical fabrication shop that uses both traditional and newly developed techniques on glass, crystals, and polycrystals, this presentation will step through the intrinsic and extrinsic material limitations, and tool, abrasive, and workpiece interactions, that give rise to classic polishing problems still relevant today.

2:10 PM

(GOMD-S4-037-2018) Fabrication of silica glasses with tailored compositions by 3D printing

R. J. Dylla-Spears*[2]; J. Destino[1]; P. R. Ehrmann[2]; D. T. Nguyen[2]; N. Dudukovic[2]; M. A. Johnson[2]; L. L. Wong[2]; T. D. Yee[2]; K. Sasan[2]; T. Fears[2]; W. A. Steele[2]; E. Duoss[2]; T. I. Suratwala[2]

1. Creighton University, Chemistry Department, USA
2. Lawrence Livermore National Laboratory, USA

The ability to control the properties of glasses spatially could promote novel system designs; however, glass optics with custom-tailored composition profiles are impracticable by conventional methods. In this work, glass materials are built to prescription using the direct-ink-writing (DIW) method of 3d printing, which allows composition to be varied spatially within the printed form. Rheologically tuned, silica-based inks of different compositions are blended inline at ratios required to deposit the desired material composition at the desired location within a near net shape, low density green body. The completed green body is then heat treated to form a full density glass structure containing the gradient in material property imparted through the composition variation. Afterward, the glass can be polished to achieve the desired surface figure and surface quality. This method has been used to create transparent, amorphous glass with directed compositional change, including gradient index (GRIN) glass optics. The 3d-printed components are compared to conventionally prepared glasses, and optical performance of DIW-printed glass optics is verified. *This work 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 16-SI-003. LLNL-ABS-742152

2:30 PM

(GOMD-S4-038-2018) AFM nanoscratching of optical materials near the elastic-plastic load boundary to mimic the mechanics of polishing particles

N. Shen*[1]; E. Feigenbaum[1]; T. I. Suratwala[1]; W. A. Steele[1]; L. L. Wong[1]; M. D. Feit[1]; P. E. Miller[1]

1. Lawrence Berkeley National Laboratory, USA

Localized mechanical loads on optical material surfaces from polishing particles can lead to surface modifications ranging from deep multi-micrometer fractures, to nanometer level plastic deformations, to a pure elastic response. To understand the material removal rate and the resulting surface roughness, it is necessary to understand both the chemical and the mechanical removal function due to individual particles. We present the use of atomic force microscope to create nanoscratches in air and aqueous environments on a range of optical material surfaces to mimic deformations resulted from individual particles during polishing. This technique is ideal for studying mechanical material removal in the small load range typical of slurry particle polishing. Nanoscratches were created on a range of materials as a function of the applied load to estimate the single particle removal functions. Combined with other experimentally measured parameters, polishing rate and surface roughness may be quantitatively predicted using model based on the microscopic Preston equation. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

2:50 PM

(GOMD-S4-039-2018) Predictive models for grinding and polishing of various optical materials

T. I. Suratwala*[1]; W. A. Steele[1]; L. L. Wong[1]; P. E. Miller[1]; N. Shen[1]; E. Feigenbaum[1]; M. D. Feit[1]; J. Destino[2]

1. Lawrence Livermore National Laboratory, Optics and Materials Science & Technology, USA
2. Creighton University, Chemistry, USA

The following study establishes quantitative rules, based on fundamental the removal mechanisms, for determining the grinding & polishing rate and grinding roughness for a given workpiece material & slurry particle composition to aid in reducing the development effort. A large variety of optical materials (glasses, glass-ceramics, & single crystals) have been processed by loose abrasive grinding and by polishing using various slurries. Using a fracture mechanics model for lateral cracks, a set of analytical expressions successfully describe the grinding rate and the resulting workpiece surface roughness as a function of the lateral crack growth constant of the workpiece, mean abrasive size, applied pressure and velocity. The polishing rate depends on the dominant removal mechanism. For the case of nanoplastic removal, the single particle nanoplastic removal depth is shown to be linearly related to the polishing rate. For the case of chemical removal, the removal rate is often limited by the condensation reaction rate. The chemical polishing rate is shown to scale exponentially with the partial charge difference between metal hydroxide of the workpiece relative to the metal hydroxide of the polishing particle. This partial charge model also explains the age-old experimental finding of why cerium oxide is the most effective polishing slurry for chemical removal for certain workpiece materials.

3:10 PM

(GOMD-S4-044-2018) Several strategies to morphologically stabilize and luminescently enhance $[Ag_m]^{n+}$-quantum-cluster contained muliti-phase glass

X. Qiao*[1]; X. Chen[1]; J. Zhao[1]; R. Ma[1]; X. Xu[1]; J. Du[2]; X. Fan[1]

1. Zhejiang University, School of Materials Science and Engineering, China
2. University of North Texas, Department of Materials Science and Engineering, USA

The molecule-like silver-quantum-clusters ($[Ag_m]^{n+}$) have shown great potential as LED lighting phosphors due to their super-broad visible emission bands with high quantum yields (QYs). Espicially, it is eary to form mono-dispersed and heavily-doped $[Ag_m]^{n+}$ active quantum clusters in some inorganic glasses due to the stabilization role of charged network tetrahedra, such as $[BO_4]$, $[AlO_4]$ and $[ZnO_4]$. It has been reported that such glass had an luminescence QY up to 96.7%. However, their QYs and CRIs cannot be improved synchronously due to luminescence quenching by energy transfers between differernt $[Ag_m]^{n+}$. Here we prepared one type of luminescent glass simultaneously containing green-white emitting $[Ag_m]^{n+}$ enriched borate nano-glassy-phases and red-emitting $[Ag_m]^{n+}$ enriched aluminate nano-glassy-phases. There is no mutual interference between different kinds of $[Ag_m]^{n+}$, thus it could enhances QY and CRI simultaneously. Aggregation degree and charge quantity could be well controlled via solubility and charge compensation strategies in the glass. The luminescence behaviors of $[Ag_m]^{n+}$ also shows phenomena similar with quantum size effects. It is further interpreted through a TDDFT simulation with B3LYP (hybrid Becke three-parameter Lee–Yang–Parr functional) and LANL2DZ basis sets.

Session 5: Optical Fabrication Science & Technology II

Room: La Vista F (22nd Fl)

Session Chairs: Rebecca Dylla-Spears, Lawrence Livermore National Laboratory; Tayyab Suratwala, Lawrence Livermore National Laboratory

3:40 PM

(GOMD-S4-040-2018) Dynamic Freeform Optics Manufacturing with Surface Error Spatial Frequency Control (Invited)

D. Kim*[1]; C. Oh[1]; H. M. Martin[2]; L. Graves[1]; I. Trumper[1]; H. Choi[1]

1. University of Arizona, College of Optical Sciences, USA
2. University of Arizona, Steward Observatory, USA

The next generation large optical systems often utilize dynamic active/adaptive freeform optics for creating a superior performance segmented optical system. Those precision optics can be efficiently produced using a computer controlled optical surfacing (CCOS) process. For instance, a large-scale surface figure error is controlled by a guided dwell-time based removal process. Smaller-scale surface errors are controlled by polishing process parameters. Various new approaches advancing the current CCOS processes have been investigated, developed and implemented to manufacture highly aspheric or freeform dynamic optics at the University of Arizona. Some exciting technologies including actively shape controlled Stressed lap, non-Newtonian fluid conformal lap, IR deflectometry using a hot wire, and dynamic freeform metrology using an iPhone with a color pattern-multiplexing are presented with actual data demonstrating their exceptional performance and capability as a precision optics manufacturing technology. Especially, the control of surface errors as a function of spatial frequency is critical during the fabrication of modern optical systems. The measurements from various metrology systems are converted to Power Spectral Density plots and combined in the spatial frequency domain. Results cover 5 orders of magnitude in the spatial frequency domain.

4:10 PM

(GOMD-S4-041-2018) Freeform Optic Manufacturing Using Advanced Magnetorheological Finishing Technology

J. A. Menapace*[1]

1. Lawrence Livermore National Laboratory, National Ignition Facility, USA

Corrective optical form an important part of high-precision optical systems. Many of these elements can be difficult to manufacture without compromise due to extreme wavefront specifications that defy conventional finishing processes. Over the past fifteen years, we have been developing freeform optic manufacturing techniques using Magnetorheological Finishing (MRF®) that deterministically addresses complicated optical fabrication. During our discussion, we will present the development of MRF techniques specifically designed to meet the demanding optical performance challenges required in complicated optical systems. Examples include MRF manufacture of ultra-precise laser beam conditioning optics to manipulate beam quality. These optics contain customized surface topography and high gradients that cannot be made using conventional processes. Large-aperture off-axis aspheric lens and freeform corrective element fabrication will also be highlighted showing how MRF is used to perform ultra-precision polishing yielding optics with nanometer level error. Lastly, we will show how sub-aperture polishing can be used to correct for internal inhomogeneity in transmissive elements to improve optical wavefront and system performance. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-742243

4:30 PM

(GOMD-S4-042-2018) Material properties for optimized lightweight space-based mirrors (Invited)

J. T. Mooney*[1]

1. Harris Corporation, Space and Intelligence Systems, USA

Future space-based telescopes are driving to enable enhanced science missions including studying the universe "first light", origin of galaxies, and exploration and imaging of habitable planets. In 2019, we will see the launch of the James Webb Space Telescope which will have a 6.5 meter aperture mirror, 6.25 times more collection area than the Hubble telescope. These future systems will be leveraging larger optical apertures to achieve their science missions. A key enabling component in these systems is the primary mirror. This presentation will discuss the high level primary mirror requirements and some of the key material properties for current and future space-based telescopes as well as advancements in mirror manufacturing to address the key schedule, weight, and cost drivers for mirror production.

5:00 PM

(GOMD-S4-043-2018) A Guide to Proper Fused Silica Selection Based on Application and Performance Needs (Invited)

T. Jaeger*[1]

1. Heraeus Tenevo LLC, USA

Fused silica is a key material in a multitude of optical applications including high power laser systems, spectroscopic instrumentation, astronomy, telecommunications, etc. Multiple techniques for fused silica production exist leading to a wide variety of natural and synthetic silica materials with varying physical and optical properties. It is often difficult to choose which variety of fused silica best matches the price and performance points of a given application. The intention of this talk is to clarify the advantages of utilizing one material or another for applications from the Near-Infrared to the Ultraviolet.

Wednesday, May 23, 2018

Award Lectures

Varshneya Frontiers of Glass Science Lecture

Room: El Mirador East (22nd Fl)

8:00 AM

(GOMD-AW-003-2018) Glass and Rare-Earth Elements (Invited)

S. Tanabe*[1]

1. Kyoto University, Japan

Many functional glasses, either passive or active, contain one or multiple kinds of rare-earth ions as a very important key element. This lecture focuses on active glasses and fibers doped with rare-earth elements, in which 4f electrons play critical role, as well as the impact of their photonic functions on many applications such as optical amplifications in fiber telecommunication. The inventions of neodymium- or erbium-doped glass lasers by E. Snitzer in 1960s can be regarded as triggers of later developments of many photonic devices of doped glasses and progress in understanding of their spectroscopy sciences. These inventions later led also to the invention of Er-doped fiber amplifier, EDFA in late 1980s. Invention of fluoride glasses led to invention of uv or visible upconversion fiber lasers, PDFA and TDFA while that of chalcogenides led to mid-IR optics and light sources. Scientific progress in rare-earth spectroscopy, and technologies of doped glasses and fibers in recent 60 years have been more than dramatic. In this lecture, I will explain my personal perspectives on glass and rare-earth elements, which have given me exciting experiences during my carrier on material research.

S1: Fundamentals of the Glassy State

Session 1: Glass Formation and Structural Relaxation I

Room: El Mirador East (22nd Fl)
Session Chairs: John Mauro, Pennsylvania State University; Ozgur Gulbiten, Corning Incorporated

9:20 AM

(GOMD-S1-091-2018) Structure and Dynamics of Viscous Liquids Subject to High Electric Fields (Invited)

R. Richert*[1]

1. Arizona State University, School of Molecular Sciences, USA

High electric fields modify the structure and dynamics of liquids, particularly when they are glass-forming liquids and near the glass transition. The approach to the state that is in equilibrium with the electric field (ac or dc) involves changes in the time constants of the system, and therefore it is analogous to the structural recovery observed during physical aging. In contrast to temperature jumps, field jumps with magnitudes of several 100 kV/cm are easily performed on the microsecond time scale, thereby facilitating relatively fast aging experiments. A variety of such field induced structural recovery experiments will be discussed, with emphasis on how these high field experiments can provide additional insight into models of physical aging. Signatures of time-aging-time superposition (TaTS) are observed, but observations also hint at limitation of TaTS. Interestingly, dynamics can become faster or slower with the application of a field, depending on whether an ac or dc type field is used, respectively. Because the magnitude of these effects are quadratic in the electric field strength, an asymmetric rise/decay behavior is observed when applying and removing the field, analogous to findings in the context of electro-optical Kerr effects.

9:50 AM

(GOMD-S1-092-2018) Physical aging of glasses: Phenomenology and structural models (Invited)

R. Golovchak*[1]

1. Austin Peay State University, Physics and Astronomy, USA

The phenomenon of physical aging or structural relaxation at below-T_g temperatures is known from the middle of 19th century, when J.P. Joule first documented the drift of zero scale for his thermometers made of silicate glass. Since that time, the physical aging of many inorganic glasses and polymers has been studied on the timescales from several hours to several decades. Its main signature includes changes in the mechanical, thermodynamic, optical properties, but excludes any phase transitions (e.g. crystallization). Despite a large amount of collected experimental data, the existing phenomenological and structural models of physical aging are ambiguous in many aspects. Their re-evaluation can be done through the analysis of physical aging in canonic chalcogenide glasses (ChG). Thus, if the ageing temperature T_a is close enough to T_g, the enthalpy recovery during physical ageing in ChG follows a sigmoidal time dependence well described by a stretch-exponential relaxation function, which stretching exponent depends on structural parameters. The farther departure of T_a from T_g causes the appearance of some plateaus in time dependence of enthalpy recovery. In addition, the external influences are shown to accelerate physical aging processes in ChG. A successful unified description/model of structural relaxation in disordered solids below T_g should be compliant also with these experimental observations.

10:20 AM

(GOMD-S1-093-2018) New understanding of collective modes and thermodynamics of the liquid state

K. Trachenko*[1]

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

A theory of liquids and liquid-glass transition requires understanding most basic thermodynamics properties of the liquid state such as energy and heat capacity. This has turned out to be a long-standing problem in physics. Landau&Lifshitz textbook states that no general formulas can be derived for liquid thermodynamic functions because the interactions are both strong and system-specific. Phrased differently, liquids have no small parameter. Recent experimental and theoretical results open a new way to understand liquid thermodynamics on the basis of collective modes (phonons) as is done in the solid state theory. There are important differences between phonons in solids and liquids, and we have recently started to understand and quantify this difference. I will review collective modes in liquids including high-frequency solid-like transverse modes and will discuss how a gap in the reciprocal space emerges and develops in their spectrum. This reduces the number of phonons with temperature, consistent with the experimental decrease of constant-volume specific heat with temperature. I will discuss the implication of the above theory for the liquid-glass transition and the change of heat capacity at Tg.

10:40 AM

(GOMD-S1-094-2018) Structure and mechanical properties of sodo-silicate glasses

W. Kob*[1]; S. Sundararaman[2]; S. Ispas[3]; L. Huang[2]

1. University of Montpellier, France
2. Rensselaer Polytechnic Institute, USA
3. University of Montpellier, France

Sodo-silicate glasses are one of the simplest binary glass-formers that can be easily produced. Despite this simplicity the properties of these systems show a surprisingly complex dependency on the Na concentration. In this talk I will present the results from computer simulations of sodo-silicate systems $x*Na_2O-(1-x)*SiO_2$ with a wide range of compositions ($0 <= x <= 0.4$). In particular I will discuss how the sodium content affects the structure, the thermal expansion coefficient, the elastic constants, as well as the vibrational properties. The x-dependence of many of these properties can be understood by recalling that pure silica has a density anomaly which influences the properties also of sodo-silicate glasses.

11:00 AM

(GOMD-S1-095-2018) Volume Strain Versus Linear Strain: Anisotropy in Dimensional Change During Low Temperature Ion Exchange

E. A. King*[1]; D. C. Allan[1]; C. Smith[1]

1. Corning Incorporated, Glass Research, USA

Chemically strengthened glasses produced via ion exchange processes are currently of great interest due to their high strength and damage resistance. Such strengthening is the result of an atomic size mismatch between exchanged alkali ions, leading to strain within the glass network and ultimately to changes in the glass dimensions. In past work we have shown how to directly measure the linear dimensional changes associated with strain during ion exchange processes. Free strain within the glass network during ion-exchange processes is generally assumed to be isotropic. Here we use our new method of direct linear strain measurement, in conjunction with volume strain measurements, to determine applicability of the aforementioned isotropic assumption in low temperature single alkali ion-exchange using glasses having a range of thermal histories.

11:20 AM

(GOMD-S1-096-2018) Modified elastic model for viscosity in glass-forming systems

S. Jaccani*[1]; O. Gulbiten[2]; D. C. Allan[2]; J. C. Mauro[3]; L. Huang[1]

1. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA
2. Corning Incorporated, USA
3. Pennsylvania State University, USA

For most glass-forming liquids, the temperature dependence of viscosity is non-Arrhenius. Despite the technological and geological importance, the origin of this non-Arrhenius temperature dependence of viscosity remains elusive to date and constitutes an important but unsolved problem in condensed-matter physics. It has become increasingly clear in recent years that high-temperature elasticity and viscosity of glass-forming liquids are strongly correlated. This work proposes a modified elastic model to predict equilibrium viscosity of glass-forming liquids. The modified elastic model considers the configurational entropy as a factor controlling the activation energy for viscous flow in addition to the high-frequency shear modulus as in the Dyre shoving model. It works much better than the shoving model in fitting equilibrium viscosity for both strong and fragile systems. The modified model also has the capability to estimate the non-equilibrium isostructural viscosity of glass from the equilibrium viscosity and the temperature-dependent elasticity of the glassy state.

11:40 AM

(GOMD-S1-097-2018) Shear-induced ultra-slow relaxation and two-step non-Newtonian behavior in supercooled selenium and related glass-forming liquids

W. Zhu*[1]; B. Aitken[2]; S. Sen[1]

1. University of California, Davis, Materials Science Engineering, USA
2. Corning Incorporated, Science & Technology Division, USA

The shear-thinning behavior of supercooled Se, As_xSe_{100-x} ($10 \le x \le 20$) and $As_xSe_{100-x-y}I_y$ ($10 \le x \le 20$, $10 \le y \le 20$) liquids is studied using oscillatory parallel plate rheometry at various temperatures. Master curves of rheological properties of all samples as a function of normalized shear rates (Weissenberg number Wi = shear rate*structural relaxation time) are obtained by time-temperature superposition over nearly 11 orders of magnitudes. While all supercooled liquids display non-Newtonian shear thinning behavior at the expected onset $Wi \ge 1$, a second low-frequency onset accompanied by a "rubbery plateau" in storage modulus is observed around $Wi \sim 10^{-2}$ in Se and $As_{10}Se_{90}$ liquids. Increasing the Se chain length of $As_{20}Se_{80}$ by incorporating I in the network also progressively introduces the "rubbery plateau" and brings the system to the edge of two-onset separation. The low-frequency onset is a novel dynamic effect related to the shear induced formation of anisotropic structural configurations with characteristic relaxation rates that are orders of magnitude slower than the a-relaxation rate of the liquid.

Session 3: Structural Characterizations of Glasses III

Room: El Mirador West (22nd Fl)

Session Chairs: Mario Affatigato, Coe College; Randall Youngman, Corning Incorporated

9:20 AM

(GOMD-S1-098-2018) Amorphous Tantala and its Relationship with the Liquid State (Invited)

O. L. Alderman*[1]; C. J. Benmore[4]; J. Neuefeind[3]; S. Sendelbach[1]; A. Tamalonis[1]; L. Gallington[4]; C. Elodie[2]; A. Mermet[2]; V. Martinez[2]; R. Weber[1]

1. Materials Development Inc., R&D, USA
2. Institut Lumière Matière, Université Claude Bernard Lyon 1, France
3. Spallation Neutron Source, Oak Ridge National Laboratory, USA
4. Argonne National Lab, X-ray Science Division, USA

Amorphous tantala films have been used in the successful detection of gravitational waves, where they act as high index layers within the multilayer mirrors of large scale interferometers. From a glass science perspective, a-Ta_2O_5 is an intriguing material, being composed of an 'intermediate' oxide which has not been melt-quenched to form glass, but is typically formed by ion-beam sputtering. Nonetheless, glasses containing large molar amounts of Ta_2O_5 have been formed from melts of e.g. $46Ta_2O_5.54Al_2O_3$ and $30Ta_2O_5.35La_2O_3.35Nb_2O_5$ suggesting that Ta may well partake in network formation. Here we use high-energy x-ray and neutron diffraction to study liquid Ta_2O_5 and its putative isomorph – molten Nb_2O_5. These measurements are then compared to the x-ray diffraction pattern of a-Ta_2O_5 obtained in transmission geometry through a 15μm film, where the silicon substrate has been removed by ion beam milling. Whilst the liquids are dominated by metal cations coordinated by 5 or 6 oxygen, the amorphous solid has a local structure more akin to the crystalline solids built from primarily 6- and 7-fold polyhedra. These results will be discussed in terms of the temperature dependence of the liquid structure and the known structural changes occurring upon annealing and doping of the amorphous films, and glass-formation from heavily modified tantalate melts. This work was partially funded under DOE contract number DE-SC0015241.

9:50 AM

(GOMD-S1-099-2018) Lorentzian lineshapes and linewidths of symmetric stretch peaks (800-1200 cm^{-1}) in the Raman spectra of alkali glasses and melts

M. Bancroft[2]; W. Nesbitt[3]; G. Henderson*[1]; C. O'Shaughnessy[1]; T. Withers[3]; D. R. Neuville[4]

1. University of Toronto, Earth Sciences, Canada
2. University of Western Ontario, Chemistry, Canada
3. University of Western Ontario, Earth Sciences, Canada
4. IPGP, Geomaterials, France

Raman spectra of the SiO_4 symmetric stretch region (800-1200 cm^{-1}) for low alkali (M) silicate glasses (5 and 10 mol% M_2O) yield intense well-resolved Q^3 peaks at ~1100 cm^{-1} with mostly Lorentzian character (>90% at 298K), in contrast to previous Gaussian fits for silicate glasses. The spectra of both Na and Li glasses show an additional Q^3 peak. It results from close approach of the alkali (M) to the bridging oxygens (BO), which alters Raman shifts of the Q species to somewhat lower frequencies. The linewidths (FWHM) of fitted Q^1, Q^2 and Q^3 species peaks are similar (35-55 cm^{-1}) at 298K for all alkali silicate glasses. However, there appears to be a small systematic increase ine linewidth from Q^1 to Q^2 and Q^3. The Q species FWHM of 5 and 10 mol% Cs_2O silicate glasses show a T dependence similar to those of crystal silicate spectra: both increase by 35-45 cm^{-1} from 298K to 1200K. The T dependence and the Lorentzian lineshapes can be explained on theoretical grounds considering Heisenberg lifetime linewidths and the Balkanski formulation. The 30 mol% K_2O glass and the 50 mol% Na_2O spectra are then readily fit with two or three Q^2 or Q^3 peaks of mainly Lorentzian character, which yield reasonable linewidths and separations between peaks.

10:10 AM

(GOMD-S1-100-2018) Structural evolution of glasses with their thermal history (Invited)

D. de Ligny*[1]; M. Bergler[1]; A. Veber[1]; S. Schuller[2]; F. Angeli[2]

1. University Erlangen-Nürnberg, Materials Sciences and Engineering, Germany
2. CEA, Marcoule, France

The dependence of the structure of different families of glasses with their thermal history will be presented. It will include results on titano silicates, borosilicates, borate, phosphate glasses. The glass samples were equilibrated at different temperatures or obtained with control undercooling from 0.1 to 300K/min. The evolution of the structure of the glass was investigated on all range order from short to long by recording their Raman spectra from 5 to 1600 cm^{-1}. Complementary Brillouin spectroscopy observations were realized to prove the effect of the heat treatment on the global elastic properties. In a general rule it appears that the sensitivity of the short range order is strongly correlated to the polymerization. At the opposite on highly polymerized glasses structural modifications are very tenious and difficult to characterize. Moreover it will also be shown as already mentioned by other authors that the concept of fictive temperature needs to be used with care since different structural units of a glass can present different relaxation behavior. At the end the new knowledge of the structural modifications of these glasses with their thermal history will be used as a tool to found back their cooling history. This approach will be applied as well on hyperquenched samples as glass fibers or glasses submitted to different laser treatment.

10:40 AM

(GOMD-S1-101-2018) Investigation of Nucleation and Growth in Liquid and Glass Materials using Extended Range X-ray Pair Distribution Function Measurements

R. Weber*[1]; O. L. Alderman[1]; C. J. Benmore[2]; A. Tamalonis[1]; D. Robinson[2]

1. MDI, USA
2. Argonne National Lab, Advanced Photon Source, USA

Recent advances in the generation, focusing and detection of synchrotron x-rays enable new types of in-situ measurements. By using a novel arrangement of two large area x-ray detectors placed at different distances from the sample, small and wide angle scattering measurements can be made simultaneously over a broad and contiguous range of reciprocal space. Measurement of both nearest neighbor atomic bonding and mesoscale structure in near real time provides a powerful tool to study phase changes, onset of crystal nucleation, phase separation and development of nanoscale heterogeneities. In combination with various sample environments, nucleation and growth in supercooled liquids, heat treated glasses and supersaturated solutions can be investigated in a systematic way. Simultaneous detection enables fast measurements to study structural relaxation and evolution in time resolved measurements. This contribution will describe the instrument and illustrate its application with examples of measurements made during the development and commissioning stages of the work. This work is funded by the Department of Energy grant number DE-SC-001645.

11:00 AM

(GOMD-S1-102-2018) Molecular dynamics study of correlations between IR peak position and bond parameters of silica and silicate glasses: Effects of fictive temperature, temperature, and mechanical stress

J. Luo[1]; Y. Zhou[1]; S. Milner[1]; C. G. Pantano[2]; S. H. Kim*[1]

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

In the IR spectra of silica and silicate glasses, the shifts of the maximum intensity position of the $n_{Si\text{-}O\text{-}Si,as}$ band due to fictive temperature, temperature, and mechanical stress could be attributed to changes in the distribution of bond parameters such as bond length and bond angle. At different fictive temperatures, density of glass changes. Upon heating, isotropic expansion occurs and the density changes; upon applying mechanical stress, anisotropic strain is induced and a significant change in the Si-O-Si bond angle is observed. From molecular dynamics simulations of silica glasses, it was found that the peak position shift correlates better with the asymmetric change in the Si-O bond length distribution, rather than the Si-O-Si bridge angle, the O-Si-O tetrahedral angle, or the density change. This new finding provides an insight into how and why the $n_{Si\text{-}O\text{-}Si,as}$ IR peak of soda lime silica (SLS) glass shifts upon chemical strengthening via ion exchange and thermal tempering.

11:20 AM

(GOMD-S1-103-2018) Structure of Mixed Anion Salt Glasses

E. T. Nienhuis*[1]; M. Saleh[1]; J. Marcial[1]; M. Naji[2]; A. Goel[2]; J. McCloy[1]

1. Washington State University, USA
2. Rutgers University, USA

This study seeks to understand the melt structure of molten salts in relation to the low temperature reactions and melts that occur during the vitrification of Hanford Low Activity Waste (LAW). Salts (such as nitrates, sulfates, carbonates, halides) play a key role in these low temperature reactions as they form complex eutectic mixtures during early stage melting in the cold cap. Sulfates are of particular interest as they have limited solubility in the final glass waste form and can be detrimental to the long-term durability. To better understand these low temperature processes, melts of several simple binary and ternary salt systems were studied. In one example, salt melts consisting of varied amounts in the ternary K_2SO_4-$ZnSO_4$-NaCl were melted and rapidly quenched to retain the amorphous melt structure. Synchrotron x-ray diffraction data was then obtained and reduced to determine the pair distribution function (PDF). Empirical Potential Structure Refinement (EPSR) was used to model the pair distribution function data. From this model, the individual atom pair distribution functions and coordination numbers were determined. Additional information was determined from infrared absorption spectroscopy and thermal analysis.

Session 8: Glass Under Extreme Conditions - High Pressure

Room: La Vista A/B (22nd Fl)
Session Chair: Morten Smedskjaer, Aalborg University

9:20 AM

(GOMD-S1-104-2018) Impact of pressure on plastic yield in amorphous solids with open structure (Invited)

A. Tanguy*[1]

1. INSA Lyon, LaMCoS, France

Plasticity in amorphous silica is unusual: The yield stress decreases with hydrostatic pressure, in contrast to the Mohr-Coulomb response commonly found in more compact materials. We present in this talk different calculations of yield surfaces in sodo-silicate glasses, together with the analysis of the signature of pressure effect on their vibration modes. Finally, we relate the plastic yield of silica based glasses upon pressure to the buckling behaviour of their silicon skeleton.

9:50 AM

(GOMD-S1-105-2018) Intermediate state of SiO_2 glass during pressure-induced phase transformation (Invited)

T. Sato*[1]

1. Hiroshima University, Japan

SiO_2 glass shows various interesting behavior under high pressure. In our recent studies, we have summarized the high-pressure behavior of silica glass at room temperature as follows: (i) SiO_2 glass behaves as a single amorphous polymorph having a fourfold-coordinated structure below 10 GPa. (ii) Irreversible changes in the intermediate-range order occur at 9 ~ 13 GPa. (iii) It behaves as a fully densified fourfold-coordinated phase (20% denser than the ambient phase) up to 20 GPa. (iv) Changes in the short-range order occurs at around 20 ~ 40 GPa and the coordination number continuously increases from four to six. (v) A sixfold-coordinated phase persists up to at least 100 GPa. However, how these transformations proceed is not fully understood yet. By using a high-pressure in situ small-angle x-ray scattering method, we have found that the structure of SiO_2 glass is inhomogeneous during the phase transformation in the short-range order, i.e., fourfold- and sixfold-coordinated domains coexist at the (iv) stage.

10:20 AM

(GOMD-S1-106-2018) Pressure-induced structural changes in silicate glasses and liquids at high pressures (1 to 3 GPa)

S. Bista*[1]; J. Stebbins[1]

1. Stanford University, Geological Sciences, USA

In this work, we will provide an overview of pressure-induced structural changes in wide-ranging compositions of aluminosilicate and aluminoborosilicate glasses. We will discuss the role of various structural factors such as oxygen speciation, modifier cation field strength and interactions among network cations in pressure-induced network cation coordination increases. We will also talk about interactions between these structural parameters, which further complicates the role of each of these parameters. For instance, the role of non-bridging oxygen in network cation coordination increases with pressure becomes systematically less important as we replace low-field strength alkali modifiers with high-field strength alkaline-earth modifiers in a glass. Finally, we present our analysis of structural and density data using a computational geometric approach.

10:40 AM

(GOMD-S1-107-2018) Spectroscopy as a tool for local density measurement in vitreous silica

C. Weigel[1]; M. Foret[1]; R. Vacher[1]; B. Hehlen[1]; B. Ruffle*[1]

1. Montpellier University, Physics Department, France

The paper will discuss the possibility for light spectroscopies, e.g. Brillouin Light Scattering or Raman Scattering, to locally monitor the densification of amorphous silica. It is indeed well-known that silica significantly densifies under high stresses, either elastically as for example during a high-pressure experiment in a diamond-anvil cell below about 10 GPa or plastically above that limit. Further, this elastic limit strongly depends on the temperature. Irradiation-induced density changes are also observed using ultra-short laser pulses, neutrons or other particles. All these different routes lead to substantial structural modifications which in turn alter the response of silica to light spectroscopy in a complex manner.

11:00 AM

(GOMD-S1-108-2018) Mechanical Response of Borosilicate Glass During Spherical Nanoindentation and Diamond Anvil Cell Testing: Relation to Constitutive Equation Modeling

B. L. Hackett*[1]; R. C. Gallagher[2]; B. A. Oistad[2]; A. Wereszczak[2]; G. M. Pharr[3]

1. University of Tennessee, USA
2. Oak Ridge National Laboratory, USA
3. Texas A&M University, USA

Formulating constitutive relations that comport well with experimental observations of glasses that deform by both volume and non-volume conserving mechanical processes and that exhibit densification-dependent elastic properties is not a trivial undertaking. While progress has been made in devising new continuum mechanical descriptions thereof, comparison and validation of models to the experimental behavior of real materials has been limited to high-purity vitreous silica. Here, the mechanical response of borosilicate glass is probed using spherical nanoindentation and double-toroid diamond anvil cell compression. Parameters defining a linear and an elliptical hydrostatic pressure and shear co-dependent yield criterion are found experimentally from the stress state beneath the indenter at yielding and pressure-density data from diamond anvil cell compression. The two yield criteria, accounted for with companion finite element modeling, are compared and discussed.

11:20 AM

(GOMD-S1-109-2018) Pressure Induced Densification and Compression in a Reprocessed Borosilicate Glass

K. J. Ham*[1]; Y. Vohra[1]; Y. Kono[2]; P. Patel[3]; S. Kilczewski[4]

1. University of Alabama at Birmingham, Physics, USA
2. Carnegie Institution of Washington, HPCAT, Geophysical Laboratory, USA
3. U.S. Army Research Laboratory, Ceramics and Transparent Materials Branch, USA
4. Bennett Aerospace, Inc., USA

A reprocessed sample of borosilicate glass has been studied by X-ray radiography and energy-dispersive X-ray diffraction to 4.94 GPa using a Paris-Edinburgh (PE) press at a synchrotron X-ray source. Gold foil pressure markers were used to obtain the sample pressure by X-ray diffraction, while X-ray radiography provided a direct measure of sample volume. The X-ray radiography method for volume measurements at high pressures was validated for a known sample of pure α-Iron. The experimentally measured bulk modulus of the reprocessed borosilicate glass was determined as $B_0 = -V(dP/dV)$ using the low pressure experimental points, which remain in the elastic region of compression. The bulk modulus of 30.34 ± 0.01 GPa obtained from experimental volume data is in good agreement with the 32.9 GPa value derived from the measured elastic constants. An additional sample of reprocessed borosilicate glass was compressed to 12.2 GPa, and the flotation density measured is 2.755 gm/cc and shows an increase in density of 24%, as compared to the starting sample.

S3: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 4: Glass-based Optical Devices I

Room: La Vista C (22nd Fl)
Session Chairs: Juejun Hu, Massachusetts Institute of Technology; Hongtao Lin, Massachusetts Institute of Technology

9:20 AM

(GOMD-S3-027-2018) Fs-laser processing of glass-based optical waveguide devices (Invited)

D. Krol*[1]

1. University of California, Davis, Materials Science and Engineering, USA

Fs-laser processing of glass allows for the modification of material properties within the sample, notably the refractive index, with three-dimensional freedom and (sub)micrometer resolution. By selective modification of various geometrical structures it is possible to fabricate a wide range of photonic elements and devices, such as waveguides, splitters, couplers, gratings, nanogratings, three-dimensional memory arrays, photonic crystals, and waveguide lasers and amplifiers. In this presentation I will review the state-of –the-art of fs-laser fabrication of glass-based optical waveguide devices as well as the role of glass composition, laser pulse repetition rate and laser wavelength. The physical processes during laser-matter interaction and materials modification will also be discussed.

9:50 AM

(GOMD-S3-028-2018) Photochromic windows

N. Lonnroth*[1]; N. F. Borrelli[1]; G. Brown[1]; M. Price[1]; J. Grochocinski[1]

1. Corning Incorporated, USA

Window sizes and the window-to-wall area ratio in commercial and residential buildings continue to increase, while building energy codes require higher efficiency. This has driven the development of technologies, such as thermochromic and electrochromic windows, to reduce excess heat and light penetration through the windows, while still allowing a view outdoors. Corning developed photochromic glasses a half a century ago, mainly used for sun glasses but the application to architectural windows was contemplated from the start. The physical mechanism and kinetics of photochromic glass darkening and fading is temperature dependent and makes utilization in single pane windows impractical. Most new windows installed are double or triple pane windows, where the inside pane is more insulated from the outdoor environment. Reduced temperature swings allow the use of photochromic glass in a window. Due to energy requirements all windows are further equipped with a low-e coating to cut down the UV and IR radiation that penetrates through the window. Photochromic glass is darkened mainly by UV wavelengths, 320-410 nm. Thus, performance of a photochromic glass inner pane can be limited by a low-e coated outer pane. We demonstrate in this work the performance of photochromic glass when used in a low-e coated multipane window, the range between clear and dark state and show the degree of glare reduction it delivers.

10:10 AM

(GOMD-S3-029-2018) Chalcogenide Glass Waveguide-integrated Black Phosphorus Mid-Infrared Photodetectors

S. Deckoff-Jones*[1]; H. Lin[1]; D. Kita[1]; H. Zheng[1]; W. Zhang[2]; D. Li[1]; J. Hu[1]

1. Massachusetts Institute of Technology, USA
2. Ningbo University, China

Black phosphorus (BP) is a promising 2D material that has unique in-plane anisotropy and a 0.3 eV direct bandgap in the mid-IR. However, waveguide integrated black phosphorus photodetectors have been limited to the near-IR on top of Si waveguides that are unable to account for BP's crystalline orientation. In this work, we employ mid-IR transparent chalcogenide glass (ChG) both as

a broadband mid-IR transparent waveguiding material to enable waveguide-integration of BP detectors, and as a passivation layer to prevent BP degradation during device processing as well as in ambient atmosphere. Our ChG-on-BP approach not only leads to the first demonstration of mid-IR waveguide-integrated BP detectors, but also allows us to fabricate devices along different crystalline axes of black phosphorus to investigate, for the first time, the impact of in-plane anisotropy on photoresponse of waveguide-integrated devices. The best device exhibits responsivity up to 40 mA/W and noise equivalent power as low as 30 $pW/Hz^{1/2}$ at 2185 nm wavelength. We also found that photodetector responsivities changed by an order of magnitude with different black phosphorus orientations. This work validates black phosphorus as an effective photodetector material in the mid-IR, and demonstrates the power of the glass-on-2D-material platform for prototyping of 2D material photonic devices.

10:30 AM

(GOMD-S3-030-2018) High-performance flexible chalcogenide glass waveguide-integrated photodetectors

L. Li*[1]; H. Lin[1]; Y. Huang[1]; R. Shiue[2]; A. Yadav[3]; J. Li[1]; J. Michon[1]; D. Englund[2]; K. Richardson[3]; T. Gu[1]; J. Hu[1]

1. Massachusetts Institute of Technology, Materials Science and Engineering, USA
2. Massachusetts Institute of Technology, Electrical Engineering and Computer Science, USA
3. University of Central Florida, The College of Optics & Photonics, USA

Chalcogenide glasses have recently been demonstrated as a promising material for novel on-chip integrated photonic circuits thanks to their wide transparency, tunable high refractive indices, low processing temperature and the amorphous characteristics enabling monolithic integration on different material platforms. Here we describe the design and experimental demonstration of chalcogenide glass waveguide integrated on InGaAs nanomembrane photodetectors on flexible polymer substrate. The realized devices present a measured responsivity of 0.35 A/W and a 3-dB bandwidth of 1.4 GHz at 1530 nm wavelength. Besides, the devices exhibit extraordinary mechanical flexibility which can sustain 1000 bending cycles at sub-millimeter bending radius without measurable performance degradation by using the developed multi-neutral -axis micro-mechanical design.

10:50 AM

(GOMD-S3-031-2018) Thermally Drawn Glass Fibers with Conductor-Semiconductor Structured Core

S. Chen*[1]; F. Tan[1]; J. Kaufman[1]; H. Ebendorff-Heidepriem[2]; R. M. Gaume[1]; A. Abouraddy[1]

1. University of Central Florida, College of Optics and Photonics, USA
2. The University of Adelaide, Australia

One of the long-standing goals in the burgeoning field of multi-material fibers is to incorporate functionalities associated with electronic devices – that necessitate conductor, semiconductor and insulator materials – into thermally drawn optical fibers. Such task faces severe obstacles stemming from complicated material system that may undergo capillary break-up and unstable mixing between adjacent crystalline materials within micro-scale cross-sectional compartments, especially at the interface between metal electrodes and semiconductors. We present a thermally drawn fiber composed of four distinct material phases: an insulating glass, a crystalline metal, a crystalline semiconductor and an amorphous electrically conductive glass composite. The fiber architecture was designed to parallel that of a planar electronic device, with the semiconducting phase at the fiber center and two metallic electrodes above and below running the length of the fiber. The composite glass acts as a viscous barrier during the draw between the semiconducting and metallic phases, preventing mixing of the two phases and preserving the preform architecture in the final fiber. Studies of the fiber microstructure, carrier transport properties at the contact barrier between composite and semiconductor, and simulations of the electronic band structure may pave the road for the future fiber-based thermally drawn electronic devices.

11:10 AM

(GOMD-S3-032-2018) Improving the thermal stability of phosphor in a white light-emitting diode (LED) by glass-ceramics: Effect of Al_2O_3 dopant

T. Zhang*[1]; H. Su[1]; J. Yan[1]

1. Fuzhou University, College of Materials Science and Engineering, China

In this work, a phosphor for white light-emitting diode (LED) application, Ce^{3+}-doped yttrium aluminum garnet (YAG:Ce^{3+}), was successfully packaged using a P_2O_5-ZnO-Na_2O-Al_2O_3 glass-ceramic system, through a vertical deposition method. Here, we found that white light can be achieved by combining the packaged phosphor with a blue chip (e.g. InGaN). The specimen doped with 4 mole% Al_2O_3 showed a luminous efficacy (LE) of 125.8 $lm*W^{-1}$, at a correlated color temperature (CCT) of 5769K, with a color rendering index (CRI) of 68. In addition, the LE loss of the specimen doped with 4 mole% Al_2O_3 was only 3.6% after heat treatment at 150 °C for 1200 h, which is significantly lower than that of traditional resin (19.3%). Moreover, a possible mechanism for reducing the LE loss using glass-ceramics was proposed.

S4: Glass Technology and Cross-Cutting Topics

Session 3: Challenges in Manufacturing I

Room: La Vista F (22nd Fl)

Session Chairs: Irene Peterson, Corning Incorporated; Michael Josh Snyder, Corning Research and Development Corporation

9:20 AM

(GOMD-S4-044-2018) Critical Considerations in Modeling of Radiative Heat Transfer in Glass Melts (Invited)

M. K. Choudhary*[1]

1. International Commission on Glass and MKC Innovations LLC, USA

At high temperatures encountered in glass manufacturing, thermal radiation plays an important role and impacts parameters such as energy efficiency, environmental emissions, furnace life, and product quality. The lecture will critically assess approaches for modeling radiative transfer in glass melts. We will begin with background information on heat transfer in an absorbing medium such as a glass melt and discusses the implications of using the Rosseland or diffusion approximation for modeling thermal radiation. This will be followed by an overview of the Discrete Ordinates Model (DOM) that accounts for the spectral dependence of the radiation heat flux. Next, we will review selected high temperature absorption spectra and photon or radiation conductivity values calculated from them. Finally, we will present results from numerical modeling to assess the consequences of using the DOM versus the Rosseland approach on temperature distribution in glass furnaces and delivery channels. These results will be used to critically assess conditions under which the approximate or the detailed modeling approach would be appropriate. In summary, the lecture will describe the conceptual framework for analyzing radiative heat transfer in glass melts, provide insights, present results on flow and heat transfer in glass melting and delivery, and discuss criteria for selecting modeling approaches.

9:50 AM

(GOMD-S4-045-2018) Computational Fluid Dynamics and Heat Transfer Modeling of a Waste Glass Melter (Invited)

D. P. Guillen*[1]; A. Abboud[1]; R. Pokorny[2]

1. Idaho National Laboratory, Materials Science and Engineering, USA
2. UCT Prague, Czechia

A high-fidelity computational model of a waste glass melter is being developed wherein multiphase fluid flow and heat transfer is solved simultaneously in the plenum, cold cap, and molten glass regions. The physics incorporated into the melter model includes forced convection from bubbling, ohmic heating, and thermal radiation. Because the melter operates at high temperatures, contains opaque fluids, and is enclosed within refractory-lined, water-jacketed steel, obtaining suitable validation data is challenging. A suite of models at different scales ranging from laboratory to pilot-scale has been developed wherein specific physics are examined and validated against experimental data. A tiered approach to model validation is implemented consisting of a series of progressively more complex test cases designed to model the physics occurring in the full-scale system. Four successive levels are defined in a validation pyramid and built up in levels of increasing complexity from unit problems to subsystem cases, to pilot-scale systems, and then to the full-scale system.

10:20 AM

(GOMD-S4-046-2018) Alumina and Silica Sources for Continuous Reinforcement Glass Fiber Manufacturing - Melting Energy Aspect (Invited)

H. Li*[1]

1. Nippon Electric Glass, USA

There are two types of major alumina sources used in commercial production of E-Glass fiber products (primarily composed on CaO, Al_2O_3, and SiO_2) as reinforcements for plastic composite materials; they are Kaolinite, $Al_4Si_4O_{10}(OH)_8$, and Pyrophyllite, $Al_4Si_8O_{20}(OH)_4$. The Al_2O_3 : SiO_2 ratio is 1 : 2 for Kaolinite as compared with 1 : 4 for Pyrophyllite. Relative to Kaolinite, to make a glass of the same chemistry, the use of Pyrophyllite enables the batch free from sand to meet, whiles about 30% sand must be added to the E-Glass batch using Kaolinite. In turn, fast batch-to-melt conversion process can be achieved by using the Pyrophyllite-derived, sand-free batch. Another type of continuous reinforcement glass fibers (P-Glass) contains higher SiO_2 and appreciable amount of alkalis. The use of natural, amorphous Perlite has been recently utilized by using electric melting technology. The glassy Perlite derived batch, plus the batch being nearly free from sand, also enables fast batch-to-melt conversion process as compared with E-Glass case using Kaolinite. The presentation will focus on characterizations of kinetics of the batch-to-melt conversion, including intermediate phases formed, and the associated conversion energy differences.

10:50 AM

(GOMD-S4-047-2018) Impact of calcination of briquette on batch to melt conversion process (Invited)

T. Maehara*[1]; Y. Doi[1]; S. Hyodo[1]; D. Kikutani[1]; M. Yamamoto[1]

1. Asahi Glass Co., Ltd., Production Technology Division, Japan

Batch to melt conversion process is known as a complex process affected not only by chemical reactions but also by physical phenomena like heat transfer through a layer of glass batch. Briquetting (pelletizing by rotated twin rolls) is one of the most effective way to improve glass batch properties like thermal conductivity, contact area between ingredient particles and so on. As an additional practical benefit, briquetting enable us to handle 'easy to melt' raw materials with fine grain size without dust problem. Preheating of glass batch briquette have been well known idea to improve melting kinetics. When we chose adequate grain size distributions of each ingredient, briquette can be preheated up to 850°C without adhesion of briquette to one another. Furthermore, fully calcined briquettes can be obtained by heat treatment at around 900°C. Adhesion between calcined briquettes after the heat treatment are weak enough to be broken by hammering. Melting behavior of calcined briquette is very different than that of normal briquette. In the presentation, impacts of the absence of CO_2 release from glass batch on batch to melt conversion process will be discussed.

11:20 AM

(GOMD-S4-048-2018) In-situ analysis of formulation of silicate glass melt using Raman spectroscopy and X-ray Computed Tomography (Invited)

T. Yano*[1]; R. Kado[1]; T. Miyawaki[1]; T. Kishi[1]; N. Matsushita[1]

1. Tokyo Institute of Technology, Department of Materials Science and Engineering, Japan

Glass formulation from batch in silicate glass system has been investigated using in-situ analysis techniques; Ramam spectroscopy and X-ray Computed Tomography(XCT). Raw materials of silicate glass batch in crucible were heated up to melting temperature at the constant heating rate, and their vitirification process was observed through these techniques. Vibrational spectra indicates the phase changes and reactions of materials on heating in atomic level, while 3D images of XCT reveals the macroscopic alteration of materials. In this paper, the silicate glasses, especially soda-lime glass, are given main attention, and behavior of the formulation of melts are discussed.

Session 4: Waste Immobilization - Structure

Room: La Vista D/E (22nd Fl)
Session Chair: Stephane Gin, CEA

9:20 AM

(GOMD-S4-049-2018) Recent advances in understanding self-irradiation damage and gas bubble formation in nuclear waste matrices (Invited)

A. Mir*[1]; J. A. Hinks[1]; S. Donnelly[1]

1. University of Huddersfield, Electron Microscopy and Materials Analysis, United Kingdom

Nuclear waste matrices are subjected to self-irradiation damage due to electrons, alpha-particles and recoil nuclei resulting from transmutation reactions. The combination of radiation damage and, helium accumulation can result in bubble formation. The classical approach to address these issues has relied on using single-beam irradiation of the surrogate waste glasses. However, more recent studies have shown that such irradiations do not simulate well the actual multi-irradiation scenario of the waste matrices. It is now understood that as well as creating defects, this self-irradiation can also induce partial defect annealing. Furthermore, studies on noble gas implantation and bubble formation in different glass systems using in-situ TEM and ion irradiation has shed light on the conditions necessary for bubble formation. Using MD simulations, it is now possible to simulate cavity formation under ballistic damage where bubbles can nucleate and, using Monte-Carlo simulations it is then also possible to ascertain the physical state of the gas bubbles/precipitates within the host matrix. This presentation is aimed at highlighting the importance of studying the radiation damage using multi-beam irradiations and will include recent developments in our understanding of bubble-nucleation in waste matrices and in the use of Monte-Carlo for the simulation of bubbles in glasses.

9:50 AM

(GOMD-S4-050-2018) Raman and X-ray Absorption Spectroscopy of Network Modifying Tetrahedral Species in Borosilicate Waste Glasses (Invited)

D. A. McKeown*[1]; H. Gan[1]; I. S. Muller[1]; A. C. Buechele[1]; K. S. Matlack[1]; I. L. Pegg[1]

1. Catholic University, Vitreous State Laboratory, USA

S, V, Cr, Mo, and Tc found in various nuclear wastes can be problem elements to incorporate homogeneously in borosilicate glass. Raman and X-ray absorption spectroscopy (XAS) of glasses frequently indicate that these elements are in TO_4 tetrahedra (where: T = S, V, Cr, Mo, Tc, or Re as a Tc surrogate) surrounded by network-modifying Li^+, Na^+, or Ca^{2+}. Both techniques have important strengths and limitations to recognize. Due to large Raman cross-sections of these tetrahedral species and relatively weak cross-sections of the borosilicate network, glass Raman spectra are sensitive to the presence of $S^{6+}O_4$, $V^{5+}O_4$, $Cr^{6+}O_4$, $Mo^{6+}O_4$, $Tc^{7+}O_4$, or $Re^{7+}O_4$. The T-O stretch mode frequency varies with surrounding network-modifying cation type, and area is proportional to element concentration, if the element is solely in tetrahedra; this is typical of oxidizing conditions. More reducing conditions can produce lower valence, higher coordination cations that may have weak or no associated Raman features (e.g., $Cr^{3+}O_6$ or $Tc^{4+}O_6$ octahedra). XAS is usually sensitive to all valence and local coordination environments of an element, and may or may not contain longer-range information. Strengths and weaknesses of Raman and XAS will be reviewed, where examples will be shown using both techniques to provide a more complete picture of an element's bonding characteristics in glass.

10:20 AM

(GOMD-S4-051-2018) Structure and properties of cesium loaded Mo-Fe-phosphate glasses

J. Bai*[1]; J. Hsu[1]; R. Brow[1]; C. Kim[2]; J. Szabo[2]; A. Zervos[2]

1. Missouri University of Science & Technology, USA
2. MO-SCI Corporation, USA

Chemically durable iron phosphate glass is a promising candidate for hosting nuclear wastes containing constituents like Cs_2O and MoO_3 that have lower solubilities in more conventional borosilicate glasses. In this work, two series of Cs_2O-MoO_3-Fe_2O_3-phosphate glasses were characterized. Both series have the same nominal O/P ratio of 3.4. In the first series, the Mo/(Mo+Fe) ratio was fixed (0.26) and the Cs_2O content varied from 0 to 22.5 mol%, and in the second series, the Cs_2O content was fixed (15 mol%) and the Mo/(Mo+Fe) ratio was varied from 0 to 1. Raman spectroscopy reveals that the preferred Mo coordination environment changes from octahedral to tetrahedral with increasing Cs_2O content. Information about the phosphate anions that constitute the glass structure was obtained by high-pressure liquid chromatography. Density and molar volume, glass transition temperature, thermal expansion coefficient, and dissolution rate in water were determined and their relation to glass structure information will be described in detail. This work was supported by the US Department of Energy, SBIR/STTR phase I &II contract DE-SC0011906.

10:40 AM

(GOMD-S4-052-2018) Structural role of iron in sodium aluminosilicates and sodium silicates

M. Ahmadzadeh*[1]; P. A. Bingham[2]; J. McCloy[1]

1. Washington State University, Mechanical and Materials Engineering, USA
2. Sheffield Hallam University, Materials & Engineering Research Institute, United Kingdom

As a significant element in high-level nuclear waste (HLW) glasses as well as natural silicates, iron can change the structure, crystallization, and properties of silicate glasses. However, the detailed nature of iron in silicates is still under debate. Here, we report systematic investigations of $NaAlSiO_4$–$NaFeSiO_4$ join as well as other important Fe-silicate compositions (aegirine – $NaFeSi_2O_6$, 5.1.8 – $Na_5FeSi_4O_{12}$, and Fe-albite – $NaFeSi_3O_8$), for both glasses and crystallized samples. In addition to these simplified stochiometric samples, the effects of Fe addition on the crystallization of the "A4" composition (a known simulant HLW glass) upon canister centerline cooling (CCC) is discussed. Substituting Fe for Al in the aluminosilicate compositions decreases glass transition and crystallization temperature, as Fe additions depolymerizes and weakens the glass structure. It is found that Fe substitutes for Al in the structure of nepheline crystals (Nominally $NaAlSiO_4$) up to $NaAl_{0.63}Fe_{0.37}SiO_4$. Iron redox determination reveals that, while the valence state of Fe is mostly Fe^{3+} in these silicate glasses, Fe^{2+}/Fe^{3+} ratio is higher in low-Fe glasses. While varying Fe additions to A4 glass does not significantly affect nepheline crystallization upon CCC, more Fe additions considerably change Li partitioning from eucryptite (Nominally $LiAlSiO_4$) to a Li-containing spinel phase ($LiFe_5O_8$).

11:00 AM

(GOMD-S4-053-2018) Effect of zirconia substitution on the short- and medium-range structures of soda lime borosilicate glasses

X. Lu*[1]; L. Deng[1]; J. Du[1]

1. University of North Texas, Material Science and Engineering, USA

Zirconia is an important component in vitrification of nuclear wastes, where small amount of ZrO_2 significantly increases density, viscosity and glass transition temperature. It was found recently that it enhances long-term dissolution by inhibiting the alteration layer formation, even though ZrO_2 decreases the initial dissolution rate. In this study, glasses with composition of $xZrO_2$-$(61-x)SiO_2$-$17B_2O_3$-$18Na_2O$-4CaO with x=0, 1, 2, 4, 6 and 8 were simulated using classical molecular dynamics (MD) simulations with recently developed composition-dependent potential sets. Local environments of cations, such as bond distance, bond angle distribution and coordination numbers were systematically studied and compared with experimental values. Bond distance of Zr-O is ~2.11 Å, and slightly distorted $[ZrO_6]$ octahedra appear in all the glass compositions. $[ZrO_6]^{2-}$ is charge compensated by both Na^{1+} and Ca^{2+} with a slightly higher preference of Ca^{2+}. Medium-range structural information altered by ZrO_2 substitution was also investigated. ZrO_2/SiO_2 substitution increases the overall network connectivity and the amount of smaller sized rings thus decreases the initial dissolution rate by stronger network and limit water diffusivity. Furthermore, diffusion and dynamic properties of the ions were studied and discussed for better understanding the chemical durability of these glasses.

11:20 AM

(GOMD-S4-054-2018) Sulfate Sequestration by Ba-Sn Composite Materials to Increase Re Retention in Low-Activity Waste Glass

J. George*[1]; P. Cholsaipant[1]; D. Kim[1]; T. Levitskaia[1]; M. Fujimoto[1]; I. Johnson[1]; A. A. Kruger[2]

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

Difficulty incorporating radioactive Tc-99 into glass during vitrification of low-activity waste (LAW) at the Hanford Site is a concern. Previous studies suggested that the presence of sulfate salts in the melt hinder the incorporation of Re, a non-radioactive surrogate for Tc-99, into nuclear waste glass. In this study, we assessed the capability of a Ba-Sn composite to sequester sulfate during vitrification of an LAW feed and the resulting effects on Re retention in the glass. AN-102 simulated LAW was prepared and the Ba-Sn composite material was added to sequester sulfate. Glass formers and modifiers were then added to the feed, which were dried, crushed, and heated to temperatures between 400-1000 °C at 5 °C/min and air-quenched to room temperature. X-ray diffraction (XRD) was performed on the heated samples. The heated samples and dried feeds were leached in deionized water. The solution from the leach test were analyzed

by Raman spectroscopy and Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) to determine the amount of soluble sulfate salts as a function of temperature and the resulting solids were analyzed for Re retention. The effect of the Ba-Sn composite material on sulfate during vitrification and Re incorporation into the glass will be discussed.

S1: Fundamentals of the Glassy State

Session 1: Glass Formation and Structural Relaxation II

Room: El Mirador East (22nd Fl)
Session Chairs: John Mauro, Pennsylvania State University; Ozgur Gulbiten, Corning Incorporated

1:20 PM

(GOMD-S1-110-2018) Glass formation in highly unstable and fragile systems: The case of phase change materials (Invited)

P. Lucas*[1]; J. Pries[2]; S. Wei[2]; C. Persch[2]; W. Warfel[1]; M. Wuttig[2]

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

Phase change materials (PCMs) such as $Ge_2Sb_2Te_5$ are ideal candidates for memory technologies due their extremely fast phase transformation kinetics and the high contrast in conductivity and reflectivity between the two phases. These contrasts have been mainly attributed to the atypical resonant bonding mechanism of the crystalline phase which has been extensively characterized. The amorphous phase on the other hand, has received considerably less attention. Amorphous PCMs are unstable by design to enable the ultrafast phase change necessary for PC-RAM applications. They can only be obtained through extreme cooling rates and are therefore trapped in a hyperquenched state of high fictive temperature. It was also shown that they exhibit unusually high fragilities among network glass formers. This combination of high fragility and high fictive temperature results in unique relaxation and crystallization dynamics which are yet another peculiarity of these unusual materials.

1:50 PM

(GOMD-S1-111-2018) Variability in the relaxation behavior of glass: Impact of thermal history fluctuations and fragility

J. C. Mauro*[1]; Q. Zheng[2]

1. Pennsylvania State University, Materials Science & Engineering, USA
2. Qilu University of Technology, China

Glasses are nonequilibrium materials that continuously relax toward the metastable supercooled liquid state. As such, the properties of a glass depend on both its composition and thermal history. When an initially cooled glass is subjected to additional thermal cycles, relaxation during the heat treatment is accelerated, leading to changes in the macroscopic properties of the glass. This relaxation behavior is intrinsic to the glassy state and of critical interest to the high-tech glass industry. In many practical cases, the magnitude of the relaxation is less important than the variability of the relaxation effects due to slight variations in the thermal history experienced by the glass. These fluctuations in thermal history can occur either during the initial glass formation or during the subsequent heat treatment cycle(s). Here we calculate the variation in relaxation behavior using a detailed enthalpy landscape model, showing that the relaxation variability can be reduced dramatically by increasing the fragility of the system.

2:10 PM

(GOMD-S1-112-2018) Investigation of Relaxation Processes by MDSC

O. Gulbiten*[1]

1. Corning Incorporated, Science & Technology Division, USA

Heat Capacity Spectroscopy, utilized by modulated differential scanning calorimetry(MDSC), has been recently demonstrated to be used in the low-frequency range to evaluate the response of dynamic processes during the isothermal annealing. Complex heat capacity approach allows us to de-convolute the independent contribution of different dynamic domains and the imaginary part of the complex heat capacity is directly linked to the distribution of the relaxation times. In this study, structural relaxation processes are investigated by heat capacity spectroscopy and macroscopic first order thermodynamic property measurements.

2:30 PM

(GOMD-S1-113-2018) Multicomponent diffusion in calcium and sodium aluminosilicate melts

E. Gouillart*[1]; C. Claireaux[1]; E. Burov[1]; M. Toplis[2]; M. Roskosz[3]

1. Joint Unit CNRS/Saint-Gobain, Surface, Glass and Interfaces, France
2. Observatoire Midi-Pyrénées, France
3. Muséum d'Histoire Naturelle, France

The effect of temperature on multicomponent chemical diffusion in liquids of the quaternary system CaO-Na2O-Al2O3-SiO2 has been studied. Diffusion-couple experiments were performed for three temperatures far above the glass transition as well as 30°C above the glass transition. For each temperature, we determined the diffusion matrix of the system. Strong multidiffusive effects were observed for all temperatures, with significant uphill diffusion of calcium, demonstrating that uphill diffusion happens close to the glass transition as well as at high temperature. Little variation of the eigenvectors of the diffusion matrix was observed as a function of temperature, with a dominant eigenvector corresponding to the exchange of sodium with calcium, and the two other eigenvectors corresponding to the exchange of calcium with network formers. For the temperature range 1200-1360°C, the eigenvalues of the diffusion matrix have an Arrhenian dependence on temperature, with an activation energy consistent with electrical conductivity for the exchange of sodium and calcium, and an activation energy consistent with viscosity for eigenvectors involving network formers. Close to the glass transition, some diffusion profiles are asymmetric due to strong viscosity contrasts resulting in concentration-dependent eigenvalues. Moreover, we observe some departure from Eyring relation close to the glass transition.

2:50 PM

(GOMD-S1-114-2018) Viscosity surging in accordance with phase-separation of boroaluminosilicate glass

H. Tokunaga*[1]; J. Konishi[1]; K. Hayashi[1]; S. Urata[2]

1. Asahi Glass Co., Ltd., New Product R&D Center, Japan
2. Asahi Glass Co., Ltd., Innovative Technology Research Center, Japan

Viscosity is one of key properties to design a manufacturing process of sheet glasses production. Recently, there has been considerable interest in phase-separated glasses (PSG) as a component of electronic devices. However, there are few published data about viscosity of the molten phase-separated glasses. This is considered that the molten PSG must show non-Newtonian behavior, that is, non-linear behavior between shear stress and shear rate, and as a result, measuring the viscosity of such inhomogeneous melt is difficult. We therefore developed a custom designed rotating viscometer, which enables us to measure viscosity of a boroaluminosilicate glass up to $10^{6.5}$ Pa.s. By use of newly developed apparatus, we found several intriguing behaviors owing to phase segregation on viscosity of the glass. One is sudden viscosity jump associated

with phase segregation at phase separation temperature. In addition, the viscosity surging is more significant if we apply faster shear rate during the measurement. The other finding is, more interestingly, the ascent rate of viscosity is decreasing with temperature decreasing. These unpredictable behaviors of viscosity of the molten PSG were studied by using molecular dynamics (MD) simulation with modeling a spherical hard core inclusion embedded into soft matrix glass. The results of MD simulations will be discussed in the presentation.

3:10 PM

(GOMD-S1-115-2018) Heating rate effect and activation of the heterogeneous structural relaxation in sodium silicate glass

Y. P. Vaills*[1]

1. CNRS-CEMHTI, Physics, France

Relaxation phenomena take place differently in glass, depending on the temperature of stabilization and of the heating rate which is imposed to the glass to reach this temperature. Several relaxation phenomena can take place, and the number of them is generally difficult to appreciate because most of the time measurements are global and take into account all of them in one unique measured value. In any case the glass reaches a new state undergoing several structural relaxation phenomena. Is there de discrete or de continuous distribution of phenomena? We can report on the variation of acoustic wave frequency for example by a discrete modelization or take into account the idea of a time relaxation distribution function. The case of a binary alkaline silicate glass will be reported, studying relaxation just below the glass transition, and using several heating rates.

Session 3: Structural Characterizations of Glasses IV

Room: El Mirador West (22nd Fl)
Session Chairs: Sabyasachi Sen, UC Davis; Randall Youngman, Corning Incorporated

1:20 PM

(GOMD-S1-116-2018) Structure of chalcogenide glasses: Partial structure factors by neutron diffraction with isotope substitution (Invited)

A. Zeidler*[1]; P. S. Salmon[1]

1. University of Bath, Department of Physics, United Kingdom

Chalcogenide glasses (those containing S, Se or Te) can be formed over a wide compositional range, and feature networks that are built from a rich variety of structural motifs that include homopolar bonds and edge-sharing tetrahedral units. It is therefore a formidable challenge to solve the structure of these materials by diffraction methods, especially when the chemical species in a given material have similar neutron scattering lengths or x-ray form factors. In this talk, I will present new results on the structure of Ge-S, Ge-Se and As-Se based glasses as obtained by using the method of neutron diffraction with isotope substitution. I will show how the technique can be used to gain site-specific information on the coordination environments of selected chemical species over multiple length scales, thus providing essential information on the glass structure. I will also show how advances in neutron diffraction now make it possible to measure the full set of partial structure factors for an enhanced range of glassy materials over a wide compositional range. The results are compared to those obtained from first-principles molecular dynamics simulations. Future challenges for experiment and simulation are discussed.

1:50 PM

(GOMD-S1-117-2018) Structural Origin of Intermediate Glasses

S. Jaccani*[1]; L. Huang[1]

1. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA

In contrast to normal glasses like window glass and anomalous glasses such as silica glass, intermediate glasses show nearly constant elastic moduli with temperature and/or pressure. Although a few intermediate glasses have been reported, the structural origin for this behavior remains elusive. We combined in-situ high-temperature and high-pressure Raman and Brillouin Light Scattering (BLS) to understand the structural origin underlying the intermediate elastic response in sodium silicate, sodium aluminosilicate, sodium titanium silicate and borosilicate glass systems. Our experiments reveal that the intermediate elastic behaviors come from the delicate balance between conformation changes in the medium range order and bond anharmonicity in response to temperature and/or pressure. In-situ high-temperature and high-pressure Raman and BLS experiments can help identify as well as understand intermediate glasses that hold great promise in sensing applications and in applications where a broad range of thermal and mechanical stimulation is expected.

2:10 PM

(GOMD-S1-118-2018) Structure of Bi and Ga modified $GeSe_4$-$GeTe_4$ glasses via Neutron Scattering

J. R. Oelgoetz*[1]; J. Allen[1]; J. Bunton[1]; J. Kelly[1]; T. L. Hodge[1]; R. Golovchak[1]; A. Kovalskiy[1]; Y. Shpotyuk[2]

1. Austin Peay State University, Physics & Astronomy, USA
2. University of Rzeszow, Center for Innovation and Transfer of Natural Sciences and Engineering Knowledge, Faculty of Mathematics and Natural Sciences, Poland

Bi and Ga modified GeSe4-GeTe4 glasses have been shown to have band gaps below 1eV and a large enough attenuation coefficient that samples of ~mm thickness are opaque to visible and infrared light, yet are still semiconductors. The structure of these non-binary chalcogenide glasses is an open subject. Questions such as how the atoms are interconnected as well as basic parameters such as bond lengths and angles are all of interest. A selection of these non-binary chalcogenide glasses ($Bi_1Ga_5Ge_{18.8}Se_{37.6}Te_{37.6}$, $Bi_5Ga_5Ge_{18}Se_{36}Te_{36}$, and $Bi_{10}Ga_5Ge_{17}Se_{34}Te_{34}$) have been studied using the NOMAD beamline at the Spallation Neutron Source at Oak Ridge National Laboratory. In this talk we present structural models built from these neutron diffraction studies using Reverse Monte Carlo modeling. The interconnection of atoms, their lengths and other structural parameters will be presented.

2:30 PM

(GOMD-S1-119-2018) Cavities, chemical disorder and polymorphic transitions in chalcogenide liquids and glasses from diffraction studies and modelling (Invited)

E. Bychkov*[1]

1. University of Littoral, LPCA – EA 4493, France

Chalcogenide glass systems have been widely studied over the last decades stimulated by various and promising applications in optics, electronics, data and energy storage. Recent advances in NMR and vibration spectroscopy, high-energy x-ray and pulsed neutron diffraction techniques combined with computer modelling revealed many previously hidden structural features and trends in glassy chalcogenides. The present contribution will be focused on (i) cavity analysis for sulfide binary systems in relation to ionic diffusion and ion exchange, (ii) chemical ordering in non-stoichiometric compositions and chemical disorder in stoichiometric binaries, and (iii) polymorphic transitions in chalcogenide and chalcohalide liquids and glasses as a function of temperature, pressure or chemical potential. The experimental x-ray and neutron diffraction results, RMC and DFT structural modelling will be compared with complementary Raman data and tracer experiments.

3:00 PM

(GOMD-S1-120-2018) Probe Medium-range Structure of Glass Materials by First Sharp Diffraction Peak from Total Scattering Analysis

Y. Shi*[1]

1. Corning Incorporated, Charaterization Science, USA

The structure of a glass is very important for determining its properties. The first sharp diffraction peak (FSDP), a feature in the total scattering pattern of glass materials, has long been associated with the medium range structure and various studies have investigated the origin of FSDP. Here we propose a method to derive the medium range (4-5 Å) structure information from first sharp diffraction peak (FSDP) of neutron total scattering structure function developed from neutron measurements of more than one hundred silicate and aluminosilicate glasses.

Session 8: Glass Under Extreme Conditions - Crack, Shock and Damage

Room: La Vista A/B (22nd Fl)

Session Chair: Mohamed Naji, Rutgers, The State University of New Jersey

1:20 PM

(GOMD-S1-121-2018) Structural change under deformation in aluminosilicate glasses (Invited)

H. Inoue*[1]

1. The University of Tokyo, Institute of Industrial Science, Japan

Crack resistance by chemical composition design is one of important developments for oxide glasses. High modulus, high hardness and high crack resistance have been achieved in the glass $40SiO_2$-$60Al_2O_3$ prepared by gas levitation furnace. However, the glass forming ability is low. Therefore, there is a great limitation for practical use. Also, the mechanism of resistance to that crack is not sufficiently understood. In this study, the structural models are prepared by using molecular dynamics technique and the atomic level structural change in deformation is investigated. The structural models of SiO_2, Na_2O-SiO_2 and Al_2O_3-SiO_2 glasses were made and their elastic moduli were evaluated. For the uniaxial deformation the structural models with free surface were prepared. The calculated Young's, Bulk and Shear moduli of the Al_2O_3-SiO_2 glass are were 98 GPa, 86 GPa and 38 GPa, respectively. These values were 70-86% of the experimental ones. Under uniaxial tension, in large deformation, voids are formed in SiO_2 and Na_2O-SiO_2 glasses. The voids are connected and grew into cracks. On the other hand, in the structural models of Al_2O_3-SiO_2 glass, there was no void and it did not break even at an elongation of 200%. During the uniaxial tension test, the coordination number of Si was almost unchanged at 4. On the other hand, the coordination number of Al decreased from five-fold to four-fold coordination.

1:50 PM

(GOMD-S1-122-2018) Impact-induced crack patterns in brittle materials: A peridynamics based investigation

J. Rivera[2]; J. Berjikian[2]; M. Bauchy[2]; N. Krishnan*[1]

1. Indian Institute of Technology, Civil Engineering, India
2. University of California, Los Angeles, Civil and Environmental Engineering, USA

Glasses are constantly exposed to impact loading during their service life. In many cases, these impacts lead to the formation of cracks and ultimately the failure of the material. Understanding the role of geometric and material properties on the formation of crack patterns is essential to design tailored glass compositions for impact-related applications. Here, using peridynamics, we simulate the effect of projectile impact on a brittle glass plate. To this extent, we use copper and glass bullets with velocities varying from 5 m/s to 100 m/s. First, we investigate the role of geometric properties, such as plate thickness and radius, on the crack patterns. Then, we investigate the effect of material properties, such as elastic modulus and fracture energy, by considering values over different orders of magnitude. Interestingly, we observe that the overall damage exhibits a power-law dependence with respect to the fracture energy of the material. The origin of this power-law is found to be linked to the velocity of radial cracks, which leads to a crack-branching behavior.

2:10 PM

(GOMD-S1-123-2018) Impact of pressure on the structure of glass (Invited)

P. S. Salmon*[1]; A. Zeidler[1]

1. University of Bath, Department of Physics, United Kingdom

High pressures have a significant impact on the structure-related properties of glass and are encountered in scenarios ranging from fracture mechanics, where stresses in the gigapascal regime are easily generated by sharp-contact loading, to the manufacture of permanently densified materials with tuned physical characteristics. Here, we show how the nature of the structural changes under load in oxide and chalcogenide glasses can be elucidated by combining neutron and x-ray diffraction results with molecular dynamics simulations. Example systems include the network-formers SiO_2, GeO_2, $GeSe_2$ and $GeSe_4$, and the modified silicates $MgSiO_3$ and $CaSiO_3$. In the case of oxide materials, the oxygen-packing fraction is an important indicator of when pressure-induced transformations to the network-forming motifs are likely to occur. Densification occurs in stages, where a plateaux of stability for a given type of network-forming motif is followed by a regime of change. The conversion of tetrahedral AO_4 to octahedral AO_6 motifs starts at an oxygen-packing fraction of 0.58, and fivefold coordinated AO_5 units act as important intermediaries during this transformation. It appears that the position of the first-sharp diffraction peak in measured diffraction patterns is sensitive to the oxygen-packing fraction, enabling it to be used as a marker for structural change.

2:40 PM

(GOMD-S1-124-2018) Network Dilation Anomaly in Ion-Exchanged Glasses Quenched under Pressure

M. Wang[1]; M. M. Smedskjaer[2]; J. C. Mauro[3]; G. Sant*[1]; M. Bauchy[1]

1. University of California, Los Angeles, USA
2. Aalborg University, Denmark
3. Pennsylvania State University, USA

Ion exchange is commonly used to strengthen oxide glasses. However, the resulting stuffed glasses usually do not reach the molar volume of as-melted glasses of similar composition—a phenomenon known as the network dilation anomaly. This behavior seriously limits the potential for the chemical strengthening of glasses and its origin remains one of the mysteries of glass science. Here, based on molecular dynamics simulations, we investigate the effect of pressure-quenching on the network dilation anomaly in a sodium silicate glass. We show that the application of pressure during quenching results in permanently densified glasses that exhibit varying network topology/rigidity. In turn, the topology of the atomic network is found to control the extent of ion exchange-induced dilation. In particular, we demonstrate that optimally constrained (isostatic) glasses do not show any network dilation anomaly. This is found to arise from the combined absence of floppy modes of deformation and internal eigenstress in isostatic atomic networks. This demonstrates that finely tuning the rigidity of glass networks can enhance the effect of ion-exchange and, thereby, could lead to the design of stronger glasses.

2:40 PM

(GOMD-S1-125-2018) Glass Striae and Laser Shock Damage

A. T. Mayville*[1]; A. Wereszczak[1]; M. K. Ferber[1]; S. Toller[2]

1. Oak Ridge National Lab, Materials Science and Technology Division, USA
2. LSP Technologies, USA

Laser shock testing can be an informative method to study damage evolution in glasses. Additionally, there is anecdotal evidence to suggest that striae in float glasses may serve as preferential locations for nucleation of shock-induced damage and crack-branching. The motivation of this study was to further examine that potential relationship. Laser shock was struck on relatively thick borosilicate glass tiles containing striae. There were some indications that the striae sometimes perturbed the shock-induced damage, but it was not consistently observed. This presentation describes the laser shock experiments, the striagrams of the pre- and post-tested shocked glass, and the postmortem analyses. Research sponsored by WFO sponsor U.S. Army TARDEC-RDECOM under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

Session 8: Glass Under Extreme Conditions - Shock and High Pressure

Room: La Vista A/B (22nd Fl)
Session Chair: Benoit Ruffle, Montpellier University

3:40 PM

(GOMD-S1-126-2018) Permanent deformation and damage of shock loaded silica glass: Experimentation and modeling (Invited)

C. Dereure[1]; R. Renou[2]; D. Loison[1]; E. Lescoute[2]; R. Hall[4]; F. Baber[4]; M. Nivard[1]; I. Guven[4]; J. Sangleboeuf[1]; L. Berthe[3]; L. Soulard[2]; J. Guin*[1]

1. CNRS @ Univ Rennes, Physics Institute Rennes, France
2. CEA DAM DIF, France
3. PIMM Arts et Métiers ParisTech, France
4. Virginia Commonwealth University, Mechanical and Nuclear Engineering, USA

Mechanical behavior of materials under extreme conditions of both pressure levels and loading rates (up to 10^9 s^{-1}) is of interest for practical applications in aeronautical or planetology fields. From a scientific view, it is exciting to challenge the limits of the possible especially when such experiment loading conditions, due to their time scale compatibility, offer a real opportunity for comparison with molecular dynamic simulation or peridynamic. For silica, shock waves may induce various type of modifications in the glass such as permanent deformation (phase change, densification) or damage. Instrumented laser driven shock loading tests were performed using high power intensity laser facilities to generate such loading conditions. Compared with other shock-generating methods as plaque impact, the benefit of laser impulses is that the shock pressure is only applied to the laser-impacted zone, which allows to reach high pressures without damaging the glass in a way that it is no more recoverable for post-mortem investigation such as Raman spectroscopy, micro Xray computed tomography. Experimental set up and results will be presented and discussed: in the light of MD simulations results made under similar conditions for the permanent deformation regime; in the light of peridynamic simulations to describe the intiation and propagation of the damage (2D and 3D) for the damage regime.

4:10 PM

(GOMD-S1-127-2018) Localized atomic segregation in the spalled area of a $Zr_{50}Cu_{40}Al_{10}$ BMG induced by laser-shock experiment

B. Jodar[1]; D. Loison[1]; Y. Yokoyama[3]; M. Nivard[1]; E. Lescoute[2]; L. Berthe[4]; J. Sangleboeuf*[1]

1. Institute of Physics Rennes, France
2. CEA/DAM/DIF, France
3. Institute for Material Research, Japan
4. PIMM, France

Laser-shock experiments were performed on a ternary Zr50Cu40Al_{10}Bulk Metallic Glass. Spalling process was studied through post-mortem analyses conducted on recovered sample and spall. Scanning Electron Microscopy magnification of fracture surfaces revealed the presence of a peculiar feature known as cup-cone. Cups are found on sample fracture surface while cones are observed on spall. Two distinct regions can be observed on cups and cones: a smooth viscous-like in the center and a flat one with large vein-pattern in periphery. Energie Dispersive Spectroscopy measurements conducted on these features emphasized atomic distribution discrepancies both on sample and spall. A mechanism is proposed for the initiation and the growth of these features but also a process for atomic segregation during spallation. Cup and cones would originate from cracks arising from shear bands formation (softened paths). These shear bands result from a quadrupolarshaped atomic disorder engendered around an initiation site by shockwave propagation. This disorder turns into shear band when tensile front reaches spallation plane. During the separation process, temperature gain induced by shockwave and shear bands generation decreases material viscosity leading to higher atomic mobility. As a result, a high rate of copper is found in sample cups and high zirconium concentration is found on spall cones.

4:30 PM

(GOMD-S1-128-2018) Silica glass under pressure: A view from first principles calculations (Invited)

S. Ispas*[1]; S. Sundararaman[2]; L. Huang[2]; W. Kob[1]

1. University of Montpellier, Lab. Charles Coulomb, France
2. Rensselaer Polytechnic Institute, USA

The vibrational properties of silica glass under pressure have been intensively studied experimentally during the last four decades, in particular using Raman spectroscopy. However there are few theoretical studies of the evolution of the vibrational properties under pressure. By using a combination of classical and first principles molecular simulations, we have generated a series of structural models for amorphous silica for pressures between 0 and 12 GPa. Further, their vibrational density of states and infrared spectra have been calculated within the density functional theory framework, known to reliably predict these properties, at least at zero pressure. In this talk, we will discuss the evolution of the vibrational features (band positions and peak intensities) of our models under pressure, focusing on their correlation to the structural changes as well as to the variation of their elastic moduli.

5:00 PM

(GOMD-S1-129-2018) Understanding Cracking Behavior of Glass from its Response to Compression

S. Jaccani*[1]; R. Sun[1]; L. Huang[1]

1. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA

Under Vickers indentation, glass deforms elastically and then plastically in forms of densification, shear flow and network structure changes, which interplay with each other and lead to stress/residual stress build-up and ultimate cracking. However, it is not easy to delineate the individual contribution of each deformation mode under indentation due to the experimental difficulties associated with the in-situ investigation at a local scale (tens of microns) under very high stresses. To this end, an optical microscopy technique was

developed to measure volume of glass under pressure in a diamond anvil cell (DAC) by using liquid argon as a pressure-transmitting medium. This provided the densification and recovery of glass under hydrostatic compression and decompression. In-situ Raman and Brillouin light scattering experiments were carried out at the same time to measure the structural and elastic response of glass to pressure. A few multicomponent glasses with vastly different indentation cracking behaviors were selected to study in this work. Our experiments reveal that glass networks with a high ability to undergo reversible structure changes in response to compression and decompression show a high cracking resistance.

S3: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 4: Glass-based Optical Device II

Room: La Vista C (22nd Fl)
Session Chairs: Hongtao Lin, Massachusetts Institute of Technology; Tingyi Gu, University of Delaware

1:20 PM

(GOMD-S3-033-2018) Novel methods of glass restructuring for fabrication of devices by laser irradiation (Invited)

H. Jain*[1]

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

Glass is a metastable material that can be stimulated to transform toward stable crystalline state continuously or discretely by providing sufficient external energy. Irradiating a glass with a laser of suitable energy can produce this transformation in a narrowly focused region through the change of electronic defects, coordination defects, atomic configurations and/or local chemical composition, while rest of the glass remains unaffected. Thus, through a controlled movement of laser, one can restructure the glass in a pre-determined region and fabricate 3D micro-architecture of remarkably different properties within uniform glass matrix. Depending on glass composition and laser characteristics (such as wavelength, intensity, exposure duration, total dose and polarization), one can modify various chemical (such as etching rate in a solvent), and physical (e.g. optical, electrical) properties. This strategy of glass restructuring in oxide and chalcogenide glasses is reviewed in this presentation, especially as it applies to the fabrication of micro-optic Fresnel elements, grayscale lithography, information storage, active single crystal waveguides, microfluidic devices, etc.

1:50 PM

(GOMD-S3-034-2018) Chalcogenide Glass Waveguide On-Chip Mid-Infrared Gas Sensor Integrated with PbTe Detector

P. Su*[1]; Z. Han[1]; D. Kita[1]; P. Becla[2]; H. Lin[1]; K. Richardson[3]; L. C. Kimerling[1]; J. Hu[1]; A. Agarwal[4]

1. Massachusetts Institute of Technology, Department of Materials Science and Engineering, USA
2. CapeSym, USA
3. University of Central Florida, CREOL, USA
4. Massachusetts Institute of Technology, Materials Research Laboratory, USA

Integrated photonic sensors that can operate in the mid-infrared chemical fingerprint region promise to be sensitive, specific, and cheap chemical sensors, deployable in large sensor networks. We present a first-ever demonstration of a mid-infrared chemical sensor that includes an integrated sensing element and detector, an important step towards realizing a fully integrated sensor on a chip. The sensor is a chalcogenide glass (GeSbS) spiral waveguide with a waveguide-integrated PbTe detector. A chalcogenide glass spiral waveguide was used for its broadband transparency in the mid-infrared coupled with the long interaction length a spiral provides for the evanescent wave to interact with the chemical. PbTe was used as a detector due to its strong absorption in the mid-infrared, photoconducting behavior, and ease of deposition and patterning. All three layers - the PbTe detector, the metal contacts, and the GeSbS waveguide - were fabricated using thermal evaporation and standard liftoff techniques. Methane gas was sensed at 3.31 micron, where it has a strong absorption peak. These results show that chalcogenide glass photonic circuits with integrated PbTe detectors are a promising way to achieve fully on-chip sensing in the mid-infrared.

2:10 PM

(GOMD-S3-035-2018) Broadband spectroscopic sensing using chip-scale integrated glass waveguide and supercontinuum source

Q. Du*[1]; H. Zhong[3]; Y. Zhang[1]; Y. Huang[2]; L. Zhang[4]; W. Zhang[5]; J. Hu[1]; Z. Luo[2]

1. Massachusetts Institute of Technology, Materials Science and Engineering, USA
2. Xiamen University, China
3. Zhejiang University, China
4. Tianjin University, China
5. Ningbo University, China

Photonic integrated chemical sensors have attracted increasing attentions in portable spectroscopy application. However, a major challenge is that certain wavelengths of interest to spectroscopy are often inaccessible for on-chip laser sources. In this work, we present the first supercontinuum (SC) integrated on-chip spectroscopic sensor. Submicron GeSbSe waveguides with high optical nonlinearity and a wide transparency window were dispersion-engineered for efficient SC generation. A home-built, 1.56 μm femtosecond laser source was used to excite the SC in the GeSbSe waveguide to achieve a flat SC spectrum over half-octave bandwidth. We validated the sensing capability through chloroform sensing experiments. Chloroform sensing at various concentration levels was performed using its absorption peak at around 1695 nm. This work provides a facile method to enable on-chip spectroscopic sensors to access different spectral ranges for sensing applications.

Session 5: Optical Ceramics and Glass-ceramics I

Room: La Vista C (22nd Fl)
Session Chair: Dingyuan Tang, Nanyang Technological University

3:40 PM

(GOMD-S3-036-2018) Glass ceramic optical fibers fabricated by melt-in-tube method and successive heat treatment (Invited)

J. Qiu*[1]

1. Zhejiang University, OPtical Science and Engineering, China

In this paper, we will introduce a method for fabrication of glass ceramic optical fibers with both various optical functions and low optical attenuation. Usually, serious crystallization will occur during fiber drawing process using traditional rod-in-tube method for various glass compositions. We propose a method called melt-in-tube method and successive heat treatment which allow us to prepare precursor glass fibers at first and then precisely control the nucleation and crystallization at low temperature. By using this method, we have fabricated glass ceramic fibers with various optical functions, e.g. glass ceramic fibers with upconversion luminescence, second harmonic generation, and large third order optical nonlinearity etc. This method is a versatile and universal process for preparation of glass ceramic optical fibers.

4:10 PM

(GOMD-S3-037-2018) Rare-earth doped sesquioxide transparent ceramics for laser applications (Invited)

J. Wang[1]; D. Yin[1]; P. Liu[2]; J. Ma[1]; Y. Wang[2]; D. Tang*[1]

1. Nanyang Technological University, School of EEE, Singapore
2. Jiangsu Normal University, School of Physics and Electronic Engineering, China

Sesquioxide ceramics, such as Y_2O_3, Lu_2O_3, and Sc_2O_3, have excellent thermal conductivity, thermal expansion coefficient, and relatively small phonon energy. They are desired host materials for high power solid state lasers. In this talk, we will present our works on the fabrication of various rare-earth doped sesquioxide laser ceramics, such as Yb^{3+}:Y_2O_3, Yb^{3+}:Lu_2O_3, Nd^{3+}:Y_2O_3, Ho^{3+}:Y_2O_3, and Er^{3+}:Y_2O_3. Well dispersed Y_2O_3 and Lu_2O_3 nano-powders with good dispersibility and narrow particle size distribution were synthesized by using the chemical co-precipitation method. High optical quality sesquioxide laser ceramics were produced by the vacuum sintering plus hot isostatic pressing. Optical quality, especially, the homogeneity of the fabricated laser ceramics were experimentally characterized. Influence of sintering aids on lasing property of the ceramics was investigated. High efficient laser operations at 1.0μm, 2.0μm, 3.0μm based on the fabricated laser ceramics were successfully demonstrated.

4:40 PM

(GOMD-S3-038-2018) Microstructure-composited materials: Is the Mr. Right of materials towards extreme-laser? (Invited)

L. Zhang*[1]; B. Jiang[1]; J. Fan[1]; X. Mao[1]

1. Shanghai Intitute of Optics and Fine Mechanics, CAS, China

Partially owing to the prospect providing almost limitless carbon-free energy, researchers around the world have made great and generally unrecognized progress toward achieving inertial confinement fusion (ICF) using strong laser during the past 30 years. The laser amplified materials used in currently running ICF facilities is still Nd-phosphate glass. However, the Nd-phosphate glass is not available to the next-generation ICF systems forward the inertial fusion energy, which requires the laser driver to have the enough high repetition rate (~10Hz) and efficiency. Facing the trend of the next-generation strong laser systems, laser crystals (like Ti:sapphire, Yb:YAG, Nd:CaF_2, ete.) towards the large-size fabrication have been absorbed considerable attentions. Recently, we proposed a new type laser material - crystalline/glass Microstructure-composited materials. Such materials were prepared by a ceramic-like procedure, based on the nanoparticle crystalline and glass powders with refraction index mostly identical to composited crystalline. In this talk, we will report our progress in developing such kind new laser materials, and compare with laser glass as well as laser crystal. We will also report our recent progress on some laser ceramics with composited microstructure, served as ICF applications to face the challenge against the ASE.

5:10 PM

(GOMD-S3-039-2018) Luminescence mechanisms and defect levels of undoped powder processed and single crystalline ZnS (Invited)

M. Saleh*[1]; E. Walter[2]; K. Lynn[3]; J. McCloy[4]

1. Washington State University, Materials Science and Engineering Program, USA
2. Pacific Northwest National Laboratory, USA
3. Washington State University, Center for Materials Research, USA
4. Washington State University, School of Mechanical and Materials Engineering, USA

The broader aim of this study is to gain insight into defects contributing to the luminescence behavior of ZnS, which would aid in optimizing the properties of ZnS based materials for radiation detection applications. The scintillation behavior for bulk ZnS has not been sufficiently studied for materials made by current industrial processes. Several pure commercial ZnS single crystals and powder processed materials are compared to identify the active defects for luminescence and decay and to gain insight into the effect of ZnS structure and processing method on its properties. Materials studied are commercial single crystals made by vapor phase transport and high pressure vertical Bridgman with different crystallographic orientations, and legacy and recent powder processed materials. This study couples optical, electrical, and magnetic resonance techniques such as UV-VIS transmission, temperature-dependent Photoluminescence (PL) and PL Excitation (PLE), Thermoluminescence (TL), Optical Deep Level Transient Spectroscopy (ODLTS), and Electron Paramagnetic Resonance (EPR). The investigated materials show complex and diverse luminescence behavior which is compared to the processing method, structure, and defects and reference the literature to identify some of those defects and their contribution to ZnS performance.

Session 6: Glasses and Glass-ceramics in Detector Applications

Room: El Mirador West (22nd Fl)

Session Chairs: Jacqueline Johnson, UTSI; Mario Affatigato, Coe College; S. Sundaram, Alfred University

3:40 PM

(GOMD-S3-073-2018) Luminescent Glasses and Glass Ceramics for Radiation Detection in Imaging Applications (Invited)

R. L. Leonard*[1]; C. W. Bond[1]; A. Evans[1]; J. E. King[1]; A. R. Lubinsky[2]; J. A. Johnson[1]

1. University of Tennessee Space Institute, Mechanical, Aerospace, and Biomedical Engineering, USA
2. Stony Brook University, Department of Radiology, USA

The versatility of luminescent glasses and glass ceramics enables their use as radiation detectors in many types of imaging applications, including medical imaging, contraband detection, and nondestructive evaluation. In particular, the ability to tailor the composition and shape of these materials allows for the optimization of their performance for different types of ionizing radiation. Typically, they are employed as scintillators in radiography applications, spontaneuously emitting visible light in the presence of ionizing radiation, which is processed by an array of sensors to create an image. However, certain glass ceramics may also function as storage phosphor materials that can be used in computed radiography applications. The authors present imaging results from their glasses and glass ceramics under exposure to low- and high-energy x-rays and cold neutrons. Future opportunities for these materials will also be discussed.

4:10 PM

(GOMD-S3-074-2018) In-Situ Characterization of Crystallite Growth in Glass-Ceramic Scintillators (Invited)

B. Beckert*[1]; S. Lombardo[1]; C. Struebing[1]; B. Wagner[1]; Z. Kang[1]; J. Nadler[1]

1. Georgia Institute of Technology, Georgia Tech Research Institute, USA

Composite scintillators are developed to advance the capabilities and reduce the cost of systems for medical imaging, homeland security, and non-destructive evaluation. Glass and glass-ceramic materials are particularly well-suited for this problem because their optical behavior can be controlled via composition modifications, and straightforward processing methods simplify the transition to commercial scale. However, their scintillation efficiency and timing have lagged behind single crystals, and limited widespread implementation. The present study sought to overcome these limitations by developing a more in depth understanding of the growth reaction in which scintillating crystallites precipitate from an oxide host glass

matrix. Multiple glass formulations were prepared and heat treated at a range of temperatures and dwell periods to identify the process parameters needed to achieve the desired crystallite size (<30nm) and composition. Crystal phase evolution was observed in-situ via hot stage X-ray diffraction experiments, and the resulting crystallites were imaged and further analyzed via transmission electron microscopy and energy dispersive X-ray spectroscopy. The temperature range for crystallite growth was narrower than anticipated, with most crystallites forming within a 150°C range. Size became self-limiting after dwelling for approximately 8 hours at the growth temperatures investigated.

4:40 PM

(GOMD-S3-075-2018) Thin Film Storage Phosphors for Computed Radiography Applications

C. W. Bond*[1]; R. L. Leonard[1]; Y. J. Shin[2]; A. R. Lubinsky[3]; A. K. Petford-Long[2]; J. A. Johnson[1]

1. University of Tennessee Space Institute, Department of Mechanical, Aerospace, and Biomedical Engineering, USA
2. Northwestern University, Materials Science and Engineering, USA
3. SUNY Stony Brook, Department of Radiology, USA

We have developed novel thin film storage phosphors for computed radiography applications. In applications of computed radiography using conventional granular storage phosphor materials to medical and dental imaging for example, the desire for high spatial resolution drives a need for thinner detector layers with high performance. These films consist of multiple layers of orthorhombic phase barium chloride nanocrystals doped with europium, separated by nanoscale layers of fluoride glass. The films are deposited on fused silica substrates via the pulsed laser deposition method using a multi-component target. This method allows for precision control of layer thickness and doping level for optimized performance. In addition, a higher concentration of luminescent centers can result as compared to glass ceramic imaging plates produced in bulk form. We report performance characteristics for the films including stimulation spectra, stimulated emission spectra, stimulation efficiency, and gain – the number of detected electrons per absorbed x-ray. Readout is accomplished using a custom, high-resolution telecentric scanner. Sample radiographs of line pair phantoms and test materials will be presented. This research was supported by the National Science foundation under grant # DMR 1600783.

5:00 PM

(GOMD-S3-076-2018) Scintillating Glasses for Digital Radiography Flat Panel Imagers

A. R. Lubinsky*[1]; A. Howansky[1]; R. L. Leonard[2]; S. Dow[1]; J. A. Johnson[2]; W. Zhao[1]

1. Stony Brook University, Radiology, USA
2. University of Tennessee Space Institute, USA

In recent years digital radiography (DR) has become a predominant technology for medical x-ray imaging. In a flat panel imager (FPI) for DR, an image captured by an x-ray scintillating or photoconducting layer is read out by a self-scanning array of pixels, each containing a photosensing or charge sensing element and a thin film transistor (TFT) switching element. The TFT readout array is constructed on a thin glass substrate. In an "indirect" FPI imager, the primary x-ray sensing layer comprises a scintillating phosphor such as Gd2O2S:Tb or CsI:Tl; in a "direct" imager the corresponding layer is typically amorphous selenium. The x-ray illumination is typically from the "front", i.e. passing first through the x-ray sensing layer. Alternative indirect imager configurations have recently been considered, for example where the imager contains two phosphor layers ("front" and "back" screens) sandwiched around a single TFT array. In the present work, an alternative system is proposed in which a layer of scintillating glass serves as the support for the TFT readout array and also plays the role of an active sensor layer (back screen). The image quality and x-ray dose improvements and tradeoffs expected in such a system are quantified in cascaded linear system model calculations. In addition, the scintillating glass specifications required to achieve a successful result are discussed.

5:20 PM

(GOMD-S3-077-2018) Molecular Dynamics Simulation of Composition-Structure-Property Correlation of Aluminoborosilicate Glasses

R. Dongol[1]; A. Tandia[2]; S. K. Sundaram*[1]

1. Alfred University, USA
2. Corning Incorporated, USA

We have studied the composition-structure-property correlation of aluminoborosilicate glasses using classical molecular dynamics. In our study, the glass compositions were statistically designed within the compositional space of the commercial photomultiplier (PMT) glasses for neutrino detection. Glass structures and Young's modulus were calculated for these glasses subjected to different temperature and pressure conditions. The densities calculated of the simulated glasses for all temperature and pressure conditions showed no statistical variations. Similarly, the Young's modulus calculated for the glasses also showed no statistical variations. In this work, various composition-structure and structure-property relationship were explored. Coordination number analysis of the simulated glasses showed that silicon was found almost entirely in 4-coordination, boron was observed in 3- and 4-cooridination and aluminum was mostly found between 4- and 5- coordination with a small amount of 6-coordination. The Young's modulus was calculated by using a linear regression of the stress-strain curve generated by uniaxial tensile simulation. Our results showed that the E dependent on the amount of bridging and non-bridging oxygen concentrations and sodium concentration.

5:40 PM

(GOMD-S3-078-2018) Time-Dependent Microstructural and Optical Evolutions of Ge-Sb-S Chalcogenide Glasses upon Gamma Irradiation for Mid-Infrared Photonics Applications

M. Kang*[1]; B. Sohn[2]; S. Novak[1]; D. Ma[3]; Q. Du[3]; R. Pujari[3]; C. Blanco[1]; L. Sisken[1]; A. Yadav[1]; C. Schwarz[4]; J. Hu[3]; D. T. Tan[2]; A. Agarwal[3]; K. Richardson[1]

1. University of Central Florida, CREOL, College of Optics & Photonics, 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. Ursinus College, Department of Physics and Astronomy, USA

Chalcogenide glasses (ChGs) have been studied extensively for mid-infrared photonics applications, benefiting from their broadband transmission and widely tunable optical properties. Our team has aimed to use Ge-Sb-S ChGs that can align with photonic links for chip-scale microphotonic chemical sensors or countering weapon of mass destruction applications. We seek to understand the effect of gamma irradiation on their properties that could impact device performance, as these devices could be deployed in high radiation environments. Since the sensing devices rely on low optical loss and shifts in the refractive index due to the presence of an analyte, an understanding of the gamma-induced effects on the optical properties is crucial. Our study has focused on bulk glass radiation where post-irradiation modifications of physical and optical properties have been examined. Specifically, we report the radiation-induced effects that have been studied through a variety of characterizations including XEDS, XRD, UV-Vis transmittance spectroscopy, and linear and nonlinear refractive index measurements at a range of exposure doses. We correlate their time-dependent response and proposed mechanisms to radiation-induced, metastable defect states which relax following short term (weeks) periods at room temperature.

S4: Glass Technology and Cross-Cutting Topics

Session 3: Challenges in Manufacturing II

Room: La Vista F (22nd Fl)
Session Chairs: Jennifer Mawdsley, Corning Incoporated; Irene Peterson, Corning Incorporated

1:20 PM

(GOMD-S4-055-2018) MAS-NMR Investigation of Structural Changes during Melting in a Multicomponent Sodium Aluminophosphosilicate Glass

J. Rygel*[1]; C. Hogue[1]

1. Corning Incorporated, USA

Magic Angle Spinning Nuclear Magnetic Resonance (MAS-NMR) is an established technique that has been used extensively to study the structural changes that occur in glass as a function of composition, pressure, and glass transition temperature. This technique can also be used to understand the structural changes that occur in glass during the melting process. Samples of glass were extracted from below the surface scum layer in a continuous melter at several locations, from the back to the front of the tank. ^{31}P, ^{29}Si, ^{27}Al, and ^{23}Na MAS-NMR as well as ^{29}Si Static NMR spectra were gathered from each of the samples. As glass progressed through the tank, phosphorus polymerization was found to increase as well as concomitant chemical shifts in the other cations which indicate increasing phosphorus incorporation into the glass network, i.e. structural homogenization.

1:40 PM

(GOMD-S4-056-2018) Change of Viscosity of the Liquid Phase during Batch Melting

A. Priven*[1]; I. Peterson[2]

1. Corning Korea, Republic of Korea
2. Corning Incorporated, USA

One of the most important factors affecting kinetics of the batch melting process is the viscosity of the liquid phase. However, this quantity is hard to determine. In this presentation, we suggest an approach to resolving this problem by using in-situ measurements of the phase composition at high temperatures by using the method of neutron diffraction. The method allows the use of industrial (coarse) batch materials and determines the amounts of all crystalline phases and the amorphous (liquid) phase. We studied the dynamics of batch melting for an earlier published Na_2O-MgO-Al_2O_3-SiO_2 glass composition and determined the compositions of the liquid phase as a function of time. The tests were performed for several batches with different particle sizes of materials at two different time-temperature regimes. Then we selected the best of the known models to predict the viscosity; for that, we compared the predictions of different known models with the available data about similar compositions taken from the worldwide literature. Applying the selected models, we calculated the viscosity values corresponding to different temperatures. To validate the predictions, several compositions were melted and characterized. The results of study give the information about the effects of mentioned factors on the viscosity of the liquid phase during melting.

2:00 PM

(GOMD-S4-057-2018) Near Isostatic Sintering of Infrared Glass in a Carbon-Free Environment

D. J. McGill*[1]; J. Benghozi-Bouvrande[2]; L. Roumiguier[2]; C. Blanco[1]; M. Dolhen[2]; G. Delazir[2]; S. Chenu[2]; J. Duclere[2]; K. Richardson[1]; R. Gaume[1]

1. University of Central Florida, School of Optics/CREOL, USA
2. Universite de Limoges, Science of Ceramic Processes and Surface Treatments Laboratory, France

A new method to sinter glass powders under near isostatic conditions in a carbon-free environment was developed. A highly plastic pressure-transmitting medium was used to surround the 70TeO2-20WO3-10La2O3 (TWL) glass green body and create near isostatic pressure within a uniaxial press. The sintering vessel used can be prepared within a controlled atmosphere for use with air sensitive samples. Fully densified TWL samples have now been created in this carbon-free environment using this new method.

2:20 PM

(GOMD-S4-058-2018) Application of Micro-Computed Tomography for Quantification of Glass Seeds

K. Goetschius*[1]; A. Mohammadkhah[1]; C. Bischoff[1]; A. Gudde[2]; B. Pouran[2]; K. Fulton[1]

1. Guardian Glass, USA
2. UMC Utrecht, Netherlands

Glass quality, including optical homogeneity, defect count and defect size, is essential to the manufacture of industrial glasses and is usually tailored to customer requirements for the application. Float manufacturing typically uses laser and vison systems for accurate online measurements which are enabled due to the flat nature of the glass but the effectiveness of these techniques does not translate to different shapes or instances of overlapping defects. These restrictions are difficult to deal with in R&D. Micro-computed tomography, μ-CT, is a non-destructive method of scanning that generates a 3D image of seeds for the entire sample by exploiting differences in x-ray attenuation between the glass and the gas. This enables measurements of irregularly shaped samples with variable resolutions (from microns to nanometers in range) and at higher defect densities for samples produced for research and development. This work focuses primarily on the application of μ-CT to characterize seeds in SLS glass samples produced in the lab. The ability of μ-CT, along with image analysis, was evaluated as a tool to quantify the number and size distribution of seeds for non-flat samples for different levels of seeds at 40 μm resolution. It was established that μ-CT could be a useful tool to evaluate seed distribution in SLS glass samples quantitatively and accurately.

2:40 PM

(GOMD-S4-059-2018) Study of the chemical strengthening of glazes suitable for ceramic tiles by using the Mixture Design approach

M. Montorsi*[1]; S. Barbi[1]; C. Mugoni[2]; C. Siligardi[2]

1. University of Modena and Reggio Emilia, Department of Science and Methods for Engineering, Italy
2. University of Modena and Reggio Emilia, Department of Engineering Enzo Ferrari, Italy

Ion exchange have been employed in industry since many years to improve the mechanical resistance of fragile inorganic materials as soda-lime glass. The purpose of this study was to verify the applicability of this process to glazed ceramic tiles, where a significative higher number of oxide are employed with respect to a soda-lime glass. Due to its quite complex chemical formulation a rational approach have been employed to investigate the effect of different combination of oxide on the mechanical properties of glazed ceramic tile after the chemical strengthening process. Also a comparison was made with glazes already available on the market. Microstructural and mechanical properties of the glazes were determined before and

after different ion exchange processes. Only one of the commercial glazes resulted suitable to ion exchange process, thanks to its high Na_2O content, with the respect of the majority of the glazes nowadays on the market of ceramic tile production. Subsequently the mixture design approach suggests that tailored chemical formulation, were B_2O_3, Na_2O Li_2O and P_2O_5 content have been modified, are able to improve the surface hardness of +25%. The results suggest that ion-exchange process is positively affected by an appropriate combination of ions in the glaze formulation and a low amount of commercial ceramic glazes are nowadays suitable.

Session 3: Challenges in Manufacturing III

Room: La Vista F (22nd Fl)

Session Chairs: Hong Li, Nippon Electric Glass; Laura Adkins, Corning Incorporated

3:40 PM

(GOMD-S4-060-2018) Theoretical background of modeling of continuous fiber drawing (Invited)

O. Prokhorenko*[1]

1. L.G.P. International, USA

Continuous fiber drawing is one of the major processes of the modern glass industry. In order to minimize simplifications we begin the modeling with a forming section of forehearth, and end it at a winder. The present paper describes theoretical bacground of continuous fiber drawing including all physical processes while molten glass flows inside the forehearth, fills the bushing block, distributes above a bushing plate, flows through numerous tips to form menuscus, and cooled down to form a fan of fibers under the action of essential forces. At the first stage we solve a stationary-state task of drawing the fibers under a sum of forces of gravity, stretdhing force, viscous resistance, and surface tension. By taking into account heat transfer, flow, and deformation we were able to develop analytical solution of stationary-state task, which allowed to simulate drawing of, virtually, unlimited number of single filaments. At the second stage we have introduced mechanical, chemical, and thermal perturbations (having both continuous, and spontaneous character) bringing the system non-stationary behavior. As a result the system responds to perturabations by linear, resonance, or non-linear growth of the stretching force. By comparing values of momentum force with the limit of fracture of selected fibers the model can determine probability of fiber breackage alone with other important characteristics of the whole process.

4:10 PM

(GOMD-S4-061-2018) Glass-to-metal contact in glass-forming: Some new insights into sticking, friction and lubrication (Invited)

C. Roos*[1]

1. RWTH Aachen University, Glass, Germany

Visco-elastic behavior of glass and the existence of a glass-transition is essential for glass forming. The glass experiences quite a significant change of viscosity over the complete forming process from about 10^3 dPas (which reflects the viscosity at gob-cutting) to more than $10^{7,6}$ dPas. In forming, the rheological - and hence structurally and chemically dependent - properties of the glass inevitably need to be considered in combination of the tribological situation of the whole forming (e.g. the contact with the forming material). Theories propose a so-called "sticking" of the glass to the forming material at certain viscosity. And the sticking or non-sticking seems to be independent of the type of contact material and seems to be depending only on a certain viscosity value (and hence for different glass-types on different temperatures). However, the presentation will give insight into investigations of mechanisms of glass-material interactions and into an alternative theory, which shows that there indeed is a dependence between type of contact material and glass sticking.

4:40 PM

(GOMD-S4-062-2018) Development of a low friction coating for the container glass forming process

D. K. Orzol*[1]; L. Wondraczek[2]; C. Roos[3]

1. IPGR - International Partners in Glass Research e.V., Germany
2. Friedrich-Schiller-University Jena, Germany
3. RWTH Aachen University, Germany

Glass-material contacts occur at several steps during glass container forming process, for example between the gob and the shears, the delivery equipment and during forming of the container. Different solid and liquid lubricants are used in the industry for optimizing the glass-metal contact, but all of them introduce additional problems to the container glass forming process. The loading of the gob into the blank mold is a crucial step, which can be facilitated by swabbing. During the swabbing an oil and graphite based lubricant is applied in short intervals manually on the blank molds. This leads to several downsides regarding the process stability and operator safety. In this project, fundamental research is done by the installation of a special measurement device to investigate the dynamic glass-material contact. The coefficient of friction is calculated by an analytical mathematical model. Low friction materials were investigated and analyzed. Results are summarized from different theoretical aspects, for example the shear strength of the contact material. With these results, a coating system for existing forming tools is developed. A verification of the coating performance regarding container glass forming without lubrication was initiated, that also proves the transition from fundamental research to an industrial application.

Session 4: Waste Immobilization - Corrosion IV

Room: La Vista D/E (22nd Fl)

Session Chair: David McKeown, Catholic University

1:20 PM

(GOMD-S4-063-2018) Does Alpha Radioactivity Impact Glass Durability? (Invited)

M. Tribet*[1]; S. Mougnaud[1]; S. Rolland[1]; S. Peuget[1]; C. Marques[1]; V. Broudic[1]; C. Jegou[1]

1. CEA, DE2D, France

The resulting wastes from spent fuel reprocessing are immobilized into a borosilicate glass. Its long-term behavior has been investigated with a view to geological disposal, and the kinetics and mechanisms of glass alteration have been studied in aqueous media. Most of the current knowledge of the long term behavior is based on studies of non-radioactive material. To go further, the present work focuses on the effects of alpha irradiation on the long term alteration rate by studying both doped glasses and glasses submitted to external irradiation. ^{239}Pu and ^{244}Cm doped glasses are leached under static conditions (90°C, Ar atmosphere, SA/V = 30 cm^{-1}), in order to reach quickly the long term alteration rate. In addition, leachings of pre-damaged non-radioactive glasses are carried out in order to focus on the impact of alpha decay and to compare with results from doped glasses. The alteration rate of doped glasses is monitored by the releases tracer elements. Pre-damaged glass alteration is monitored on monoliths by ToF-SIMS elemental depth profiles. The alteration layer morphology is characterized by SEM and TEM. Results underline an impact of the alpha decay on the glass alteration rate (up to a factor of 4), on both doped material and pre-damaged non-radioactive glasses. These observations, consistent with SEM and TEM characterizations, highlight the importance of the initial structure of a glass on its chemical durability.

1:50 PM

(GOMD-S4-064-2018) Behavior of low-activity waste glasses at the Hanford Integrated Disposal Facility: Linking laboratory testing to performance assessment modeling

J. Neeway*[1]; D. Bacon[1]; N. Qafoku[1]; G. Tartakovsky[1]

1. Pacific Northwest National Lab, USA

Vitrification of the wide range of chemical and physical properties of the tank waste at the United States Hanford site will require a wide range of borosilicate glass compositions. The resulting immobilized low-activity waste (ILAW) glass will be disposed at the on-site, near-surface Integrated Disposal Facility (IDF). Before the ILAW can be disposed of at the IDF, a performance assessment (PA) that estimates the facility's impacts on the long-term protection of the public and the environment, must be conducted. The PA will calculate the release of the radionuclides into the environment, which is dependent on the dissolution rate of the glass. To inform PA calculations, it is necessary to understand the corrosion behavior of a wide range of glass compositions that will be disposed at IDF. To this end, we will present dissolution data on a wide range of ILAW glass compositions and we will explain how these data are implemented into IDF reactive transport models. Specifically, we will present the results of radionuclide release into backfill materials from three model ILAW glass compositions under accelerated recharge in proposed field lysimeter experiments. The discussion will also include areas of uncertainty in the modeling.

2:10 PM

(GOMD-S4-065-2018) Effects of Microstructure on the Corrosion Behavior of Borosilicate Glass-Ceramics for Waste Vitrification

N. Roberts*[1]; P. Porter[1]; R. Brow[1]

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

Spent nuclear fuel will be reprocessed into several secondary waste products, as described by the Advanced Fuel Cycle Initiative (AFCI). The secondary waste products are intended to be vitrified into environmentally acceptable waste forms. One form developed by Pacific Northwest National Laboratories (PNNL) is a borosilicate glass-ceramic; viz., J. Crum, et al., J. Nucl. Mater. 482 1–11 (2016). Borosilicate glasses provided by PNNL were re-melted and quenched with different thermal histories to produce samples with a range of microstructures, described by analytical electron microscopy and x-ray diffraction. In particular, slower quench rates and longer isothermal treatment times produced samples with greater fractions of powellite and oxyapatite crystals. Product consistency tests (PCT) were performed to characterize the effects of microstructural development, including the fraction and composition of the residual glass, on elemental release rates. Atomic force microscopy (AFM) and profilometry studies of polished, monolithic samples provide information about the relative recession rates of the residual glass and major phases, and reveal faster corrosion of the residual glass from samples with greater fractions of crystallized species. This work was supported by the US Department of Energy (NEUP 15-8112). The authors thank Jarrod Crum (PNNL) for providing the glasses.

2:30 PM

(GOMD-S4-066-2018) Role of minor element doping on the structure and dissolution of simplified glasses for nuclear waste

H. Smith[1]; A. J. Fisher[1]; R. J. Hand[1]; N. C. Hyatt[1]; C. L. Corkhill*[1]

1. University of Sheffield, Materials Science and Engineering, United Kingdom

Nuclear waste glasses have been designed to immobilise a wide range of short- and long-lived radionuclides comprising fission products, transuranics and activation products arising from reprocessing of spent nuclear fuel. Understanding the durability of these glasses is essential to support development of underground disposal options, necessitated by the presence radionuclides with long half-lives. We here present results of from an investigation of series of simplified sodium aluminoborosilicate glasses, where small additions or replacements (<5 mol%) of dopant elements have been made. Using MAS-NMR we determine the effect of these additions on the structure of the glass, and relate this to results from a durability assessment using single-pass flow-through (SPFT), product consistency test (PCT) and monolith (MCC-1) standards. Results are discussed with respect to structure-property relationships in the forward rate, and with respect to a thermodynamic assessment of glass leaching, through geochemical modelling of surface precipitates and in free energy of hydration analysis.

Session 4: Waste Immobilization - Processing I

Room: La Vista D/E (22nd Fl)

Session Chair: Claire Corkhill, University of Sheffield

3:40 PM

(GOMD-S4-068-2018) Using Glass Polymerization and Structure Combined with Quasicrystalline Theory to Produce High Level Radioactive Borosilicate Glass Remotely: A Successful and Easily Modified Statistical Process Control (SPC) System

C. M. Jantzen*[1]; T. B. Edwards[1]; C. L. Trivelpiece[1]

1. Savannah River National Laboratory, USA

The Defense Waste Processing Facility (DWPF) at the Savannah River Site has been processing High Level Waste (HLW) since 1996. The waste glass mixtures have been successfully controlled by a unique "feed forward" statistical process control (SPC) system for the last 21 years. Three individual composition-property models define the glass forming region for each batch of HLW and glass additive mixture. The composition-property models were developed based on concepts of the molecular structure of glass, polymerization theory of glass, and quasicrystalline theory of glass crystallization. These models define a glass forming region which is durable, pourable, and processable with 95% accuracy. The DWPF will soon be receiving increased concentrations of cesium and titania enriched wastes from the use of solvent extraction for cesium removal and ion exchange/sorption of ^{90}Sr and alpha-emitting radionuclides with monosodium titanate. Therefore, modifications to the DWPF SPC were necessary. The methodology for the modifications, which included the calculation of the impacts of TiO_2 on the various glass properties based on the known role of titania in glasses and fitting to the experimental data matrix developed, will be discussed.

4:00 PM

(GOMD-S4-069-2018) ORP-PNNL Research Activities to Improve Tc-99 Management during Waste Vitrification: Potential Implementation Scenarios

D. Kim*[1]; A. A. Kruger[2]

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

High volatility of Tc-99 and thus low retention in glass is one of the major technical challenges during vitrification of Hanford low-activity waste (LAW) for the U.S. DOE's Office of River Protection (ORP). The baseline plan is to recycle the off-gas stream that contains volatilized Tc back to the melter to maximize the final Tc retention in glass product. A negative impact of this recycling is that the off-gas stream also sends other volatile components such as S and Cl back to the melter. These components are known to limit the loading of waste in the glass and increase the glass volume. Therefore, it is important to develop technologies that can be used to manage Tc immobilization without recycling the off-gas. Two main research areas are being pursued at Pacific Northwest National Laboratory (PNNL) for ORP: 1) Tc separations research explores various materials that can selectively remove Tc from LAW or the off-gas scrub solution and 2) Tc retention research includes a series

of studies to understand the mechanism of Tc volatilization from, or incorporation into, glass melt during vitrification. Potential scenarios on how to implement these technologies, once successfully developed, for the Hanford Waste Treatment and Immobilization Plant (WTP) that currently is under construction will be discussed.

4:20 PM

(GOMD-S4-070-2018) Effect of Chlorine and Chromium on Sulfur Solubility in Low-Activity Waste Glass

T. Jin*[1]; D. Kim[1]; D. Mar[1]; B. L. Weese[1]; M. J. Schweiger[1]; A. A. Kruger[2]

1. Pacific Northwest National Laboratory, USA
2. U.S. Department of Energy Office of River Protection, USA

According to an empirical sulfur solubility model based on over two hundred simulated Hanford low-activity waste (LAW) glass compositions, chlorine and chromium have shown strong effects on lowering sulfur solubility. In this work, a simplified LAW glass was prepared and saturated by sodium sulfate, sodium chloride, and sodium chromate salts as single components and as mixtures with varying ratios (25 mol%, 50 mol%, and 75 mol% sulfate mixed with chloride or chromate). Nine glass samples were prepared by a crucible-scale salt-saturation method. Various salts were integrated into crushed glass powder, melted at 1150°C for one hour, and quenched. The quenched glass with a separated salt layer was crush to fine powder to repeat the mix-melt-quench cycle. A total of three cycles were used to achieve the solubility limit of sulfur in the simplified LAW glass. The compositions of the glasses saturated by sulfate/chloride and sulfate/chromate mixed salts were analyzed by inductively coupled plasma – atomic emission spectroscopy and ion chromatography. The correlation between sulfur solubility and chlorine/chromium concentrations was investigated in an effort to improve the LAW glass composition - sulfur solubility model.

4:40 PM

(GOMD-S4-071-2018) Molybdenum solubility in alkali-aluminophosposilicate glasses

H. Kamat*[1]; N. Stone-Weiss[1]; M. Naji[1]; H. Eckert[2]; J. McCloy[3]; A. Goel[1]

1. Rutgers -The State University of New Jersey, Materials Science, USA
2. University of São Paulo, Sao Carlos Institute of Physics, Brazil
3. Washington State University, School of Mechanical & Materials Engineering and Materials Science & Engineering Program, USA

An innovative glass-ceramic waste form is being developed to immobilize non-fissionable waste streams of alkali/alkaline-earths, lanthanides, and transition metals generated by the projected TRUEX plus process. The major hurdle in the development of this glass-ceramic is the high MoO_3 (~14 mass%) and alkali (Rb_2O, Cs_2O ~12 mass%) content of the waste stream. The presence of these species can lead to liquid-liquid phase separation and the uncontrolled crystallization of alkali/alkaline-earth molybdates. Literature reveals the existence of MoO_3 – P_2O_5 based glasses where the MoO_3 content can be as high as 80 mol.%. However, these glasses suffer from poor chemical durability which can be improved by the addition of aluminum oxide. Based on this analogy, we hypothesized that incorporation of P_2O_5 in an aluminosilicate glass matrix may result in higher molybdenum solubility. In order verify this hypothesis, we have synthesized a series of glasses/glass-ceramics in the system (100-x)(Na_2O-Al_2O_3-P_2O_5-SiO_2)–xMoO_3. The crystallization behavior of these glasses has been studied using X-ray diffraction, Raman/NMR spectroscopy, SEM-EDS, and EPMA, followed by liquidus temperature measurements and rotation viscometry. Based on the above results a mechanism for the effect of phosphorus addition on molybdenum solubility in alkali-aluminophosphosilicate glasses will be discussed in this presentation.

5:00 PM

(GOMD-S4-072-2018) Uranium solubility in a molten reduced glass

P. Chevreux[1]; L. Tissandier[2]; A. F. Laplace*[1]; S. Bahl[3]; E. Deloule[2]

1. CEA Marcoule, France
2. CRPG, CNRS, France
3. KIT, Germany

A new conditioning matrix is currently being developed to immobilize intermediate level nuclear waste by a vitrification process. High actinides concentrations (uranium and plutonium) are expected and the final waste package contains both a vitreous phase and a metallic phase coming from the waste. During the high temperature elaboration process, glass and metal phases are melted together which imposes a strongly reducing environment to the glass melt. This might modify actinides' oxidation state and thus affect their solubility in the glass as for uranium which solubility in silicate melts is known to be lower in reducing conditions compared to oxidizing ones. This paper presents the uranium solubility study in an aluminosilicate glass melt as a function of oxygen fugacity. Uranium oxidation state is first determined in glass samples melted under different redox conditions, using XANES measurements. In order to determine its solubility, a concentrated uranium doped glass under its uranyl U(VI) soluble form is prepared. The glass melt is then equilibrated under different redox potentials in a thermochemical reactor and uranium solubility is determined using MEB-EDS and microprobe analysis. The presented solubility data will be discussed on a thermodynamic point of view and also in the frame of the currently developed process.

Award Lectures

Norbert J. Kreidl Award for Young Scholars

Room: El Mirador East (22nd Fl)

6:10 PM

(GOMD-AW-004-2018) Fabrication of Intrinsically Low Nonlinearity Glass Optical Fibers

M. Cavillon*[1]; J. Ballato[1]; P. Dragic[2]

1. Clemson University, Materials Science and Engineering, USA
2. University of Illinois at Urbana-Champaign, Electrical and Computer Engineering, USA

Optical nonlinearities plague scaling to higher output powers in modern high energy laser (HEL) systems. Amongst the most detrimental nonlinearities are stimulated Brillouin and Raman scattering (SBS, SRS), nonlinear refractive index n_2-related wave mixing phenomena, and transverse mode instability (TMI). As opposed to the complex micro-structured large mode area (LMA) fibers typically developed to mitigate these parasitic effects, this present work advocates another approach instead; namely attacking the nonlinearities through the enabling materials from which they originate. Conventional circular core-clad fibers comprising an oxyfluoride core in the alkaline earth fluoride (AEF_2) – alumina (Al_2O_3) – silica (SiO_2) glass family with a pure silica cladding are fabricated using the molten core method and their properties discussed. AE- and Al_2O_3-doped silica glasses participate in the formation of intrinsically low Brillouin and Raman scattering materials, while fluorine lessens the linear and nonlinear refractive indices, as well as the thermo-optic coefficient. Fibers exhibiting reductions of 6-8 dB in the Brillouin gain coefficient, 1-2 dB in the Raman gain coefficient, and 2-3 dB in the thermo-optic coefficient relative to conventional silica fibers will be presented.

6:30 PM

(GOMD-AW-005-2018) Temperature-Modulated Differential Scanning Calorimetry Analysis of High-Temperature Silicate Glasses

T. K. Bechgaard*[1]; O. Gulbiten[2]; J. C. Mauro[3]; M. M. Smedskjaer[1]

1. Aalborg University, Denmark
2. Corning Incorporated, USA
3. Pennsylvania State University, Department of Materials Science and Engineering, USA

Temperature modulated differential scanning calorimetry (TM-DSC) has not been widely applied in the silicate glass community, since commercial instruments have typically been restricted to ~700°C. In this talk, we discuss how to obtain high quality data on silicate samples with high glass transition temperatures (T_g) by adjusting the experimental parameters considering T_g and liquid fragility (m) of the probed glass. Furthermore, we show how to determine m in tectosilicate CaO-Al_2O_3-SiO_2 glasses using the thermal relaxation caused by the temperature modulation to estimate the structural relaxation time. Fragility decreases with increasing silica content, consistent with trends observed from direct viscosity measurements and standard DSC using the activation energy for structural relaxation. TM-DSC thus succeeds in reproducing the trend in m, whereas the absolute values of m are systematically lower for high-m compositions and vice versa for low-m compositions. Finally, we discuss the use of TM-DSC to probe the so-called intermediate phase in silicate glasses, featuring isostatic topology with minimal structural relaxation upon heating. Our data suggests that within the tectosilicate system, the relaxation behavior can be tuned by changing the network topology. We thus infer that TM-DSC could be used to search for silicate glasses with minimal volume relaxation during heating.

Thursday, May 24, 2018

Award Lectures

Varshneya Frontiers of Glass Technology Lecture

Room: El Mirador East (22nd Fl)

8:00 AM

(GOMD-AW-006-2018) Recent research trends of chalcogenide glasses and ceramics for infrared photonics and energy applications (Invited)

X. Zhang*[1]

1. CNRS - Université Rennes 1, France

Chalcogenide glasses have been studied since several decades for infrared transmission and the most important commercial application is infrared optics for thermal imaging. Compared to the most used germanium optics, chalcogenide glass optics have two important features, which are the lower cost, especially for high volume applications, and the lower sensibility to temperature variation. Molded chalcogenide optic is one of the key elements, which are boosting the massive application of thermal imaging. These current and future applications necessitate cost reduction and materials with higher performance. Recent innovation in glass fabrication process and in the development of highly efficient optics, for example, with gradient refractive index will be presented. Chalcogenide glasses have relatively narrow and adjustable bandgap width. Through controlled crystallization, it is possible to obtain composite semiconducting materials with intern and self-organized p-n junctions, resulting in exceptional photoelectric properties. Their potential applications for energy conversion via photocatalytic or photovoltaic effect will be summarized.

S1: Fundamentals of the Glassy State

Session 4: Topology and Rigidity I

Room: El Mirador West (22nd Fl)
Session Chairs: Mathieu Bauchy, University of California, Los Angeles; Morten Smedskjaer, Aalborg University

9:20 AM

(GOMD-S1-130-2018) Topological Model for Glass Relaxation (Invited)

J. C. Mauro*[1]

1. Pennsylvania State University, Materials Science & Engineering, USA

The prediction of glass relaxation is traditionally known as one of the most challenging problems in condensed matter physics, with important implications for several high-tech applications of glass. In this study, I present a predictive model for the temperature, thermal history, and composition dependence of glassy relaxation dynamics based on topological constraint theory. The model enables, for the first time, the quantitative prediction of relaxation behavior in the design of new glass compositions.

9:50 AM

(GOMD-S1-131-2018) Low-frequency vibrational modes and Boson peak during nanoindentation: The role of structural heterogeneity in glass deformation (Invited)

L. Wondraczek*[1]

1. University of Jena, Germany

Starting from the non-Debye normalization of low-frequency vibrational modes in vitreous silica and in the binaries of SiO_2-Al_2O_3, SiO_2-P_2O_5 and SiO_2-B_2O_3, the effect of local stress such as induced during instrumented indentation on the vibrational density of states in the Boson region will be dicussed. In line with recent computational findings, our experimental observations suggest that the degree and nature of structural heterogeneity play a major part in the local damage infliction at glass surfaces, as opposed by short-range structural parameters.

10:20 AM

(GOMD-S1-132-2018) Relaxation and rigidity: Lessons from simple models (Invited)

G. Naumis*[1]

1. Instituto de Física, Mexico

One of the main questions in glass relaxations is why short-time properties can determine long time relaxation. Here we discuss the topology of the energy landscape metabasins and it relationship with glass relaxation. Then we discuss how two-level models are modified by floppy-modes and its relationship with the Kramers formula for relaxation. Some of these ideas are tested for a simple rigidity model of beta relaxation which includes non-linear interactions. The results indicate an exponential relaxation which depends upon the low-frequency modes, although the results are far from trivial since sticky states appear, in which relaxation follows a power law.

10:50 AM

(GOMD-S1-133-2018) Topological Constraint Theory as a Predictor of Hardness in Glass (Invited)

S. P. Baker*[1]

1. Cornell University, Materials Science and Engineering, USA

The "topological constraint theory" was an application of mechanical network principles to describe glass forming ability and elastic behavior of random networks. This general concept was adapted to relate the hardness of chalcogenide glasses to average coordination number, and further to correlate hardness with the average number of constraints per atom on bending and stretching motion.

This approach has been used to find good correlations between hardness and the average number of constraints per atom with composition in several different silicate glasses. However, in studies of tectosilicate calcium-aluminosilicate, magnesium-aluminoslicate and calcium-galliosilicate, glasses, it was not possible to make this correlation—even the sign was wrong! A modified calculation based on the average number of constraints per unit volume provides a correlation with the correct sign, but does not capture details of trends with composition. In this talk, we consider the physical origins of hardness and limitations of topological constraint theory as a predictor of this quantity.

11:20 AM

(GOMD-S1-134-2018) Search for a Structural or Dynamical Signature of the Intermediate Phase in the Ge-Se System

A. Zeidler[1]; P. S. Salmon*[1]

1. University of Bath, Department of Physics, United Kingdom

The topological ordering of the network structure in vitreous Ge_xSe_{1-x} was investigated across most of the glass-forming region ($0 \leq x \leq 0.4$) by using high-resolution neutron diffraction to measure the composition dependence of the mean coordination number and correlation lengths. The thermal properties of the samples were also measured by using temperature-modulated differential scanning calorimetry. The results do not point to a structural origin of the so-called intermediate phase, which in our work is indicated for the composition range $0.175(8) \leq x \leq 0.235(8)$ by a vanishingly small non-reversing enthalpy near the glass transition. The midpoint of this range coincides with the mean-field expectation of a floppy-to-rigid transition at $x = 0.20$. The composition dependence of the liquid viscosity, as taken from the literature, was also investigated to look for a dynamical origin of the intermediate phase, using the Mauro-Yue- Ellison-Gupta-Allan (MYEGA) model to estimate the viscosity at the liquidus temperature. The evidence points to a maximum in the viscosity at the liquidus temperature, and a minimum in the fragility index, for the range $0.20 \leq x \leq 0.22$. The utility of the intermediate phase as a predictor of the material properties in network glass-forming systems is discussed.

11:40 AM

(GOMD-S1-135-2018) Glass Relaxation is Controlled by the Topology of the Atomic Network

Y. Hu[1]; X. Li[1]; W. Song[1]; Z. Liu[1]; T. K. Bechgaard[2]; M. M. Smedskjaer[2]; M. Bauchy*[1]

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

Understanding, predicting, and controlling glass relaxation is of primary importance for the manufacturing of display glasses, as any small variation in volume can result in undesirable pixel misalignments. However, no clear atomistic mechanism of structural and stress relaxation is available to date, which limits our ability to identify optimal glass compositions featuring low relaxation. Here, based on molecular dynamics simulations, we study the relaxation of a series of alkali-free calcium aluminosilicate (CAS) and sodium silicate (NS) glasses with varying compositions. We observe that selected glass compositions exhibit minimal relaxation. We investigate the structural origin of this behavior by means of topological constraint theory. Based on this analysis, we demonstrate that minimal relaxation is achieved for isostatic glasses, which are both free of eigenstress and floppy modes. This highlights the crucial role of the atomic topology in controlling the propensity for relaxation.

S3: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 2: Charge and Energy Transport in Disordered Materials I

Room: El Mirador East (22nd Fl)

Session Chairs: B. Potter, University of Arizona; Krishna Muralidharan, University of Arizona; Xianghua Zhang, CNRS - Université Rennes 1

9:20 AM

(GOMD-S3-079-2018) New Solid State Li^+ and Na^+ Ion Conducting Glassy Solid Electrolytes and Their Use in All Solid State Batteries (Invited)

S. W. Martin*[1]

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

Recent challenges and problems of explosions and fires with organic liquid electrolyte based lithium batteries has renewed interest in all solid state lithium and sodium batteries which replace the highly conducting but also highly flammable and volatile organic liquid electrolyte with an all solid state electrolyte. There are many such solid electrolytes and one of particular interest due to its low cost of manufacturing are glassy solid electrolytes. In this talk, I will give an overview of glassy solid electrolytes with a particular emphasis on highly conducting sulfide-based chemistries and show recent results from our laboratory on using these solid electrolytes in new all solid state lithium batteries.

9:50 AM

(GOMD-S3-080-2018) Nitridation of $LiPO_3$ glass and reprocessing of LiPON in new glass compositions

S. R. de Souza*[1]; J. E. de Souza[1]; A. Whale[1]; S. W. Martin[1]

1. Iowa State University, MSE, USA

Lithium-ion conducting glasses are widely studied due to their potential application as solid-state amorphous electrolytes. $LiPO_3$ glass is known to be nitride after exposure to NH_3 flow to form LiPON glass, in the following reaction: $LiPO_3 + xNH_3 \rightarrow LiPO_{3-(3x/2)}N_x + (3x/2)H_2O$, by partially replacing two-fold coordinated oxygen atoms with three-fold coordinated nitrogen atoms. After nitridation the glass exhibits improved properties, such as working range and electrical conductivity. However, bubbles formation is inherent to the nitridation process, being necessary to reprocess the LiPON glass under a controlled atmosphere. In the present study $LiPO_3$ glass was prepared by the conventional melt/molding method. The nitridation processes were carried out by remelting the $LiPO_3$ glass at temperatures up to 800°C, under NH_3 flow, applying different times ranging from 3 to 12h. The nitridation was successfully confirmed by Raman and by changes in the glass transition temperatures to higher values. The quantification of N content was carried out by NCHS and XPS. The influence of nitrogen incorporation on the glass structure has been investigated by Raman and FTIR. The nitrogen content was maintained after remelting LiPON glass under N_2, preserving its local structure. Additionally, the LiPON glasses will be used to make new glass compositions as oxy-sulfide-nitride glasses.

10:10 AM

(GOMD-S3-081-2018) New NaPSON glass compositions using $NaPO_3$ and NaPON glasses

J. E. De Souza*[1]; S. R. de Souza[1]; S. Kmiec[1]; A. R. Joyce[1]; S. W. Martin[1]

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

Nitridation of sodium phosphate glasses, $NaPO_3$, has been widely studied because of the changes on its properties like glass transition temperature, density and electrical conductivity. The increase in the ionic conductivity of $NaPO_{3-3x/2}N_x$ is non-linear with respect

to the N/P ratio. New oxy-sulfide-nitride glasses may be promising for solid-state glass electrolytes applications. In the present work $NaPO_3$ glasses were obtained by the conventional melt/molding method at 800°C using Pt/Au crucible. The nitridation processes were carried out by remelting the $NaPO_3$ glass at 750°C, under NH_3 flow, for 6h. Different materials, such as graphite, vitreous carbon, alumina, boron nitride and silica glass were used as boats in order to find a way to obtain the NaPON glasses free of contaminants. The maximum in weight percentage of N incorporation was 9.6 (N/P = 0.66) as measured by CNHS. The NaPON glasses has been used in the preparation of new glass compositions in the $yNa_2S - (1\text{-}y)NaPO_{3\text{-}3x/2}N_x$ system. The influence of nitrogen incorporation on the glass structure has been investigated by Raman and FTIR.

10:30 AM

(GOMD-S3-082-2018) Properties of Lithium Oxythiophosphoborate Glasses

M. R. Hoyt*[1]; S. W. Martin[1]

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

Highly modified lithium oxythiophosphoborate (LiBPSO) glasses of the composition $xLi_2S_xO_{(1\text{-}x')} + (1 - x)[x'B_2S_3 + (1 - x')P_2O_5]$ were prepared. The glasses were made by stoichiometric mixing of $Li_2S + B_2S_3$ and $Li_2O + P_2O_5$ binaries and melting the mixture in a N_2 atmosphere glovebox. LiBPSO glasses were made with a ~10% increase in oxygen substitution of sulfur compared to the previously studied $Li_2S + B_2S_3 + B_2O_3$ glasses. The LiBPSO glasses were analyzed for weight loss, sample homogeneity, working range, and compositional purity. Weight loss was measured by twice melting the LiBPSO samples and cooling to room temperature between melts to measure weight change. Sample homogeneity was assessed by visual inspection of the sample and confirmation of a single glass transition. The working range, or difference between crystallization and glass transition onset temperatures, was measured by differential scanning calorimetry. Compositional purity was determined by infrared spectrometry, which also revealed the interatomic structures of the glasses.

10:50 AM

(GOMD-S3-083-2018) Defects and Lithium ion diffusion behaviors in $Li_{1+x}Al_xGe_{2-x}(PO_4)_3$ ($0.1 \leq x \leq 0.8$) glass-ceramics from computer simulations

P. Kuo*[1]; J. Du[1]

1. University of North Texas, Material Science and Engineering, USA

Lithium aluminum germanium phosphate (LAGP), $Li_{1+x}Al_xGe_{2-x}(PO_4)_3$, glass-ceramics have been investigated as a promising solid state electrolytes for its low activation energy and 3D ion migration path. In this paper, glass and crystalline $Li_{1+x}Al_xGe_{2-x}(PO_4)_3$ (x = 0.1 to 0.8) were studied comparatively using classical molecular dynamics (MD) simulations to understand the diffusion mechanism. Firstly, intrinsic and extrinsic defect formation energies were calculated using the energy minimization method. The structural features were studied in terms of the coordination number, pair distribution function and bond angle distribution. Then, lithium ion diffusion coefficients were obtained from mean square displacement (MSD) calculations. A binding energy of 0.88 eV was found between positive charged Li^+_i and negatively charged Al'_{Ge}, implying the formation of defect cluster in LAGP. Structural features were compared with experimental measurement to prove the validation of simulation cell. Lithium ion trapping i.e. Li^+ trapped around Al'_{Ge} was observed in dynamic simulations. Diffusion coefficients at various temperatures were used to find the energy barrier. The results showed a minimum of energy barrier of 0.47eV at x=0.5. Li^+ diffusion mechanism was studied and diffusion pathway identified. Simulation results provide insight on the diffusion of Li^+ in LAGP.

11:10 AM

(GOMD-S3-084-2018) Atomistic Interpretation of the ac-dc Crossover Frequency in Ionic Conductors: Results from Electrical Impedance and NMR Spectroscopy (Invited)

S. Sen*[1]; M. A. Marple[1]

1. University of California, Davis, USA

The ionic transport properties of crystalline and glassy solids are at the heart of their application as solid-state electrolytes for energy storage, conversion and chemical sensing. It is well known that the frequency dependence of the electrical conductivity of these ionic conductors can be described by the Jonscher expression: $\sigma_\nu = \sigma_{dc}[1+(\nu/\nu_H)^\alpha]$. In this expression, σ_{dc} is the frequency-independent dc conductivity, $0 \leq \alpha \leq 1$ is a constant and ν_H is the frequency marking the onset of frequency-dependent ac conductivity. Almond and West identified ν_H with the hopping frequency of the mobile ions. Such a suggestion is consistent with the expectation that the ionic motion will be localized and sub-diffusive only at observation frequencies higher than the hopping frequency. However, it may also lead to major inconsistencies if ν_H is associated with the frequency of elementary hops. We will present a comprehensive analysis of our recently published results on ionic dynamics in a variety of crystalline and glassy ionic conductors using a combination of electrochemical impedance and NMR spectroscopic techniques. These results will demonstrate that a reinterpretation of ν_H as the frequency of "successful" hops between the mobile species "sites" in the structure yields a consistent atomistic picture for frequency-dependent ionic transport in solids.

11:40 AM

(GOMD-S3-085-2018) Mixed anion effect in Li-ion conducting chalcogenide glasses

M. A. Marple*[1]; S. Kim[1]; B. Aitken[2]; S. Sen[1]

1. University of California Davis, Chemical Engineering and Materials Science, USA
2. Corning Incorporated, USA

Recent studies have indicated that glassy solid electrolytes with more than one type of anion can have significantly higher cationic conductivity compared to their single-anion counterparts. However, systematic studies varying the mixing of anions between the pure extremes have been lacking due to the instability of mixed-anion glasses against crystallization. We have recently observed continuous and stable glass formation in the stoichiometric $Li_2X\text{-}GeX_2$ (X= S, Se) system between pure sulfur and pure selenium end members. These glasses, at a fixed modifier content, display an increase in the ionic conductivity with increasing S/Se ratio with a corresponding decrease in the activation energy and the pre-exponential factor, which go through a minimum at S:Se=1:1. Raman spectroscopic measurements indicate that the structure of these glasses is composed of $GeS_{4/2}$, $GeSe_{4/2}$, and mixed anion GeS_xSe_{4-x} tetrahedra with non-bridging Se and S. The concentration of these mixed anion tetrahedra are maximized around S:Se=1:1 and leads to the non-linear changes in activation energy and the pre-exponential factor. When taken together, these results suggest a strong connection between the glass structure and the activation entropy for ionic transport.

Session 5: Optical Ceramics and Glass-ceramics II

Room: La Vista C (22nd Fl)
Session Chair: John McCloy, Washington State University

9:20 AM

(GOMD-S3-086-2018) Sintering via a stress-induced polymorphic transition: A novel approach to the fabrication of transparent ceramics

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1. University of Central Florida, CREOL, USA
2. US Army Research Laboratory, RDRL-WMM-E, USA

The fabrication of transparent scintillator ceramics of both hygroscopic and birefringent materials is extremely challenging. Fundamental limits to optical transparency are determined by scattering due to mismatch in refractive index at grain boundaries as well as residual porosity. Additionally, air contamination and high processing temperatures favor the formation of defects, which interrupt the energy transfer in the scintillation process. In an attempt to circumvent these issues, this work investigates a new sintering concept based on a stress-induced polymorphic phase transition to fabricate ceramics of Eu:$BaCl_2$, a recently-identified high-performance gamma-ray scintillator. Densification experiments were carried out to demonstrate the feasibility of this approach and understand the conditions for phase-change sintering. These experiments, supported by x-ray diffraction, electron microscopy, and thermal analysis, lead to the production of optically isotropic cubic barium chloride ceramic samples. The optical and scintillation properties of Eu:$BaCl_2$ ceramic samples were investigated and revealed an energy resolution of 6% at 662 keV, an unprecedented value for a halide ceramic scintillator.

9:40 AM

(GOMD-S3-087-2018) Large Magneto-optical Effect of Random Oxides in Short Wavelength Range (Invited)

K. Tanaka*[1]

1. Kyoto University, Department of Material Chemistry, Japan

Magneto-optical materials are useful for practical applications such as an optical isolator, sensing of a magnetic field or an electric current, a holographic memory, and so forth. For the infrared region including the wavelength for optical telecommunications, single-crystalline garnet-type ferrites have been practically utilized as an optical isolator, because they show large Faraday effect and high transparency in the infrared region. In contrast, less materials of high practicality have been developed in a shorter wavelength range such as the visible to ultraviolet region. We have prepared random oxides which show rather large Faraday effect in such a wavelength region; they are random spinel-type zinc ferrite, amorphous oxides containing a large amount of divalent europium ions, and silica glass thin films embedded with very small metallic iron crystals or clusters. For example, amorphous divalent europium titanate thin films prepared by pulsed laser deposition method show Verdet constant comparable to those of crystalline magnetic semiconductors such as EuSe. The structural analysis of the thin films reveals that the local environment of divalent europium ion in the titanate thin films is very similar to that of EuO that is a ferromagnet with high Curie temperature, leading to the large Faraday effect in the visible region as well as ferromagnetism of the amorphous divalent europium titanates.

10:10 AM

(GOMD-S3-088-2018) Upconversion color tunability and white light generation in $Tm^{3+}/Er^{3+}/Yb^{3+}$ doped CaF_2 single crystal (Invited)

L. Su*[1]

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

Here, we report a simple method to produce white light from single crystal matrices, made with Yb^{3+}, Er^{3+} and Tm^{3+} ion co-doped CaF_2 single crystal. The tri-doped CaF_2 single crystal was synthesized via temperature Gradient Technique (TGT) method. Figure 1a displays the up-conversion luminescence spectra of La^{3+}:CaF_2 single crystal. The strong blue, green and red emission lines centered at 408nm, 478nm, 550nm and 670nm are well agree with the transitions $^4F_{9/2}\rightarrow{}^4I_{15/2}$ of Er^{3+}, $^1G_4\rightarrow{}^3H_6$ of Tm^{3+}, $(^2H_{11/2}, ^4S_{3/2})\rightarrow{}^4I_{15/2}$ of Er^{3+}, and $^4F_{9/2}\rightarrow{}^4I_{15/2}$ of Er^{3+}, respectively. The color coordinates of the multicolor upconversion fluorescence in sample are indicated in Figure 1b. With increasing Tm concentration, we obtained the optimal concentrations of 10 mol % Yb^{3+}, 0.1 mol % Er^{3+}, and 0.05 mol % Tm^{3+} in tri-doped CaF_2 single crystal for generating ideal upconverted cool white light with color coordinates of (0.33, 0.2565) under 980 nm pump with power density of 500 mW.

10:40 AM

(GOMD-S3-089-2018) High Power Urtrashort Pulse Laser Based on Yb-doped Ceramic Materials (Invited)

S. Kitajima*[1]; A. Shirakawa[1]; H. Yagi[2]; T. Yanagitani[2]; H. Ishizawa[3]

1. University of Electro-Communications, Institute for Laser Science, Japan
2. Konoshima Chemical Co., Ltd., Japan
3. Nikon Co., Ltd., Japan

In the past twenty years, Yb-doped gain media has attracted great attention as high power, highly efficiency laser due to its simple energy level structure, small quantum defect and appropriate pump sources. Especially in the field of ultrashort pulse laser and amplifier, Yb-doped solid state laser is being increasingly used in many applications as an alternative of Ti:sapphire laser. Meanwhile, along with the progress of highly transparent ceramics technology, ceramic laser have demonstrated good results as high power CW laser and ultrashort pulse laser. Ceramic material as laser gain media has several advantages such as high fracture toughness, mitigation of concentration quenching problem and high compositional homogeneity. Moreover, most ceramics sintering process has lower cost, shorter processing time and higher flexibility compare with the ordinary single crystal fabrication process. In our labs, we have studied various new ceramic laser gain media such as Yb:YAG, Yb:LuAG, Yb:Lu_2O_3 and Yb:CaF_2. In this talk, I mainly focuse on high power mode-locked thin-disk ceramic laser. Recently, we demonstrated Kerr-lens mode-locked thin-disk laser based on Yb:Lu_2O_3 ceramic. The oscillator had the output power of 17 W with 588 fs pulse duration or 3.2 W output with 177 fs pulse duration, respectively. Best of our knowledge, this is the first demonstration of KLM ceramic thin-disk laser.

11:10 AM

(GOMD-S3-090-2018) Hot Isostatic Pressing as a way of processing of luminescent alumina polycrystalline ceramics with high in-line transparency (Invited)

K. Maca*[1]; K. Drdlikova[1]; T. Spusta[1]; D. Drdlik[1]; R. Klement[2]; D. Galusek[2]

1. Brno University of Technology, Czechia
2. Alexander Dubcek University of Trencin, Centre for Functional and Surface Functionalized Glass, Slovakia

A new processing method for preparation of transparent doped alumina ceramics with luminescent properties has been developed. The method is based on proper treatment of dopants (various rare-earth oxides) combined with novel pressure-less pre-sintering followed by Hot Isostatic Pressing. Moreover, the grain growth,

which is a limiting factor for transparency of birefringent polycrystalline ceramics, was thoroughly studied during the pre-sintering as well as during Hot Isostatic Pressing, which helped to optimize the whole sintering process. The final product was characterized in terms of real in-line transmission, measurement of photoluminescence spectra in visible and NIR spectral region, and also by hardness measurement. The combination of superior optical (RIT > 50%), luminescent and mechanical (Vickers hardness > 25 GPa) properties makes this material a promising candidate for number of hi-tech applications. These transparent aluminas are currently tested as a host material in solid state lasers, or as a material for stabilization of laser frequency in atomic clocks.

Session 7: Rare-earth and Transition Metal-doped Glasses and Ceramics for Photonic Applications I

Room: La Vista A/B (22nd Fl)

Session Chairs: Setsuhisa Tanabe, Kyoto University; Shibin Jiang, AdValue Photonics Inc; Kohei Soga, Tokyo University of Science

9:20 AM

(GOMD-S3-091-2018) Optical fiber waveguide designs enabling efficient laser amplification on weak optical transistions (Invited)

J. W. Dawson*[1]; P. Pax[1]; V. Khitrov[1]; L. Kiani[1]; D. Drachenberg[1]; M. Messerly[1]

1. Lawrence Livermore National Lab, NIF&PS, USA

Many rare earth ions have multiple laser transistions, but typically only the strongest transistion is practical for use by laser designers. We have developed a microstructured optical fiber waveguide design capable of providing large distributed losses in predetermined wavelength bands. This waveguide design permits low loss guiding at both longer and shorter wavelengths. Application of this waveguide design to a Nd^{3+} based optical fiber has enabled demonstration of efficient laser operation both in the 900-940nm wavelength band and in the 1400-1500nm wavelength band. In Nd^{3+}, the 1060-1100nm is the strongest optical transistion and the 1400-1500 nm band is approximately 10x weaker. Prior to our work, the 1400-1500nm wavelength band was not accessable in fused silica based optical fibers. We have now demonstrated >20dB of optical gain and >10W of optical power in this wavelength band. These results have particular applicability to future telecom systems. We believe this waveguide design could greatly enhance the operating ranges of optical fiber amplifiers.

9:50 AM

(GOMD-S3-092-2018) Ceramic Gain Media with Tailored Doping Profile

Z. M. Seeley*[1]; T. D. Yee[1]; N. Cherepy[1]; S. A. Payne[1]

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

Polycrystalline transparent ceramics offer a range of advantages over single crystal or glass optical materials. A unique opportunity that optical ceramics fabrication provides is the ability to form a tailored dopant concentration profile throughout the 3-dimensional bulk of the optic. Unlike most glass and single crystal optics, ceramics are fabricated from a solid preform and densified through a solid state sintering process. This process allows a preform with tailored composition, such as a doping gradient, to retain its compositional profile in the final optic. To demonstrate this advantage, we are using the Direct Ink Write (DIW) additive manufacturing process to create optics with tailored composition. The application of tailoring the dopant concentration gradient to match the pumping profile in laser gain media will improve the efficiency and stabilize the TEM_{00} mode. At the same time, we can compensate for the change in refractive index by adding an inert dopant thereby controlling the wavefront. We have successfully fabricated transparent ceramic laser rods with a Nd:YAG core and Lu:YAG cladding by this method, and are working to improve the doping profile and optical scatter. Compositionally tailored optics will soon find uses in other applications. This work was performed under the auspices of the U.S. DOE by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

10:10 AM

(GOMD-S3-094-2018) Luminescent ceramics for solid state light sources (Invited)

M. Raukas*[1]; J. Kelso[1]; A. Lenef[1]; Y. Zheng[1]

1. OSRAM Opto Semiconductors, Materials, USA

Truthful rendering or identification of objects typically requires a broad wavelength range of incident radiation and therefore efficient conversion of light in semiconductor-based sources is of interest in applications. From general illumination to projection or automotive lighting it is important to have the performance and quality of light sources on top level. Over 95% of lumens (contribution of radiation to our sense of vision) in Light Emitting and/or Laser Diode (LED, LD) based lighting comes from various spectral conversion materials. These wavelength 'converters' range from phosphor or semiconductor particles in organic or inorganic matrix materials (e.g. glass) to monolithic crystals and ceramics. Microstructure and composition of the latter vary depending on the application, which in turn give rise to different physical properties like spectral and spatial power distribution or thermal conductivity. Green and yellow emitting garnets are used next to oxy-nitride and nitride materials that extend the spectral range to red. Physical parameters (light scattering, absorption and emission as well as mechanical and thermal behavior) that influence the choice of material type and determine the performance of such ceramic bodies in comparison with glass or organics are reviewed. Work continues towards fine-tuning property-performance relationships, bringing along technological challenges from materials science point of view.

10:40 AM

(GOMD-S3-095-2018) Optical Characterization of Lanthanides Local Structure in Mo Containing Borosilicate Glasses and Glass-Ceramics

M. Saleh*[1]; D. S. Patil[2]; J. McCloy[2]

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

The aim of this study is to understand the effect of lanthanides (Ln) on the phase separation and crystallization in borosilicate glasses for nuclear waste applications using optical techniques. Mo, which is present in some high level nuclear waste, has low solubility in borosilicate glasses leading to phase separation and crystallization of Mo-rich components with low chemical durability. One proposal being studied is to form durable Mo-containing crystals in glass which can incorporate alkaline earths and Ln, such as $CaMoO_4$; thus, it is important to study the effect of the Ln on crystallization. In this study, UV-VIS-NIR absorption, Photoluminescence (PL), and PL Excitation (PLE) are used to study local structure of Ln in simplified nuclear waste borosilicate glass to understand the compositional dependence of the crystallization and phase separation. The effects of composition, heat treatment, and Ln identity (La, Ce, Nd, Sm, Er, Eu, and Yb) are studied. Luminescence and absorption techniques are used to infer the charge state of some of the Ln and the bandgap of the materials studied. The PL/PLE of samples containing Er, Sm, and Eu is used to infer the symmetry of the Ln sites. The UV-VIS-NIR absorption is used to calculate the Judd-Ofelt parameters in samples containing Sm, Er, and Nd which gives insight into the local symmetry and environment of those Ln.

11:00 AM

(GOMD-S3-096-2018) Photo-ionization of polyvalent ions in glasses – defect recovery and long-term stability

D. Möncke*[1]

1. National Hellenic Research Foundation / Linnaeus University, Theoretical and Physical Chemistry Institute / Department of Built Environment and Energy Technology, Greece

Interaction of radiation with glasses often modifies properties of the glasses, such as the color or the refractive index. Most noticeable is a loss in transmission, which is welcome for photo-sensitive applications such as dosimeters, but is to be avoided in many other cases. To better understand the processes of defect generation a systematic comparison of defect formation in fluoride-phosphate glasses doped with low concentrations of various d- and post transition metal elements was attempted. A series of samples doped with 10–5000 ppm cations were irradiated in the UV range by excimer lasers. Additionally, phosphate, silicate, borate and borosilicate glasses containing various polyvalent ions were studied after X-ray or UV-lamp irradiation. Defects form at low concentrations (ppm), but can be analyzed with high sensitivity using optical and/or electron spin resonance spectroscopy. Polyvalent dopants were either photo-oxidized or photo-reduced. Photo-oxidation is prevalent for all ions that can reach the empty valence shell of a d^0 ion (Ti^{3+}, V^{4+}, W^{5+}, Zr^{3+}). However, Mn^{2+}, Fe^{2+}, Co^{2+} or Ni^{2+} can be photo-oxidized to the trivalent ion. In low basicity glasses e.g. fluoride phosphate glasses, Ni^{2+} was however photo-reduced. In the decade following the irradiation experiment increased the number of photo-oxidized species as intrinsic hole center transform into e.g. $(Co^{2+})^+$.

11:20 AM

(GOMD-S3-097-2018) Intense Red Luminescence by Near-UV Excitation in $YSiO_2N:Eu^{3+}$

Y. Kitagawa*[1]; J. Ueda[1]; S. Tanabe[1]

1. Kyoto University, Graduate School of Human and Environmental Studies, Japan

Many red phosphors like $CaAlSiN_3:Eu^{2+}$ have been developed for the improvement of color rendering index of white-LEDs. Nevertheless, the luminous efficacy of Eu^{2+}-doped red phosphors is not high because of the broad emission band extending longer than 650 nm. Considering wavelength dependence of photopic vision, narrow red emission bands of Eu^{3+} are more suitable for getting higher luminous efficacy. However, conventional Eu^{3+}-doped oxide phosphors have an intense excitation band only in deep-UV light (~260 nm) due to charge transfer (CT) from O^{2-} to Eu^{3+}, and low symmetry around Eu^{3+} is required for intense luminescence. In prospect of valence band (VB) energy shift and asymmetry of Eu^{3+} sites by partial N^{3-} coordination, Eu^{3+}-doped oxynitride $YSiO_2N:Eu^{3+}$ phosphor was fabricated. The sample was excited efficiently by near-UV light (280~360 nm). The CT band was redshifted more than 50 nm, compared with $Y_2Si_2O_7:Eu^{3+}$, because the VB top increases due to the N 2p orbital. In the PL spectrum, strong luminescence bands were observed at 624 nm due to the hypersensitive transition of $^5D_0 \rightarrow {}^7F_2$, the transition probability of which depends on asymmetry of Eu^{3+} sites. Thus, Eu^{3+} sites in the mixed-anion coordination of N^{3-} and O^{2-} result in low symmetry as we expected. As a result of temperature dependence of fluorescence lifetime, it was found the Eu^{3+} red luminescence has a good stability against thermal quenching up to 500 K.

S4: Glass Technology and Cross-Cutting Topics

Session 2: Sol-Gel-derived Processing of Glasses and Ceramics I

Room: La Vista F (22nd Fl)
Session Chairs: Lisa Klein, Rutgers University; Gang Chen, Ohio University

9:20 AM

(GOMD-S4-073-2018) Wear resistant and multifunctional sol-gel coatings for mechanical protection of glass (Invited)

A. Durán*[1]; Y. Castro[1]

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

The surface state of glasses plays a key role for different applications, such as vehicles windshields, protective glass sheets of solar panels, solar mirrors, or every type of glazings. The glass surface maybe exposed to a variety of external aggressive conditions that significantly reduce the mechanical and optical properties. Typical examples are sandstorms in Sahara, responsible for the surface degradation of glass substrates and mirrors. The erosion of glass provokes the formation of defects randomly distributed on the exposed surface that greatly reduced the fracture strength; roughness increases and the optical transmission decreases by light scattering, critically affecting the use of windscreens and solar panels. The development of inorganic coatings is a good alternative to obtain transparent and hard coatings with high durability for protecting functions. Sol-gel presents many advantages being appropriate for preparing inorganic films adding the variety of possible deposition techniques. In particular, SiO_2, TiO_2, and ZrO_2 containing films are successfully prepared by sol-gel for different applications, including photocatalytic, anticorrosion or scratch resistance coatings. Different functionalities can be also added as hydrophilic/hydrophobic behaviour and/or antireflective properties.

9:50 AM

(GOMD-S4-074-2018) Effect of the sol-gel matrix on the luminescence properties of lanthanide ions (Invited)

R. M. Almeida*[1]

1. Instituto Superior Tecnico, Univ. Lisboa, Centro de Quimica Estrutural, Portugal

In applications like lasers and optical amplifiers, or up- and down-converting coatings for efficient photovoltaic solar cells, the nature of the matrix determines to a large extent the luminescence properties of lanthanide (Ln) dopant ions. In particular, whether the host matrix has glassy or crystalline nature will determine the fine structure of the emission spectra of these ions. Sol-gel processing is an increasingly popular technique to deposit films and coatings on different substrates, including multilayer thick coatings in the form of 1-D photonic crystals which may enhance the photoluminescence (PL) properties of Ln ions. In this work, sol-gel derived materials like aluminosilicate glass, TiO_2, YAG ($Y_3Al_5O_{12}$) and YF_3 have been doped/co-doped with different concentrations of Er, Er/Yb and Tb/Yb and their structure and properties have been investigated by SEM, GIXRD, Ellipsometry, FTIR/Raman and PL spectroscopies, in order to determine their morphology, glassy/crystalline nature, refractive index/thickness, atomic scale structure and PL properties, respectively. In particular, Er^{3+} was found to be more sensitive than Tb^{3+} or Yb^{3+} to the effects of the glassy/crystalline nature and the maximum phonon energy of sol-gel derived matrices with respect to their luminescence properties, including PL emission and excitation spectra plus relevant lifetimes.

10:20 AM

(GOMD-S4-075-2018) New Insights into the Condensation Kinetics and Structure of Sol-Gel Silicate Glasses

T. Du*[1]; M. M. Smedskjaer[2]; H. Li[1]; M. Bauchy[3]

1. Harbin Institute of Technology, School of Civil Engineering, China
2. Aalborg University, Department of Chemistry and Bioscience, Denmark
3. University of California, Los Angeles, Department of Civil and Environmental Engineering, USA

The sol-gel method is an attractive technique to synthesize homogeneous glasses with high purity while relying on lower processing temperatures than in the melt-quench method. The sol-gel method can also be used to synthesize unusual glasses that are likely to be inaccessible from direct quenching. However, the role of the composition and concentration of the sol-gel precursors remain unclear. Here, based on reactive molecular dynamics simulations, we investigate the sol-gel formation of calcium silicate glasses exhibiting various Ca/Si ratios. The structure of the obtained sol-gel glasses is compared to that of their isochemical melt-quenched counterparts. The role of the fraction of Ca cations on the condensation kinetics is discussed.

10:40 AM

(GOMD-S4-076-2018) SAXS Characterization of Structure and Properties of Sol-gel Glasses

G. Chen*[1]; M. Sundararajan[1]

1. Ohio University, USA

Small-angle X-ray Scattering (SAXS) is a powerful tool for studying inhomogeneity of materials at the nanoscale. In addition to the nanoscale structure, SAXS can also be used to study physical properties of materials. In this talk, I will discuss our recent development on the SAXS characterization of mechanical and thermal properties of sol-gel-derived glasses. Mesoporous silica was used as a prototype material to demonstrate the feasibility of SAXS characterization of its mechanical properties such as Young's modulus and Poisson's ratio and thermal property such as thermal expansion coefficient. The observed anomalies of the material will be discussed.

11:00 AM

(GOMD-S4-077-2018) Solution processed nanostructured materials for functional applications (Invited)

A. Martucci*[1]

1. University of Padova, Industrial Engineering, Italy

Solution processing is a rapidly growing area in the field of materials science owing to the potential to reduce production costs of high-quality thin films and bulk materials at relatively low temperatures. Among the different wet chemistry techniques, sol-gel chemistry is probably the most used for the realization of nanostructured materials. Hydrophobic coatings obtained by sol-gel chemistry were used for increasing the efficiency of heat transfer in two-phase heat exchanger. It is possible to increase the heat transfer coefficient by several times, substituting the classic film wise condensation (FWC) with the dropwise condensation (DWC). We developed sol-gel hydrophobic coatings based on alkoxysilane modified with hydrophobic groups for DWC demonstrating their efficiencies in improving the thermal heat transfer coefficient. Silk Fibroin, the protein extracted from the silk fiber, has been used successfully during the last few years as a platform for optics and high tech application with performances comparable to that of the other polymer used in optics. To increase the performances of silk as a material for optics the refractive index is the most important parameter. Here we report on the synthesis of easy tailored refractive index nanocomposite made of silk and titanate nanosheets, which are 2D crystals of sub-stoichiometric TiO_2, with high refractive index, and small size that prevents scattering.

Session 4: Waste Immobilization - Processing II

Room: La Vista D/E (22nd Fl)
Session Chair: John Vienna, Pacific Northwest National Lab

9:20 AM

(GOMD-S4-078-2018) Numerical and Experimental Study of Crystal Accumulation in Melter Discharge Riser

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1. Idaho National Laboratory, Materials Science and Engineering, USA
2. Savannah River National Lab, USA

Accumulation of spinel crystals in the melter vessel, discharge throat and riser of a waste glass melter is a possible concern wherein clogging and/or subsequent failure of the melter may occur. A computational model is used in concert with experiments in a full-scale, room temperature test platform to predict crystal settling and accumulation. The experimental system consists of a plexiglass discharge riser and throat attached to a feed tank that is agitated to homogenize and suspend the crystals. Silicone oil with a kinematic viscosity of 5000 cSt and magnetite particles with a size range of 125-149 μm were used as simulants for the molten glass and spinel crystals, respectively. Crystal settling in the riser and throat at reduced and target pouring rates were quantified. A bubbling air lance inserted in the riser is evaluated for its effectiveness in resuspending settled crystals. The ability to reliably predict the settling and accumulation of crystals could allow for higher waste loading in the glass by means of different operational and idling strategies.

9:40 AM

(GOMD-S4-079-2018) Understanding the Mechanisms Governing the Crystallization of Spinels in High Level Nuclear Waste Glass

M. Naji*[1]; M. Ahmadzadeh[2]; D. P. Guillen[3]; G. Sterbinsky[4]; C. J. Benmore[4]; J. McCloy[2]; A. Goel[1]

1. Rutgers, The State University of New Jersey, Materials Science and Engineering Department, USA
2. Washington State University, School of Mechanical and Materials Engineering and Materials Science & Engineering Program, USA
3. Idaho National Laboratory, Materials Science and Engineering Department, USA
4. Argonne National Lab, Advanced Photon Source, USA

Radioactive waste from underground tanks in Hanford site is to be vitrified at the Waste Treatment and Immobilization Plant currently under construction. Since the cost of vitrifying radioactive waste is directly proportional to the volume of glass to be produced, it is desired to maximize the waste loading in glass without posing unacceptable risk for melter operation. The major problem facing the processing of HLW glasses is the crystallization of spinel crystals (Fe, Ni, Mn, Cr) in the melt which can result in clogging of the melter discharge channel. To address this challenge, we have investigated the impact of the melt chemistry and environment on nucleation-crystal growth of spinels in a series of simplified HLW glasses. We have performed a systematic study on the impact of iron redox and other transition metal oxides on the nucleation and crystal growth of spinels. A multi-spectroscopic approach has been adopted to probe the magnetic, electronic and structural features of the glass to gain an in-depth understanding of the mechanisms governing the nucleation and growth of spinels. In this presentation, we will discuss complementary results obtained from Fe(K-edge) XANES-EXAFS, VSM, PDF, Raman, and SEM-EDS on a series of simple-to-complex HLW glasses with an aim to build a fundamental knowledge of nucleation and crystallization of spinels in HLW glasses.

10:00 AM

(GOMD-S4-080-2018) Effect of redox on crystallization of spinel crystals in HLW borosilicate glasses

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1. Pacific Northwest National Lab, Radiological Materials & Detection, USA
2. Pacific Northwest National Lab, Materials Characterization, USA
3. Rutgers University, USA
4. DOE-Office of River Protection, USA

The effectiveness of high-level waste vitrification at Hanford's Tank Waste Treatment and Immobilization Plant may be limited by precipitation/accumulation of spinel crystals [$(Fe, Ni, Mn, Zn)^{II}(Fe, Cr)^{III}_2O_4$] in the glass discharge riser of Joule-heated ceramic melters during idling. These crystals do not affect glass durability; however, if accumulated in thick layers, they can clog the melter and prevent discharge of molten glass into canisters. A high temperature reactor was employed to investigate the effect of redox on crystal accumulation and crystal size, morphology, and composition. Borosilicate glasses were heat treated at 850°C in H_2/Ar or in air for different times up to three weeks and analyzed with X-ray diffraction, SEM-EDS, image analysis. A wet chemical method and Mössbauer spectroscopy were used for glass redox measurement. In addition, atom probe tomography was used to quantify the concentration gradient of various elements in the crystals at the crystal/glass interface, and in the immediate vicinity in the glass. The presentation will discuss the findings and their effect on development of highly waste loaded crystal-tolerant glasses.

10:20 AM

(GOMD-S4-081-2018) Crystallization behavior of iron- and boron-containing nepheline based glasses: Implications for the performance of high level nuclear waste glasses

A. A. Deshkar*[1]; M. Ahmadzadeh[2]; A. Scrimshire[3]; E. Han[1]; P. A. Bingham[3]; D. P. Guillen[4]; J. McCloy[2]; A. Goel[1]

1. Rutgers University, Materials Science & Engineering, USA
2. Washington State University, School of Mechanical & Materials Engineering, USA
3. Sheffield Hallam University, Materials and Engineering Research Institute, United Kingdom
4. Idaho National Lab, USA

The present study focuses on understanding the compositional and environmental dependence of iron redox in nepheline-based simplified, inactive high-level nuclear waste glasses designed in the quinary $Na_2O–Al_2O_3–B_2O_3–Fe_2O_3–SiO_2$ system. The impact of composition and different heating atmospheres (air, inert and reducing) on the crystallization behavior and iron redox chemistry of glasses have been investigated using X-ray diffraction, electron microscopy, Mössbauer spectroscopy and vibrating sample magnetometry. The results indicate that while iron coordination changed as a function of glass chemistry, the heating atmosphere exhibited a minimal effect on the redox behavior in the glass-ceramics, thus leading to a minimal impact on the crystalline phase assemblage. However, the heating atmosphere had a significant impact on the microstructural evolution of these glasses as the formation of an iron-rich layer of crystals on the surface of the glass-ceramics was observed when heated in air or inert atmospheres. Details of these results, along with an explanation on the basis of diffusion kinetics of oxygen and network modifiers in glasses, and the plausible implications on the chemical durability of high-level nuclear waste glasses will be discussed in the presentation.

10:40 AM

(GOMD-S4-082-2018) Determination of Crystal Size, Crystal Fraction, and Glass Forming Constraints in Spinel Forming Simulated High Level Waste Glasses

C. Lonergan*[1]; V. Gervasio[1]; K. Akinloye-Brown[1]; N. L. Canfield[1]; M. Schweiger[1]; J. Vienna[1]; A. A. Kruger[2]

1. Pacific Northwest National Lab, USA
2. Office of River Protection, USA

Crystallization is a major concern during the vitrification of high-level waste (HLW) glasses. One crystal of particular importance is spinel as it can accumulate at the bottom of the HLW melters. The presence of spinel layers can cause processing issues that can result in delays during the vitrification process. The imposition of compositional- and parameter-based constraints when determining glass compositions help to mitigate failures and extend melter lifetimes. To support the development of accurate glass formulation algorithms, aided by producing robust and representative models, compositional dependence of the crystal size and crystal fraction is explored. In this work, simulated HLW glasses underwent heat treatments for 72 hr at the following temperatures: 850, 900, and 950 °C and specimens were examined with optical and scanning electron microscopies and X-ray diffraction. All glasses contained crystals after heat treatment and the average spinel sizes were $\langle$ 10 um. Of the 33 glasses in this study, 32 formed spinel crystals and 15 precipitated crystals of other phases. The total crystal fraction present in the glasses varied from 0.2 wt% to 41.0 wt% with the primary phases of spinel, hematite, and nepheline. The resulting data was used to produce models to predict crystal fraction and size as a function of temperature and composition.

11:00 AM

(GOMD-S4-083-2018) Crystallization Kinetics and Microstructural Development in a Complex Borosilicate Glass-Ceramic for Waste Vitrification

P. Porter*[1]; N. Roberts[1]; R. Brow[1]

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

We have studied the effects of controlled quench rates and isothermal holds on the evolution of the microstructure of a complex borosilicate glass-ceramic developed by Pacific Northwest National Lab for nuclear waste vitrification; viz., J. Crum, et al., J. Nucl. Mater. 482 1–11 (2016). Glass melts were quenched from 1300°C to room temperature at rates between 3°C/sec and 50°C/sec, using a melt-wedge technique, and at rates from 150°C/s to 25°C/s using a hot thermocouple device. Other melts were quenched in a roller cooler (~100°C/sec) and in furnaces cooled as slowly as 0.01°C/sec. In a second set of experiments, melts were rapidly quenched into tin baths set between 600 and 1100°C and isothermally held for up to 60 minutes. Analytical scanning electron microscopy, Raman spectroscopy, and quantitative X-ray diffraction techniques were used to characterize the development of microstructural features, including the formation of Mo-rich amorphous droplets from which powellite crystals nucleate and grow, and the development of rare-earth containing oxyapatitic crystals. This work was supported by the US Department of Energy (NEUP 15-8112). The authors thank Jarrod Crum (PNNL) for providing the glasses for this study.

11:20 AM

(GOMD-S4-084-2018) Calculation of Spinel Settling from High Level Waste Glass Using Stoke's Law

C. Lonergan*[1]; J. Matyas[1]; P. Hrma[1]; J. Vienna[1]

1. Pacific Northwest National Lab, USA

The Hanford Tank Waste Treatment and Immobilization Plant is being constructed to vitrify radioactive waste into borosilicate glass. The loading of Hanford's high-level waste (HLW) in glass is limited by glass composition and property constraints. Significant among

them are constraints aimed at minimizing the adverse effects of crystallization in the melter. If crystals accumulate in the melter, they can cause issues with pouring, including clogging the pour spout riser. Previously, a constraint involving the melt liquidus temperature was utilized but this approach significantly reduced the waste loading. Another approach of limiting the fraction of crystals to an arbitrary 1 vol% was pursued, which improved the potential waste loading but lacks technical justification. This work seeks to develop a constraint that minimizes the risk of crystal accumulation on melter life while allowing for an increase in waste loadings. The proposed approach applies crystal fraction and size data to estimate crystal accumulation rate through a modified Stoke's Law. The model will be described along with initial predictions for mock Hanford HLW pour spout riser data.

11:40 AM

(GOMD-S4-085-2018) Thermodynamic and kinetic assessment of nepheline crystallization in Na_2O-Al_2O_3-B_2O_3-SiO_2 glasses: Impact of mixed network former effect

A. A. Deshkar*[1]; M. Naji[1]; O. Gulbiten[2]; R. Youngman[2]; A. Goel[1]

1. Rutgers University, Materials Science & Engineering, USA
2. Corning Incorporated, USA

Vitrification of sodium and alumina-rich high-level radioactive waste (HLW) into borosilicate glasses faces the problem of nepheline ($NaAlSiO_4$) crystallization, which is detrimental to the durability and long-term stability of the final waste form. Studies show the suppressing effect of B_2O_3 on nepheline crystallization, but its precise mechanism has not yet been fully understood. The change in glass viscosity and fragility arising from the variation of B_2O_3 as well as its excess of enthalpy during glass to liquid transition are expected to impact the tendency of nepheline crystallization. Therefore, the present study aims towards understanding the thermodynamic-kinetic behavior governing the crystallization of nepheline based Na_2O-Al_2O_3-B_2O_3-SiO_2 glasses. Accordingly, the crystallization behavior of the synthesized glasses has been studied by conducting non-isothermal and isothermal heat treatments, while the thermodynamic-kinetic behavior has been investigated by probing the temperature-dependence of the equilibrium and non-equilibrium viscosity. The latter was conducted near the glass-transition range to obtain the fragility index. The sharpness of the glass transition has been measured and expressed in terms of change in heat capacity and excess of enthalpy and results have been correlated with fragility and crystallization behavior.

S1: Fundamentals of the Glassy State

Session 4: Topology and Rigidity II

Room: El Mirador West (22nd Fl)

Session Chairs: Mathieu Bauchy, University of California, Los Angeles; Morten Smedskjaer, Aalborg University

1:20 PM

(GOMD-S1-136-2018) Topological nano-engineering of cement hydrates (Invited)

N. Krishnan*[1]; B. Wang[2]; M. Bauchy[2]

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

Calcium–silicate–hydrate (C–S–H), the binding phase of concrete, has a complex layered-but-disordered atomic structure exhibiting a wide range of compositions. This unique structure is complimented with remarkable properties such as creep or relaxation of the atomic network under constant stress, and radiation resistance. However, among different C–S–H structures, the degree of structural relaxation and radiation resistance is found to vary. Understanding the composition–structure–property relationships in C–S–H is essential to reconcile these observations and to design better cement compositions. Herein, relying on molecular dynamics simulations and topological constraint theory, we analyze the response of C–S–H structures—with Ca/Si ratio varying between 1.1 and 1.9—to external stress and radiation. We observe that the structures with Ca/Si around 1.5 exhibit maximum creep modulus and radiation resistance representing an optimal network. Based on a topological analysis, we demonstrate that the optimal composition corresponds to an isostatic atomic network, which is characterized by the absence of zero energy floppy modes and eigenstress. Altogether, we demonstrate that an isostatic network features superior radiation- and creep-resistant properties. Such an improved understanding based on atomic topology can lead to the design of cement compositions with improved durability and sustainability.

1:50 PM

(GOMD-S1-137-2018) Entropy favors heterogeneous network structures near the rigidity threshold (Invited)

L. Yan*[1]

1. University of California, Santa Barbara, Kavli Institute for Theoretical Physics, USA

Amorphous materials like glasses and concretes are ruled mainly by the elastic aspect of their microscopic structures. In network glasses, this structural elasticity can be set on and off by tuning the composition of chemicals with different valences, which also controls the covalent network topology. For homogeneous networks, such a rigidity transition is expected to be regulated by a critical threshold at the balance between the degrees of freedom of atoms and the number of covalent constraints. The actual plot in chalcogenides, for example, is however complicated by the presence of structural heterogeneity: instead of a point, a homogeneous intermediate phase of critical features sits in between two heterogeneous phases. Counterintuitively, this mysterious heterogeneity has an entropic origin. Here we show that the vibrational entropy gains from creating separated rigid and floppy regions in a network when the connectivity is close to the rigidity onset of homogeneous structures. While the stress-energy on contrary penalizes the heterogeneity and dominates a smaller vicinity of the rigidity threshold at the glass transition, which results in the homogeneous intermediate phase.

2:20 PM

(GOMD-S1-138-2018) Statistical Mechanical Model of Bonding in Mixed Modifier Glasses

S. Goyal*[1]; J. C. Mauro[2]

1. Corning Incorporated, USA
2. Pennsylvania State University, Material Science, USA

Oxide glasses often consist of multiple network formers that create the backbone of the glass network and modifiers that serve as either charge compensators or creators of non-bridging oxygens. The variety of bonding preferences results in very rich composition-property relationships. In this work, we present a statistical description of the glass structure governed by the relative enthalpic and entropic contributions to the bonding preferences in a glassy system. Using the proposed model, we derive an analytical expression to represent the bonding in mixed modifier glasses and explain the role of composition and fictive temperature on glass structure. The model is able to provide the criteria for nonlinearity in bonding preference and reveals regions where high fluctuations in local structure are predicted. We then apply dilute solution theory to calculate the free energy for varying glass mixtures, resulting in derivation of the glass mixing zone for model glasses. Finally, we apply the derived model, along with a non-linear optimizer to predict structure for alkali silicates with high accuracy.

2:40 PM

(GOMD-S1-139-2018) Physical properties of $Ge_xGa_ySe_{1-x-y}$ chalcogenide glasses and their correlation to topological structure

J. M. Lonergan*[1]; C. Lonergan[2]; K. Richardson[2]; J. McCloy[1]

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

This study analyzed the structure and properties of chalcogenide materials in the glass-forming region of the Ge_x-Ga_y-Se_{1-x-y} ternary. Topological constraint theory, <r>, was used to semi-empirically analyze trends in properties. Ten compositions covering a range of coordination numbers from <r>=2.3 to <r>=2.8 were melt quenched and analyzed. Sharp inflections near the average coordination number of <r> = 2.67 were observed for many properties. Heat capacity and thermal conductivity continuously increased with coordination number with maximum values of 0.305 J/g•K and 0.313 W/m•K measured at <r> = 2.8 respectively. Observations indicate thermal, physical, and optical properties in these chalcogenide glasses are highly sensitive to the chemical ratio of Ge(Ga)-Se versus Se-Se bonds, as well as the ratio of tetrahedral $GaSe_{4/2}$ to $GeSe_{4/2}$ units. Theoretical predictions of fracture toughness, heat capacity, and thermal conductivity were generated to provide additional insights. This talk will detail the melt process, the resulting structure, and its effects on properties in the resulting $Ge_xGa_ySe_{1-x-y}$ glasses.

3:00 PM

(GOMD-S1-140-2018) Topological Dependence of Chemical Durability in Densified Glasses

N. Mascaraque Alvarez[1]; M. Bauchy[2]; M. M. Smedskjaer*[1]

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. University of California, Los Angeles, USA

Glasses gradually dissolve and corrode when they are exposed to aqueous solutions, and for many applications it is necessary to understand and predict the kinetics of the glass dissolution. Recent studies have indicated that the dissolution rate of oxide glasses with different chemical compositions is controlled by their atomic topology. That is, the dissolution rate exponentially decreases with the number of topological constraints per atom acting within the molecular network. Here, to further understand the topological origin of chemical durability, we study the effect of permanent densification on dissolution kinetics. Specifically, we study the bulk glass dissolution rate of phosphate, silicophosphate, borophosphate, borosilicate, and aluminoborosilicate glasses, which have been compressed at 0.5, 1.0, and 2.0 GPa at the glass transition temperature. We perform weight loss and supplementary modifier leaching measurements of bulk samples immersed in acid (pH 2) and neutral (pH 7) solutions. Compression generally improves the chemical durability as measured from weight loss, but the effect is highly composition- and pressure-dependent. As such, we show that the dissolution mechanisms depend on the topological changes induced by permanent densification, which in turn are a function of the changes in the number of nonbridging oxygens and the network cross-linking.

3:20 PM

(GOMD-S1-141-2018) Hydrophilic-to-Hydrophobic Transition in Glassy Silica is Driven by the Atomic Topology of its Surface

Y. Yu[1]; N. Krishnan[2]; M. M. Smedskjaer[3]; G. Sant*[1]; M. Bauchy[1]

1. University of California, Los Angeles, USA
2. Indian Institute of Technology Delhi, India
3. Aalborg University, Denmark

The surface reactivity and hydrophilicity of silicate materials are key properties for various industrial applications. However, the structural origin of their affinity for water remains unclear. Here, based on reactive molecular dynamics simulations of a series of glassy silica surfaces annealed at various temperatures and subsequently exposed to water, we show that silica exhibits a hydrophilic-to-hydrophobic transition driven by its silanol surface density. By applying topological constraint theory, we show that the surface reactivity and hydrophilic/hydrophobic character of silica are controlled by the atomic topology of its surface. This suggests that novel silicate materials with tailored reactivity and hydrophilicity could be developed through the topological nanoengineering of their surface.

S3: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 2: Charge and Energy Transport in Disordered Materials II

Room: El Mirador East (22nd Fl)

Session Chairs: B. Potter, University of Arizona; Krishna Muralidharan, University of Arizona; Xianghua Zhang, CNRS - Université Rennes 1

1:20 PM

(GOMD-S3-098-2018) Functional Chalcogenide Glass-ceramics for Photovoltaic and Ionic Conduction

B. Fan*[1]; X. Bai[1]; Y. Xv[2]; Q. Shen[3]; H. Fu[4]; Z. Luo[4]; H. Ma[5]; X. Zhang[5]

1. Shenzhen University, College of Physics and Energy, China
2. College of Materials Science and Engineerging, China Jiliang University, China
3. College of Materials Science and Engineering, Zhejiang University, China
4. College of Chemistry and Environmental Engineering, Shenzhen University, China
5. Institute of Chemical Science, University of Rennes 1, France

Chalcogenide glass-ceramics which are originally designed to improve the mechanical properties, are now developed to be used for energy conversion and storage. Two examples are presented. $GeSe_2$-Sb_2S_3-CuI glass-ceramics showing significantly improved photoelectrical response can be fabricated from the base glass by careful composition design and crystallization procedure controlling. The co-precipitation of I:Sb_2Se_3 and Cu_2GeSe_3 in the glass matrix, as a result of kinetically allowed eutectoid crystallization, can create nano-scaled heterojunction networks and improve the photoelectrical response. These novel selenide glass-ceramics are expected to be used in solar cells. GeS_2-Ga_2S_3-Li_2S-LiI glass-ceramics with elaborately controlled crystallinity shows improved ionic conductivity compared with the base glass. Typically, a crystallinity around 30% results in several times higher ionic conductivity, that is proposed to be associated with the easy ion path formed at the glass/crystal interface. In a word, using controllable crystallization to create special micro-structure in glass-ceramics provides a novel way to develop functional materials for energy applications.

1:40 PM

(GOMD-S3-099-2018) Structure and Properties of Highly Modified Mixed Anion Chalcogenide Glasses in the Na_2S-SiS_2-$SiSe_2$-$PS_{5/2}$ System

S. Kmiec*[1]; A. R. Joyce[1]; S. W. Martin[1]

1. Iowa State University, USA

The SiS_2-$SiSe_2$ isoelectronic substitution was investigated in the [65 Na_2S+ 22.5$SiS_{(2-x)}Se_{(x)}$ +12.5 $PS_{5/2}$] glass series to determine the effect selenium has on the physical and electrical properties. Studies have shown the addition of a different anionic species to sulfide glass can have a large effect on its properties such as the glass transition temperature (T_g), and ionic conductivity. To better understand this effect, the short range order (SRO) of these glasses was characterized using Raman and ^{29}Si & ^{31}P Magic Angle Spinning NMR (MAS NMR) spectroscopies to identify the role of selenium in the glass structure. Evidence suggests that the addition of selenium causes de-polymerization of the silicon structure though the formation

of mixed sulfur-selenium tetrahedra. These units allow for greater uptake of sodium ion to the system leading to a large change in properties and can be seen most notably in the glass transition temperatures and ionic conductivity.

2:00 PM

(GOMD-S3-100-2018) Porous aluminosilicate structures with tunable thermal transport properties

G. Gupta[2]; P. Rao[1]; M. Momayez[2]; K. Runge[1]; K. Muralidharan*[1]

1. University of Arizona, Materials Science and Engineering, USA
2. University of Arizona, Mining and Geological Engineering, USA

The thermal transport properties of porous amorphous aluminosilicate structures are investigated using a combination of molecular dynamics simulations and finite element methods in conjunction with targeted experimental synthesis and characterization techniques, and their applications as thermal insulation coatings for buildings are examined. Specifically, the interplay between the choice of charge balancing cations (Na, K, Ca) and the extent of porosity on the thermal conductivity of the aluminosilicate (AS) structures are characterized. It is seen that the thermal conductivity of the AS structures show a monotonic dependence on the system porosity for densities varying between 2.45 to 0.5 g/cc. Interestingly, for a given density (i.e. for a given volume of pores introduced), a larger distribution of smaller pores results in a lower thermal conductivity. This observation is correlated to more phonon-scattering centers in such systems. Further, the choice of the cation also plays a part in controlling the thermal conductivity of the AS structures, Replacing Na by either K or Ca leads to a further decrease in thermal conductivity by approximately 10 %. This is attributed to the respective diffusivities of the corresponding cations. In conclusion, mechanically robust, low density porous AS structures provide an inexpensive route for fabricating large-scale thermal insulation coatings.

2:20 PM

(GOMD-S3-101-2018) Conducting pathways in silver-doped chanlcogenide glasses (Invited)

K. Prasai*[2]; G. Chen[1]; P. Biswas[3]; D. Drabold[1]

1. Ohio University, Physics and Astronomy, USA
2. Stanford University, Applied Physics, USA
3. The University of Southern Mississippi, Physics and Astronomy, USA

Silver-doped chalcogenides acquire a reversible conducting phase when subjected to a bias voltage between suitable electrodes. This property has been utilized to design memory elements, commonly known as conducting bridge random access memory or CBRAM. But, the atomic level structure of the conducting phase is still being actively explored. In this work, we explore the microscopic origin of electronic conductivity in $GeSe_3Ag$ glass using first principles modeling method. We show here that the models that are rich in Ag_2Se phase are conducting and the conduction pathways include Se-atoms that are primarily bonded to Ag-atoms. We develop a crude way to estimate the space-projected conductivity and to identify "conductive paths" within disordered systems. We show that for higher concentrations of Ag, the electronic conduction can be projected onto filament-like region of space that is continuously connected from one end of the cell to another. We follow this with a more rigorous approach to space resolved conductivity. Finally, we show that continuous Ag nanowires of sufficiently low thickness don't conduct by an explicit modeling of such wires into our model.

2:50 PM

(GOMD-S3-102-2018) Electrical properties of Cu-As-Te

G. Coleman*[1]; B. G. Potter[1]; P. Lucas[1]

1. University of Arizona, Materials Science, USA

Cu-As-Te glasses are a unique class of chalcogenide glass due to their ability to incorporate greater than 30atm% Cu, high conductivities while maintaining its amorphism. They have potential applications in/as thermoelectric devices, infrared detectors, and field-effect transistors. However, their performance are usually limited in these applications because chalcogenide glasses suffer from a negative correlation energy, which effectively inhibits defect formations to contribute to their electrical conductivity. We explore the connection between defect formation, electrical properties, and structural origins within the Cu-As-Te network.

3:10 PM

(GOMD-S3-103-2018) Electrical Conduction in Cu-doped Ge-Se Glasses

G. Chen*[1]; B. Bhattarai[1]; D. Drabold[1]

1. Ohio University, USA

Glasses are usually poor electrical conductors. However, upon addition of metal ions into chalcogenide glasses, the materials become not only ionically conducting but also, sometimes, electrically conducting. This unusual electrical property is the basis behind the Conductive-bridging Random Access Memory (CBRAM), a type of resistive random access memory that shows threshold switching in resistance under external disturbance. To understand the structure and electrical property relation of metal-doped chalcogenide glasses, we synthesized Cu-doped Ge-Se thin films and CBRAM devices by magnetron sputtering. The electrical property was studied as a function of Cu concentration and correlated with the structure of the materials obtained by X-ray scattering. MD simulations were also performed to understand the correlation between the atomic structure and the observed unusual electrical property.

3:30 PM

(GOMD-S3-104-2018) High electrical conductivity in carbon-nanofiber glass composites

S. Chen*[1]; G. Tao[1]; S. J. Pandey[1]; M. Molinari[2]; L. Tetard[3]; H. Ebendorff-Heidepriem[4]; A. Abouraddy[1]; R. M. Gaume[1]

1. University of Central Florida, College of Optics and Photonics, USA
2. University of Reims Champagne Ardenne, France
3. University of Central Florida, NanoScience Technology Center, USA
4. The University of Adelaide, Australia

Glass composites have important applications in diverse fields including waste management, the automobile industry, healthcare, and in the elimination of electromagnetic interference, among other possibilities. Here we present a thermoformable glass/carbon-nanofiber composite with controllable electrical conductivity achieved by varying carbon loading. The surface chemistry of a polymer surfactant that facilitates the dispersion of the carbon nanofibers before thermal densification plays a pivotal role in achieving the highest reported room-temperature electrical conductivity (1800 S/m) in a bulk oxide glass corresponding to the theoretical limit for the conductive-phase volume-fraction. Densification and dispersion were confirmed by SEM and further supported by electrical nanoscale characterization. Conductive-AFM measurements provide a micron-scale conductivity mapping and delineates distinct barrier-contact behavior in carbon-loaded and non-loaded samples. Electron transport modeling studies estimates a percolation threshold of 1.9 vol% and suggest a carbon nanofiber aspect ratio and a tunneling length consistent with SEM observation and literature reports. The temperature dependency of electrical conductivity for composites with different carbon loading is found to be governed by a combination of different carrier transport mechanisms.

3:50 PM

(GOMD-S3-105-2018) Crystallization behavior under hydrogen and its electrochemical property of bismuth borate glass

T. Honma*[1]; Y. Omori[1]; T. Komatsu[1]

1. Nagaoka Univeristy of Technology, Department of Materials Sciencs and Technology, Japan

Bismuth borate glass is interesting optical glass system bacause its high refractive index, third order optical nonlinearlity, and low temperature fluidity. On the other hand, Bi_2O_3 is also kown to be focused as anode materials for lithium ion battery. In this study, We examined crystallization bahavior under hydrogen-argon mixture atmosphere, electrical conductivity, and alkali ion insersion properties. We confirmed that $70Bi_2O_3$-$30B_2O_3$ glass forms bismuth meal particle in glass matrix by heat treatment at glass transition temperature. And we also confirmed that glass-ceramics anode exhibits over 300mAh/g for lithium metal.

Session 5: Optical Ceramics and Glass-ceramics III

Room: La Vista C (22nd Fl)

Session Chair: Yiquan Wu, Alfred University

1:20 PM

(GOMD-S3-106-2018) Fabrication and Optical Properties of Transparent Nd-doped BaF_2 Ceramics

X. Chen*[1]; Y. Li[1]; Y. Wu[1]

1. Alfred University, Materials Science and Engineering, USA

Nd:BaF_2 transparent ceramics have been fabricated via vacuum sintering of nanopowders prepared via co-precipitation. First, a Nd:BaF_2 precursor powder was synthesized through co-precipitation, which was subsequently calcined at 600°C for 5h in an Ar atmosphere. The resulting powder was analyzed via SEM, XRD, and BET surface area methods, with its average particle size determined by BET and SEM observations to be approximately 100-200nm. Transparent ceramics were then fabricated through consolidation of the nanopowder via vacuum sintering at 1200°C for 10h. The average grain size of the consolidated ceramic was determined through SEM observations of its polished and thermally-etched microstructure to be 420μm. Photoluminescence and transmission spectra measurements of the Nd:BaF_2 ceramic revealed an emission peak located at 1058nm; excited by 800nm excitation, and a maximum transmittance of ~67%; observed at a wavelength of 1058nm.

1:40 PM

(GOMD-S3-107-2018) Study on the Consolidation of Sulfide-Based Infrared Optical Ceramics (Invited)

Y. Li[1]; Y. Wu*[1]

1. Alfred University, Kazuo Inamori School of Engineering, USA

Zinc sulfide (ZnS) and calcium lanthanum sulfide ($CaLa_2S_4$) are sulfide-based infrared (IR) optical materials known for their favorable IR transmittance properties. In this study, pressure-assisted sintering techniques were applied to fabricate ZnS, $CaLa_2S_4$, and ZnS-$CaLa_2S_4$ composite IR optical ceramics. The effects of varying different processing parameters, in both the powder synthesis and consolidation stages, were studied to develop a procedure for fabricating sulfide-based ceramics with enhanced optical and mechanical properties. XRD phase composition analysis was performed to unveil the influence of starting powder particle size, sintering temperature, and applied pressure on the sphalerite-wurtzite phase transition of ZnS. The sintering mechanisms associated with the different sintering techniques applied to the single-phase ZnS and $CaLa_2S_4$ ceramics, as well as the composite sulfide-based ceramics, were investigated through microstructural characterization and sintering behavior analysis. A study of photoluminescence behavior was also conducted to investigate the nature of the intrinsic defects present in the ceramics. The development of a comprehensive understanding of the relationships between processing, microstructure, and properties may shed new light on both the experimental and theoretical aspects of developing sulfide-based infrared optical ceramics.

2:10 PM

(GOMD-S3-108-2018) Field-Assisted Consolidation of Gallium Oxide Optical Ceramics

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As a semiconductor with a wide band gap of 4.9 eV, gallium oxide (Ga_2O_3) has attracted significant research interest due to its promise as a transparent conductive oxide material. In the present research, Ga_2O_3 optical ceramics were consolidated through field assisted sintering of Ga_2O_3 nanopowders. X-ray diffraction analysis of the sintered ceramics revealed them to be single-phased β-Ga_2O_3. The effects of varying different sintering parameters were investigated in order to optimize the properties of the consolidated Ga_2O_3 ceramics. The densification behavior and grain growth of the Ga_2O_3 ceramics were studied through sintering curve analyses and microstructural observations. In addition, the optical and mechanical properties of the ceramics were characterized to establish the relationships between different variables of the consolidation process, and the end microstructural features and properties of the ceramics. Studies of the photoluminescence properties of the ceramics were also performed to investigate the nature of the intrinsic vacancy and interstitial defects present in the Ga_2O_3 ceramics.

Session 7: Rare-earth and Transition Metal-doped Glasses and Ceramics for Photonic Applications II

Room: La Vista A/B (22nd Fl)

Session Chairs: Setsuhisa Tanabe, Kyoto University; Shibin Jiang, AdValue Photonics Inc; Kohei Soga, Tokyo University of Science

1:20 PM

(GOMD-S3-109-2018) Developing narrow red LED downconverters for display and lighting applications (Invited)

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The nature of the human eye sensitivity makes the spectral position and width of the red component of white light critical for acheiving color quality (whether that be color gamut in displays or color rendering in lighting) and energy efficiency simultaneously. Over the past five years, there have been multiple narrow red phosphors and downconverters that have been proposed for use in LED lighting and displays. In this presentation, we will briefly review some of the more industrially relevant materials, including semiconductor quantum dots, Eu^{2+}-doped nitrides, and Mn^{4+}-doped complex fluorides. In addition, we also discuss in greater detail some initial issues in implementing Mn^{4+}-doped complex fluorides into commercial LED packages for lighting and displays. Many of these issues have been addressed in GE's TriGain phosphors based upon K_2SiF_6:Mn^{4+} compositions, and we will briefly discuss the luminescence properties of these phosphors along with their performance in LCD backlights and general illumination.

1:50 PM

(GOMD-S3-110-2018) Nitride and oxynitride phosphors for LED lighting (Invited)

N. Cherepy*[1]; R. Osborne[1]; Z. M. Seeley[1]; D. Aberg[1]; S. A. Payne[1]; T. Wineger[1]; A. Srivastava[2]; H. Comanzo[2]; D. Schlagel[3]; T. Lograsso[3]

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Phosphor-converted white light LEDs (pc-LEDs) offer significant advantages over fluorescent lighting, such as higher efficiency (lumens/watt) and less phosphor per lamp, meaning much less rare earth element usage. In pc-LEDs, the light from the blue LED is partially converted with green- and red-emitting phosphors to produce the white light. New Eu-doped nitride and oxynitride phosphors offer high quantum yield, low thermal quenching, reasonably short excited state lifetimes (to avoid excited state absorption), strong absorption at 450 nm, and long-term chemical stability under ambient conditions. Optimized combinations of nitride phosphors can achieve high color rendering (CRI and R9), while offering high efficiency. New synthesis methods to reduce cost of nitride phosphors are being explored as well as methods of implementation to mitigate thermal quenching and droop. Acknowledgements: This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344, and funded by the DOE EERE Critical Materials Institute.

2:20 PM

(GOMD-S3-111-2018) Nanomaterials for OTN-NIR Biophotonics

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Over-1000 nm Near Infrared (OTN-NIR), in other words, second biological window or NIR II/III, wavelength range is attracting much interests of both users and developers of biophotonics since the range gives a minima of the loss of the propagation of electromagnetic wave in biological tissues. The authors have developed fluorescent imaging probes for the OTN-NIR small animal fluorescence imaging together with functional materials for medical use. One of them is the OTN-NIR fluorescence nano-sensor for measuring temperature or parameters as pH by detecting the fluorescence spectrum of the nano-material. Another example is the OTN-NIR phototheranostic nanoparticles, which can be applied for photodynamic therapy and fluorescence in vivo imaging by using the OTN-NIR excitation light. This presentation will review the development of materials development, namely rare-earth doped ones, and system of the OTN-NIR biophotonics.

2:40 PM

(GOMD-S3-112-2018) Frequency Conversion in Lanthanide-based Molecules and Materials (Invited)

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Based on their outstanding optical properties, Ln^{3+}-based compounds have been suggested for a wide range of applications including the field of biomedicine and solar energy conversion. For instance, the capability of Ln^{3+}-based materials to emit visible and near-infrared (NIR) light under NIR excitation is highly sought after when aiming for biomedical applications. This is due to the fact that NIR light penetrates deeper into biological tissue when compared to UV or visible light. Fluorides, such as $NaGdF_4$, are commonly considered as suitable host materials for upconverting and NIR emitting Ln^{3+} ions (e.g. Er^{3+}) and their preparation via the thermal decomposition process has been widely studied. The microwave-assisted approach offers a promising alternative for the synthesis of Ln^{3+}-nanoparticles of controlled size and crystalline phase. Ln^{3+}-based compounds have also been suggested to reduce efficiency loss in solar cells. In this context, Ln^{3+} ions such as Eu^{3+} or Tb^{3+} are suitable candidates emitting visible light under UV excitation. Moreover, Eu^{3+} is a model ion of particular interest since its emission spectrum allows us to draw conclusions about the chemical environment of Eu^{3+} ions as shown on the example of a Tb^{3+}/Eu^{3+}-complex. This presentation will shine a light on the versatile landscape of Ln^{3+}-based materials and molecules focusing on materials synthesis and Ln^{3+}-specific optical features.

3:10 PM

(GOMD-S3-113-2018) Rare Earth Doped Nanoparticles: Core/Multi-Shell Structures for Multifunctionality (Invited)

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In the last decade, the field of rare earth doped nanoparticles has progressed from the basic understanding of the photophysical properties governing their nanoscale luminescence to their use in a variety of applications, with considerable focus in biology and medicine. This interest stems primarily from the ability to stimulate these luminescent nanoparticles with near-infrared (NIR) light as well as their diverse emission wavelengths spanning the UV to the NIR regions. Therefore, with a single NIR excitation wavelength, it is possible to observe anti-Stokes emission, known as upconversion, or single photon (Stokes) NIR emission in the three biological windows (BW-I: 700-950 nm, BW-II: 1000-1350 nm, BW-III: 1550-1870 nm) where tissues are optically transparent. Here, we present methods for controlling the luminescence of these nanoparticles through core/shell nanostructures/nanoplatforms and demonstrate how their various emissions could be harnessed for applications in biology and nanomedicine.

S4: Glass Technology and Cross-Cutting Topics

Session 2: Sol-Gel-derived Processing of Glasses and Ceramics II

Room: La Vista F (22nd Fl)
Session Chairs: Gang Chen, Ohio University; Lisa Klein, Rutgers University

1:20 PM

(GOMD-S4-086-2018) Fabrication of Micro- and Nanostructured Materials using Microreactor-Assisted Chemical Processes (Invited)

C. Chang*[1]; Y. He[1]; A. Chang[1]; M. TorresArango[2]; R. Malhotra[3]; K. Sierros[2]

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2. West Virginia University, USA
3. Rutgers University, USA

The Microreactor-Assisted Nanomaterial Deposition (MAND) process combines the merits of microreaction technology and solution phase synthesis of nanomaterials. This technique uses microreactors for the synthesis, assembly and deposition of nanomaterials. In synthesis, microreactor offers large surface-area-to-volume ratios within microchannel structures to accelerate heat and mass transport. This feature allows for rapid changes in reaction temperatures and concentrations leading to more uniform heating and mixing. Synthesis of nanomaterials in the required volumes at the point-of-application eliminates the need to store and transport potentially hazardous materials, while providing new opportunities for tailoring novel nanostructures. In our laboratory, MAND process was used to implement sol-gel chemistry for the fabrication of micro- and nanostructured based materials. In particular, the possibility of controlling the reaction kinetics and dynamics of the sol-gel

chemistry and process were explored and demonstrated. In this presentation, I will discuss the results of using microreactor-assisted chemical processes for the fabrication of functional nanoparticles, micro- and nanostructured thin films, and three-dimensional sol-gel glasses. In particular, the unique capability to tailor micro- and nanostructures through kinetics and dynamic control of the process will be addressed.

1:50 PM

(GOMD-S4-087-2018) Novel Approaches towards Create Colored Nanoporous Sol-Gel Glasses

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In this study, aluminum doped silica glass was prepared via a sol-gel method. The obtained sol-gel glass showed colors ranging from clear, light amber, dark brown and back to clear at different thermal annealing temperatures. This amber color has been briefly mentioned in the literature, but has not been carefully studied. Sol-gel aluminum-doped silica glasses of different colors were synthesized and characterized to better understand their structural and chemical natures. The results ruled out the possibility of carbon formation, elemental composition differences, and contamination by other elements such as Fe or S. The data suggest that the amber color could be either related to the porosity of the glass as the amorphous array of air pores with short-range order in the silica glass results in noniridescent colors or to defect centers. Another interesting finding from this study is a new approach to fabricate nanoporous, opaquely white glass by adding nanosized polystyrene spheres to the aluminum-doped silica glass. The original attempt was to intentionally create porous photonic glass. Surprisingly, opaquely white glasses were obtained after high-temperature sintering. Worm-like nanoporous structure along with micron-size air cavities were clearly shown from scanning electron microscopy images. It is believed that the worm-like nanoporous structure served as light scatters to render the opaquely white color.

2:10 PM

(GOMD-S4-088-2018) Silica Melting Gels Modified by Gold Nanospheres

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Organic-inorganic hybrid gels, in particular melting gels, have been studied for over a decade as a replacement for inorganic sealing glasses for microelectronics. By using melting gels, the sealing temperature is decreased significantly from 600ºC to 150ºC. Melting gels have the unique characteristic that their viscosity can be repeatedly decreased and increased by heating them up to 110ºC and cooling them down to 25ºC, until the network is fully crosslinked in a consolidation treatment. In order to tune the properties of this unique coating material, we used gold nanospheres, exploiting their optical and thermal properties. Methyltriethoxysilane (MTES) and dimethyldiethoxysilane (DMDES) were used to obtain melting gels with three different molar ratios, 65-35%, 70-30% and 75-25% (MTES-DMDES). Gold nanospheres were successfully incorporated in gels of all three ratios. FTIR, Raman, and UV-Vis spectroscopies and rotational rheometry were used to investigate the interface of the melting gels with the nanoparticles. The doped melting gels exhibit optical properties originating from the embedded (monodispersed) gold nanospheres and have altered rheological properties. Each ratio has a different way of incorporating the nanoparticles thus revealing intrinsic differences among the various silica networks.

2:30 PM

(GOMD-S4-089-2018) Silica Melting Gels Applied by Electrospraying

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Electrospray deposition is a convenient method for producing textured thin and thick films. According to the electrostatic breakup phenomenon in a uniform liquid stream, electrospraying results in the formation of uniform droplets of liquid. By generating micro-droplets, it is possible to deliver very small quantities of material at a continuous rate. The parameters that can be controlled include the spray composition, flow rate, solvent evaporation rate, distance to substrate and substrate temperature. Melting gels were prepared with methyl triethoxysilane (MTES) and dimethyl diethoxysilane (DMDES). The composition 65 mol% MTES-35 mol% DMDES was chosen, which has a glass transition temperature of -15.7°C. It was dissolved in 2-butanone at a 1 wt% loading. Because of the low T_g, it behaves as a thermoplastic liquid before it is converted into an irreversible structure at about 150°C. In this study, we deposited melting gel materials using different experimental conditions. We observed the systematic ways that the conditions affect the final morphologies of the films. The results show that electrospray can be used to generate structures from smooth, to rough, or cellular.

Session 4: Waste Immobilization - Processing III

Room: La Vista D/E (22nd Fl)

Session Chair: Charmayne Lonergan, Pacific Northwest National Lab

1:20 PM

(GOMD-S4-090-2018) Low-Activity Waste Vitrification and Off-Gas Sampling in a Laboratory-Scale Melter

D. Dixon*[1]; W. Eaton[1]; C. Stewart[1]; D. Cutforth[1]; J. Peterson[1]; J. Lang[1]; M. Hall[1]; J. Venarsky[1]

1. Pacific Northwest National Lab, USA

The path for immobilizing Hanford tank low-activity waste (LAW) for long-term storage is to mix these concentrated salt solutions with additive chemicals and minerals and then vitrify the LAW slurry feed in an electric melter. Small-scale melter tests are typically useful for gathering information about melting and off-gas behavior without requiring high volumes of slurry feed as used for large-scale melter tests and limit the committed resources for testing while providing dynamic information that can be difficult to acquire from crucible tests. An externally heated, laboratory-scale melter (LSM) with glass pouring capabilities and a unique off-gas treatment and sampling system has been fabricated at Pacific Northwest National Laboratory. The LSM vessel was constructed from Inconel 690 with an octagonal cross sectional area of 0.011 m^2. The off-gas system design allowed the total off-gas stream to be diverted to a sample loop consequently preventing the inherent issues related to required off-gas piping geometry for slip-stream sampling. Operational challenges and solutions as well as improvements to the LSM system during testing are discussed. Performance characteristics of the LAW glass production and melting behavior are planned between the LSM and other melter systems.

1:40 PM

(GOMD-S4-091-2018) Maximising waste volume reductions through vitrification of both waste clinoptilolite and Magnox sludge

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2. Sellafield Ltd., United Kingdom

Waste effluent from spent fuel storage ponds at the Sellafield site, U.K., is treated by passing through sand bed filters followed by ion exchange with clinoptilolite (a zeolite mineral). This generates significant quantities of both clinoptilolite and sand waste as well as significant quantities of sludge that is filtered by the sand beds (in total ~3700m^3). This sludge is primarily composed of $Mg(OH)_2$ and uranium oxide(s) from corrosion of Magnox fuel cladding and uranium metal fuel respectively. By combing the two waste streams together and conditioning via vitrification significant waste volume reductions are achieved as well as producing a waste form with a high chemical durability. Here we present results on lab-scale vitrification studies of the waste using several different glass formulations. Characterisation techniques include SEM/EDX, XRD with Rietveld, DTA, PCT chemical durability studies and XANES analysis. The key factor in the glass formulation is maximum magnesium solubility within the glass as, at high sludge waste loadings, forsterite crystallises. Forsterite is a nesosilicate composed of isolated silica tetrahedra, thus taking glass-formers away from the residual glass network. The main theme of this work is studying crystallisation of magnesium-containing phases from the glass and the effect this has on the material properties of the final waste form.

2:00 PM

(GOMD-S4-092-2018) Rheology of the cold cap

B. McCarthy*[1]; J. George[1]; D. Dixon[1]; M. Wheeler[1]; P. Hrma[1]; D. Linn[1]; J. Chun[1]; D. Cutforth[1]; A. A. Kruger[3]; M. Hujova[2]; R. Pokorny[2]

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During the vitrification of radioactive waste in a Joule-heated melter, aqueous melter feed slurry forms a cold cap, a reacting material, which floats on the surface of the molten glass while undergoing complicated physicochemical changes. The rheological behavior of the feed to glass conversion affects cold cap formation and shape, and is vital for modeling the conversion process. Slurry feed simulant and fast dried slurry solids representing the cold cap were used to investigate the rheological behavior of the feed as it transforms into glass. Both low-temperature and high-temperature rheometry were performed, with a new scheme applied to obtain rheological responses for the feed and estimate its viscosity. Our study, provides physical insights to feed to glass conversion process that proceeds in four stages that form distinct regions in the cold cap: (i) a fast-spreading boiling slurry that evaporates at the cold cap top surface, (ii) a porous solid region (viscosity > 10^8 Pa s) containing reacting solids and molten salts, (iii) a plastic region in which glass-forming melt connects the refractory solids (~10^8 to ~10^6 Pa s), and (iv) a viscous foam layer in which the viscosity drops from ~10^5 to ~10^1 Pa s.

2:20 PM

(GOMD-S4-094-2018) Heat Capacity of Simulated LAW Waste Glass

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The Hanford site in Washington State is home of the Tank Waste Treatment and Immobilization Plant (WTP), which will separate the wastes into High Level Waste and Low Activity Waste (LAW) fractions and vitrify each fraction into borosilicate glasses for disposal. In nuclear waste vitrification, a mixture of radioactive waste and glass formers is charged into a continuous fed electric glass-melting furnace and the molten glass is then poured into stainless steel canisters to cool for future disposal. The heat contained in the hot glass must be removed from the containers and this must be accomplished within the production schedule constraints of the plant operation. The heat release depends on the thermal properties of the glass and the data analysis of these properties will validate the cooling calculations used for facility design and operation. A long term goal is to develop a larger database of waste glass thermal properties in an effort to improve the overall understanding of composition effects on such properties from a fundamental level. Heat capacity of ten Low Activity Waste Hanford waste glasses with systematic variation in composition were measured and analyzed. The resulting data are valuable in the design of the pour cave and overall operation of the WTP.

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