August 13-16, 2018
Ruth Pike Auditorium, University Park, PA

PROGRAM

Thank you to our sponsors:
This August, under the direction of John C. Mauro and sponsorship by the American Ceramic Society, The Pennsylvania State University (Penn State) will host the 20th University Conference on Glass Science. Announcement of this conference brought to mind the 6th in this series also held at Penn State in 1981 when a historic debate on the atomic structure of glass took place between two of the foremost and highly respected materials scientists of that time – the late Rustum C. Roy and Alfred R. Cooper. More about this debate below.

For the record, under the leadership of Delbert E. Day and the late Norbert J. Kreidl, this series of conferences originated at The University of Missouri - Rolla, now Missouri University of Science and Technology (Missouri S&T). The first three in this series were convened in Rolla. In 1977, upon agreement reached by L. David Pye, Delbert E. Day, and the late Robert H. Doremus and Guy E. Rindone, the series was expanded to include Alfred University, Rensselaer Polytechnic Institute (RPI) and Penn State. The 4th in this newly formalized series was held at Alfred in 1977, the 5th at RPI in 1979, the 6th at Penn State in 1981, and, after several rotations, the 14th at Lehigh University in 1997. The 21st is scheduled to be convened by Missouri S&T in 2020 with the theme “Water in Glass and Glass in Water.” As an aside, this series was inspired by another rotated among Alfred University, The
University of Notre Dame, The University of California, and The University of North Carolina only in this series, the theme was ceramic science.

The conference theme of the 1981 Penn State meeting was “Glass Microstructure: Surface and Bulk.” At the suggestion of Cooper, the opening session of this conference was dedicated to William H. Zachariasen who had authored fifty years earlier arguably one of the most profound scientific contributions in the history of glass science, “The Atomic Arrangement in Glass.” Intensely debated over its meaning and validity compared to other structural models, it gave rise to what would become known as the random network model (RNT) of glass structure. Cooper presented the keynote address of this session he entitled “W.H. Zachariasen – The Melody Lingers On.”

Therein lies the origin of the debate alluded to above. Shortly after the start of Cooper’s presentation, Roy entered the conference room joining those in attendance. At the end of Cooper’s presentation, the usual polite questions were raised and answered with corresponding politeness. Breaking with standard presentation protocol, Roy then joined Cooper on the presentation stage and proclaimed he fully agreed that the “Zachariasen melody lingers on - the only trouble it is off key.” Game on! Given the worldwide professional standing of Cooper and Roy, it was a time for assistant professors to listen, learn, and remain silent.

Multiple overhead transparencies were utilized in support of respective points and counterpoints, beliefs and counter beliefs, conclusions and counter conclusions either for or against the validity of the Zachariasen model. In his presentation material, Cooper fully embraced the model which he believed gave significant insight into the properties of glass and glass formation not only in oxide systems but metallic ones as well. Whereas, ostensibly opposed to what he believed was an over embracement of the Zachariasen model by the international glass science community, Roy argued several objections could be raised including the existence of inherent thermodynamic driving forces in glass forming systems which give rise to more ordered atomic structures - a viewpoint supported in part by theories of amorphous phase separation and homogenous crystal nucleation. He further argued that glass formation is more of a kinetic than structure-based phenomenon as set forth in the Zachariasen model.

In the end, the debate seemed to result in an amical draw between the two internationally renowned scientists. That so many of us remember this moment to this day speaks to a belief we had witnessed a seminal moment in the history of glass science.

The enduring and perhaps greater meaning of this debate is in realizing it was but one chapter in the on-going saga of the development of theory related to the structure, properties, processing and application of glass.

We should also be mindful that while there are many desired outcomes of science as a discipline, by far the greatest is developing theory for what can be observed, measured, and validated. That is, the essence of science is to predict. To obtain a full understanding of glass structure theory, predications should involve both characterization and property measurements which in turn support processing and applications. Further, new theories are built on past successes. Thus, with its emphasis on chemical bonding, localized structure and ion size, the RNT gave rise to the development of the band and ligand field theories of glass and the strengthening of glass by ion exchange. Similarly, structural information obtained through advanced characterization methods, including computer simulations, are readily interpreted in terms of the localized structure described by Zachariasen and later expanded by G.N. Greaves with his “modified random network theory” for glass structure. This structure-based approach coupled with the kinetic theory of glass formation promoted by Roy and developed by D.R. Uhlmann and others, has proved to be very useful in exploring new glass-forming systems. Collectively, both considerations have paved the way for a greater understanding of the properties of glass and by extension, success or failure of industrial processing for the making of glass for specific applications.

A scheduled presentation by Adriano C. Wright at this year’s Glass and Optical Materials Division meeting in San Antonio entitled “Oxide Glass Structure: Towards a Working Hypothesis for the 21st Century,” and the planned program for next year’s International Congress on Glass forecasts there will be further refinements of various theories related to structure and glass formation in general.

In summary, the intent of this communication was to stop and take a look back at a seminal moment in the history of glass science at the time which some believe is the arrival of the Glass Age and others - the emergence of the nanotechnology paradigm. Equally important was reaffirming the role glass plays in nearly all aspects of everyday life including communications, transportation, architecture and healthcare among others. A recent article in the Atlantic declaring glass as “Humankind’s Most Important Material” gives support and meaning to all of the above.

Contact: L. David Pye is Dean Emeritus at Alfred University. Contact him at pye@alfred.edu.

Note—The essentials of this history will be published as a Letter to the Editor in the American Ceramic Society Bulletin, August 2018.
## PROGRAM AT A GLANCE

### Monday 2018 August 13

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
<th>Presenter</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>7:30</td>
<td>Registration/breakfast</td>
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<tr>
<td>8:30</td>
<td>Opening remarks</td>
<td>John C. Mauro</td>
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<tr>
<td>8:40</td>
<td>Opening Session (Session Chair: John C. Mauro)</td>
<td>Arun Varshneya</td>
<td>Chemically Strengthened Glass (T)</td>
</tr>
<tr>
<td>9:40</td>
<td></td>
<td>Mario Affatigato</td>
<td>Thermophysical Properties of Glasses Measured using Aerolevitation (T)</td>
</tr>
<tr>
<td>10:40</td>
<td>Break</td>
<td>Shiv Prakash Singh</td>
<td>Nanoglass: A prospective nanostructured glassy materials (T)</td>
</tr>
<tr>
<td>11:00</td>
<td>Lunch</td>
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<tr>
<td>12:00</td>
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<tr>
<td>1:20</td>
<td>Glass Mechanics</td>
<td>Emily Aaldenberg</td>
<td>Permanent Bending of Thin Glass Plates (R)</td>
</tr>
<tr>
<td>1:40</td>
<td></td>
<td>Nathan Card</td>
<td>Design and testing of a large sub-hemispherical glass port for a deep-sea camera housing (R)</td>
</tr>
<tr>
<td>2:00</td>
<td></td>
<td>Kuo-Hao Lee</td>
<td>Crack Initiation in an Indented Metallic Glass with Embedded Nanoparticle (R)</td>
</tr>
<tr>
<td>2:20</td>
<td></td>
<td>Nisha Sheth</td>
<td>The effects of acid leaching on the mechanical properties of soda lime glass (R)</td>
</tr>
<tr>
<td>2:40</td>
<td></td>
<td>Xinyi Xu</td>
<td>Flexural strength testing in lithium disilicate glass-ceramics (R)</td>
</tr>
<tr>
<td>3:00</td>
<td>Break</td>
<td></td>
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</tr>
<tr>
<td>3:20</td>
<td>Glass Relaxation (Session Chair: Arun K. Varshneya)</td>
<td>John Mauro</td>
<td>Glass Transition and Relaxation Behavior (T)</td>
</tr>
<tr>
<td>4:20</td>
<td></td>
<td>Ozgur Gulbiten</td>
<td>Viscous flow of medieval cathedral glass (R)</td>
</tr>
<tr>
<td>4:40</td>
<td>Optical Glasses (Session Chair: Arun K. Varshneya)</td>
<td>Claudia Goncalves</td>
<td>Ge20Te80-xSex Glasses as Materials for Far-Infrared Applications: a Theoretical and Spectroscopic Investigation (R)</td>
</tr>
<tr>
<td>5:00</td>
<td></td>
<td>Myungkoo Kang</td>
<td>Ultra-Low Dispersion Multicomponent Thin Film Chalcogenide Glass for Broadband Gradient Index Optics (R)</td>
</tr>
</tbody>
</table>

### Tuesday 2018 August 14

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
<th>Presenter</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:00</td>
<td>Breakfast</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8:40</td>
<td>Glass Structure (Session Chair: Jincheng Du)</td>
<td>Nicholas Smith</td>
<td>Important Aspects of Glass Surfaces in Modern Applications (T)</td>
</tr>
<tr>
<td>9:40</td>
<td></td>
<td>Seong Kim</td>
<td>XPS and IR Analysis of Silicate Glass Network (T)</td>
</tr>
<tr>
<td>10:40</td>
<td>Break</td>
<td>S.K. Sundaram</td>
<td>Terahertz Glass Science and Engineering (T)</td>
</tr>
<tr>
<td>11:00</td>
<td>Lunch</td>
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<td>12:00</td>
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<tr>
<td>1:20</td>
<td></td>
<td>Alexis Clare</td>
<td>Bond-Type Influence on Glass Structure (T)</td>
</tr>
</tbody>
</table>

Thank you to our sponsors: pg. 4 (T) Tutorial Presentation (R) Research Presentation
## PROGRAM AT A GLANCE

### Wednesday 2018 August 15

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Speaker(s)</th>
<th>Presentation Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>2:20</td>
<td><strong>Glass Structure cont.</strong></td>
<td>Gabriel Cocking</td>
<td>The Introduction of 4+ cations in Nepheline glasses (R)</td>
</tr>
<tr>
<td>2:40</td>
<td></td>
<td>Nicholas Stone-Weiss</td>
<td>Impact of pressure on structure and properties of sodium aluminoborosilicate glasses (R)</td>
</tr>
<tr>
<td>3:00</td>
<td><strong>Break</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3:20</td>
<td></td>
<td>Manzila Tuheen</td>
<td>Structures of Lanthanum Phosphate and Aluminophosphate Glasses from Molecular Dynamics Simulations (R)</td>
</tr>
<tr>
<td>3:40</td>
<td></td>
<td>Zhe Wang</td>
<td>Structure of Glassy Silica: Role of the Synthesis Method (R)</td>
</tr>
<tr>
<td>4:00</td>
<td><strong>Bioactive Glasses</strong> (Session Chair: Liping Huang)</td>
<td>Yinan Lin</td>
<td>Long-term bone regeneration, mineralization and angiogenesis in rat calvarial defects implanted with strong porous bioactive glass (13–93) scaffolds (R)</td>
</tr>
<tr>
<td>4:20</td>
<td><strong>Ionic Conductivity</strong> (Session Chair: Liping Huang)</td>
<td>Steve W. Martin</td>
<td>New developments in fast in conducting glasses: Towards enabling a new paradigm of high energy density and battery safety (T)</td>
</tr>
<tr>
<td>5:20</td>
<td></td>
<td>Steven J. Kmiec, Adriana Joyce</td>
<td>Ionic conductivity and short range order structures of new oxy-sulfide sodium thiophosphate glasses (R)</td>
</tr>
<tr>
<td>8:00</td>
<td><strong>Breakfast</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8:40</td>
<td><strong>Surfaces &amp; Durability</strong> (Session Chair: Seong Kim)</td>
<td>Richard Brow</td>
<td>Dissolution Studies of Specialty Glasses for Nuclear Waste and Biomedical Applications (T)</td>
</tr>
<tr>
<td>9:40</td>
<td></td>
<td>Ashutosh Goel</td>
<td>Nuclear Waste Vitrification - Grand Challenges and Open Questions (T)</td>
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<tr>
<td>10:40</td>
<td><strong>Break</strong></td>
<td></td>
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</tr>
<tr>
<td>11:00</td>
<td><strong>Lunch</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12:00</td>
<td><strong>Chemical Durability cont.</strong> (Session Chair: Nicholas Smith)</td>
<td>Minoru Tomozawa</td>
<td>Water and Glasses (T)</td>
</tr>
<tr>
<td>1:20</td>
<td></td>
<td>Nikhila Balasubramanya</td>
<td>The Effect of Mixed Network Former on the Spinel Formation in High Level Nuclear Waste Glasses (R)</td>
</tr>
<tr>
<td>2:20</td>
<td></td>
<td>Huseyin Kaya</td>
<td>Effect of Surface Conditions on Glass Corrosion (R)</td>
</tr>
<tr>
<td>3:00</td>
<td></td>
<td>Hongshen Liu</td>
<td>Effects of surface initial condition on aqueous corrosion of glass (R)</td>
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<tr>
<td>3:20</td>
<td><strong>Break</strong></td>
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</tbody>
</table>
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PROGRAM AT A GLANCE

3:40 **Chemical Durability cont.** Dien Ngo  
Spectroscopic Study of ISG Glass Corroded in Aqueous Solutions (R)

4:00  
Arron Potter  
The alkali leaching mechanism in soda-lime silicate glass (R)

4:20 **Crystallization** (Session Chair: Mathieu Bauchy) Volkmar Dierolf  
Crystal Lattice Engineering during Laser-induced Single Crystal Growth (T)

5:20  
Courtney Au-Yeung  
In situ observation of Sb2S3 crystal formation in Sb2S3 glass by micro x-ray diffraction (R)

5:40  
Alessio Zandona  /New insights into the crystallization mechanism of TiO2-nucleated cordierite glass-ceramics: a multi-analytical approach (R)

6:30 **Reception/Dinner** Hintz Alumni Center

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**Thursday 2018 August 16**

8:00 **Breakfast**

8:40 **Glass Synthesis** (Session Chair: Ashutosh Goel) Liping Huang  
In-situ Light Scattering Studies of Glasses under High Temperature and/or High Pressure Conditions (T)

9:40  
Paul Miller  
Evaluation of wet silicon oxidation mechanisms using infrared spectroscopy (R)

10:00  
Ye Luo  
Synthesis and Characterization of GeO2-SiO2-ZnO-K2O Optical (R)

10:20  
Carly Mathewson  
Efficacy of Fining Agents in Extremely Viscous and High Melting Aluminosilicate Glass (R)

10:40 **Break**

11:00 **Glass Modeling** (Session Chair: John C. Mauro) Jincheng Du  
Molecular Dynamics Simulations in Glass Research: From Structure of Bioactive Glasses to Surface Reaction and Properties of Nuclear Waste Glasses (T)

12:00 **Lunch**

1:20  
Mathieu Bauchy  
The surface reactivity of sodium silicate glasses in aqueous environment under varying pH: a ReaxFF molecular dynamics study (R)

2:20  
Seung Ho Hahn  
Topological Constraint Theory of Glass (T)

2:40  
Amreen Jan  
Molecular dynamics simulation of ballistic effects in simplified nuclear waste glasses (R)

3:00 **Break**

3:20  
Katelyn Kirchner  
Statistical Mechanics of Topological Fluctuations in Glass-Forming Liquids
<table>
<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Presenter</th>
<th>Presentation Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>4:00</td>
<td></td>
<td>Siddharth Sundararaman</td>
<td>New interaction potentials for multi-component oxide glasses (R)</td>
</tr>
<tr>
<td>4:20</td>
<td></td>
<td>Yongjian Yang</td>
<td>Understanding of Structure and Properties of ZIF Glass via Computational Modeling (R)</td>
</tr>
<tr>
<td>4:40</td>
<td></td>
<td>Collin Wilkinson</td>
<td>A topological constraint model is developed to elucidate the coordination environment of tellurite glasses (R)</td>
</tr>
<tr>
<td>5:00</td>
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<td>Junjie Zhao</td>
<td>Use Molecular Dynamics Simulations to Predict Possible Crystal Phases from Oxyfluoride Glass Phase Separation (R)</td>
</tr>
<tr>
<td>5:20</td>
<td>Closing Remarks</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Emily Aaldenberg, T.A. Blanchet, Arron Potter, and Minoru Tomozawa  
Rensselaer Polytechnic Institute  
**PERMANENT BENDING OF THIN GLASS PLATES**  
Relaxation of stress in glass typically occurs at or above the glass transition range, however, relaxation of surface stress was found to occur at temperatures far below the Tg of the glass. Previously, the kinetics of surface stress relaxation for various glasses were measured from the permanent bend of a released fiber after being heat-treated with a prescribed bend. In these studies, the prescribed bend was a “U-shape,” where the ends of the fiber came into contact parallel with the faceplates which apply the bend. From these measurements, it was observed that increased water vapor pressure and elevated temperature both led to an increase in the permanent bending of the fiber. In the present study, permanent bending of thin soda-lime silicate glass plates with the edge of the sample not parallel to the faceplate is analyzed and the rate of surface stress relaxation for these samples is compared to the rate calculated from the fiber bending experiments. This geometry allows the use of short samples bent to low stresses with a larger area under uniform stress. Additionally, the cumulative relaxation of the same sample can be measured by using the thin plates with a rectangular cross-section.

Mario Affatigato, Coe College  
**THERMOPHYSICAL PROPERTIES OF GLASSES MEASURED USING AEROLEVITATION**

Courtney Au-Yeung, Lehigh University  
**IN SITU OBSERVATION OF Sb2S3 CRYSTAL FORMATION IN Sb2S3 GLASS BY MICRO X-RAY DIFFRACTION**  
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 lattice formation that proceeds via crystal nucleation and growth. Here we present in situ observation during Sb2S3 crystal formation under laser/X-irradiation, which provides insight of the origin of the rotating lattice within these single crystal architectures. 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. Crystal lines were fabricated using the x-ray beam and a rotation along the scanning direction was identified. A computational model was created to determine the temperature gradient of the x-ray beam during crystallization. The implications of these observations for lattice rotation and crystal growth in a confined medium will be discussed.

Nikhila Balasubramanya, Mohamed Naji and Ashutosh Goel  
Rutgers-The State University of New Jersey  
**THE EFFECT OF MIXED NETWORK FORMER ON THE SPINEL FORMATION IN HIGH LEVEL NUCLEAR WASTE GLASSES**  
During the processing of high level wastes, Fe, Cr, Ni, Mn, Zn, and Ru precipitate into spinels. The vitrification of high Fe, Ni and Cr containing waste faces the problem of the crystallization of spinel in the melter cold cap that poses a threat to the efficiency of the melter and also brings down the volumetric efficiency of the vitrified waste. The objective of this study is to bring a fundamental understanding of the effects of melt chemistry on nucleation and crystallization of spinels in HLW glasses formulated from a simplified composition.
representing the AZ-101 tank. The research focuses on understanding the impact of the mixed network former on the spinel formation in the glass compositions of the system Na2O-Al2O3-B2O3-SiO2-Fe2O3-MnO-NiO-Cr2O3. Glass compositions of the above mentioned system were synthesized and the effect of varying Al2O3/SiO2 and B2O3/SiO2 ratios on the spinel crystallization tendencies were studied. The compositions were synthesized using two different heat treatment techniques, one representing the melter operating conditions and the other, the melter idling conditions. The synthesized glasses have been characterized for their amorphous and crystalline content using X-ray diffraction, followed by their microstructural evaluations by electron microscopy. An attempt has been made to correlate the crystallization behavior of these glasses with the octahedral site preferential energy and crystal field stabilization energy which have been found to play a very determining role in predicting spinel formation.

**Mathieu Bauchy, University of California**

**TOPOLOGY CONSTRAINT THEORY OF GLASS**

Rigidity and topology concepts have proved to be powerful tools for predicting the composition, temperature, and pressure dependence of glass properties. Topological constraint theory reduces complex atomic networks into simpler mechanical trusses and, thereby, elegantly captures the important features of glasses’ atomic networks while filtering out unnecessary second-order structural details that do not affect macroscopic properties. In this tutorial, I will introduce basic concepts of molecular rigidity and present how topological constraint theory can be used to predict the glass-forming ability, hardness, and dissolution rate of oxide and chalcogenide glasses.

**Richard Brow, Missouri University of Science and Technology**

**DISSOLUTION STUDIES OF SPECIALTY GLASSES FOR NUCLEAR WASTE AND BIOMEDICAL APPLICATIONS**

Silicate, aluminosilicate, and borosilicate compositions constitute the (Nittany) lion’s share of commercial oxide glass products, and their interactions with aqueous environments determine their suitability for a variety of applications from nuclear waste encapsulation (e.g., the International Simple Glass and SON68) to biomedical applications (e.g., 45S5). Less-well known are dissolution studies of glasses based on borate and phosphate chemistries, although these types of glasses have also found recent applications as waste hosts and biomedical materials. In this lecture, I will review the relationships between composition and molecular-level structures of simple Na-Ca-phosphate, Na-Fe-phosphate, and Na-Ca-borate glasses, then show how their structures control dissolution rates in various aqueous solutions. Factors that control dissolution kinetics include solution chemistry, temperature, and pH, as well as the precipitation of phases like hydroxyapatite.

**Nathan Card, Francois Cazenave, Eric Baker, George D. Quinn, Paul Remijan, Jonathan Salem, and Arun K. Varshneya**

Saxon Glass Technologies

**DESIGN AND TESTING OF A LARGE SUBHEMISPHERICAL GLASS PORT FOR A DEEP-SEA CAMERA HOUSING**

A dome-shaped H-K9L glass port was developed for a sub-sea camera for use on an autonomous underwater vehicle at water depth to 2,000m. The unusually large (250mm diameter) and flattened shape of the dome was dictated by optical requirements. Using finite element analysis and fractography to guide, a design that would pass 2,750 psi pressure was developed. Weibull parameters, fracture toughness and slow crack growth parameters of the glass were measured. 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, larger deep-water camera domes of newer shapes having better optical quality with predictable reliability can be made.

**Alexis Clare, Kathryn Russell, Alfred University**

**Bond-Type Influence on Glass Structure**

Zachariesens original hypothesis of melt quenched glasses needing to be a majority of covalent compounds that have small coordination numbers and form a disordered network. There have been a number of melt quenched glasses that don’t appear to fit this description such as heavy metal fluoride glasses and some bulk metallic glasses that appear to favor the “confusion principle” for glass structure; i.e. if enough different atoms/ions are together and quenched, usually faster than their covalent compound counterparts they will make a glass. However, many ionic compounds, for example, beryllium fluoride which is a good glass former, show significant covalency to their bonding, as do some metallic glasses; for example, refractory metals. To what extent the degree of covalency affects the glass formation and stability against devitrification versus the variation of size and types of atoms/ions in the melt quenched glass will be discussed.

**Gabriel Cocking, Emily Nienhuis and Dr. John McCloy**

**Washington State University**

**The Introduction of 4+ Cations in Nepheline Glasses**

Crystallization of aluminosilicates in Hanford high-level nuclear waste (HLW) glass is problematic, as it decreases the chemical durability of the remaining glass. The purpose of this study is to determine how the addition of Sn affects the crystallization of nepheline (NaAlSiO4) in a simplified HLW glass — specifically, if Sn promotes or hinders crystallization upon cooling. In this study, Sn was substituted for Si in the simplified glass to give a glass composition of NaAl6xSn1-xO4. Sn4+ was targeted and selected based on its hypothesized ability to replace the Si atoms in the glass, and potential crystalline phases, as Sn and Si can have similar coordination numbers with oxygen. The resulting glasses were heat treated and subjected to quantitative x-ray diffraction (XRD) and Rietveld Refinement to determine if increasing Sn addition hindered or promoted crystallization upon cooling, and what crystal phases formed. Additionally, TGA-DTA was performed to measure the glass transition temperature of the glasses (Tg) to determine the effect of Sn on the glass formability of the system.


**Lehigh University**

**Crystal Lattice Engineering during Laser-Induced Single Crystal Growth**

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 and 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 method for fabricating single crystal waveguides in glass 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 nonreciprocal optical devices.
Jincheng Du, University of North Texas

**MOLECULAR DYNAMICS SIMULATIONS IN GLASS RESEARCH: FROM STRUCTURE OF BIOACTIVE GLASSES TO SURFACE REACTION AND PROPERTIES OF NUCLEAR WASTE GLASSES**

Computational materials play an increasingly important role in materials research and discovery, with ever-increasing computing power and development of new methodologies. Molecular dynamics simulation is an established atomistic simulation method that is widely used in various scientific fields. Due to the lack of long-range order like crystalline materials, understanding the structure of glasses (and other amorphous materials) poses a significant scientific challenge. MD simulations, in particular, is a unique and powerful technique that is capable of generating atomistic-level structures of glasses and correlating them to different properties and behaviors with structure features. As a result, MD and related simulation methods find applications in glass research from university labs to industrial environments. In this talk, I will present a brief history of MD simulations of glasses. Then the basics of MD simulations of glasses: from the choice of empirical potentials to the procedure to generate glass structure will be presented. Two examples of applications of MD simulations based on the research results of our group will then be presented: the first one is on the simulations of phosphosilicate bioactive glasses, where the structural features of bioactive glasses and how to correlate them with bioactivities discussed. The second example is on the study of borosilicate nuclear waste glasses, where the bulk and surface structure features from MD simulations will be presented. Additional topics such as simulations water-glass interactions using reactive potentials will be discussed. Lastly, challenges of MD simulations of glasses such empirical potential development and validation of simulation results will be presented.

Claudia Gonçalves, Raphaël Mereau, Eric Furet, Michaël Deschamps, Laurent Le Pollès, Claire Roiland, Pierre Florian, Lila Bouéssel du Bourg, Virginie Nazabala, Catherine Boussard-Pledel, Marc Dussauze, and Bruno Bureau
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**GE20Te80-xSex GLASSES AS MATERIALS FOR FAR-INFRARED APPLICATIONS: A THEORETICAL AND SPECTROSCOPIC INVESTIGATION**

We report results of a study to rationalize the substituent effect on the glass structure and physical properties for a new generation of far-infrared transmitting telluride materials. This field is currently receiving increased attention because of the potential applications of such glasses in photonic systems such as perimeter monitoring, night vision or in the control of greenhouse gas emissions. [1]. Despite their intrinsic qualities, limited structural information has been published for materials within this glassy system. A multi-technique approach has been employed which utilizes solid-state NMR to probe local order of the telluride glasses, combined with vibrational spectroscopic techniques including Raman and Infrared, which provide insight into the organization of the structural network and provide an understanding of the structural and physical properties of new families of telluride glasses [2, 3].

An important objective of the work is comparison of spectroscopic data with results of theoretical analysis, which involves calculation of spectral parameters within experimental spectra. An in-depth knowledge of the organization in glasses is essential for any rationalization and optimization of their physical properties. In this context, we report the first solid-state NMR results for ternary glasses Ge20Te80-xSex. The work involves rather unusual nuclei such as 73Ge and 77Se with atypical spectroscopic characteristics (low gamma, strong anisotropy, and strong quadrupole constant). The assignments of vibratory modes are proposed thanks to DFT calculations implemented using Gaussian software. This coupling between calculation and spectroscopic measurements provides insight into the complex spectral evolution. Findings of our effort show the first structural assessment of the overall Ge20Te80-xSex glass series. For
the selenium-rich glasses, when tellurium is added, Te is shown to fit into the homopolar Se-Se chains, forming mixed chains, with Se-Te type units. From a certain %mol of tellurium, we show binding of germanium to form mixed tetrahedral units. In the case of tellurium-rich glasses, we shown that when selenium is added, formation of mixed tetrahedra connected to each other by Te-Te homopolar chains occurs. Moreover, no vibrational signature of the mixed-chain modes (210 cm$^{-1}$) is observed, which confirms the only presence of the vibration mode $\nu_{Te-Te}$. A summary of these observations are presented.

Ozgur Gulbiten, John C. Mauro, Xiaoju Guo, and Olus Boratav
Corning Incorporated

VISCOUS FLOW OF MEDIEVAL CATHEDRAL GLASS

A popular urban legend concerns the apparent flow of stained glass windows in medieval cathedrals, where the glass windows are commonly observed to be thicker at the bottom than they are at the top. Advances in glass transition theory and experimental characterization techniques now allow for us to address this urban legend directly. In this work, we investigate the dynamics of a typical medieval glass composition used in Westminster Abbey. Depending on the thermal history of the glass, the room temperature viscosity is on the order of $10^{24}$ to $10^{25}$ Pas, about 16 orders of magnitude lower than found in a previous study of soda lime silicate glass. Despite this significantly lower value of the room temperature viscosity, the viscosity of the glass is much too high to observe measurable viscous flow on a human time scale. Using analytical expressions to describe the glass flow over a wall, we calculate a maximum flow of ~1 nm over a billion years.

Seung Ho Hahn, The Pennsylvania State University

THE SURFACE REACTIVITY OF SODIUM SILICATE GLASSES IN AQUEOUS ENVIRONMENT UNDER VARYING pH: A REAXFF MOLECULAR DYNAMICS STUDY

The initial stages of the glass-water reaction in different aqueous environment (varying pH) were investigated using reactive molecular dynamics (MD) simulation. The MD framework used in this work is based on the ReaxFF reactive force field with the parameters that were recently developed to correctly describe the detailed chemical dissolution mechanisms of silicate glasses. In this work, the modeling of sodium silicate glass-water interface focused on the chemical modifications which are followed by the ion-exchange process between sodium ions (Na$^+$) from glasses and protons (H$^+$) from water. From the simulation results, it is observed that chemical reactions involving the Na$^+$/H$^+$ ion-exchange is stoichiometrically met after several hundred picoseconds of the simulation time scale in case for the neutral pH conditions. This indicates that the formation of silanol groups (Si-OH) may depend of the surface sites, and that the water dissociation pathway is relevant to the initial dominance of Na$^+$-water interactions upon contact with water. The simulation results with acid or base environments showed that the abundance or lack of proton species in the aqueous medium resulted in different number in evolution of silanol concentration, thereby affecting the overall density profile of the alkali-leached surface. In addition, the penetration of water molecules to the bulk sodium silicate was captured. Depending on the size of the channel formed by long-range disordering of Si-O network, protons diffuse into the surface through the hopping mechanism from one NBO (non-bridging oxygen) sites to the other or as an intact water molecule without affecting nearby glass network.

Liping Huang, Rensselaer Polytechnic Institute

IN-SITU LIGHT SCATTERING STUDIES OF GLASSES UNDER HIGH TEMPERATURE AND/OR HIGH PRESSURE CONDITIONS

Characterizing the disordered structure of glass at the atomic level remains a grand challenge. On the macroscopic level, glass is structurally homogenous and isotropic; only two independent elastic constants are
needed to characterize its elasticity. Elastic constants are simple to define and easy to measure, and are directly related to the interatomic forces and potentials, embodying the local structure and bonding information. Therefore, perturbing the glass with thermal or mechanical agitation (e.g., temperature or pressure) and measuring the changes in elastic moduli, can be used as a probe to gain insights into the atomic level structure of glass. We developed in-situ Brillouin light scattering technique to study the elastic properties of glass under high temperature or high pressure conditions. High temperature measurements were carried out in an optical furnace up to 1500 degree Celsius, a diamond anvil cell was used to carry out high pressure experiments up to 30 GPa. Our studies show that elastic properties of glass, and their temperature and pressure dependence are very sensitive to the structure and bonding of glass, as confirmed from in-situ Raman scattering experiments. Therefore, in-situ Brillouin and Raman light scattering can be used as non-contact and non-invasive techniques to study the atomic structure of glass from its elastic and dynamic response to external stimuli.

Amreen Jan, CEA Marcoule, France and PNNL, USA

Molecular Dynamics Simulation of Ballistic Effects in Simplified Nuclear Waste Glasses

Immobilization of High Level Waste (HLW) in borosilicate matrix and further disposal into geological repository has been regarded as one of the best way for long term isolation of HLW from biosphere [1]. Radionuclides are expected to stay confined until glass matrix has been breached by water and it begins to alter. Recently, an increase in glass alteration rate was observed in irradiated samples (with dominant ballistic dose) as compared to non-irradiated samples [2] [3]. Other studies using doped glasses, external irradiation techniques and molecular dynamics have now confirmed that ballistic effects caused by recoil nuclei, on alpha decay, will be the dominant source of irradiation damage on the long term. Ballistic effects have been observed to induce macroscopic and microscopic structural changes e.g. swelling, decrease

in hardness, increase in fracture toughness and structural disorder and depolymerisation in the glasses [4]. Thus, it becomes necessary to study such changes and their impact on the physical and chemical durability of this glass. In the current study, molecular dynamics simulation of ballistic effects have been investigated in simple sodium borosilicate \((Na_{2}BO_{2})n=1\) and sodium alumino-borosilicate \((Al_{2}O_{3}–Na_{2}BO_{2})n=1\) glass compositions, by exposing such glasses to series of displacement cascades, wherein heavy projectiles cause atomic displacements by elastic collisions and progressively damage the bulk glass. The accumulated pressure or stored energy inside the glass was found to saturate with deposited energy. Furthermore, structural analysis of the irradiated glasses revealed a decrease in density, depolymerisation, increase in intermediate, short range disorder and randomness. The magnitude of damage was found to depend on the glass composition and, in general, aluminosilicate glasses were found to be slightly less damaged, after irradiation, as compared to borosilicate glasses. An ongoing study on, impact of such structural evolutions under irradiation, on alteration of glass will also be discussed.


Ultra-Low Dispersion Multicomponent Thin Film Chalcogenide Glass for Broadband Gradient Index Optics

Microlens arrays have become increasingly important for a wide range of applications, such as compact imaging, optical sensing, and fiber coupling. As a result, there has been growing demand for the development of low-cost, scalable fabrication techniques capable of manufacturing such high performance components. Although significant
progress has been made using conventional spherical lenses, chromatic aberration and small operational bandwidth remains a lingering problem for infrared imaging. These challenges are difficult to overcome due to the lack of materials capable of broadband transmission as well as the feasibility for manufacturing multi-element/multi-material systems with micro-scale dimensions. Novel gradient refractive index (GRIN) materials have been engineered to provide dispersive properties which lie far outside those found in nature, providing new degrees of freedom for optical design as well as the potential for use in new applications. This work reports progress on a novel photo-thermal process to spatially modulate high-index nanocrystals within a meta-stable thin film chalcogenide glass, composed of Ge-As-Pb-Se (GAP-Se) constituents, thereby achieving ultra-low dispersion over an unprecedented bandwidth of 1 to 12 µm wavelength while enabling control of an arbitrary index gradient required for GRIN optics [1]. Spatially tailorable refractive index change is induced using a two-step fabrication approach, capable of fabricating achromatic optical components. Sub-bandgap laser exposure is used to create non-bonded, atomic defects in the metastable, homogeneous thin film GAP-Se glass which lead to the formation of Pb-rich amorphous secondary phases within the film. These phases are subsequently crystallized into a high-index crystal phase by thermal treatment. The nanocrystal density is modulated by the laser dose, providing a spatially tailorable index change up to ~ 0.1. The measured chromatic properties after the index change were found to be superior to conventional homogeneous infrared media throughout the entire extent of the bandwidth. Finally, employing the knowledge of laser-material modification and the correlation to phase conversion and index modification, the technique was successfully used to create and demonstrate clear optical functionality in the form of an infrared diffraction grating.

Huseyin Kaya, The Pennsylvania State University

**EFFECT OF SURFACE CONDITIONS ON GLASS CORROSION**

Alteration layer, which forms at the surface as a result of corrosion, acts as a passivating layer by limiting diffusion of chemical species that take place in the corrosion reactions causing a significant decrease in corrosion rate. Properties and stability of this layer are extremely important as it determines corrosion rate. In the case of the breakdown of the alteration layer, a corrosion rate resumption occurs. To date, studies have characterized glass corrosion from mass balance of the chemical species that dissolve from glass, and surface conditions effects haven’t been understood yet. Structure of the alteration layer and how it evolves are important to uncover to understand the stability of this layer. Moreover, aqueous species within the layer need to be characterized as they are primary actors of the corrosion reactions. All these changes in the surface layer can be observed remarkably with spectroscopic characterization techniques such as, specular reflection infrared (SR-IR) spectroscopy, spectroscopic ellipsometry (SE), attenuated total reflection infrared (ATR-IR) spectroscopy and vibrational sum frequency generation (SFG) spectroscopy.

Glass corrosion is a complicated phenomenon as it involves multiple processes, namely ion exchange, network hydrolysis and dissolution, taking place simultaneously. In ion exchange, water soluble alkali and alkaline earth ions in glass are exchanged with protons from the solution. These ions leach out of the glass into the solution, and protons take their places. As a result, composition of glass becomes different in the altered layer than that of bulk. Glass network forming bonds, as Si-O-Si, Si-O-B, and Si-O-Al, tend to break forming silanol groups (Si-OH) in the presence of –OH groups. That is network hydrolysis. These formed silanol groups can further react with each other and form new network linkages. Bond dissociations and formations and ion exchange lead to a structurally different, porous and silica-rich alteration layer. The porous nature of this layer is thought to be controlling the diffusion rate of the chemical species in and out of the glass affecting overall corrosion rate.
Due to ability to obtain information on the molecular level, spectroscopic characterization techniques are imperative to inspect glass corrosion. SR-IR peak positions are significantly sensitive to bond strength. Any change in the bond length or bond angle of the network forming bonds would manifest itself in the spectrum. Therefore, SR-IR is a very useful tool to observe evolution of the network structure. As the composition and structure of the alteration layer is different than that of bulk, optical properties of it are also different. This lets to utilization of SE to determine the thickness and porosity of the alteration layer. Determination of entrapped water molecules and silanol groups requires a higher surface specificity. Therefore, ATR-IR and SFG are employed for aqueous specious characterization. With ATR-IR, these species are quantified, and with SFG, hydrogen bonding interactions of these species are investigated.

Seong H. Kim, The Pennsylvania State University

**XPS AND IR ANALYSIS OF SILICATE GLASS NETWORK**

The surface properties of silicate glass materials are highly influenced by the connectivity of silicate network. Although it is easy to analyze the network connectivity in the surface region in computational simulations, it is quite difficult to get such information through experimental measurements. This lecture explains how the areal density of bridging oxygen (BO), non-bridging oxygen (NBO), and hydroxyl (OH) can be obtained quantitatively from x-ray photoelectron (XPS) spectroscopy measurements. It also teaches how the distribution of such species influences the vibrational spectral features probed with specular reflection infrared (SR-IR) and attenuated total reflection infrared (ATR-IR) spectroscopy. This talk will also invokes questions and limitations of conventional peak assignments and suggests a more meaningful way of interpreting silicate vibrational features.

Katelyn A. Kirchner, The Pennsylvania State University

**STATISTICAL MECHANICS OF TOPOLOGICAL FLUCTUATIONS IN GLASS-FORMING LIQUIDS**

All liquids are topologically disordered materials; however, the degree of disorder can vary as a result of internal fluctuations in structure and topology. These fluctuations depend on both the composition and temperature of the system. Most prior work has considered the mean values of liquid or glass properties, such as the average number of topological degrees of freedom per atom; however, the localized fluctuations in properties also play a key role in governing the macroscopic characteristics of any glass-forming system. Our work proposes a generalized approach for modeling topological fluctuations in glass-forming liquids by linking the statistical mechanics of the disordered structure to topological constraint theory. In doing so we introduce the contributions of localized fluctuations into the calculation of the topological degrees of freedoms in the network. With this approach the full distribution of properties in the disordered network can be calculated as an arbitrary function of composition, temperature, and thermal history (for the nonequilibrium glassy state).

Steven Kmiec, Adriana Joyce

Iowa State University

**IONIC CONDUCTIVITY AND SHORT RANGE ORDER STRUCTURES OF NEW OXY-SULFIDE SODIUM THIOPHOSPHATE GLASSES**

Sodium based thio-phosphate glasses exhibit extraordinarily high ionic conductivities, and have received a lot of attention as potential electrolyte materials in solid state batteries. However due to the poor chemical and electrochemical stability of sulfide materials efforts have been made to improve these properties though the incorporation of oxygen. The short-range order (SRO) structures of glasses in the Na$_4$P$_2$S$_7$-(7-x)O$_x$, 0 ≤ x ≤ 7 system were investigated on samples prepared by melt quench technique. The short range order (SRO) structure of the glasses were characterized using FT-IR, Raman and $^{31}$P Magic Angle Spinning NMR (MAS NMR) spectroscopies to identify the role of oxygen in the glass structure. Evidence suggests
that the addition of oxygen causes a disproportionation reaction to occur in the structure though the formation of mixed oxy-sulfide 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 ionic conductivity.

Kuo-Hao Lee, Yongjian Yang and John C. Mauro The Pennsylvania State University

**CRACK INITIATION IN AN INDENTED METALLIC GLASS WITH EMBEDDED NANOPARTICLE**

Nanoindentation was performed on metallic glass with embedded glassy nanoparticle using molecular dynamics (MD) simulations to investigate the effect of the second phase on shear band formation and crack initiation. It was found that the addition of a nanoparticle underneath the indenter centralizes the region of shear strain below the indenter and increases the peak tension on the plastic/elastic boundary. With the increase of the nanoparticle size, deformation becomes more severe, decreasing the critical load and effective hardness of the composite.

Yinan Lin, The Pennsylvania State University

**LONG-TERM BONE REGENERATION, MINERALIZATION AND ANGIOGENESIS IN RAT CALVARIAL DEFECTS IMPLANTED WITH STRONG POROUS BIOACTIVE GLASS (13–93) SCAFFOLDS**

There is growing interest in the use of bioactive glass scaffolds for repairing structural bone defects but data on the capacity of the scaffolds to regenerate bone in vivo, particularly over a long-term duration, are limited. In this study, bone regeneration in rat calvarial defects implanted with strong porous scaffolds of silicate 13–93 glass (porosity=47±1%) was investigated at 12 and 24 weeks post-implantation and compared with previous results from a similar study at 6 weeks. Three groups of implants, composed of as-fabricated scaffolds, scaffolds pretreated in a phosphate solution to convert a thin surface layer (5 μm) to hydroxyapatite (HA) and pretreated scaffolds loaded with bone morphogenetic protein-2 (BMP2) (1 μg/defect) were used. Bone regeneration, bioactive glass conversion to HA and blood vessel formation in the defects implanted with the three groups of scaffolds were evaluated using histology, histomorphometopic analysis and scanning electron microscopy. When compared to the as-fabricated scaffolds, the pretreated scaffolds enhanced bone regeneration at 6 weeks but not at 12 or 24 weeks. In comparison, the BMP2-loaded scaffolds showed a significantly better capacity to regenerate bone at all three implantation times and they were almost completely infiltrated with lamellar bone within 12 weeks. The amount of glass conversion to HA at 24 weeks (30–33%) was not significantly different among the three groups of scaffolds. The area and number of blood vessels in the new bone that infiltrated the BMP2-loaded scaffolds at 6 and 12 weeks post implantation were significantly greater than those for the as-fabricated and pretreated scaffolds. However, there was no significant difference in blood vessel area and number among the three groups of scaffolds at 24 weeks. The results indicate that these strong porous bioactive glass (13–93) scaffolds loaded with BMP2 are promising candidate implants for structural bone repair.

Hongshen Liu, The Pennsylvania State University

**EFFECTS OF SURFACE INITIAL CONDITION ON AQUEOUS CORROSION OF GLASS**

Being a non-equilibrium material, the structure of glass varies with the sample history. Thus, the initial surface condition of a glass can vary with the preparation condition and have a large impact on its reactivity. This study shows how the initial surface state of international simple glass (ISG) affects the aqueous corrosion behavior. The ISG glass samples were prepared as-polished-only and polished-then-annealed and they were immersed in pH 7 aqueous solution saturated with soluble SiO2 at 30 °C for 21 days (modeling a mild condition) and at 90 °C for 7 days (a severe condition). The surface structures of as-prepared and corroded ISG samples were analyzed using vertical scanning
interferometry (VSI), atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS), specular reflection infrared (SR-IR) spectroscopy, attenuated total reflection infrared (ATR-IR) spectroscopy and spectroscopic ellipsometry (SE). In addition, molecular dynamics (MD) simulations were performed to obtain atomic structure models of ISG to assist oxygen speciation from XPS data. Only the oxygen speciation with XPS showed discernable differences between two surfaces with different preparation histories; all other analysis methods could not differentiate the surface preparation history. Such minor difference in chemical structures was found to have a large impact on corrosion behaviors in the mild condition. In the harsh condition, the surface history dependence was not as drastic as the corrosion in the mild condition. The analysis results from XPS, SR-IR, ATR-IR and AFM of the corroded surfaces suggested that the thickness and structure of the alteration layer formed on ISG in aqueous corrosion can vary with the initial surface state.

Han Liu, Yipeng Li, Nazreen Ahmad Sabri, Zipeng Fu, and Mathieu Bauchy
University of California

**DEVELOPMENT OF EMPIRICAL FORCE-FIELDS FOR GLASS SIMULATIONS USING MACHINE LEARNING**

Molecular dynamics simulations are especially well-suited to investigate the atomic structure of glasses, which is usually challenging to access using conventional experiments. Yet, the development of accurate and transferable interatomic potentials remains a major bottleneck. Here, we report the development of a new set of empirical potentials for silicate glasses, whose parametrization is derived from first principle ab initio simulations combined with machine learning optimization methods. We demonstrate that this method is highly efficient and yields a force-field that shows a good transferability to various disordered silicate systems. This study highlights that combining atomistic simulations and artificial intelligence is a promising route toward the discovery of novel glass formulations with unusual properties.

Ye Luo, Arshiya Bhadu and John C. Mauro
The Pennsylvania State University

**SYNTHESIS AND CHARACTERIZATION OF GeO2-SiO2-ZnO-K2O OPTICAL**

Germania-silica glasses are essential in the manufacture of low attenuation glass waveguides for communication. However, the high price of GeO2 precludes their use in many other applications. In this study, thirteen samples centered around 40 mol% GeO2-20 mol% SiO2-20 mol% ZnO-20 mol% K2O were melted in alumina crucibles and the composition-property relationships were investigated. The densities are in the range of 3.18–3.53 g/cm³ and the refractive index (RI) are between 1.586 and 1.612. Density and RI values increase with GeO2 contents. ZnO powder, with band gap at 3.37 eV is used as UV shield in these glass samples. The cut-off edge of UV-Vis is around 310 nm, significantly higher compared with 157 nm in typical soda lime glass. A shift toward the visible region is observed when more ZnO is added. Fragility and glass transition temperature (T_g) were calculated by fitting viscosity data with the MYEGA equation. The T_g from the MYEGA equation is in good agreements with results from DSC.

Carly Mathewson, The Pennsylvania State University

**EFFICACY OF FINING AGENTS IN EXTREMELY VISCOUS AND HIGH MELTING ALUMINOSILICATE GLASS**

When making a glass, bubbles are often formed. These bubbles are the result of the evolution of gases as a product of the formation of the glass; the air present between the particles of powdered reagent or pieces of cullet; the diffusion of gases through the crucible during melting; and the presence of moisture in the reagents or the crucible itself. In extremely viscous glasses that melt at high temperatures, such as aluminosilicate glass, small bubbles, called seeds, are unable to rise or dissolve into the melt, and a fining agent is needed. Here is presented an experimental study of various non-toxic fining agents and their efficacy in fining the seeds of an aluminosilicate glass. Tin oxide, cerium oxide, and iron (III) oxide are
compared, as are the effects of using aluminum hydroxide in place of alumina to generate water, the addition of a nitrate to oxidize and recycle fining agents, and the substitution of calcium oxide for calcium carbonate as a reagent to reduce the amount of carbon dioxide released during glass formation. The efficacy of the glass is determined in terms of the number and size of the bubbles present. In order to determine any effects the fining agents might have on the glass product, the coefficient of thermal expansion, glass transition temperature, viscosity, and UVvis spectrum were obtained.

John Mauro, The Pennsylvania State University

**GLASS TRANSITION AND RELAXATION BEHAVIOR**

As a nonequilibrium material, a glass is continually relaxing towards its metastable supercooled liquid state. A comprehensive understanding of glass transition and relaxation behavior is of critical importance for many high-tech applications of glass, including optical fiber, glass substrates for liquid crystal displays, and chemically strengthened cover glass for electronic devices. In this tutorial, I will review the current state-of-the-art in understanding the dynamics of glass transition and relaxation phenomena, including the physical origins of its non-Arrhenius and non-exponential characters.

Paul Miller, Minoru Tomozawa

**EVALUATION OF WET SILICON OXIDATION MECHANISMS USING INFRARED SPECTROSCOPY**

Surface stress relaxation of oxide glasses was found to take place much more rapidly than bulk stress relaxation in the presence of a trace amount of water vapor. Correspondingly, the surface stress relaxation of silica glass can take place at a temperature much lower than the glass transition (\(\sim 1150°C\)), while the bulk stress relaxation usually takes place at or higher temperature than the glass transition temperature. This surface stress relaxation has been used to make a stronger silica glass fibers and to explain various anomalous phenomena such as surface compressive stress degradation and the fatigue limits of glasses. The possible role of this fast surface stress relaxation in the kinetics of oxidation kinetics of silicon in wet atmosphere was examined. Silicon oxide films formed by oxidation of silicon wafer are under biaxial compressive stress, which is expected to reduce the diffusion coefficient of oxidants such as molecular water. This compressive stress, along with fictive temperature changes, shifts the wavenumber of a silica asymmetric stretching vibration bands in the IR absorption spectrum. Silicon wafers were oxidized to measure this wavenumber and oxidation kinetics in wet atmosphere at 700°C - 1000°C. This data was used to generate a profile of wavenumber from which the stress state of the oxide can be interpreted. Comparison between oxidation kinetics and the peak shift suggests the onset of the surface stress relaxation corresponds to the transition of the linear kinetics to parabolic kinetics of the oxidation. This indicates an important role of surface stress relaxation.

Dien Ngo, The Pennsylvania State University

**SPECTROSCOPIC STUDY OF ISG GLASS CORRODED IN AQUEOUS SOLUTIONS**

Corrosion of International Simple Glass (ISG), a 6-oxide borosilicate glass, in aqueous solutions with or without electrolyte has been studied using different spectroscopic techniques. A significant change of the surface network structure was revealed through infrared spectroscopy and the surface layer is rich in silica. Results from spectroscopic ellipsometry show that the corroded layers are porous with pore size distribution depending on the corrosion time in aqueous solution. The change of pore size while the layer thickness is relatively constant implies a structural rearrangement during the corrosion process. The long-time corroded layers are depleted of mobile elements such as boron, sodium as shown by photoelectron spectroscopy (XPS).
**Carlo Pantano**, The Pennsylvania State University  
**GLASS SURFACES AND INTERFACES**

This lecture will focus primarily on fundamental aspects of glass surface structure. How does the bulk structure of the glass terminate at the surface? What happens to the dangling bonds and how do they influence the surface atomic structure, reactivity and other properties? What is the surface of glass? Subsequently, the formation of stable interfaces between glass surfaces and other materials will be exemplified.

The chemical and physical adsorption of water is a fundamental aspect of surface reactivity and structure of silicate glasses. Much is known about these surface reactions in the case of amorphous silica, and to a lesser extent silica glass, whereas our knowledge is still emerging in the case of multi-component glass surfaces. The chemical reactions between glass surfaces and water vapor depend on the glass composition and how the surface was created. There are no direct experimental methods for characterization of atomic structure at multicomponent glass surfaces. The use of computer simulations is absolutely essential for the development of new or improved models, as well as for interpretation of experiments.

Understanding the surface reactivity of multicomponent glass is important for many reasons. Glass is widely used as a substrate for thin films and coatings including metals, semiconductors, polymers and biology. The structure, chemistry and reactivity of the glass substrate surface can influence the deposition process, adhesion, chemical and mechanical stability and optics. In many cases, thermal treatments and/or silane coatings are required create a functional interface.

**Arron Potter**, Rensselaer Polytechnic Institute  
**THEALKALILEACHINGMECHANISMINSODA-LIMESILICATEGLASS**

Glass corrosion is important in many fields, particularly in nuclear waste processing. The leaching of alkali species into water in either liquid or vapor forms is a key step in the corrosion of alkali-containing oxide glasses. The exchange of alkali ions with hydronium ions (H$_3$O$^+$) has been suggested as a mechanism for this. Supporting of this mechanism, it was demonstrated that concentration of hydrogen in the leached layer of soda-lime silicate glasses was three times that of alkali ions existed in the glass. However, further studies of various oxide glass leaching layers indicated that this is not a ubiquitous phenomenon, with many glasses exhibiting a hydrogen-to-alkali ratio far lower than three. An alternate mechanism of alkali leaching has been proposed wherein water diffusion is followed by alkali ion-proton exchange, and thus water diffusion becomes the rate-controlling step for glass corrosion. To test this hypothesis, the low-temperature water diffusion rate for soda-lime silicate glass has been measured in a vapor environment and compared to the corrosion rate at various temperatures.

**Nisha Sheth**, Pennsylvania State University  
**THE EFFECTSOFACTICILEACHINGONTHE MECHANICAL PROPERTIESOF SODA LIME GLASS**

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 (bridging oxygen, non-bridging oxygen, hydroxyl groups) and incorporation of molecular water into the glass structure. One may expect that water in the acid leached surface facilitates mecha-nochemically-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 mecha-nochemical properties of silicate glasses. Differences in the mechanical behavior including crack initiation, crack propagation, hardness, and indentation fracture resistance in different environments will be discussed.
Shiv Singh, Herbert Gleiter and Horst Hahn
Institute of Nanotechnology, Karlsruhe Institute of Technology

**NANOGGLASS: A PROSPECTIVE NANOSTRUCTURED GLASSY MATERIALS**

Since the beginning of mankind history, most of materials in use are crystalline as it is most stable state of solid. In modern age, nanocrystalline materials have attracted renew interest for crystalline materials. The main reason for the preference of nanocrystalline materials is the fact that one can control their properties by modifying their defect microstructures as well as their chemical microstructures at nanoscale. Another popular material known as glass also exists since the civilization but with limited applications. The glasses are considered as a metastable and disordered material. Hence, it is difficult to introduce any defects like grain boundaries similar as in crystalline materials.

However, recently the group of Prof. Herbert Gleiter has proposed a new concept of nanoglass [1-4]. It is the idea of nanoglasses to fabricate a new kind of glass that will allow to modify the defect and the chemical microstructures of glasses in a way comparable to the methods that are used for nanocrystalline materials. A nanocrystalline material with a high density of defects in the form of grain boundaries is obtained by consolidating nanometer-sized crystals. The idea behind nanoglasses is to apply an analogous approach, i.e., the consolidation of nanometer-sized glassy clusters under high pressure to obtain a high density of interfaces between adjacent glassy regions with either the same or with different chemical compositions. In other words, by consolidating nanometer-sized glassy clusters, it generate a solid material that consists of nanometer-sized glassy regions connected by interfaces with an enhanced free volume due to the misfit between the atoms at the surfaces of adjacent glassy clusters. Due to the analogy of the nanometersized microstructures, the above glassy materials obtained is called as nanoglass. The above nanoglasses have demonstrated some interesting properties in compare to the conventional melt spinning glass ribbons of same composition. The glassy alloy of Fe90Sc10 shows paramagnetic for nanoglass whereas it is ferromagnetic for the melt spun ribbon [3]. Mössbauer spectra for the nanoglass and the melt spun ribbon of same composition of Fe90Sc10 have shown different spectra which indicate the different electronic states in both the cases [3]. The nanoglass of Sc75Fe25 have shown higher plastic flow (≈15 %) in compare to melt spun ribbons (≈1 %) [4]. In view of above, the proposed nanoglass will open a new door to the materials science community.

Nicholas Smith, Corning Incorporated

**IMPORTANT ASPECTS OF GLASS SURFACES IN MODERN APPLICATIONS**

In many commercial applications of glass, the surface provides a—if not, the—critical function for performance. From the surface strength of cover glasses for mobile devices, to contaminant-free substrates for modern displays, to durable surfaces for pharmaceutical packaging, many valuable attributes of glass can be traced to its surface. Here, we provide a tutorial discussion on several key aspects and properties of multicomponent glass surfaces that factor into its use in modern applications, with particular highlights on display glass substrates, water interactions and chemical durability at surfaces, and the application of some newer surface characterization techniques to understand surface properties and their physical origins.

Nicholas Stone-Weiss, Nicholas J. Smith, Randall E. Youngman, Michal Bockowski, Liping Huang, and Ashutosh Goel, Rutgers University

**IMPACT OF PRESSURE ON STRUCTURE AND PROPERTIES OF SODIUM ALUMINOBOROSILICATE GLASSES**

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 ultrastrong cell phone touch displays and thermal resistant glasses to glasses for nuclear waste immobilization.
Applying high pressure to glasses near the glass transition has been shown to significantly affect glass structure and properties, as varied pressure can induce polymorphism in the glass network due to density alterations. We aim to elucidate the effects that pressure has upon structure and mechanical / elastic properties in sodium aluminoborosilicate glasses. By measuring glass structure via NMR spectroscopy and properties of samples prepared at both ambient and 1 GPa pressures, we expect to gain a complete understanding of the role that pressure plays in inducing polymorphic changes across a broad composition space and in turn how these changes impact glass performance and characteristics.

S.K. Sundaram, Alfred University

**TERAHertz GLASS SCIENCE AND ENGINEERING**

Siddharth Sundararaman, Simona Ispas, Walter Kob and Liping Huang
Rensselaer Polytechnic Institute

**NEW INTERACTION POTENTIALS FOR MULTI-COMPONENT OXIDE GLASSES**

In this work, a new optimization scheme was developed to parameterize effective pairwise potentials for molecular dynamic (MD) simulations of various multi-component oxide glasses including alkali silicates, aluminates and borates. Our approach was to fit to results from accurate first principles calculations and explicitly incorporate the radial distribution function (RDF) of the equilibrium liquid at multiple temperatures and compositions, the vibration density of states (VDOS) of glass and the density of glass at different pressures into the cost function of the fitting scheme. These improved potentials for oxide glasses 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 yield surface to better understand the plastic deformation of multi-component oxide glasses.

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Minoru Tomozawa, Rensselaer Polytechnic Institute

**WATER AND GLASSES**

Most oxide glasses contain impurity water which has disproportionately large influence on glass properties. For example, a trace amount of water impurity increases optical loss in silica glass fibers and reduces the glass viscosity. Furthermore, water or water vapor in atmosphere can influence mechanical strength greatly and causes glass corrosion. Thus, water appears to have mainly adverse effects on glass properties. There are some beneficial effect of water on glass properties, also. The radiation coloration of glasses can be diminished greatly by impurity water. Recently, we found that the surface relaxation, both stress and structural, takes place much more rapidly than bulk relaxation, in the presence of a trace amount of water vapor in atmosphere. The fast surface stress relaxation of glass fibers under tensile stress was used to make stronger glass fibers. The fast surface stress relaxation was also used to explain long standing mysteries of glass science, e.g. mechanical fatigue limit, coaxing effect, and surface compressive stress degradation of ion-exchange strengthened glasses. The fast surface relaxation is expected to play an important role in anomalous phenomena observed in glasses with large surface area, such as thin films and thin fibers: growth kinetics of silica by oxidation of silicon and birefringence appearance in thin fibers. In order to understand the role of water in these variety of phenomena of glasses, details of glass-water interaction such as water diffusion into glass, effects of water on glass property and structure have been investigated. After spending many years on the research of water and glasses, the author has scratched the surface of this difficult but fascinating subject related to glass science and technology and has high hope that some bright and young people will pursue this challenging and rewarding research activities.
Manzila Islam Tuheen, Jincheng Du
University of North Texas

**STRUCTURES OF LANTHANUM PHOSPHATE AND ALUMINOPHOSPHATE GLASSES FROM MOLECULAR DYNAMICS SIMULATIONS**

Rare-earth phosphate glasses have recently gained significant attention in the realm of glass research due to their usefulness in various optical and optoelectronic applications. This work reports structural studies of alkaline phosphate and aluminophosphate glasses on addition of lanthanum using classical molecular dynamics simulations. Short and medium range structure information of phosphate glasses in xLa₂O₃ (100-x) NaPO₃: (x=0, 3, 5, 7.5) and aluminophosphate glasses in xLa₂O₃- yAl₂O₃ - (100-x-y) NaPO₃ : (0≤ x ≤5 and 5≤y≤15) series were obtained performing molecular dynamic (MD) simulations using a combination of constant temperature and pressure (NPT) and microcanonical (NVE) ensembles. Change in the cation local environments due to the presence of lanthanum was analyzed in the short range studying partial distribution functions, bond angle distributions and coordination number. It was found that, coordination number of lanthanum, NLaO in the phosphate glasses ranges from 6.7 to 7 and in the aluminophosphate glasses it is slightly increased above 7. Unaffected by the presence of lanthanum, in both of the series phosphorus is four coordinated whereas aluminum coordination number, NAlO varies. The bond distance La-O is found to be ~2.43Å with a sharp peak indicating a well-defined coordination shell. Also, the larger average coordination number of lanthanum (~7.2Å) compared to sodium (~6.75Å) indicates the stronger ability of La to attract oxygen than Na. Distribution of lanthanum ions in the glasses were also analyzed as a function of composition.

Arun K. Varshneya, Saxon Glass Technologies, Inc.

**CHEMICALLY STRENGTHENED GLASS**

This tutorial describes the science, technology and some applications of glass chemical strengthening by ion exchange. Kinetics of interdiffusion between two alkali ions are discussed. Stress development due to ion size difference is calculated and compared with those measured. Fast and slow relaxation processes that act to reduce the surface compression are explored. Technology and some applications are briefly reviewed.

Arun K. Varshneya, Saxon Glass Technologies, Inc.

**GLASS TECHNOLOGY**

If you have never had a formal course on glass technology, this is for you. We will briefly cover glass formulation, raw materials, batch calculation, laboratory glass melting, commercial scale melting, furnaces and fuels, mixing and homogenization, fining of glass, colors in glass, redox equilibria, thermal efficiency, pollution control, the making of glass containers, flat glass, tube/rod, insulation and optical fiber glass, secondary processes, sol-gel coatings, and annealing and tempering.

Zhe Wang, Tao Du, Hui Li, and Mathieu Bauchy
University of California

**STRUCTURE OF GLASSY SILICA: ROLE OF THE SYNTHESIS METHOD**

Amorphous and glassy materials can be synthesized via various techniques, e.g., melt-quenching, sol–gel, vapor deposition, or irradiation. Although all these techniques yield a disordered atomic network, the effect of the synthesis method on the structure of the resulting disordered material remains unclear. Here, based on molecular dynamics simulations, we compare the structural features of four disordered silica glasses obtained by melt-quenching, sol–gel condensation, vapor deposition, and irradiation, respectively. We show that the structure of glassy silica significantly depends on the synthesis method. Overall, our results suggest that these alternative synthesis methods can be used to produce “forbidden” glasses, that is, with a structure that cannot be achieved with conventional thermal treatments.
Collin Wilkinson, The Pennsylvania State University

**NEUTRON DETECTION AND TRACK RECONSTRUCTION ARE highly desirable due to applications in the oil industry, homeland security, and others**

It is also known to be difficult, due to its neutral charge and the fact that only a few elements have a capture mechanism, which produces only a small number of highly localized secondary particles. A simulation combining neural network-based machine learning, compact layered bar detector design described in Wilkinson *et al.*, and a borate based glass that exploits the $^{10}$ neutron capture mechanism $[10B + n → 7Li + α (6\%) or 10B + n → 7Li + α + γ (94\%) ]$ achieved 98.8% classification accuracy and sub-1% radial positioning error for neutron sources. Glass development, detector architecture, neural network implementation, and simulation results will be discussed.

Collin Wilkinson, The Pennsylvania State University

**A TOPOLOGICAL CONSTRAINT MODEL IS DEVELOPED TO ELUCIDATE THE COORDINATION ENVIRONMENT OF TELLURITE GLASSES**

The model is derived from temperature-dependent constraint theory and provides a quantitative connection between the connectivity of the glass network and its compositional dependent of the glass transition temperature ($T_g$). Our model gives support to the coordination proposed by Barney *et al.* and confirms their model of coordination of alkali tellurites while simultaneously developing a frame work that can be used in binary alkali glass formers to predict the expected coordination of the network forming cation in an oxide based glass. The model, the method, and the applications will be discussed.

Xinyi Xu, Ashutosh Goel
Rutgers State University

**FLEXURAL STRENGTH TESTING IN LITHIUM DISILICATE GLASS-CERAMICS**

Glass-ceramic based on Li$_2$O-SiO$_2$ system have been wildly used in dental applications for its high chemical durability and high bioactivity. Flexural strength as one of the mechanical properties is also close relevant for dental supplies. But thing is that some compositions perform relatively low flexural strength which can be influenced by some external factor such as the shape. This research is aimed to develop and evaluate LD glass-ceramic with relatively good mechanical performance. For this purpose, this study focuses on the effects of two factors, chamfering and tapes, on the flexural strength. The composition of starting glass of the LD glass-ceramic comprises Li$_2$O, K$_2$O, Al$_2$O$_3$, P$_2$O$_5$, SiO$_2$. After subjected to two heat treatments for sintering and hot-pressing, glass-ceramics bars which contain lithium disilicate as the major crystalline phase are obtained. Some chemical and structural properties such as crystallinity and micro-morphology are investigated by XRD and SEM before and after hot-pressing. The total prepared bars are divided into four parts, further processed to either chamfering, pasting to two different tapes or remaining the same as the original group. The flexural strength data of all the four group samples show that LD glass-ceramic of this composition performs good machinability satisfying the requirement of dental restorations.

Yongjian Yang, John Mauro
The Pennsylvania State University

**UNDERSTANDING OF STRUCTURE AND PROPERTIES OF ZIF GLASS VIA COMPUTATIONAL MODELING**

As chemically flexible metal-organic frameworks (MOFs), zeolitic imidazolate frameworks (ZIFs) have diverse applications in gas storage and separation, catalysis, drug delivery, etc. New ZIF materials are created by node/linker substitution, defect introduction and glass formation from melt-quench processing. Very recently, glass formation has been discovered in several ZIF chemistries, providing a new way of functionally tuning ZIF materials. The melt-quench process makes it possible to cast ZIFs into desirable solid forms. Additionally, the non-equilibrium nature of glass will further extend the design space of ZIFs. For example, Bennett *et al.* [1–4] have successfully synthesized a series of ZIF glasses from melt-quench of ZIF-62, ZIF-4, etc. ZIF-62 has also demonstrated an ultrahigh glass-forming ability with $T_g/T_m$ higher than 0.8 [5]. While ZIF materials with tunable porosity and mechanical properties have intriguing features critical to their applications, these features are not yet well understood [6]. Despite the experimental efforts, a
ABSTRACTS

In Alphabetical order by Speaker Last Name

molecular-level understanding of the glass structure and properties is lacking. While density functional theory (DFT) is useful for studying crystalline ZIFs, classical molecular dynamics (MD) or first-principles molecular dynamics (FPMD) are more suitable for studies of ZIF glasses, where thousands of atoms are required for the simulations. In this study, we will demonstrate that MD can yield similar structural and mechanical property trends for ZIF crystals as from DFT. Our results show that a little difference of volume (~1%) of ZIF-62 between classical MD and DFT can be achieved by using an appropriate force field tuned for MOF materials. The decrease in volume and increase in bulk modulus of ZIF-62 with increasing Co substitution can be reproduced in MD for the crystalline ZIF-62. In addition, MD can be also used to study the glassy phase, which is less accessible to DFT. Our study shed lights on the application of MD to the study of ZIF glasses and node/linker effect on their elastic properties.

Alessio Zandona, B. Rudinger, O. Hochrein, and J. Deubener, TU Clausthal

NEW INSIGHTS INTO THE CRYSTALLIZATION MECHANISM OF TiO2-nUCLEATED CORDIERITE GLASS-CERAMICS: A MULTI-ANALYTICAL APPROACH

Cordierite glass-ceramics are a widespread technical material and have been known to necessitate rather high amounts of TiO2 to undergo efficient volume crystallization. However, the essential mechanism underlying this behavior has been long ignored or overlooked. Within the present study, samples of stoichiometric cordierite glass, doped with variable amounts of TiO2 (from to 8mol%), were investigated through the combination of several in- and ex-situ analytical techniques (DSC, optical dilatometry, XRD, Raman and SEM). Due to their different sensitivities, it was possible to analyze the ceramization process in all its steps, from various perspectives and at multiple scales. Integration of the different data sets and comparison among the samples allowed to identify the crucial role of the seed former phases, Al-Mg-titanate and rutile, in directing all ceramization stages. They appeared not only to act as simple heterogeneous nuclei for the volume crystallization, but to affect also the general composition of glass and, in turn, that of the aluminosilicate phases crystallizing out of it. As a result, their influence extended beyond the formation of high quartz solid solution, including its transformation into indialite and the Al-Si-ordering in the structure of cordierite.

Junjie Zhao, Jianbei Qiu, Xvsheng Qiao, Xianping Fan, and Jincheng Du
Zhejiang University

USE MOLECULAR DYNAMICS SIMULATIONS TO PREDICT POSSIBLE CRYSTAL PHASES FROM OXYFLUORIDE GLASS PHASE SEPARATION

Knowing which type of crystals will precipitate from the oxyfluoride glass is a significant challenge in preparing the rare-earth doped optical glass ceramics. In most cases, this is a trial-error based process. Recently, due to the development of effective potentials, Molecular Dynamics simulations have been proved to be a useful tool to study the phase separation behavior in oxyfluoride glasses. Owing to the close relation between phase separation and crystallization in this type of glass, we hypothesize that we can predict the potential crystals precipitating from the corresponding phase separation.

In this study, we simulated a series of La3+, Ba2+, and Na+ containing aluminosilicate oxyfluoride glass. We found that, with LaF3 substitutions of BaF2, the elements enriching in fluoride phase change from Ba, La, F to La, F. Correspondingly in experiments, the precipitating crystals change from Ba2LaF7 to Ba2LaF7/LaF3 coexisting and to finally the LaF3, when all the BaF2 get replaced. This study shows that the rare-earth ions (represented by La3+ here) can be enriched in fluoride phase, which can efficiently enhance their luminescent properties due to the low phonon energy environment of fluoride. It also shows that MD simulations can be a practical method to predict the crystallization phases based on the structure information of phase separation.