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2022 ALL IOWA GLASS CONFERENCE

Welcome to the All-Iowa Glass conference.

We're happy to welcome everyone to Iowa State University after another fantastic year of glass science and research. This year is the International Year of Glass, and like many others across the globe we will be celebrating with some special events during the conference.

This schedule has been put together by Nick Oldham and Virginia Walker. Victor Torres and Jacob Wheaton are the creators of all art used in this program. We encourage all questions and insights you might have, and we hope everyone has a great time.

Iowa State University Department of Material Science and Engineering

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International Year of Glass All Iowa Glass Conference Schedule, July 28th 2022

Page Number for Abstract	Time	Event
	8-8:45am	**Breakfast** in the Hoover Atrium
	8:45-8:55am	**Setup time**(Poster Session)
	8:55am-9am	**Intro** by Steve Martin
3	**9-9:15am**	**Invited Speaker 1:** Steve Feller
4	**9:15-9:30am**	**Invited Speaker 2:** David Sidebottom
5	**9:30-9:45am**	**Speaker 1:** Presley Phillips
6	**9:45-10am**	**Speaker 2:** Stuart Leland
	10-11am	**Poster session**
7	**11-11:15am**	**Speaker 3:** Jacob Wheaton
8	**11:15-11:30am**	**Speaker 4:** Tyler, Salrin
9	**11:30-11:45am**	**Speaker 5:** Victor Torres
10	**11:45-12pm**	**Speaker 6:** Yi Wei, Aaron Phillips
	12-12:20pm	**Group Photo**
	12:20-1:30pm	**Lunch** in the Howe Atrium
11	**1:45-2pm**	**Invited Speaker 3:** Joel Destino
12	**2-2:15pm**	**Speaker 7:** Madison Olson
13	**2:15-2:30pm -**	**Speaker 8:** Owen Eichhorn and Dillon Zimmerman
14	**2:30-2:45pm**	**Speaker 9:** Casey Walsh, Johanna Hayes
15	**2:45-3pm**	**Speaker 10:** Virginia Walker
16	**3-3:15pm**	**Speaker 11:** Mathew Walton
	3:15-3:30pm	**Outro** by Steve Martin

The oral presentations will be held in Marston 2155, the poster presentations in Marston 2200

Poster Session		
Page	**Name**	**Title**
18	Julia Radtke	Improving the Anderson-Stuart Model for Ionic Conductivity in Alkali Borate Glasses
20	Logan Johnson	Using LAMMPS to Shed Light on Haven's Ratio: Current Data
21	Andrew Fernandes	Controlling GeO2 Nanoparticle Growth with Polyol Surfactants: Improving Tunability for Glass 3D Printing
29	Grace Dirks	Photon Correlation Spectroscopy on Phosphate Glasses
26	Nick Oldham	Mixed Oxy-sulfide Nitride Glassy Solid Electrolyte Materials: Electrochemical Impedance Spectroscopy and density of $Na_4P_2S_{7-6x}O_{4.62x}N_{0.92x}$
19	Harry Hawbaker	Studies of Interatomic Structures of Binary Li2S + B2S3 Glasses
22	Harsh, Uppala	Photon Correlation Spectroscopy In Potassium Borate Glass Melts
23	Rebekah Vires	Network evolution and chemical speciation in glass materials derived from hybrid sol-gel nanoparticles
24	Sahrai Luna	Designing Various Hybrid Architectures for the Fabrication of 3-D Printable GeO2-SiO2 Glasses
25	Alexander Pajak	Electrochemical properties of bulk glass series [0.58 Na_2S+0.42(0.75(1-a)SiS_2+aP_2S_5)+0.25NaPAl_0O] and the effect of the quality of starting material silicon sulfide
27	Virginia Walker	Low Frequency Impedance Spectroscopy at Low temperatures of R Li2O B2O3
28	Will Fettkether	Reconstitution of methanol dissoluted Li-Si-P-S-O glasses for improved performance in composite cathodes
17	Thomas Radke	DC Conductivity and Raman Spectroscopy in Ternary Systems of Tellurium Vanadate Glasses
30	Alec Wakefield	Sodium Titanium Phosphate Synthesis and Processing for Use as a Na-Ion Battery Active Material

Recent Raman and NMR Studies of Lead Borate Glasses

Konstantinos I. Chatzipanagis,, Nagia S. Tagiara, Efstratios I. Kamitsos , (NHRF, Athens), Nathan Barrow (Johnson Mathey, Reading UK), Ian Slagle, Robert Wilson,, Tyler Greiner, Martha Jesuit, Nicholas Leonard, Aaron Phillips, Bryce Reynolds, Brock Royle, Katherine Ameku, Steve Feller (Coe College, Cedar Rapids, IA)

Lead borate glasses were studied by Raman spectroscopy, 207Pb Static NMR and 11B MAS NMR. The range of compositions examined was extremely wide spanning 20 to 80 mol. % PbO. The results indicate that, as lead concentration increases, the presence of two glass networks emerges including those containing Pb-rich and B-rich structural units. A comparison to alkali borates is presented as well.

We acknowledge the NSF through grants DMR-1746230 and DMR-2203142.

Dynamic Light Scattering in Sodium Borate Glass Melts

David L. Sidebottom
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We report measurements of the dynamic structure factor in sodium borate glass melts with alkali contents from x = 0 mol% to x = 10 mol% Na_2O. The structural relaxation is characteristically non-exponential (characterized by a KWW exponent) and non-Arrhenius (characterized by the fragility index) and displays variations with alkali content owing to variations in the network structure. In addition to the viscous relaxation, the PCS often display an secondary relaxation which we show to be the result of diffusion of alkali ions that is coupled with the viscous relaxation.

Structure-property relationship in mixed oxy-sulfide glassy solid electrolyte material: $0.58Li_2S + 0.42 [(1–y)SiS_2 + yLiPO_3]$

Presley J. Philipp, Victor Torres III, Steve W. Martin
Department of Materials Science and Engineering, Iowa State University, Ames, Iowa 50010, USA

Mixed oxy-sulfide (MOS) glassy solid electrolytes have proved to be a strong contender for use in solid-state batteries because of their high ionic conductivity and electrochemical stability. The MOS series $0.58Li_2S + 0.42 [(1-y)SiS_2 + yLiPO_3]$ ($y = 0.0 – 0.5$) was prepared via melt quench-synthesis. Differential scanning calorimetry (DSC) was used to determine the glass transition and crystallization temperature of these glasses. To characterize the structure, Fourier Transform Infrared Spectroscopy (FTIR), Raman Spectroscopy, and 29Si & 31P Magic Angle Spinning NMR (MAS NMR) were employed. Electrochemical Impedance Spectroscopy (EIS) was used to determine the conductivity of the glasses. The conductivity initially increases until it reaches a maximum at $x = 0.3$ of $2.10*10^{-3}$mS/cm and subsequently decreases to 2.8410^{-3}mS/cm following the mixed glass former effect trend.

Crystallization and fragility behavior in sulfide, oxy-sulfide, and oxy-sulfide-nitride glassy electrolytes

Stuart Leland, Jacob Wheaton, Steve W. Martin
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The favorable electrochemical properties of glassy solid-state electrolytes in the $Li_2S + SiS_2$ system warrant further exploration into the effects of various dopants on the thermal properties of the systems. With the intent to draw glassy solid-state electrolytes into thin films (<100 μm), an estimate of sample viscosity and crystallization behavior is necessary for ideal processing. Three systems were created through doping lithium thiometaphosphate (LiPS¬¬3), lithium metaphosphate ($LiPO_3$), and lithium phosphorus oxynitride glass (LiPON) at near-eutectic compositions. $LiPS_3$ was synthesized via planetary ball milling, $LiPO_3$ was synthesized through melt-quenching, and LiPON was synthesized via ammonolysis of $LiPO_3$. Glassy samples in this series were synthesized via melt-quenching of mechanically milled powders. Initial glass transition and crystallization temperatures measured through differential scanning calorimetry (DSC) indicate potentially favorable characteristics for thin film drawing of the $LiPO_3$ doped system. Isothermal crystallization behavior was characterized using the Johnson-Mehl-Avrami (JMA) model. Further DSC experiments were conducted on the glass system to determine the kinetic fragility and viscosity of the three systems using the Mauro-Yue-Ellison-Gupta-Allan (MYEGA) model.

This work is supported by funding from DOE EERE VTO DE-EE0008852 and NASA EPSCoR 80NNSSC20M0219.

Drawn Thin-Film Mixed Oxy-Sulfide Glassy Electrolytes for Solid-State Battery Applications

Jacob Wheaton, Stuart Leland, and Steve W. Martin
Materials Science and Engineering, Iowa State University, Ames, Iowa 50010.

Next-generation batteries utilizing solid-state electrolytes are one of the more promising avenues to meet energy storage needs. Glassy solid-state electrolytes present several advantages over traditional crystalline materials due to their low temperature forming abilities, highly tunable chemistries, and lack of grain boundaries. Glasses in the Li_2S – SiS_2 – Li_xMO_y phase space present several desirable properties including high ionic conductivity (~ 10^{-3} S/cm), large electrochemical stability windows (0 – 5 V vs Li/Li^+), and strong glass forming character. For these glasses to be used on a commercial level though, the thickness of the electrolyte must be lowered to around 50 μm while still maintaining its mechanical strength. Utilizing a process known as redrawing, a rectangular preform of a glassy solid-state electrolyte can be reheated to above the glass transition temperature and drawn into thin glass ribbons. The selection of a candidate material in the Li_2S – SiS_2 – $LiPO_3$ glass system will be discussed through its crystallization and viscosity behaviors. The films were tested using electrochemical impedance spectroscopy to determine the temperature-dependent ionic conductivity, and through symmetric cell galvanostatic cycling. These results show that thin-film glasses made through the glass redraw method are a valuable research direction for solid-state battery technology.

This work is supported by funding from DOE EERE VTO DE-EE0008852 and NASA EPSCoR 80NNSSC20M0219

Using LAMMPS to Shed Light on Haven's Ratio: Determining the Parameters

Tyler Salrin[1], Logan Johnson[1], Caio Barca Bragatto[1]
1 Physics Department, Coe College, Cedar Rapids, IA 52402, USA

As a means to understand the unclear mechanisms behind ionic conductivity, Haven and Verkerk introduced a concept now known as Haven's Ratio (HR). This ratio relates tracer diffusion coefficient (D_T) of ions to the diffusion coefficient from steady-state ionic conductivity (D_σ). It can be challenging to obtain D_σ experimentally since the number of charge carriers has to be estimated. Molecular dynamics (MD) allows for the direct measurement of the mean squared displacement (MSD) of diffusing cations, which can then be used to calculate D, avoiding the definition of a charge carrier. However, using MD can be challenging since there is a drastic time constraint compared to experimental tests. Because of this compressed time scale, it is difficult to draw immediate correlations between real and simulated temperature and electric field. This work focuses on determining the correct parameters to accurately simulate $0.3Li_2O•0.7SiO_2$ at different temperatures and with an appropriate electric field so that HR can be calculated. Other parameters considered were the interatomic potential, the ensembles used, simulation size, and timescale. Once parameters were determined work began on calculating HR in simulated glasses.

The authors would like to thank NSF (grant no. NSF-DMR-1746230) for sponsoring this work.

Preparation of Li-Si-P-S-O-N glasses: The incorporation LiPON has on ionic conductivity

Victor Torres III, Presley Philipp, Steve W. Martin
Department of Materials Science and Engineering, Iowa State University, Ames, Iowa 50010, USA

Lithium glassy solid electrolytes (GSEs) are a potential alternative to liquid electrolytes in the advancement of battery technology. Mixed oxy-sulfide nitride glasses incorporate the advantageous properties of oxide glasses which display excellent chemical stability, of nitride glasses which exhibit good electrochemical stability and of sulfide glasses, which show high ionic conductivity. In the analysis of these new GSEs, the following compositional series was explored Li_2S + SiS_2 + [(1-*x*)$Li_{0.67}PO_{2.83}$ + *x*LiPON]. Differential scanning calorimetry (DSC) was employed to determine glass temperatures of these GSEs. In addition, electrochemical impedance spectroscopy (EIS) was used to determine the temperature-dependent ionic conductivity of theses GSEs. Spectroscopy such as x-ray photoelectron spectroscopy was conducted on the glasses to further elucidate the presence of nitrogen.

Support of this research by NSF Grant NSF-DMR-1936913 is acknowledged.

Extending the Glass Formation of Alkali Tellurites

Yi Wei[1], Aaron Philips[1], Nils Empen[1], Brittany Thompson[2], Lisa Tarman[3], Ethan Frana[1], Lauren Meyer[1], Caio Bragatto[1], and Steve Feller[1]
[1]Coe College Department of Physics
[2]Northeast Community College, Lincoln, NE
[3]William Penn High School, York, PA

The physical properties of low alkali tellurite glasses, $xM_2O \cdot (1\text{-}x)TeO_2$ ($0 \leq x \leq 0.30$) have been previously collected. The twin-roller technique within a nitrogen environment successfully extended the glass-forming range. Alkali tellurite glasses, $xM_2O \cdot (1\text{-}x)TeO_2$, were made using M = Li, Na, K, Rb, and Cs. The range has been extended from x = 0.35 up to x = 0.80. At these higher molar percentages, samples were twin-roller quenched and made in a glove box to keep water from attacking the sample. Glass transition temperatures (T_g), crystallization temperatures (T_x), and Raman spectra were obtained for these glasses. This shows structural changes in the glass as the amount of alkali modifier increases. The ionic conductivity of alkali tellurite glasses were found using a Gamry Instrument Interface 1010 Potentiostat/Galvanostat/ZRA. Samples were ground into a powder and pressed into a pellet with aluminum foil electrodes. Testing was done between 130.0° C and 235.1° C.

This work was funded by the National Science Foundation (Grant No: REU-1950337, RUI-1746230, and RUI-2203142).

3D-Printing Optical Quality Glass & Beyond

Joel F. Destino[1], Alexandra C. Chinn[1], Eric L. Marsh[1], Tim Nguyen[1], Zackarea B. Alhejaj[1,2], Matthew J. Butler[1], Bachtri T. Nguyen[1]

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The advancement of additive manufacturing (AM) or 3D printing has shown an extraordinary potential to revolutionize many fields, including glass science. Here we present a review of existing approaches to fabricating AM optical quality glass materials and recent work from the Destino Group at Creighton University. The Destino group focuses on the chemical development and characterization of novel colloids and colloidal suspensions for use in 3D printing to fabricate glass materials in new compositions and combinations. Our research has focused primarily on glass-forming oxides, such as silica (SiO_2) and germania (GeO_2). We are currently investigating multiple GeO_2-SiO_2 hybrid colloid strategies and analyzing the structural evolution from colloids to a printed glass toward understanding how colloid precursor structure influences glass network formation.

This work was supported by the Nebraska EPSCoR First Award, the Research Corporation for the Advancement of Science, Cottrell Scholar Award, and in part 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. Release: LLNL-JRNL-832069. As well as, the National Science Foundation DMR-2144453.

Structure and Thermal Properties in MOSN Phosphate Glass

Madison Olson, Steven Kmiec, and Steve W. Martin
Iowa State University

The preparation, properties, and short-range order (SRO) structures of the glasses in the series $(1-x)[2/3Na_2S + 1/3P_2S_5] + x[1/3Na_2S + 2/3NaPO_{2.31}N_{0.46}] = Na_4P_2S_{7-6x}O_{4.62x}N_{0.92x}$, where $0 \leq x \leq 0.5$ (NaPSON) are reported for the first time. In this study, these mixed oxy-sulfide-nitride (MOSN) glasses were prepared by adding the nitrided material $NaPO_{3-(3/2)y}N_y$; y=0.46 = $NaPO_{2.31}N_{0.46}$ (NaPON) to the base sulfide glass $Na_4P_2S_7$. Accordingly, large batches of bubble-free glass could be prepared making this route amendable toward scaling-up the glass melting process; though, only small amounts of nitrogen could be incorporated in the glass melts. XPS was combined with Raman, FT-IR, and 31P MAS NMR spectroscopies to determine the amount of retained nitrogen in the glass after melting and quenching and to determine the effect on the structures of the glasses of incorporating oxygen and nitrogen into the sulfide chemistry $Na_4P_2S_7$, x = 0.0. The nitrogen content increased linearly with the addition of NaPON, but was found, through quantitative 31P MAS NMR analysis, to be approximately half that expected at each value of x. Despite the small amount of nitrogen retained in these glasses, profound increases in the glass transition (T_g) and crystallization temperatures (T_c), determined using DSC, were found with increasing x. For the intermediate values of x, 0.2 and 0.3, no crystallization of the supercooled melt was observed even 250 °C above the T_g.

Development of a Polystyrene Based 3-D Dosimeter

Owen Eichhorn[1], Dillon Zimmerman[1], Ugur Akgun[1]
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A 3-D dosimeter fills the need for treatment plan and delivery verification required by every modern radiation-therapy method used today. This study builds off a water-equivalent and radiation-hard dosimeter that was developed and tested in recent years. This study focuses on building a bigger prototype with a higher resolution using Polystyrene doped with the scintillating agents P-Terphenyl and BisMSB. The readout of the final detector will be done via two CCD cameras, and a previously verified machine learning approach will be used for reconstructing the 3-dimensional dose distribution within the volume. This report summarizes the previous results, the detector design and material production procedures, as well as simulation efforts to build a machine learning training dataset.

Structural studies of a very wide range of Na_2O-SiO_2 glasses

Casey Walsh[1, 2], Johanna Hayes[1, 3], Alexa Schroder[1], and Steve Feller[1]
[1]Coe College Department of Physics
[2]Hunter College Department of Physics and Astronomy
[3]Middlebury Department of Physics

Sodium silicate glasses have been previously studied at compositions (mol%) $x$$Na_2O$.(100-$x$)$SiO_2$ where x = 20 to 70. 29Si MAS-NMR was used to study the increase in the ratio of non-bridging oxygens to bridging oxygens as Na_2O content increased.Raman spectroscopy was also used to show the breaking up of the silicate network as Na_2O content increased. Additionally, we were able to observe new bands in the Raman spectra for at x = 60, 65, and 70, which indicate symmetric C-O stretching as a result of significant CO_{3-2} in the glass. ATR FTIR has shown a lack of molecular CO_2 and bond distortion in CO_{3-2} anions. With these results, we are able to improve atomic-level models of the sodium silicate structure and understand more about CO_{3-2} presence in these glasses.

This work was funded by the National Science Foundation (Grant No: REU-1950337, RUI-1746230, and RUI-2203142).

Relationship between the boron anomaly and the ionic conductivity in lithium borate glasses explored by high-frequency and low-temperature electrochemical impedance spectroscopy

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Through the addition of a network modifier (such as an Li_2O) to B_2O_3, there is an increase in the coordination number for the boron atoms from 3 to 4, essentially meaning that there is a conversion of BO_3 triangles into BO_4 tetrahedra up to a certain concentration. This is commonly referred to in the literature as the boron-oxide anomaly and has been well studied in the past to understand changes in the glass properties. In this work, we explore the effects of this phenomenon in the ionic conductivity. In order to do so, results were analyzed using the 'universal scaling' approach, proposed by Swenson and Borjesson and by evaluating the activation energy of the ionic conductivity at low temperatures of lithium borate glasses. Preliminary results are intriguing, showing no change in the universal scaling, but a change in activation energy at lower temperature, as well as a better fitting of the Nyquist plot using two parallel RC circuits.

This work has the support of the National Science Foundation NSF-DMR-1746230, Coe College and NSF-DMR 1936913 Iowa State University

Hydrophobicity of Heavy Metal Oxide and Rare-Earth Doped Glasses

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"Rare earth oxide ceramics have been shown to be intrinsically hydrophobic" (Gisele Azimi, 2013). However, few studies have been done on the hydrophobicity of a broad range of glass compositions. Static contact angle tests were carried out on lead-containing glasses of four glass families, namely borates, silicates, germanates, and gallates. These glass families were then doped with rare earth oxides. All samples were polished to 1200 grit and cleaned with either a sodium hydroxide bath or a UV ozone cleaner. As part of this work, we have established a cleaning method for our glasses and surface polish. The contact angles were measured using deionized water, formamide, and diiodomethane as the working fluids. There is evidence to suggest that both rare earth doped and lead oxide containing glasses show intrinsic hydrophobicity of up to 100 degrees. We will also discuss what has the greatest impact on the contact angles, and preliminary explanations on the origin of this effect.

This work was supported by the National Science Foundation under grants DMR-CER-2054930

DC Conductivity and Raman Spectroscopy in Ternary Systems of Tellurium Vanadate Glasses

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There have been numerous studies on the effect of adding transition metals to vanadate glasses to impact their electrical conductivity. This work investigates the effect of titanium oxide on the conductivity of tellurium vanadate glasses at room temperature. In the glass systems being studied, the molar percent of vanadium is held constant and the amount of titanium is varied through the following stoichiometry: $0.6[xTiO_2 + (1-x)TeO_2] + 0.4V_2O_5$ where x is the molar fraction of titanium dioxide. For each specimen tested, the Raman spectrum is also gathered for comparison. The research shows that as the moar percent of titanium dioxide in the glass increases the conductivity of the glass also increases. The conductivity of the glasses ranges from 10^{-5} at 6% TiO_2 on the lower end, and 10^{-3} at 48% TiO_2 on the higher end.

This works was supported by grant numbers NSF- DMR - CER 1746230 and NSF- DMR - CER 2203142.

Improving the Anderson-Stuart Model for Ionic Conductivity in Alkali Borate Glasses

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2 Coe College, Cedar Rapids, IA

Currently, there is no widely accepted model for the ionic conductivity of glasses. The first known model for ionic conductivity, the Anderson-Stuart model, considers the ionic conductivity proportional to the elastic modulus. Nascimento's modified model relates it to the free volume within the glass; however, experimental results seem to disagree with this model. This work aims to test an improved model for the ionic conductivity of alkali borate glasses by calculating the rigid unit packing fraction (RUPF) of alkali borate glasses with different amounts of modifiers. In this RUPF model, the volume within the building units of the glass matrix is considered occupied, resulting in an overall lower free volume when compared to traditional ways of measuring packing fractions. Preliminary results indicate a better agreement between the free volume and the activation energy of alkali-borate glasses. In this work, we present the data related to x Na_2O (1-x) B_2O_3, with x being 0.2, 0.3, 0.4, and 0.6.

This work is supported by NSF grant number NSF-DMR1746230. Structure and Thermal Properties in MOSN Phosphate Glass

Studies of Interatomic Structures of Binary $Li_2S + B_2S_3$ Glasses

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Building off of Dr. Steve Martin's previous work on classifying lithium modification in thioborate glass, our efforts have been directed toward understanding the structural modifications brought about by the increase in molar modifier percentage of lithium sulfide (LiS_2) in boron sulfide (B_2S_3) glasses. We have generally well-fitting NMR powder patterns for the spectra generated from the glasses where $0.55 \leq x \leq 0.69$, where x equals the mol fraction of Li_2S modifier. We have collected N_4, chemical shift, CQ (quadrupolar coupling), and ηQ (quadrupolar asymmetry) parameters. Using these parameters, which describe the fraction of B_4 units in the glass, the distribution of chemical shielding among certain unit types, and the quadrupolar interaction, we can move forward with the characterization of this family of glass.

This work is supported by NSF-DMR 1746230 and NSF SusChEM grant number 1438223.

Using LAMMPS to Shed Light on Haven's Ratio: Current Data

Logan Johnson[1], Tyler Salrin[1], Caio Barca Bragatto[1]
1 Physics Department, Coe College, Cedar Rapids, IA 52402, USA

Ionic conductivity in glasses may have been known since the late 19th century, but the mechanisms behind ionic conductivity are unknown. Many varying models can be found in literature, falling into thermodynamic or kinematic categories. In the most basic sense, ionic conductivity is related very closely to the motion of the ions through the glass structure, which can be quantified by measuring diffusion coefficient (D) as defined originally by Fisk. Haven and Verkerk studied ionic diffusion in glass structures with and without an electric field. With their work, they introduced the Haven Ratio (HR). HR is found experimentally by the ratio of tracer diffusion to the diffusion coefficient calculated using the Nernst-Einstein equation and experimental ionic conductivity data (σ). If the HR equals one, then the mechanisms of diffusion for D_T and D_σ are the same, however, if HR < 1 then the added external electric field opens more sites within the glass structure for the ions to move. In this work, the mean squared displacement (MSD) of the alkali-ions in the SiO_2 glasses with and without an electric field was calculated using Molecular Dynamics (MD) simulations. The MSD was used to calculate D_σ, D_T , and HR after the creation of a steady state process. The results for HR that were found in this project were usually between 0.2 and 0.5 suggesting the mechanisms for diffusion are in fact different.

The authors would like to thank NSF (grant no. NSF-DMR-1746230) for sponsoring this work.

Controlling GeO_2 Nanoparticle Growth with Polyol Surfactants: Improving Tunability for Glass 3D Printing

Andrew G. Fernandes, Azriel R. Carr, Benjamin J. Schauer, Joel F. Destino
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Germania is a well-known glass former and has several desirable properties for use in glass optics. In comparison to silica, germania has higher refractive capabilities and k-dielectric properties. Additionally, it has a wider optical transparency window and a higher linear coefficient of thermal expansion. Use of germania in 3D printed glass optics has been limited, much due to the chemical challenges with synthesizing small (sub-50 nm), stable, amorphous GeO_2 nanoparticles. Here, we investigate the use of two polyol surfactants, sorbitol and mannitol, to tune GeO_2 nanoparticle growth. These two molecules are stereoisomers of one another and are significantly cheaper than known surfactants of germania such as polyvinylpyrrolidone (PVP). Duplicate samples are grown on and off heat to understand the effects that heat has on surfactant use. Dynamic light scattering (DLS) and infrared spectroscopy (IR) are used to collect data on the size and structure of the sol-gel nanoparticles. Results show the polyol's success in capping particle growth on off heat samples.

Photon Correlation Spectroscopy In Potassium Borate Glass Melts

Harsh, Uppala
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Photon correlation spectroscopy conducted on alkali borate glass melts reveals both the non-Arrhenius and non-exponential character of the structural relaxation. Spectra also reveal an unexpected secondary process that appears to be caused by the diffusion of the alkali ions.

Network evolution and chemical speciation in glass materials derived from hybrid sol-gel nanoparticles

Rebekah M. Vires, Rachel M. Wayne, Sahrai Luna, Joel F. Destino
Department of Chemistry, Creighton University, 2500 California Plaza, Omaha, NE 68178-0133

The development of hybrid sol-gel nanoparticles (NPs) has played a central role in advancing the additive manufacture, or 3D printing, of glass materials in geometries and compositions unimaginable by conventional melt quench techniques. In this presentation, we investigate how hybrid NP morphology influences glass-network formation towards improving precursor design and ultimately enabling the development of new glass systems. Our study explores three unique NP systems: (1) a mixture of encapsulated GeO_2-SiO_2 and SiO_2 NPs, (2) a mixture of independent GeO_2 and SiO_2 NPs, and (3) independent GeO_2-SiO_2 NPs. NP shape, size, and morphology were analyzed using electron microscopy and atomic force microscopy. The chemical composition of the NPs was probed by energy-dispersive X-ray spectroscopy Raman and Fourier-transform infrared spectroscopies were used to study chemical structures and bonding in the resulting NPs and glass networks. Initial findings from group (1) glasses suggest these methods can identify sub-micron Ge speciation and glass phase separation. Ongoing studies will seek to apply these methods to the other NP systems.

Designing Various Hybrid Architectures for the Fabrication of 3-D Printable GeO2-SiO2 Glasses

Sahrai Luna, Rachel M. Wayne, Rebekah M. Vires, Joel F. Destino
Department of Chemistry, Creighton University, 2500 California Plaza, Omaha, NE 68178-0133

Glass is an important material in society and plays an essential role in everyday technologies. Developing new, chemical approaches to fabricating glass materials is central to enabling innovative, additive manufacturing, or 3D-printed glass technologies. This project aims to examine the fundamental chemistry needed to synthesize various nanoparticles composed of GeO_2 and SiO_2. Here, we report various hybrid silica-germania nanoparticles designed in mixed, core-shell, and layer-by-layer compositions. The morphology of the nanoparticles was analyzed using (electron and atomic force) microscopy. The chemical composition of the particles was determined using (energy-dispersive X-ray) spectroscopy. Findings from this project could help reimagine the fabrication of glass materials. Ultimately, the project aims to enable the design of freeform optics, innovate optical system design.

Electrochemical properties of bulk glass series [0.58 Na_2S+0.42(0.75(1-*a*)SiS_2+*a*P_2S_5)+0.25 $NaPAl_0O$] and the effect of the quality of starting material silicon sulfide

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Solid-state batteries have consistently been proven to be more energy dense and a safer option than liquid electrolytes. However, for solid-state batteries to display consistent metrics of conductivity and electrochemical stability, there is a great dependence on the quality of the starting materials used. Within the glass series [0.58 Na_2S+0.42(0.75(1-*a*)SiS_2+*a*P_2S_5)+0.25 $NaPAl_0O$], *a*=0.25 was studied and different qualities of silicon sulfide were used during synthesis. Raman spectroscopy was used to determine the difference in purity and composition of the batches of silicon sulfide used in this study. Significant impurities were found in the 'low quality' silicon sulfide. Electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) measurements were used to show that a 'high quality' crafted silicon sulfide enables consistent electrochemical stability for the electrolyte cell over time. The solid-state electrolyte synthesized with 'low quality' silicon sulfide generally displayed oxidative instability and lower conductivity, specifically, shown through EIS, interfacial resistances much larger than the bulk resistance.

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Mixed Oxy-sulfide Nitride Glassy Solid Electrolyte Materials: Electrochemical Impedance Spectroscopy and density of $Na_4P_2S_{7-6x}O_{4.62x}N_{0.92x}$

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Oxy-nitride electrolyte glasses have previously been shown to exhibit large working ranges while pure sulfide electrolyte glasses have been shown to exhibit high ionic conductivities. We hypothesize that mixing these two glass types can result in a combination of their properties. In this experiment, Mixed-oxy-sulfide nitride (MOSN) electrolyte glasses are analyzed to determine how the incorporation of oxygen and nitrogen into a pure sulfide glass affects the ionic conductivity and density of the glass. The $(1-x)[(2/3)Na_2S+(1/3)P_2S_5]+x[(2/3)NaPON+(1/3)Na_2S]$ glass series($0 \leq x \leq 0.5$) was used in this experiment, where sulfur is systematically substituted for nitrogen and oxygen in $Na_4P_2S_{7-6x}O_{4.62x}N_{0.92x}$. The ionic conductivity of this series was analyzed through electrical impedance spectroscopy (EIS) using bulk glass samples at frequencies ranging from 0.1 to 10^7 hertz. Density data was also collected through the Archimedes method to further characterize the properties of this glass series and provide insight into the trends in the Ionic conductivity. These results further characterize MOSN electrolyte glasses and help determine an ideal glass in the $Na_4P_2S_{7-6x}O_{4.62x}N_{0.92x}$ glass series for thin film electrolyte glass production.

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Low Frequency Impedance Spectroscopy at Low temperatures of R Li_2O B_2O_3

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Low frequency impedance spectroscopy has been used for many years to characterize different electrical properties in ionically conductive materials. Nonetheless, high-frequency impedance spectroscopy has been used in different studies, most famously the universal scaling of Bode plots. Unfortunately, most laboratories have access to low-frequency impedance spectroscopy (up to 100 kHz), limiting the analysis range. In this work, we suggest that taking measurements at low temperatures at low frequency will have the same result as taking high frequency high temperatures scans. To test this hypothesis, we will measure the ionic conductivity of lithium borate glasses(R Li_2O + B_2O_3 with R from 0.1 to 1.5), and comparing the results with scaling results found in the literature.

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Reconstitution of methanol dissoluted Li-Si-P-S-O glasses for improved performance in composite cathodes

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The electrochemical and mechanical properties of thin-film glassy electrolytes make them viable candidates for inclusion in solid-state batteries. To enable the inclusion of these novel glass technologies, new cathode materials must be developed that can be utilized in contact with the glassy solid electrolyte (GSE). As a solution to this issue, a composite cathode blend has been created that utilizes $LiFePO_4$ as a redox active material, a mixed oxy-sulfide glass [0.58 Li_2S + 0.315 SiS_2 + 0.105 $LiPO_3$] as an ionic conductor, and carbon nanotubes as an electronic conductor. In order for this cathode to function in a battery, all three of these materials must be in contact with each other in the composite at locations dubbed tri-junction points. To create more tri-junction points and thus increase the capacity and performance of the cathode, the composite materials were dissolved and tape-casted in a methanol slurry to form ionic conductor particles of smaller size and a finer dispersion. The reconstituted glass retained its amorphous nature while changing its structure, and when included in a composite cathode created full cells capable of reversible cycling.

Photon Correlation Spectroscopy in Pyrophosphate Melts

Grace Dirks and Jack Pereira

We report dynamic light scattering studies of $(Na_2O)x(P_2O_5)100-x$ and $(ZnO)x(P_2O_5)100-x$ at x between 50 and 60 mol% modifier oxide. According to VanWazer's theory, glasses in this compositional range consist of chains of PO_4 tetrahedra with chain lengths that decrease systematically with increasing modifier. Here we contrast the dynamics of melts in which Na acts mainly a network modifier, while Zn tends to function as a network former. The resulting dynamics are interpreted in terms of these structural variations.

Sodium Titanium Phosphate Synthesis and Processing for Use as a Na-Ion Battery Active Material

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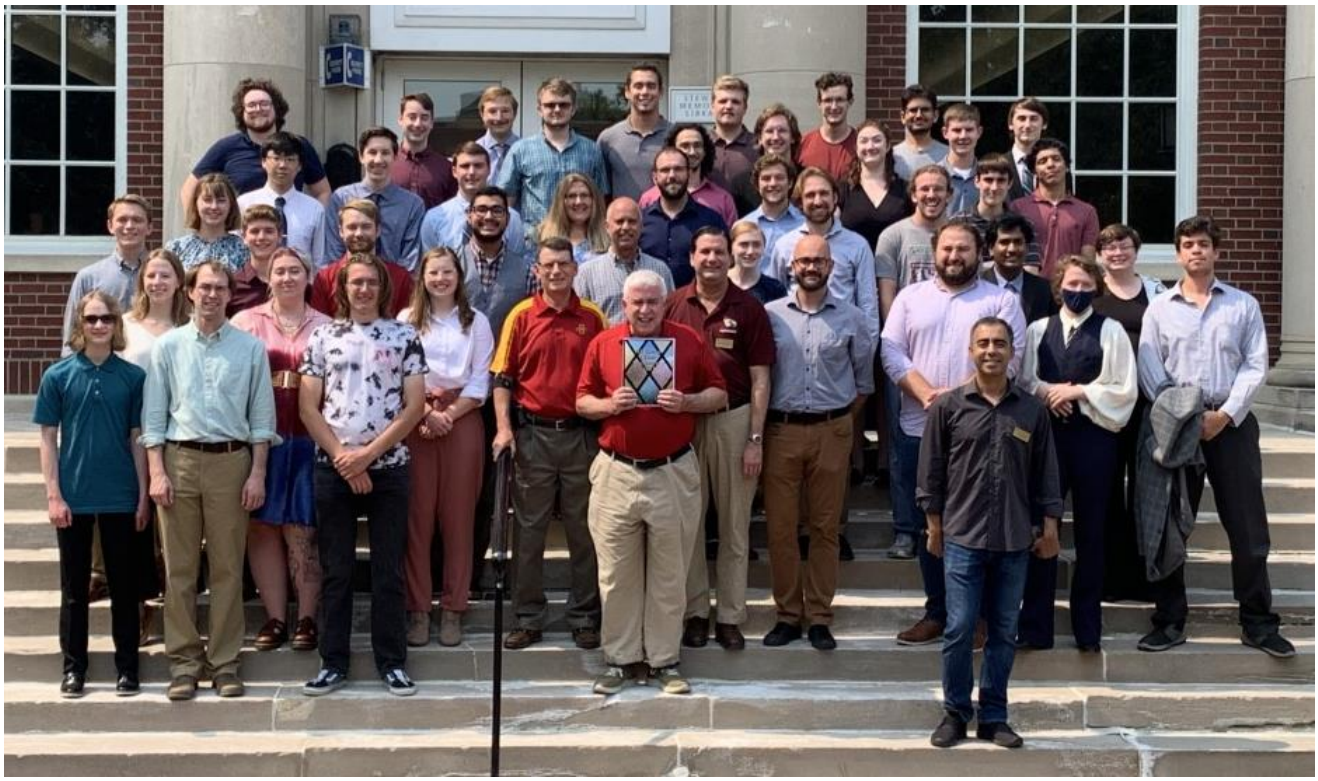
Active material choice is critical for achieving desirable properties when optimizing cathode composition for sodium-ion batteries. One popular choice for this application is sodium superionic conductors (NASICON) materials, which are highly effective for creating high-capacity and cyclable cells. This study focuses on one such NASICON active material, sodium titanium phosphate ($NaTi_2(PO_4)_3$), and its application as active material in a cathode used for a solid-state sodium-ion coin cell with a glassy solid electrolyte. The material was synthesized by combining precursors in a high-energy ball mill, followed by calcining to complete the reaction and form an in-situ carbon layer on the particle surfaces to improve electronic conductivity. After synthesis, the powder underwent XRD testing to check for the presence of the carbon coating and any unwanted sodium pyrophosphate that may have formed during the reaction. Next, the cathode composite was formed by combining the resulting active material with powdered NaPSON ion conducting glass and C45 graphite in a Thinky ball mill, followed by styrene-butadiene rubber (SBR) binder dissolved in a xylene solution. The composite-xylene solution was then tape cast onto an aluminum current-collector and used to construct coin cells for Galvanostatic cycling and SEM and EDS analysis. Characterization of the material showed it was predominantly the target active material, and saw promising results for cycling and battery performance compared to previous active materials.



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