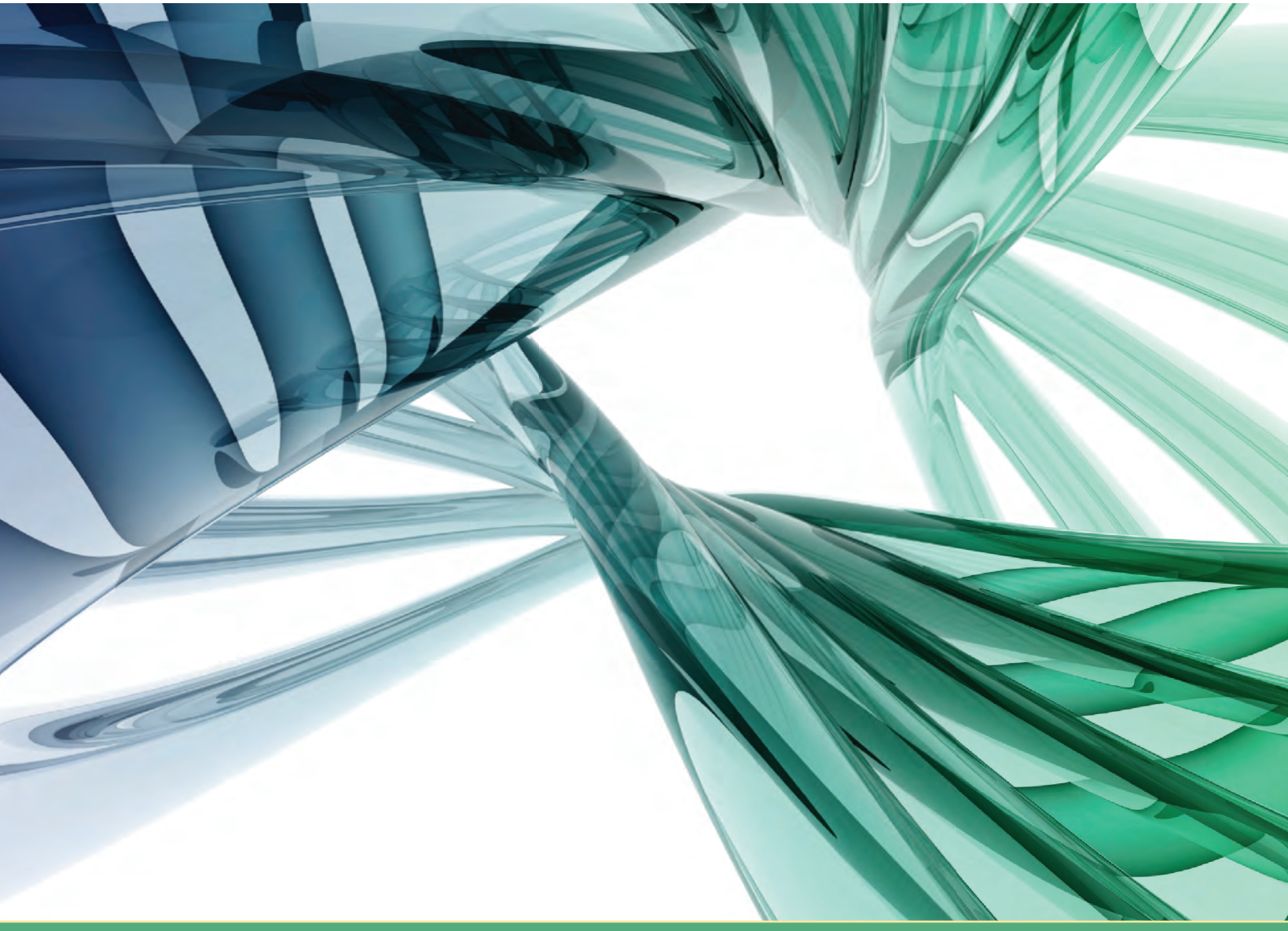
2011 GLASS & OPTICAL MATERIALS DIVISION ANNUAL MEETING

May 15-19, 2011 | Hilton Savannah DeSoto | Savannah, GA



Meeting Guide & Abstracts

Organized by:

The American Ceramic Society and the
American Ceramic Society's Glass & Optical Materials Division

The American Ceramic Society
www.ceramics.org

2011 GOMD Annual Meeting

Welcome to the 2011 Glass & Optical Materials Division Meeting (GOMD 2011)! This year's program features four symposia with sessions headed by international leaders from industry, government laboratories, and academia. You will find talks covering the latest advances in glass science, the technology of optical materials, and a focused examination of the amorphous state.

Several special activities have been planned in addition to the outstanding technical program.

- Renew acquaintances and get to know new faces within the GOMD community during the Welcome Reception held on Sunday from 5 to 7 pm.
- Students will not want to miss the "Experiences from My First Five Years in the 'Real World'" lecture planned for Monday during lunch time.
- Special Award Lectures: The Stookey Lecture of Discovery Award (Monday morning), the George W. Morey Award (Tuesday morning), and the Norbert J. Kreidl Award for Young Scholars (Tuesday at noon) consist of exceptional lectures by the honorees.
- Continue your learning experience by attending the Poster Session on Monday evening, with detailed technical presentations and top materials science students competing in the student poster contest.
- GOMD attendees are invited to be our guests and continue networking with their colleagues during the conference dinner on Tuesday evening.

After the GOMD conference, the Glass Manufacturing Industry Council (GMIC) is hosting a special symposium on "Glass Recycling in America – Challenges and Opportunities". This one-day symposium brings all stakeholders together for the common purpose of understanding how to achieve a more robust and successful recycling of glass in America. A separate registration fee is required to attend this program.

Special thanks go to our sponsors including PPG Industries, Inc. for sponsoring the George W. Morey Award; Coe College and Corning Incorporated for sponsoring the Stookey Lecture of Discovery Award; SCHOTT North America for sponsoring lunch for the Norbert J. Kreidl Award for Young Scholars; and Corning Incorporated for the Student Poster Contest. We also thank American Elements (lanyard sponsor), the *Journal of Non-Crystalline Solids* (poster session sponsor), and the *International Journal of Applied Glass Science* (welcome reception co-sponsor) for their generous support.

Savannah is located in the heart of coastal Georgia's "low-country," and we hope that you have the opportunity to enjoy the natural beauty and vibrancy of this spectacular city. The conference hotel is located in the Historic District, complete with cobblestone streets, manicured gardens, and oak-shaded parks drizzled with Spanish moss. Be sure to schedule some time for a walk through the many city gardens and down to River Street to enjoy the street performers, shops, restaurants, bars… and a great view. Other major attractions include the large Telfair Museums of Art (currently hosting an exhibit on "Optic Art, appropriately!) and the haunting, art-filled Bonaventure Cemetery, made famous by the book and movie "Midnight in the Garden of Good and Evil." Civil War-era Fort Pulaski and the endless beaches of Tybee Island are a short drive to the East.

The American Ceramic Society and the Glass & Optical Materials Division thank you for participating in this year's meeting. We hope you have a stimulating and memorable experience.

2011 GOMD Program Chairs:

Joseph V. Ryan
Pacific Northwest National Lab

Amanda Brennecka
Sandia National Labs

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Final Program

Glass & Optical Materials Division Officers

Chair
Steve W. Martin
Iowa State University

Vice Chair
Kelly Simmons-Potter
University of Arizona

Chair-Elect
John Ballato
Clemson Research Park AMRL

Secretary
Shibin Jiang
AdValue Technology

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Award Sponsors

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Poster Session Sponsor

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Program Schedule-at-a-Glance

Sunday, May 15, 2011

5:00 - 7:00 PM WELCOME RECEPTION on the pool deck (2nd floor)

Monday, May 16, 2011

Time	Cumberland	Ossabaw	Pulaski	Sapelo	Madison
8:00 - 9:00 AM	Stookey Award Lecture				
9:20 - Noon	Ion Conductors and Energy Storage Materials I	Glass Transition and Relaxation in Glasses and Glassforming Liquids I	Transparent Ceramics I	Non-Silicate Glasses I	
1:00 - 5:40 PM	Ion Conductors and Energy Storage Materials II / Glass-Ceramics	Glass Transition and Relaxation in Glasses and Glassforming Liquids II	Transparent Ceramics II / Photosensitivity and Photomodification	Non-Silicate Glasses II / Water and Glass	
5:45 - 6:30 PM	GOMD Business Meeting				
6:30 - 9:00 PM					Poster Session / Student Poster Contest

Noon - 1:00 PM STUDENT EVENT – Experiences from My First Five Years in the "Real World" – Harborview Room (15th floor)
Lunch will be available to students at no cost, on first come, first served basis.

Tuesday, May 17, 2011

8:00 - 9:00 AM	Morey Award Lecture				
9:20 - Noon	Glass Structure and Properties I	Glass Transition and Relexation in Glasses and Glassforming Liquids III	Active Optics	Glass Corrosion I	
Noon - 1:00 PM					Kreidl Award Lecture*
1:00 - 5:40 PM	Glass Structure and Properties II	Model/Experiment: Links and Limits	Optical Absorption	Glass Corrosion II	
7:00 - 10:00 PM					Conference dinner

*Boxed lunches will be available to attendees of the Kreidl Award Lecture at no cost, on first come, first served basis.

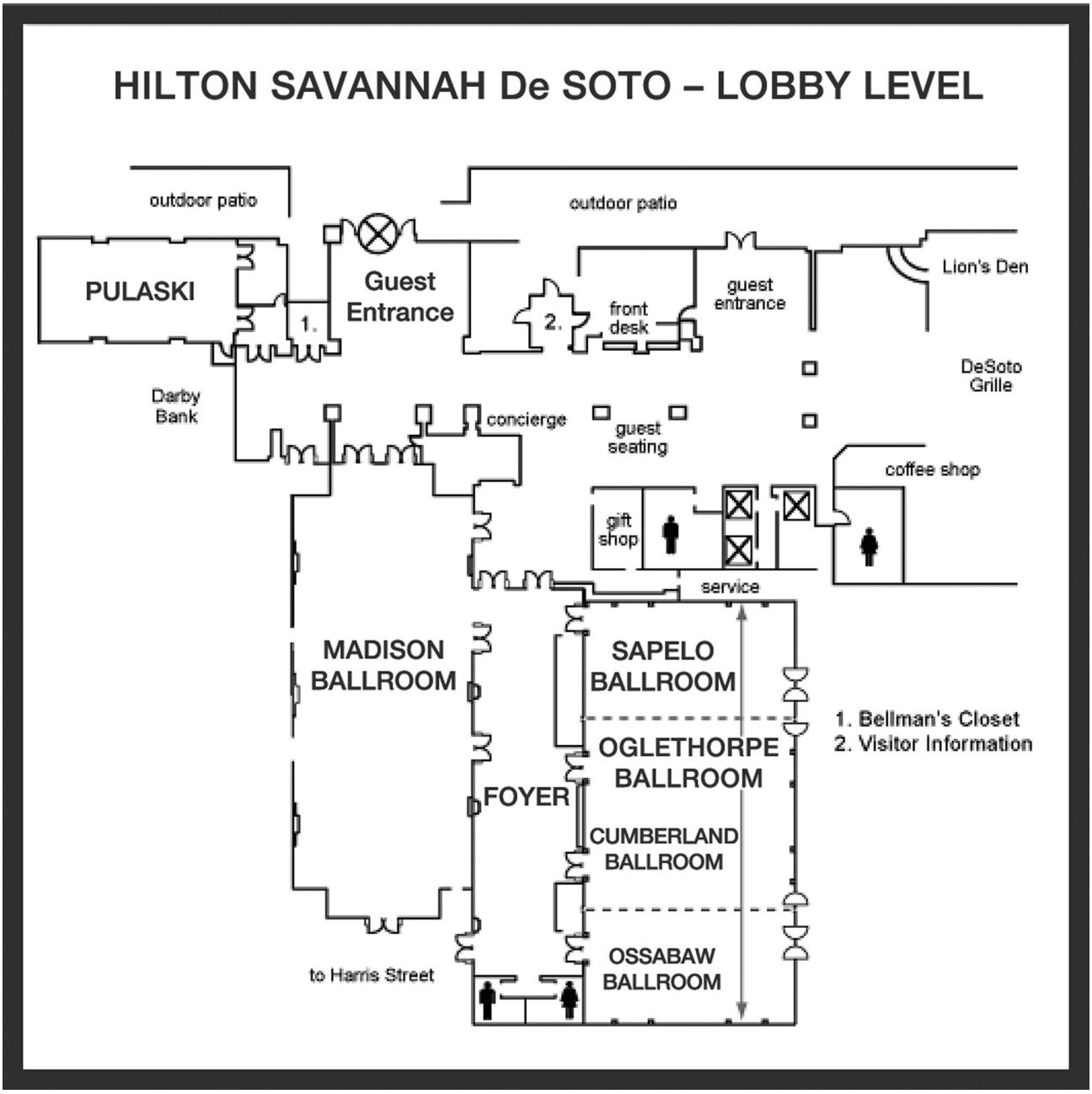
Wednesday, May 18, 2011

8:00 - Noon	Glass Strength / Sensors and Scintillators	Topology and Rigidity	Solar Energy and Photocatalysis	Surface and Interfacial Phenomena / Ancient Glasses	
1:00 - 5:40 PM	Glass Melting and Processing / Liquid Synthesis and Sol-gel Derived Materials	Medium Range Order / Medium Range Order and Amorphous Metals	Optical Coatings	Atomistic Modeling of Glass Structures and Interfaces	

Thursday, May 19, 2011

8:00 - Noon	Spin Glasses	Amorphous Metals / Glasses for Medicine and Biotechnology	Glasses for Energy and Environmental Applications		

Hilton Savannah De Soto Floor Plan



Experiences from My First Five Years in the 'Real World' – Student Activity

Monday, May 16th
12:00 p.m. – 1:00 p.m.
Kevin Fox, Savannah River National Laboratory

Kevin will provide insights on his first five years as a research scientist at the Savannah River National Laboratory. He'll address a range of early career topics such as technical adaptability, continuing education, tracking accomplishments, networking, professional societies, and funding opportunities. All students are invited to the presentation. Lunch will be available to students at no cost, on first come, first served basis.

Award Lectures

Monday, May 16 at 8 a.m. – Cumberland

The ***Stookey Lecture of Discovery***, named in honor of materials pioneer Dr. S. Donald Stookey, recognizes an individual's lifetime of innovative exploratory work or noteworthy contributions of outstanding research on new materials, phenomena, or processes involving glass, that have commercial significance or the potential for commercial impact.

Award Winner: Delbert Day, Curators' Professor of Ceramic Engineering and Senior Research Investigator Graduate Center for Materials Research
Missouri University of Science and Technology
Rolla, Missouri, USA
Presentation Title: "Repairing the Body with Glass"
Sponsored by Corning Incorporated and Coe College

Tuesday, May 17 at 8 a.m. – Cumberland

The ***George W. Morey Award*** recognizes achievements in the field of glass science and technology. The award is given for an outstanding publication on glass, either scientific or technological, published during the previous year.

Award Winner: Neville Greaves, Director and Distinguished Research Professor of Institute of Mathematics and Physics
Aberystwyth University
and
Distinguished Research Fellow
University of Cambridge, United Kingdom
Presentation Title: Glass Structure, Ion Dynamics, and the Pareto Principle
Sponsored by PPG Industries Inc.

Tuesday, May 17 at 12 p.m. – Madison Ballroom

The ***Norbert J. Kreidl Award for Young Scholars*** recognizes excellence in research by students in the fields of glass and optical materials. Dr. Kreidl's lifelong mission was to enhance the education, achievement and advancement of young people.

Award Winner: Randilynn Christensen, MSE, Iowa State University
Ames, Iowa, USA
Presentation Title: "The Mixed Glassformer Effect in Sodium Borophosphate Glass"
Boxed Lunches* sponsored by SCHOTT North America Inc.

**Note: Boxed lunches will be available at no cost on a first come, first served basis to attendees of the Kreidl Award Lecture.*

Symposium
Glass Recycling in America – Challenges and Opportunities

Presented by the Glass Manufacturing Industry Council

Thursday, May 19
8:00 a.m. – 2:30 p.m.
Madison Ballroom

Please note that a separate registration is required to participate in the Glass Recycling in America Symposium.

Glass Recycling in America has achieved only a fraction of its potential. Glass is the only common product material with an endless life cycle, yet most glass in the U.S. is not reused. Barriers to a more robust recycling utilization include both technical and economic barriers. Many constituents have an interest in the state of glass recycling, including city and state governments, waste processors, glass industry suppliers as well as glass manufacturers. This symposium brings all stakeholders together for the common purpose of understanding how to achieve a more robust and successful recycling of glass in America.

Faculty:

- Kenneth Lovejoy - VP, Environment, Health & Safety, Owens-Illinois, Inc.
- Margaret Zahller, Senior Analyst, PE Americas
- Paul J. Smith - Global Sourcing Manager – Cullet, Owens-Brockway Glass Container Inc.
- Peter Walters - Vice President, Purchasing and Distribution, Saint-Gobain Containers
- Kathleen Flight, Manager of Cullet and Recycling Procurement, Saint-Gobain Containers
- Gerhard Glawitsch – Sales Manager, BT-Wolfgang Binder GmbH
- Daniel K. Steen - Vice President, Government Affairs, Owens-Illinois, Inc.
- Gloria Hardegree, Executive Director Georgia Recycling Coalition
- Scott Mouw, Environmental Supervisor/Section Chief, North Carolina State DIPPEA
- Frank Killoran, National Business Development Manager, Pratt Industries, Inc.
- Bill Waltz, President and CEO, Strategic Materials
- Curtis Bucey, President and COO, Strategic Materials
- David Hudson, Vice President Government Affairs, Strategic Materials
- Steve Bowles, President, Reflective Recycling

Program Committee:

- Kenneth Lovejoy – Symposium Program Committee Chairman - VP, Environment, Health & Safety, Owens-Illinois, Inc.
- Paul J. Smith - Global Sourcing Manager – Cullet, Owens-Brockway Glass Container Inc.
- Ernest P. Guter - Research Associate - Glass Batch & Melting Technology, Owens Corning
- Daniel K. Steen - Vice President, Government Affairs, Owens-Illinois, Inc.
- Peter Walters - Vice President, Purchasing and Distribution, Saint-Gobain Containers
- Joseph Cattaneo – President, Glass Packaging Institute
- Robert Weisenburger Lipetz – Executive Director, Glass Manufacturing Industry Council

Program Agenda

7:00 a.m. – 8:00 a.m.	Continental Breakfast
8:00 a.m. – 8:15 a.m.	***Opening Remarks*** – Kenneth Lovejoy, VP, Environment, Health & Safety, Owens-Illinois, Inc.
8:15 a.m. – 8:45 a.m.	***Higher Societal Value of Glass Recycling*** – Margaret Zahller, Senior Analyst, PE Americas
8:45 a.m. – 9:00 a.m.	Questions & Answers
9:00 a.m. – 9:30 a.m.	***Understanding the True Valuation of Cullet*** – Paul J. Smith, Global Sourcing Manager – Cullet, Owens-Brockway Glass Container Inc. and Peter Walters, Vice President, Purchasing and Distribution, Saint-Gobain Containers
9:30 a.m. – 9:45 a.m.	Questions & Answers
9:45 a.m. – 10:15 a.m.	Morning Break
10:15 a.m. – 10:45 a.m.	***An Industry System for Quality Measurement*** – Kathleen Flight, Manager of Cullet and Recycling Procurement, Saint-Gobain and Peter Walters, Vice President, Purchasing and Distribution, Saint-Gobain Containers
10:45 a.m. – 11:00 a.m.	Questions & Answers
11: 00 a.m. – 11:30 a.m.	***Modern Technologies for Cullet Processing*** – Gerhard Glawitsch – Sales Manager, BT-Wolfgang Binder
11:30 a.m. – 11:45 a.m.	Questions & Answers
11:45 a.m. – 12:45 p.m.	Lunch Provided
12:45 p.m. – 1:30 p.m.	***State Government Perspective on Glass Recycling*** – Panel Discussion - Gloria Hardegree, Executive Director Georgia Recycling Coalition, Scott Mouw, North Carolina State Recycling Program Director, and Frank Kiloran, National Business Development Manager, Pratt Industries, Inc. - Moderated by Daniel K. Steen
1:30 p.m. – 2:15 p.m.	***Panel Discussion*** – All Faculty plus Bill Waltz, President and CEO, Strategic Materials, Curtis Bucey, President and COO, Strategic Materials, David Hudson, Vice President Government Affairs, Strategic Materials, and Steve Bowles, President Reflective Recycling – Moderated by Kenneth Lovejoy
2:15 p.m. – 2:30 p.m.	***Symposium Closing Remarks*** – Kenneth Lovejoy, VP, Environment, Health & Safety, Owens-Illinois, Inc.
2:30 p.m.	Symposium Concludes

About the Glass Manufacturing Industry Council

The Glass Manufacturing Industry Council (GMIC) is a trade association of the Glass Industry that includes among its members international representatives of all four sectors: Flat, Container, Fiber and Specialty as well as major suppliers, research institutes, universities, contractors and experienced industry professionals. GMIC promotes the interests and growth of the global glass industry.

Mission

"To facilitate, organize and promote the interests and economic growth and sustainability of the glass industry through education and cooperation in the areas of technology, productivity, innovation and the environment."

Contact Information

Glass Manufacturing Industry Council
600 N. Cleveland Avenue, Suite 210
Westerville, OH 43082
614-523-3033 Office
www.gmic.org

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Monday, May 16, 2011

Stookey Lecture of Discovery Award

Room: Cumberland

8:00 AM

Delbert Day, Missouri University of Science and Technology
Repairing the Body with Glass

Symposium I: Glass Science

Session E: Non-Silicate Glasses I

Room: Sapelo

Session Chair: Juejun Hu, University of Delaware

9:20 AM

(GOMD-SI-049-2011) EXAFS analysis of local structure of Ge in amorphous and crystallized Ge(x)Te(1-x) thin films
Y. Choi*, Lehigh University, USA; B. Cheong, Korea Institute of Science and Technology, Republic of Korea; A. Kovalskyy, H. Jain, Lehigh University, USA

9:40 AM

(GOMD-SI-050-2011) Structural models of Ag incorporation into As2S3 thin films
A. Kovalskyy, Lehigh University, USA; V. Lyubin, M. Klebanov, Ben-Gurion University of the Negev, Israel; M. Vlcek*, FCHT University of Pardubice, Czech Republic; H. Jain, Lehigh University, USA

10:00 AM

(GOMD-SI-051-2011) Analysis of Constraint Theory in Germanium Arsenic Sulfuide Glasses
P. F. Wachtel*, J. Musgraves, Clemson University, USA; N. Carlie, Schott North America, USA; J. Wilkinson, C. Ostrouchov, K. Richardson, Clemson University, USA

10:20 AM

(GOMD-SI-052-2011) Structure of S-rich Ge-S glasses by X-ray photoelectron spectroscopy
R. Golovchak, A. Kovalskyy*, H. Jain, Lehigh University, USA

10:40 AM

(GOMD-SI-053-2011) Tellurium glasses for far infrared applications
C. Boussard-Plédel*, Glasses and Ceramics group - UMR CNRS 6226, France; B. Bureau, Glasses and Ceramics group - UMR CNRS 6226, France; C. Conseil, Glasses and Ceramics group - UMR CNRS 6226, France; X. Zhang, Glasses and Ceramics group - UMR CNRS 6226, France; J. Lucas, Glasses and Ceramics group - UMR CNRS 6226, France

11:00 AM

(GOMD-SI-054-2011) Structural environments and intra-4f-configurational transitions of trivalent Dy ions in Ge–As–S and Ge–Ga–S glasses
Y. Choi*, Korea Aerospace University, Republic of Korea; H. Jain, Lehigh University, USA

11:20 AM

(GOMD-SI-055-2011) New Functionalities in Non-Oxide Glasses (Invited)
S. K. Sundaram*, B. J. Riley, H. Qiao, C. F. Windisch, Jr., M. K. Murphy, J. V. Ryan, J. S. McCloy, B. R. Johnson, Pacific Northwest National Laboratory, USA

Symposium II: The Amorphous State

Session A: Glass Transition and Relaxation in Glasses and Glassforming Liquids I

Room: Ossabaw

Session Chair: Prabhat Gupta

9:20 AM

(GOMD-SII-001-2011) The Emergence of Solid Behaviour in Amorphous Materials (Invited)
S. Williams*, D. Evans, Australian National University, Australia

10:00 AM

(GOMD-SII-002-2011) The energy landscape of glass formers and beyond (Invited)
A. Heuer*, C. Rehwald, O. Rubner, C. Schroer, Institute of Physical Chemistry, Germany

10:40 AM

(GOMD-SII-003-2011) The Interplay between Structure and Dynamics in Glass-forming Alloys (Invited)
A. Widmer-Cooper*, University of Sydney, Australia

11:20 AM

(GOMD-SII-004-2011) Spatial Correlation of the Dynamic Propensity in a Glass-Forming Binary Alloy (Invited)
M. G. Razul, G. S. Matharoo, P. H. Poole*, St. Francis Xavier University, Canada

Symposium III: Optical Materials and Devices

Session C: Transparent Ceramics I

Room: Pulaski

Session Chair: Robert Pavlacka, US Army Research Laboratory

9:20 AM

(GOMD-SIII-016-2011) The Impact of transparent ceramic materials on future lasers (Invited)
M. Richardson*, University of Central Florida, USA

10:00 AM

(GOMD-SIII-017-2011) Submicrometer-Grained Transparent Sesquioxide Ceramics
J. Ballato*, K. Serivalsatit, Clemson University, USA

10:20 AM

(GOMD-SIII-018-2011) Microstructural Characterization of Optical Ceramics using Electron Backscatter Diffraction
M. Nowell*, EDAX-TSL, USA

10:40 AM

(GOMD-SIII-019-2011) Scattering in Transparent Materials
C. Brecher, ALEM Associates, USA; S. R. Miller, R. Gurjar*, RMD Incorporated, USA; A. Lempicki, ALEM Associates, USA

11:00 AM

(GOMD-SIII-020-2011) Crystallization and second harmonic generation surface and bulk responses of lithium niobium silicate glass ceramics
H. Vigouroux*, E. Fargin, A. Fargues, ICMCB-CNRS, France; B. Le Garrec, CEA, France; M. Dussauze, V. Rodriguez, F. Adamietz, ISM, France; G. Mountrichas, E. Kamitsos, NHRF, Greece; S. Lotarev, V. Sigaev, D. Mendeleyev University of Chemical Technology of Russia, Russian Federation

11:20 AM

(GOMD-SIII-021-2011) The Quest for Large Optical Components in Multi Petawatt and Fusion Lasers (Invited)
B. J. Le Garrec*, CEA-CESTA, France

Session H: Ion Conductors and Energy Storage Materials I

Room: Cumberland

Session Chair: Steve Martin, Iowa State University

9:20 AM

(GOMD-SIII-051-2011) Superionic glass-ceramic electrolytes for all-solid-state batteries (Invited)
M. Tatsumisago*, A. Hayashi, Osaka Prefecture University, Japan

10:00 AM

(GOMD-SIII-052-2011) Predicting Glass Former Units and Transport in Ion-Conducting Network Glasses (Invited)
P. Maass*, University of Osnabrueck, Germany

*Denotes Presenter

10:40 AM

(GOMD-SIII-053-2011) Structures and properties of ion conducting glasses (Invited)
N. Greaves*, University of Cambridge, United Kingdom; E. Flikkema, CNRS- CEMHTI, France; Z. Zhou, University of Cambridge, United Kingdom; Y. Vaills, CNRS- CEMHTI, France

11:00 AM

(GOMD-SIII-054-2011) Structure of amorphous Na2S+P2S5 prepared by melt quenching and mechanical milling
S. S. Berbano*, I. Seo, C. M. Bischoff, K. E. Schuller, S. W. Martin, Iowa State University, USA

11:20 AM

(GOMD-SIII-055-2011) Crystalline phase content and ionic conductivity correlation in Li2O-Al2O3-TiO2-P2O5 glass ceramic
S. Soman*, Indian Institute of Technology Bombay, India; Y. Iwai, J. Kawamura, Institute of Multidisciplinary Research for Advanced Materials, Japan; A. Kulkarni, Indian Institute of Technology Bombay, India

Symposium I: Glass Science

Session E: Non-Silicate Glasses II

Room: Sapelo

Session Chair: Andriy Kovalskyy, Lehigh University

1:00 PM

(GOMD-SI-056-2011) Infrared Quantum Dot Chalcogenide Films for Integrated Light Sources
N. Patel*, S. Geyer, J. Scherer, M. Bawendi, Massachusetts Institute of Technology, USA; N. Carlie, J. D. Musgraves, K. Richardson, Clemson University, USA; J. Hu, P. Lin, P. Becla, Massachusetts Institute of Technology, USA; C. Dimas, Masdar Institute of Science, United Arab Emirates; L. C. Kimerling, A. Agarwal, Massachusetts Institute of Technology, USA

1:20 PM

(GOMD-SI-057-2011) Novel Methods for the Preparation of High Purity Chalcogenide Glass for Optical Fiber Applications (Invited)
D. W. Hewak*, K. Huang, K. J. Knight, University of Southampton, United Kingdom

2:00 PM

(GOMD-SI-058-2011) Conductive chalcogenide glasses for sensing applications
P. Lucas*, Z. Yang, K. Reynolds, B. Bureau, University of Arizona, USA; M. Anne, University of Rennes, France

2:20 PM

(GOMD-SI-059-2011) Solid Glass Electrolyte Enabled In-situ X-ray Absorption Spectroscopy of Electroactive Elements in Working Li-ion Batteries (Invited)
F. Alamgir*, Georgia Institute of Technology, USA

3:00 PM

Break

Session F: Glass-Ceramics

Room: Cumberland

Session Chair: Amanda Brennecka, Sandia National Laboratories

3:20 PM

(GOMD-SI-060-2011) Crystallization behavior of chromium doped CaO-ZrO2-SiO2 glass-ceramics system
M. Bahman, Imam Khomeini International University, Islamic Republic of Iran; B. Mehdikhani*, Institute of Standards & Industrial Research of Iran, Islamic Republic of Iran

3:40 PM

(GOMD-SI-061-2011) Crystallisation of powellite phase in aluminoborosilicate glasses
T. Taurines*, B. Boizot, UMR 7642 CEA-CNRS-Ecole Polytechnique, France

4:00 PM

(GOMD-SI-062-2011) Critical assessment of DTA/DSC methods to study glass crystallization kinetics
V. M. Fokin, A. A. Cabral, R. M. Reis, E. D. Zanotto*, Fed. University Sao Carlos, Brazil

4:20 PM

(GOMD-SI-063-2011) Fluorescence Properties of Rare-Earth Co-Doped Fluorochlorozirconate Glasses
M. Vu*, University of Tennessee Space Institute, USA; C. Passlick, Martin Luther University of Halle-Wittenberg, Germany; J. A. Johnson, C. E. Johnson, University of Tennessee Space Institute, USA; S. Schweizer, Fraunhofer Center for Silicon Photovoltaics, Germany

4:40 PM

(GOMD-SI-064-2011) TeO2-Bi2O3-ZnO glass ceramic with high transparency in NIR region
X. Hu*, D. Musgraves, D. Vanderveer, J. Boerstler, N. Carlie, P. Wachte, Clemson University, USA; S. Raffy, University of Bordeaux, France; R. Stolen, K. Richardson, Clemson University, USA

5:00 PM

(GOMD-SI-065-2011) Glass Ceramic Waste Form Development for Combined Fission Products Waste Streams from Used Nuclear Fuel
J. Crum*, Pacific Northwest National Lab, USA; A. Kossoy, Los Alamos National Lab, USA; B. Riley, Pacific Northwest National Lab, USA; M. Tang, Los Alamos National Lab, USA; L. Turo, Pacific Northwest National Lab, USA

Symposium II: The Amorphous State

Session A: Glass Transition and Relaxation in Glasses and Glassforming Liquids II

Room: Ossabaw

Session Chairs: Sabyasachi Sen, University of California at Davis; Ulrich Fotheringham, SCHOTT AG

1:00 PM

(GOMD-SII-005-2011) Particle dynamics in dense colloidal suspensions with short-ranged attractive potential
P. Habdas*, A. Latka, Saint Joseph's University, USA; P. Yunker, M. Lohr, A. G. Yodh, University of Pennsylvania, USA

1:20 PM

(GOMD-SII-006-2011) The Predictive Power of Three Parameter Viscosity Models
U. G. Fotheringham*, F. Lentes, SCHOTT AG, Germany; D. B. Dingwell, LMU-University of Munic, Germany

1:40 PM

(GOMD-SII-007-2011) A discussion of iso-structural viscosity based on trap-dynamics
P. Gupta*, A. Heuer, The Ohio State University, USA

2:00 PM

(GOMD-SII-008-2011) Universal characteristics of the liquid-liquid critical point (Invited)
N. Greaves*, University of Cambridge, United Kingdom

2:20 PM

(GOMD-SII-028-2011) Heat capacity at the glass transition
K. Trachenko*, Queen Mary University of London, United Kingdom

2:40 PM

(GOMD-SII-009-2011) Structural Relaxation Mechanism Associated with Glass Transition in Ge-Se Liquids
T. Edwards*, S. Sen, University of California at Davis, USA

3:00 PM

Break

3:20 PM

(GOMD-SII-010-2011) Ideal glassformers and glass transition paradigms (Invited)
C. Angell*, V. Kapko, D. Matyushov, Arizona State University, USA

4:00 PM

(GOMD-SII-011-2011) Revisit of entropy issues in non-equilibrium states
A. Takada*, Asahi Glass Company, Japan

4:20 PM

(GOMD-SII-012-2011) On the Dependence of the Properties of Glasses on Cooling and Heating Rates (Invited)
J. Schmelzer*, Germany

5:00 PM

(GOMD-SII-013-2011) Energy correlations in supercooled states of silicon
X. Mei, W. Mohamed, J. Eapen*, NC State University, USA

5:20 PM

(GOMD-SII-014-2011) Experimental and Computer Investigation of Thermal Relaxation in AsxSe1-x Glasses
E. A. King*, R. G. Erdmann, P. Lucas, University of Arizona, USA

Session G: Water and Glass

Room: Sapelo

Session Chairs: Minoru Tomozawa, Rensselaer Polytechnic Institute; Minoru Tomozawa, Rensselaer Polytechnic Institute

3:20 PM

(GOMD-SII-059-2011) Diffusion and redox reactions of water-related species in silicate melts (Invited)
H. Behrens*, Leipniz University of Hannover, Germany

4:00 PM

(GOMD-SII-060-2011) Effect of Water Penetration on the Strength and Toughness of Silica Glass (Invited)
S. Wiederhorn*, NIST, USA; T. Fett, Karlsruhe Institute of Technology, Germany; J. Guin, University of Rennes, I, France

4:40 PM

(GOMD-SII-061-2011) Effect of Water on Internal Friction for a SiO2-Al2O3-Na2O-MgO Glass
T. Tsujimura*, M. Nishizawa, A. Koike, Y. Kuroki, Asahi Glass Co., Ltd., Japan

5:00 PM

(GOMD-SII-062-2011) Nanostructure of water-containing glass by MD simulation
S. Ito*, Tokyo Institute of Technology, Japan; T. Taniguchi, Asahi Glass Co., Ltd., Japan

5:20 PM

(GOMD-SII-063-2011) Water diffusion in silica glass and wet oxidation of Si: A new interpretation for the high speed of wet oxidation
M. Tomozawa*, Rensselaer Polytechnic Institute, USA

Symposium III: Optical Materials and Devices

Session C: Transparent Ceramics II

Room: Pulaski

Session Chair: Robert Pavlacka, US Army Research Laboratory

1:00 PM

(GOMD-SIII-022-2011) Ceramic Scintillators for Computed Tomography (Invited)
H. Jiang*, J. Gent, M. Prescott, GE Healthcare, USA; S. Duclos, J. Vartuli, R. Lyons, C. Vess, R. Hagerdon, K. Mcevoy, A. Setlur, GE Global Research, USA

1:40 PM

(GOMD-SIII-023-2011) Strength-Size Scaling and Flaw Tolerance in Coarse-Grained Transparent Magnesium Aluminate Spinel Windows
J. Swab, R. Pavlacka*, S. Kilczewski, G. Gilde, US Army Research Laboratory, USA

2:00 PM

(GOMD-SIII-024-2011) Forming Transparent Ceramics for Al-rich Formulations of $MgO.nAl_2O_3$ (n>1)
A. Sutorik*, J. Swab, G. Gilde, C. Cooper, R. Gamble, E. Shanholtz, R. Pavlacka, US Army Research Laboratory, USA

2:20 PM

(GOMD-SIII-025-2011) Highly transparent Al-rich MgO.nAl2O3 spinel ($1 \leq n \leq 2.5$) by reaction sintering of MgO and Al2O3
K. Waetzig*, A. Krell, A. Michaelis, Fraunhofer Institute for Ceramic Technologies and Systems, Germany

2:40 PM

(GOMD-SIII-026-2011) Reversible optical properties of an infrared transparent Y2O3-MgO nanocomposite
D. Jiang*, A. K. Mukherjee, University of California-Davis, USA

3:00 PM

Break

Session B: Photosensitivity and Photomodification

Room: Pulaski

Session Chair: Pierre Lucas, University of Arizona

3:20 PM

(GOMD-SIII-010-2011) Optical agility of chalcogenide films using their photosensibility (Invited)
V. Nazabal*, Chemistry Sciences Center of Rennes, UMR 6226, University of Rennes, France; P. Nemec, Faculty of Chemical Technology, University of Pardubice, Czech Republic; M. Cathelinaud, UPS CNRS 2274, France; G. Boudebs, Université d'Angers, France; M. Chauvet, UMR CNRS 6174, Département d'optique, France; F. Charpentier, Chemistry Sciences Center of Rennes, UMR 6226, University of Rennes, France; M. Lequime, UMR6133, CNRS-ECM-UPCAM-UP, France; X. Zhang, Chemistry Sciences Center of Rennes, UMR 6226, University of Rennes, France

4:00 PM

(GOMD-SIII-011-2011) Atomistic nature and dynamics of optically and thermally induced changes in chalcogenide glass thin films
D. Zhao*, H. Jain, Lehigh University, USA

4:20 PM

(GOMD-SIII-012-2011) Direct Femtosecond Laser Writing in silver-containing glass
T. Cardinal*, K. Bourhis, ICMCB-CNRS, France; A. Royon, CPMOH-CNRS, France; M. Treguer, Y. Petit, J. Videau, ICMCB-CNRS, France; J. Choi, M. Richardson, UCF, USA; L. Canioni, CPMOH-CNRS, France

4:40 PM

(GOMD-SIII-013-2011) Ultrafast Laser Processing of Hybrid Micro- and Nano-Structures in Silicate Glasses
P. Mardilovich*, L. Fletcher, N. Troy, S. Risbud, D. Krol, University of California, USA

5:00 PM

(GOMD-SIII-014-2011) Mechanisms of NaF growth in photo-thermo-refractive glass
K. Chamma, J. Lumeau*, L. Glebova, L. B. Glebov, University of Central Florida, USA

5:20 PM

(GOMD-SIII-015-2011) 3D temperature distribution and crystallization mechanisms of ferroelectric LaBGeO5 during femtosecond laser irradiation inside bulk glass
A. Stone*, M. Sakakura, Y. Shimotsuma, Lehigh University, USA; K. Miura, K. Hirao, Kyoto University, Japan; V. Dierolf, H. Jain, Lehigh University, USA

Session H: Ion Conductors and Energy Storage Materials II

Room: Cumberland

Session Chair: Steve Martin, Iowa State University

1:00 PM

(GOMD-SIII-056-2011) Understanding the alkali dynamics in silicate systems for small and large electric fields (Invited)
A. Heuer*, H. Lammert, L. Lühning, Institute of Physical Chemistry, Germany

1:40 PM

(GOMD-SIII-057-2011) First and second universalities in ion-conducting glasses (Invited)
K. Funke*, University of Muenster, Germany

2:20 PM

(GOMD-SIII-058-2011) Structure/Property Correlations in the Ionic Conductivity of Mixed Glass Former Glasses in the $Na_2S+GeS_2+P_2S_5$ Glass System
C. Bischoff*, K. Schuller, S. W. Martin, Iowa State University, USA

2:40 PM

(GOMD-SIII-059-2011) Structural Studies and Models of Sodium Borophosphate Mixed Glass Former Glasses
R. B. Christensen*, S. W. Martin, G. Olson, Iowa State University, USA

3:00 PM

Break

Posters

Room: Madison

6:30 PM

(GOMD-SI-P001-2011) Influence of Structural changes on the ESR Spectra of Mn2+ doped Lead Phosphate Glasses
C. Dayanand*, Tirumala Engineering College, India

(GOMD-SI-P002-2011) Laser Aerolevitation Manufacturing of Alkaline Earth Silicates
C. Nie*, W. Trull, P. Dulal, S. Feller, M. Affatigato, Coe College, USA

(GOMD-SI-P003-2011) The Production of Cesium Borate Glass for Use in Atomic Clocks
E. Wiese Moore*, Coe College, USA; J. Bernstein, Massachussetts Institute of Technology, USA; A. Ramm, J. North, J. Maldonis, J. Alberts, S. Feller, M. Affatigato, Coe College, USA; M. Mescher, W. Robbins, R. Stoner, B. Timmons, Massachussetts Institute of Technology, USA

(GOMD-SI-P004-2011) Alumina Effect on Enthalpy of Mixing of Mixed Alkali Silicate Glasses
P. J. Lezzi*, M. Tomozawa, RPI, USA

(GOMD-SI-P005-2011) Glass-Forming Ability of Soda Lime Borate Liquids
Q. Zheng*, Aalborg University, Denmark; J. C. Mauro, Corning Incorporated, USA; M. M. Smedskjaer, Aalborg University, Denmark; M. Potuzak, Corning Incorporated, USA; R. Keding, Max Planck Institute for the Science of Light, Germany; Y. Yue, Aalborg University, Denmark

(GOMD-SI-P006-2011) Spherical bioactive glass particles and their interaction with human mesenchymal stem cells in vitro
S. Labbaf*, O. Tsigkou, M. M. Stevens, A. E. Porter, J. R. Jones, Imperial College London, United Kingdom

(GOMD-SI-P007-2011) Aqueous Corrosion of Polyphosphate Glasses
C. Smith*, R. Brow, Missouri University of Science and Technology, USA

(GOMD-SI-P008-2011) Engineered Corrosion-induced Passivation Layers for Glass Waste Forms
D. C. Skorski*, J. Ryan, Pacific Northwest National Laboratory, USA

(GOMD-SI-P009-2011) Dissolution Behavior of Na/Ca-Phosphate Glasses In in Aqueous Solutions
L. Ma*, R. K. Brow, M. E. Schlesinger, Missouri University of Science and Technology, USA

(GOMD-SI-P010-2011) Analytical modeling of thermodynamic iron redox equilibria and aqueous dissolution behavior of iron phosphate glasses
M. L. Schmitt*, R. K. Brow, Missouri S&T, USA

(GOMD-SI-P011-2011) A Raman Spectroscopy Study of the Structure of Iron Phosphate Glasses
L. Zhang*, R. Brow, Missouri University of Science and Technology, USA

(GOMD-SI-P012-2011) Microstructure and physical properties of the GexAsySe1-x-y glasses with the same mean coordination number of 2.5
R. Wang*, A. Smith, D. Choi, S. Madden, B. Luther-Davies, Australian National University, Australia

(GOMD-SI-P013-2011) Stabilization of Second Harmonic Generation in Thermally Poled, Alkali Doped Chalcogenide Glasses
T. Shoulders*, K. Richardson, Clemson University, USA; M. Dussauze, University Bordeaux 1, France; D. Musgraves, Clemson University, USA

(GOMD-SI-P014-2011) Influence of imprinting conditions on the surface morphology of chalcogenide glasses
B. Jin, Y. Choi*, Korea Aerospace University, Republic of Korea; W. Chung, Kongju National University, Republic of Korea; D. Shin, Hanyang University, Republic of Korea; H. Jain, Lehigh University, USA

(GOMD-SI-P015-2011) Thermal expansion investigation of iron sodium silicate glass
B. Mirhadi, B. Mehdikhani*, Imam Khomeini International University, Islamic Republic of Iran

(GOMD-SI-P016-2011) Optical absorption and Crystallisation of sodium desilicate glasses containing chromium oxide
B. Mehdikhani*, B. Mirhadi, Imam Khomeini International University, Islamic Republic of Iran

(GOMD-SII-P017-2011) Relaxation dynamics of supercooled silicon using molecular dynamics simulations
X. Mei*, W. Mohamed, J. Eapen, NC State University, USA

(GOMD-SII-P018-2011) A low-cost electrometer for measuring conductivity and glass transition in sugar glass
W. R. Heffner*, Lehigh University, USA; N. Ward, Oakwood University, USA

(GOMD-SII-P019-2011) Electronic Consequences of Electron-Phonon Interaction in Impurity States of Doped Semiconductors
B. Cai*, M. Zhang, D. Drabold, Ohio University, USA

(GOMD-SIII-P020-2011) Optical spectra of DIVALENT and TRIVALENT iron in sodium silicate glasses
B. Mirhadi, Imam Khomeini International University, Islamic Republic of Iran; B. Mehdikhani*, Institute of Standard and Industrial Research of Iran (ISIRI), Islamic Republic of Iran

(GOMD-SIII-P021-2011) Role of manganese as a oxidizing agent in sodium silicate glasses containing iron oxide
B. Mirhadi, B. Mehdikhani*, Imam Khomeini International University, Islamic Republic of Iran

(GOMD-SIII-P022-2011) UV-Vis spectroscopy of transition metals in sodium silicate glasses
B. Mirhadi, Imam Khomeini International University, Islamic Republic of Iran; B. Mehdikhani*, Institute of Standard and Industrial Research of Iran (ISIRI), Islamic Republic of Iran

(GOMD-SIII-P023-2011) Infrared absorption of polyvalent oxides in glass
B. Mirhadi, B. Mehdikhani*, Imam Khomeini International University, Islamic Republic of Iran

(GOMD-SIII-P024-2011) Optical properties of Mn2+ doped Lead phosphate Glasses
C. Dayanand*, Tirumala Engineering College, India

(GOMD-SIII-P025-2011) Does photoinduced anisotropy in chalcogenide glasses have atomic structure signature?
D. Zhao*, H. Jain, Lehigh university, USA

(GOMD-SIII-P026-2011) Laser-induced anomalous plasmonic evolution in silver nanocomposite glass: An in situ optical microspectroscopy study
J. A. Jimenez*, M. Sendova, New College of Florida, USA

(GOMD-SIII-P027-2011) Relation between structure and photochemistry of silver-containing phosphate glasses
K. Bourhis, Y. Petit, M. Treguer, C. Labrugere, J. Videau, ICMCB-CNRS, France; A. Royon, G. Papon, L. Canioni, LCMCP-CNRS-ENSCP, France; L. Binet, D. Caurant, CPMOH-CNRS, France; B. Revel, L. Montagne, USTL-CNRS, France; T. Cardinal*, ICMCB-CNRS, France

(GOMD-SIII-P028-2011) Pulsed Laser Deposited Ga-Ge-Te Amorphous Thin Films
P. Nemec*, University of Pardubice, Czech Republic; V. Nazabal, A. Moreac, Université de Rennes 1, France

(GOMD-SIII-P029-2011) The effects of sintering aids on defects and densification in transparent Nd:YAG ceramics
A. Stevenson*, G. L. Messing, The Pennsylvania State University, USA

(GOMD-SIII-P030-2011) Phase separation and crystallization mechanism in non linear optical LiNbO3-SiO2 glasses
G. Mountrichas, E. Kamitsos, NHRF, Greece; H. Vigouroux*, A. Fargues, E. Fargin, ICMCB-CNRS, France; B. Le Garrec, CEA, France; M. Dussauze, F. Adamietz, V. Rodriguez, ISM, France; S. Lotarev, V. Sigaev, D. Mendeleyev University of Chemical Technology of Russia, Russian Federation

(GOMD-SIII-P031-2011) The Effect of Silica on Emission Property of Various Cr4+-Doped Glass Ceramics
J. Wang*, F. Shen, NSYSU, Taiwan

(GOMD-SIII-P032-2011) Processing and Mechanical Properties of Transparent Lu2O3 Laser Host Ceramics
R. Pavlacka*, S. Kilczewski, A. Lidie, G. Gilde, US Army Research Laboratory, USA

(GOMD-SIII-P033-2011) Compositional and structural changes in thermally poled borosilicate glass and their link to non linear optical properties
T. Cremoux*, D. Marc, Univ. Bordeaux 1 - CNRS, France; E. Fargin, T. Cardinal, CNRS, France; T. Shoulders, K. Richardson, Clemson university, USA; V. Rodriguez, Univ. Bordeaux 1 - CNRS, France

(GOMD-SIII-P034-2011) Development of Pr3+-doped ZBLA fluoride waveguide for compact laser source emitting in visible
M. Olivier, P. Pirasteh, J. Doualan, Chemistry Sciences Center of Rennes, France; P. Camy, UMR 6252, CEA, CNRS, ENSICAEN et Université de Caen, France, UMR 6252, CEA, CNRS, ENSI-CAEN et Université de Caen, FranceUniversité Rennes1, France; H. Lhermite, J. Adam, V. Nazabal*, Chemistry Sciences Center of Rennes, France

(GOMD-SIII-P035-2011) Size Effects on Properties of Novel High Z Scintillators
J. V. Branson*, P. Yang, S. Thoma, P. Doty, T. J. Boyle, L. Ottley, B. A. Hernandez-Sanchez, Sandia National Laboratories, USA

(GOMD-SIII-P036-2011) Monitoring of the geological storage of CO2 using chalcogenide waveguides
M. Brandily*, University of Rennes1, France; V. Nazabal, F. Charpentier, Université Rennes1, France; H. Lhermite, University of Rennes1, France; J. Charrier, UMR 6082, France; C. Boussard-Plédel, B. Bureau, Université Rennes1, France; J. Doualan, P. Camy, CIMAP, France

(GOMD-SIII-P037-2011) The Effect of Gold Doping on the Conductivity of Sodium Trisilicate Glass
M. Wojciechowski*, C. Saiyasombat, H. Jain, Lehigh University, USA; R. Küchler, Technische Universität Dortmund, Germany

(GOMD-SIV-P038-2011) Chalcogen-based aerogels as a multifunctional platform for remediation of radioactive waste
B. Riley*, J. Chun, J. Ryan, S. K. Sundaram, D. Strachan, PNNL, USA

(GOMD-SIV-P039-2011) Evaluation of nepheline formation in nuclear waste glasses
C. P. Rodriguez*, M. J. Schweiger, A. E. Winschell, J. S. McCloy, Pacific Northwest National Laboratory, USA

(GOMD-SIV-P040-2011) Utilization of a Laboratory-Scale Melter to Determine Melting Rate of Waste Glass Feeds
J. Das Gupta*, D. Kim, M. Schweiger, W. Buchmiller, J. Vienna, Pacific Northwest National Laboratory, USA

(GOMD-SIV-P048-2011) The DHS database for High Performance Materials
G. Fischman*, Future Strategy Solutions, LLC, USA

(GOMD-SIV-P049-2011) Sorting of glass, plastics and minerals
A. Schnehen*, C. Makari, Binder & Co. AG, Austria

(GOMD-SIV-P041-2011) Soda-lime silicate glass under hydrostatic pressure and indentation: a micro-Raman study
T. Deschamps*, CEA, France; C. Martinet, LPCML, Université Lyon1, France; J. Bruneel, Université Bordeaux1, France; B. Champagnon, LPCML, Université Lyon1, France

(GOMD-SIV-P042-2011) Borate Based Bioactive Glasses for Soft Tissue Regeneration
S. Jung*, Mo-Sci Corporation, USA

(GOMD-SIV-P043-2011) Effect of temperature on UV-Vis spectroscopy of sodium silicate glasses contained nanoparticle iron oxide
B. Mirhadi, B. Mehdikhani*, Imam Khomeini International University, Islamic Republic of Iran

(GOMD-SIV-P044-2011) Preparation of CaO-MgO-SiO2 Glass-Ceramic Using Na2SiO3 Waste Solution
C. Yamagata, O. Z. Higa, Instituto de Pesquisas Energeticas e Nucleares, USA; A. D. Rodas, Instituto de Pesquisas Energeticas e Nucleares, Brazil; S. T. Reis*, Missouri University of Science and Technology, USA

(GOMD-SIV-P045-2011) Synthesis and Characterization of Phase-change Nanowires Confined in Periodic Mesoporous Silica
C. Ihalawela*, B. Prasai, G. Rosen, G. Chen, Ohio University, USA

(GOMD-SIV-P046-2011) Nanoparticle-incorporated indium tin oxide (ITO) thin films obtained through sol-gel process
H. Yavas*, M. T. Kesim, C. Durucan, Middle East Technical University, Turkey

(GOMD-SIV-P047-2011) Sol-gel derived silver-incorporated hybrid ITO thin films
M. T. Kesim*, H. Yavas, C. Durucan, Middle East Technical University, Turkey

Tuesday, May 17, 2011

George W. Morey Award Lecture

Room: Cumberland

8:00 AM

Neville Greaves, University of Cambridge
Glass Structure, Ion Transport, and the Pareto Principle

Symposium I: Glass Science

Session B: Glass Structure and Properties I

Room: Cumberland

Session Chair: Randall Youngman, Corning Incorporated

9:20 AM

(GOMD-SI-010-2011) Perfect glasses with novel mechanical properties (Invited)
N. Greaves*, L. L. Greer, University of Cambridge, United Kingdom; G. Sankar, University College London, United Kingdom

10:00 AM

(GOMD-SI-011-2011) Structural characteristics of low- and high-density amorphous phases in yttrium aluminate glasses: results from multinuclear NMR spectroscopy
N. Nasikas, ICEHT/FORTH, Greece; S. Sen*, University of California at Davis, USA; G. Papatheodorou, ICEHT/FORTH, Greece

10:20 AM

(GOMD-SI-012-2011) Composition dependence of the viscosity and other physical properties in the arsenic selenide glass system
J. Musgraves*, P. Wachtel, S. Novak, J. Wilkinson, K. Richardson, Clemson University, USA

10:40 AM

(GOMD-SI-013-2011) Electrical Transport Properties of Bulk Amorphous Semiconductors
B. R. Johnson*, J. S. McCloy, B. J. Riley, J. V. Crum, J. V. Ryan, S. K. Sundaram, Pacific Northwest National Laboratory, USA; D. N. Hebert, A. A. Rocket, University of Illinois, Urbana-Champaign, USA

11:00 AM

(GOMD-SI-014-2011) Raman and X-ray Absorption Studies of the Structure of Alkali Tungstate Glasses
C. W. Ponader*, K. Adib, B. Aitken, Corning Incorporated, USA

11:20 AM

(GOMD-SI-015-2011) The Structure and Properties of Polyphosphate glasses from the ZnO-MgO-P2O5 and ZnO-Al2O3-P2O5 Systems
C. Smith*, R. Brow, Missouri University of Science and Technology, USA

11:40 AM

(GOMD-SI-016-2011) Structure-Property Relationships in Cerium Aluminophosphate and Silicophosphate Glasses
J. L. Rygel*, C. G. Pantano, The Pennsylvania State University, USA

Session C: Glass Corrosion I

Room: Sapelo

Session Chair: Stephane Gin, CEA

9:20 AM

(GOMD-SI-028-2011) Development of first-principles-based models for glass dissolution
P. Zapol*, H. He, J. Cunnane, Argonne National Laboratory, USA

9:40 AM

(GOMD-SI-029-2011) Filling the Gaps from Atomistic to Continuum Modeling to Better Predict Nuclear Waste Glass Dissolution
L. J. Criscenti*, Sandia National Laboratories, USA

10:00 AM

(GOMD-SI-030-2011) Modeling of Glass Dissolution with Transition-State Theory
D. Strachan*, Pacific Northwest National Laboratory, USA

10:20 AM

(GOMD-SI-031-2011) Why glasses with high dissolution rates may undergo low corrosion? (Invited)
C. Cailleteau*, CEA/DEN, France; F. Devreux, Ecole Polytechnique-CNRS, France; O. Spalla, CEA/DSM, France; F. Angéli, S. Gin, CEA/DEN, France

10:40 AM

(GOMD-SI-032-2011) Evidence for a New Glass Corrosion Mechanism from Isotope Tracer Experiments (Invited)
T. Geisler*, University of Muenster, Germany; A. Janssen, Institute for Transuranium Elements, Germany; R. Denkler, University of Muenster, Germany; M. Kilburn, University of Western Australia, Australia; A. Putnis, University of Muenster, Germany

11:20 AM

(GOMD-SI-033-2011) Solid-State NMR Investigations of Nuclear Waste Glass Corrosion
K. A. Murphy*, K. T. Mueller, C. G. Pantano, The Pennsylvania State University, USA; J. V. Ryan, N. M. Washton, Pacific Northwest National Laboratory, USA

11:40 AM

(GOMD-SI-034-2011) Kinetic evaluation of aqueous dissolution of P0798 simulated HLW glass as a function of dissolved silica concentration by using micro-channel flow-through test method
Y. Inagaki*, K. Sakanani, Kyushu University, Japan; S. Mitsui, Japan Atomic Energy Agency, Japan; K. Idemitsu, T. Arima, Kyushu University, Japan; K. Noshita, Hitachi Ltd., Japan

Symposium II: The Amorphous State

Session A: Glass Transition and Relaxation in Glasses and Glassforming Liquids III

Room: Ossabaw

Session Chair: Prabhat Gupta

9:20 AM

(GOMD-SII-015-2011) What have we learned from experiments about relaxation in silica glass? (Invited)
M. Tomozawa*, Rensselaer Polytechnic Institute, USA

10:00 AM

(GOMD-SII-016-2011) What have we learned about relaxation in glass forming liquids from light scattering experiments? (Invited)
D. Sidebottom*, Creighton University, USA

10:40 AM

(GOMD-SII-017-2011) Silicate glasses under pressure (Invited)
B. Champagnon*, T. Deschamps, C. Martinet, C. Sonneville, D. de Ligny, Université Lyon1, France

11:20 AM

(GOMD-SII-019-2011) Kinetic and Thermodynamic Effects of Nanoconfinement on Glass Transition in Glycerol
S. Sen*, University of California at Davis, USA

Symposium III: Optical Materials and Devices

Session D: Active Optics

Room: Pulaski

Session Chair: David Scrymgeour, Sandia National Laboratories

9:20 AM

(GOMD-SIII-027-2011) Nonlinear photonic crystals utilizing ferroelectric oxide thin films and their application in tunable photonic circuits (Invited)
P. T. Lin*, MIT, USA; B. W. Wessels, Northwestern University, USA

10:00 AM

(GOMD-SIII-028-2011) Fs-Laser Micro Machining of Waveguide Amplifiers Inside Er-Yb Doped Zinc Polyphosphate Glass
L. B. Fletcher*, J. J. Witcher, N. Troy, University of California Davis, USA; R. K. Brow, Missouri University of Science and Technology, USA; D. M. Krol, University of California Davis, USA

10:20 AM

(GOMD-SIII-029-2011) Influence of Silver ions injection and SHG by thermal poling on sodium and niobium borophosphate glasses
E. Fargin*, A. Delestre, A. Fargues, M. Lahaye, ICMCB, France; V. Rodriguez, M. Dussauze, F. Adamietz, ISM, France; L. Canioni, A. Royon, M. Bellec, CPMOH, France

10:40 AM

(GOMD-SIII-030-2011) Thermally poled oxide glasses: correlation between polarization mechanisms and non linear optical properties
D. Marc*, V. Rodriguez, Univ. Bordeaux 1 - CNRS, France; E. Fargin, T. Cardinal, G. Guimbretiere, CNRS, France; T. Cremoux, Univ. Bordeaux 1 - CNRS, France; T. Shoulders, Clemson university, USA; E. Kamitsos, NHRF, Greece; K. Richardson, Clemson university, USA

11:00 AM

(GOMD-SIII-031-2011) Structure and Optical Properties of Pulsed Laser Deposited Ge-Sb-Te Thin Films by Raman Scattering Spectroscopy and Spectroscopic Ellipsometry
P. Nemec*, University of Pardubice, Czech Republic; V. Nazabal, A. Moreac, Université de Rennes 1, France; J. Gutwirth, M. Frumar, University of Pardubice, Czech Republic

11:20 AM

(GOMD-SIII-032-2011) Crystal coherence length effects on the infrared optical response of MgO thin films (Invited)
J. Ihlefeld*, J. C. Ginn, Sandia National Laboratories, USA; D. J. Shelton, University of Central Florida, USA; V. Matias, Los Alamos National Laboratory, USA; P. G. Kotula, M. A. Rodriguez, Sandia National Laboratories, USA; G. D. Boreman, University of Central Florida, USA; P. G. Clem, M. B. Sinclair, Sandia National Laboratories, USA

Norbert J. Kreidl Award Lecture

Room: Madison

12:00 PM

Randilynn Christensen, Iowa State University
The Mixed Glassformer Effect in Sodium Borophosphate Glass

Symposium I: Glass Science

Session B: Glass Structure and Properties II

Room: Cumberland

Session Chair: Randall Youngman, Corning Incorporated

1:20 PM

(GOMD-SI-017-2011) Yb3+ doped SiO2-Al2O3-P2O5 fiber performs: the role of Al and P on clusters dissolution
T. Deschamps*, N. Ollier, T. Charpentier, CEA, France; H. Vezin, CNRS, France; C. Gonnet, Draka, France

1:40 PM

(GOMD-SI-018-2011) High-temperature ^{11}B Magic Angle Spinning Nuclear Magnetic Resonance Spectroscopy Study of Network Dynamics in Borosilicate and Borate Glass-forming Liquids
J. Wu*, N. Kim, J. F. Stebbins, Stanford University, USA

2:00 PM

(GOMD-SI-019-2011) Diffusion of Sodium in Sodium Boroaluminosilicate Glasses: Impact of Mixed Network Formers and the Influence of Water
X. Wu*, Cornell University, USA; Q. Zheng, J. Mauro, M. Potuzak, A. J. Ellison, Corning Incorporated, USA; R. Dieckmann, Cornell University, USA

2:20 PM

(GOMD-SI-020-2011) Sodium Environments in Binary and Ternary Oxide Glasses
R. Youngman*, C. Hogue, J. Dickinson, A. Ellison, B. Aitken, Corning Incorporated, USA

2:40 PM

(GOMD-SI-021-2011) Comparison of the Structure and Properties of Normal, Abnormal and Intermediate Glasses
Q. Zhao, L. Huang*, Rensselaer Polytechnic Institute, USA

3:00 PM

Break

3:20 PM

(GOMD-SI-022-2011) Structure and bonding in oxide liquids and glasses using in-situ x-ray and neutron diffraction
R. Weber*, MDI, USA; C. J. Benmore, Argonne National Laboratory, USA; J. Neuefeind, L. Santodonato, Oak Ridge National Laboratory, USA; L. Skinner, Stony Brook University, USA; M. Wilding, Aberystwyth University, United Kingdom; S. Tumber, MDI, USA; L. Lazareva, J. B. Parise, Stony Brook University, USA

3:40 PM

(GOMD-SI-023-2011) First experiments at Nanoscale Ordered Materials Diffractometer (NOMAD) at the Spallation Neutron Source (SNS)
J. Neuefeind*, ORNL, USA

4:00 PM

(GOMD-SI-024-2011) X-ray absorption spectroscopy analysis of formation and structure of Au nanoparticles in sodium trisilicate glass
C. Saiyasombat*, M. Wojciechowski, H. Jain, Lehigh University, USA

4:20 PM

(GOMD-SI-025-2011) Hydrogen formation observed during high pressure treatment of silica glass
C. Li*, J. Price, M. Tomozawa, E. Watson, Rensselaer Polytechnic Institute, USA

4:40 PM

(GOMD-SI-026-2011) Generalized thermodynamic approach for determining the fictive temperature of glasses with arbitrary thermal history
X. Guo*, M. Potuzak, J. Mauro, D. Allan, T. Kiczenski, Corning Inc., USA; Y. Yue, Aalborg University, Denmark; R. Stewart, Corning Inc., USA

5:00 PM

(GOMD-SI-027-2011) Network Modeling of Glass Structures
P. Kroll*, M. Mwania, UT Arlington, USA

Session C: Glass Corrosion II

Room: Sapelo

Session Chair: Stephane Gin, CEA

1:00 PM

(GOMD-SI-035-2011) Characteristics of alteration layers formed on simulated HLW glass under silica-saturated solutions
T. Maeda*, Japan Atomic Energy Agency, Japan; K. Hotta, Radiation Application Development Association, Japan

1:20 PM

(GOMD-SI-036-2011) Glass Corrosion in Solution Exchange Tests
W. Ebert*, Argonne National Laboratory, USA

1:40 PM

(GOMD-SI-037-2011) Water dynamics in nuclear waste glass during corrosion: A quasi-elastic neutron scattering study
K. J. Alvine*, J. V. Ryan, Pacific Northwest National Lab, USA; M. Tyagi, NIST, USA

2:00 PM

(GOMD-SI-038-2011) Isotopic tracing to highlight glass dissolution mechanisms
A. Verney-Carron*, LISA, France; S. Gin, CEA, France; G. Libourel, CRPG, France; P. Jollivet, CEA, France

2:20 PM

(GOMD-SI-039-2011) Comparison of Glass Leaching Behavior Using a Variety of Test Methods (Invited)
I. S. Muller*, A. Papathanassiu, A. Barkatt, I. L. Pegg, The Catholic University of America, USA

3:00 PM

Break

3:20 PM

(GOMD-SI-040-2011) Reprise of Alteration of the Simulated HLW Glass at High Temperature in Beishan Underground Water (Invited)
Z. Zhang*, China Institute of Atomic Energy, China

3:40 PM

(GOMD-SI-041-2011) The dissolution behavior of simple borate glasses in aqueous environments
K. Goetschius*, R. K. Brow, Missouri S&T, USA

4:00 PM

(GOMD-SI-042-2011) A long-term glass leaching experiment in a granitic environment: importance of reactive-transport processes
S. Gin*, C. Guittonneau, J. Mestre, N. Godon, CEA Marcoule, France

4:20 PM

(GOMD-SI-043-2011) Glass corrosion in cement waters
S. Depierre*, F. Angeli, F. Frizon, S. Gin, CEA Marcoule, France

4:40 PM

(GOMD-SI-044-2011) Nuclear waste glass alteration at high pH
K. Ferrand, K. Lemmens, M. Aertsens*, Belgian Nuclear Research Centre, Belgium

5:00 PM

(GOMD-SI-045-2011) Corrosion of Phosphate-doped Alkali Borosilicate Glasses in Alkaline Solutions
X. Cheng*, R. K. Brow, G. Chen, Missouri University of Science and Technology, USA

Symposium II: The Amorphous State

Session B: Model/Experiment: Links and Limits

Room: Ossabaw

Session Chair: David Drabold, Ohio University

1:00 PM

(GOMD-SII-020-2011) Electric and Magnetic Fields Applied to Materials: Computed Response by First Principles (Invited)
J. Zwanziger*, Dalhousie University, Canada

1:40 PM

(GOMD-SII-021-2011) XAFS Study of Electrodeposited Ge-Sb-Te Phase-change Memory Materials
B. Prasai, D. A. Drabold, G. Chen*, Ohio University, USA

2:00 PM

(GOMD-SII-022-2011) Resolving the vibrational and configurational contributions to thermal expansion in isobaric glass-forming systems
M. Potuzak*, J. C. Mauro, T. J. Kiczenski, A. J. Ellison, D. C. Allan, Corning Incorporated, USA

2:20 PM

(GOMD-SII-023-2011) Thermal conductivity of amorphous ceramics from first principle calculations
B. Kouchmeshky, P. Kroll*, UT Arlington, USA

2:40 PM

(GOMD-SII-024-2011) Electronic consequences of B and P in a-Si:H: an ab initio simulation
D. Drabold*, B. Cai, Ohio U, USA

3:00 PM

Break

3:20 PM

(GOMD-SII-025-2011) Computing Transport coefficients for amorphous semiconductors using the Microscopic Response Method (Invited)
M. Zhang*, D. A. Drabold, Ohio University, USA

4:00 PM

(GOMD-SII-026-2011) Bond Percolation in C- and N-Doped Silica Glass
P. Kroll*, UT Arlington, USA

4:20 PM

(GOMD-SII-027-2011) Ab-initio simulation of solid electrolyte glasses
B. K. Prasai*, D. A. Drabold, G. Chen, Ohio University, USA

4:40 PM

(GOMD-SII-018-2011) Characterization of Shear Stress Relaxation of Glass Using a Parallel Plate Viscometer
V. Y. Blouin*, G. Vallet, H. Kadali, J. Musgraves, K. Richardson, P. Joseph, Clemson University, USA

5:00 PM

(GOMD-SII-029-2011) Statistical mechanics of glass-forming systems
R. J. Loucks*, Alfred University, USA; J. C. Mauro, Corning Incorporated, USA; S. Sen, University of California-Davis, USA

5:20 PM

(GOMD-SII-030-2011) Universality of the High Temperature Viscosity Limit of Glass-Forming Liquids
Q. Zheng*, Aalborg University, Denmark; J. C. Mauro, A. J. Ellison, M. Potuzak, Corning Incorporated, USA; Y. Yue, Aalborg University, Denmark

Symposium III: Optical Materials and Devices

Session A: Optical Absorption

Room: Pulaski

Session Chair: Mark Davis, SCHOTT North America, Inc.

1:00 PM

(GOMD-SIII-001-2011) Suppression of stimulated Brillouin scattering through multi-tone phase modulation
J. Mauro*, S. Raghavan, A. Ruffin, Corning Incoporated, USA

1:20 PM

(GOMD-SIII-002-2011) Absorption loss management in telluride glass fibers
P. Lucas*, Z. Yang, University of Arizona, USA; S. Jiang, T. Luo, Advalue Photonics, USA

1:40 PM

(GOMD-SIII-003-2011) Glass-Clad Semiconductor Core Optical Fibers
S. Morris*, J. Ballato, T. Hawkins, P. Foy, C. McMillen, R. Stolen, Clemson University, USA; R. Rice, Northrop Grumman Space Technology, USA

2:00 PM

(GOMD-SIII-004-2011) Polarized absorption characterization of spheroid-shaped nanoparticles embedded in a mesostructured silica film
D. Vouagner, Université Lyon1, France; L. Bois, UCB LYON I, France; E. Nardou, S. Sirotkin, B. Champagnon*, Université Lyon1, France; F. Chassagneux, UCB LYON I, France

2:20 PM

(GOMD-SIII-005-2011) Studying Loss Mechanisms in Chalcogenide Glass Planar Structures
V. Singh*, Massachussetts Institute of Technology, USA; J. Hu, University of Delaware, USA; J. Musgraves, N. Carlie, Clemson University, USA; A. Agarwal, Massachussetts Institute of Technology, USA; K. Richardson, Clemson University, USA; L. C. Kimerling, Massachussetts Institute of Technology, USA

2:40 PM

Break

3:00 PM

(GOMD-SIII-006-2011) Temperature dependent absorption and Urbach tail scaling in LuAG single crystals
M. Letz*, Schott AG, Germany; A. Gottwald, M. Richter, Physikalisch-Technische Bundesanstalt (PTB), Germany; V. Liberman, Massachusetts Institute of Technology, USA; L. Parthier, Schott Lithotec AG, Germany

3:20 PM

(GOMD-SIII-007-2011) Absorption in photo-thermo-refractive glass: metrology, contributions and mitigation
J. Lumeau*, K. Chamma, L. Glebova, L. Glebov, University of Central Florida, USA

3:40 PM

(GOMD-SIII-008-2011) Optical Properties of Vanadyl doped [VO2+(VS)and VO2+(VS)] Lead Phosphate Glass System
C. Dayanand*, Tirumala Engineering College, India

4:00 PM

(GOMD-SIII-009-2011) Optical absorption and crystallization of Na2O. SiO2.V2O5
B. Mehdikhani*, Institute of Standard and Industrial Research of Iran (ISIRI), Islamic Republic of Iran; B. Mirhadi, Imam Khomeini International University, Islamic Republic of Iran

4:20 PM

(GOMD-SIII-060-2011) PbS Quantum Dots Formation in Glasses Controlled by Ag Nanoclusters
K. Xu, J. Heo*, Pohang University of Science and Technology, Republic of Korea

Wednesday, May 18, 2011

Symposium I: Glass Science

Session G: Surface and Interfacial Phenomena

Room: Sapelo

Session Chair: Carlo Pantano, Penn State University

8:00 AM

(GOMD-SI-066-2011) Understanding and controlling environmental effects on friction and wear behaviors of silica and glass surfaces (Invited)
S. H. Kim*, C. G. Pantano, L. C. Bradley, Z. R. Dilworth, Pennsylvania State University, USA

8:40 AM

(GOMD-SI-067-2011) Adsorption Reactions on Multicomponent Silicate Glass Fiber Surfaces
J. Stapleton*, C. Pantano, K. Mueller, The Pennsylvania State University, USA

9:00 AM

(GOMD-SI-068-2011) Effect of glass composition on chemisorption mechanisms of probe molecules on sodium aluminosilicate glasses
K. Adib*, J. E. Dickinson, Corning Incorporated, USA

9:20 AM

(GOMD-SI-069-2011) The Effect of the Water-Silica Interface on Enhanced Hydronium Ion Formation and Transport
S. Garofalini*, G. Lockwood, Rutgers University, USA

9:40 AM

(GOMD-SI-070-2011) The influence of coupling agents at a glass/polymer interface
J. Banerjee*, J. Stapleton, C. Pantano, Pennsylvania State University, USA

10:00 AM

Break

Session D: Ancient Glasses

Room: Sapelo

Session Chair: Denis Strachan, Pacific Northwest National Laboratory

10:20 AM

(GOMD-SI-046-2011) Pattern Formation during the Alteration of Ancient Glasses: Insights from Static Corrosion Experiments (Invited)
T. Geisler*, R. Denkler, University of Muenster, Germany; A. Janssen, Institute for Transuranium Elements, Germany; M. Kilburn, University of Western Australia, Australia; A. Putnis, University of Muenster, Germany

11:00 AM

(GOMD-SI-047-2011) Chemico-mineralogical studies on impact glass from Lonar Crater: its suitability as natural analogue for nuclear waste glass (Invited)
N. RANI*, J. P. Shrivastava, University of Delhi, India; R. K. BAJPAI, BARC, India

11:20 AM

(GOMD-SI-048-2011) Long term alteration of archaeological slags: An analogue for nuclear waste glasses
A. Michelin*, CEA Marcoule, France; D. Neff, CEA Saclay, France; S. Gin, CEA Marcoule, France; P. Dillmann, CEA Saclay, France

Symposium II: The Amorphous State

Session C: Topology and Rigidity

Room: Ossabaw

Session Chairs: Pierre Lucas, University of Arizona; John Mauro, Corning Incoporated

8:00 AM

(GOMD-SII-031-2011) Understanding Glass Hardness from Constraint Theory (Invited)
M. M. Smedskjaer*, Aalborg University, Denmark; J. C. Mauro, Corning Incorporated, USA; Y. Yue, Aalborg University, Denmark

8:40 AM

(GOMD-SII-032-2011) Topological constraints in glass from Molecular Dynamics Simulations
M. Micoulaut*, M. Bauchy, UPMC, France

9:00 AM

(GOMD-SII-033-2011) Distribution of temperature dependent topological constraints
B. Mathieu*, M. Micoulaut, UPMC, France

9:20 AM

(GOMD-SII-034-2011) 2D NMR in germanium-selenium chalcogenide glasses (Invited)
M. Deschamps*, Université d'Orléans, France; C. Roiland, F. Charpentier, G. Yang, B. Bureau, Université de Rennes, France

10:00 AM

Break

10:20 AM

(GOMD-SII-036-2011) Correlation between topology and physical properties in As-Se glasses
P. Lucas*, University of Arizona, USA; G. Yang, B. Bureau, T. Rouxel, University of Rennes, France; O. Gulbiten, University of Arizona, USA; J. Sangleboeuf, University of Rennes, France

10:40 AM

(GOMD-SII-037-2011) Effects of Rigidity Percolation on Structural Relaxation in Supercooled Germanium Selenide Liquids
S. Sen*, E. Gjersing, University of California at Davis, USA

11:00 AM

(GOMD-SII-038-2011) Structure and Topology of Na2O-B2O3-Al2O3-SiO2 Mixed Network Glasses
Q. Zheng*, Aalborg University, Denmark; R. E. Youngman, C. L. Hogue, J. C. Mauro, M. Potuzak, A. J. Ellison, Corning Incorporated, USA; M. M. Smedskjaer, Y. Yue, Aalborg University, Denmark

11:20 AM

(GOMD-SII-039-2011) Twinkling Fractal Theory of the Glass Transition: Experimental Proof and Applications (Invited)
R. P. Wool*, University of Delaware, USA

Symposium III: Optical Materials and Devices

Session G: Solar Energy and Photocatalysis

Room: Pulaski

Session Chair: Matthew Lloyd, NREL

8:00 AM

(GOMD-SIII-045-2011) Organic photovoltaic cells: material processing, device structure and light management (Invited)
J. Xue*, University of Florida, USA

8:40 AM

(GOMD-SIII-046-2011) Interfaces in organic photovoltaic devices (Invited)
B. Kippelen*, Georgia Tech, USA

9:20 AM

(GOMD-SIII-047-2011) Overcoming Degradation in Organic Photovoltaic Devices with Air Stable Electrodes
M. Lloyd*, NREL, USA

9:40 AM

(GOMD-SIII-048-2011) Electrical and optical properties of CdTe-ZnO nanocomposite thin films as tunable optoelectronic materials for photovoltaic energy conversion
B. G. Potter*, R. Beal, G. Shih, C. Swanborg, C. G. Allen, University of Arizona, USA

10:00 AM

Break

10:20 AM

(GOMD-SIII-049-2011) PbS and PbSe quantum dot Schottky junction and heterojunction solar cells (Invited)
J. Luther*, National Renewable Energy Lab, USA

11:00 AM

(GOMD-SIII-050-2011) Oxyfluoride and sulfide based glass ceramics for LED lighting and for improving solar cells' efficiency (Invited)
X. Zhang*, University of Rennes I/CNRS, France; X. Fan, Zhejiang University, China; B. Fan, C. Point, L. Calvez, J. Adam, University of Rennes I/CNRS, France

Symposium IV: Glass Technology

Session B: Glass Strength

Room: Cumberland

Session Chair: Elam Leed, Johns Manville

8:00 AM

(GOMD-SIV-010-2011) Factors Affecting the Reliability of Glass (Invited)
S. Freiman*, Freiman Consulting, USA

8:40 AM

(GOMD-SIV-011-2011) Using the Hertzian Ring Crack Initiation Approach to Measure Surface Flaw Size
R. Tandon*, Sandia National Laboratories, USA

9:00 AM

(GOMD-SIV-012-2011) A Fracture Mechanics View of the Practical Strength of Glass (Invited)
R. Bradt*, The University of Alabama, USA

9:40 AM

(GOMD-SIV-013-2011) Two Point Bend Studies of Fatigue Effects in Silicate Glasses
Z. Tang*, R. K. Brow, Missouri S&T, USA; C. R. Kurkjian, University of Southern Maine, USA

10:00 AM

Break

Symposium III: Optical Materials and Devices

Session F: Sensors and Scintillators

Room: Cumberland

Session Chair: Mary Bliss, Pacific Northwest National Laboratory

10:20 AM

(GOMD-SIII-040-2011) Laser formation of micro to nano-scale 2D and 3D SbSI single crystal ferroelectric features in chalcogenide glass for device integration
P. Gupta*, A. Stone, N. Woodward, Lehigh University, USA; L. Ding, East China University of Science and Technology, China; M. Sakakura, Y. Shimotsuma, K. Miura, K. Hirao, Kyoto University, Japan; V. Dierolf, H. Jain, Lehigh University, USA

10:40 AM

(GOMD-SIII-041-2011) Novel chalcogenide glasses for nano-cavity photothermal chem-bio detection
J. Hu*, University of Delaware, USA; D. J. Musgrave, Massachusetts Institute of Technology, USA; N. Carlie, Clemson University, USA; A. Agarwal, Massachusetts Institute of Technology, USA; K. Richardson, Clemson University, USA; L. Kimerling, Massachusetts Institute of Technology, USA

11:00 AM

(GOMD-SIII-042-2011) Fabrication and Scintillation Response of Rare Earth Doped Transparent Ceramics
L. G. Jacobsohn*, K. Serivalsatit, S. A. Roberts, Clemson University, USA; E. G. Yukihara, Oklahoma State University, USA; T. A. DeVol, J. Ballato, Clemson University, USA

11:20 AM

(GOMD-SIII-043-2011) Synthesis and Properties of Transparent (Gd,Lu)x(Ga,Al)yO12:Ce Ceramic Scintillator
Y. Wang*, G. Baldoni, RMD, USA; C. Brecher, W. Rhodes, ALEM Associates, USA; K. Shah, RMD, USA; N. Cherepy, J. Kuntz, S. Payne, Lawrence Livermore National Laboratory, USA

11:40 AM

(GOMD-SIII-044-2011) Scintillating glasses for slow and fast neutron detection
M. Bliss*, D. A. Haas, S. M. Bowyer, L. Smith, D. S. Barnett, J. A. Stave, Pacific Northwest National Laboratory, USA

Symposium I: Glass Science

Session A: Atomistic Modeling of Glass Structures and Interfaces

Room: Sapelo

Session Chair: Jincheng Du, University of North Texas

1:00 PM

(GOMD-SI-001-2011) The Role of the Water-Silica Interface on the High Thermal Expansion of Nanoconfined Water (Invited)
S. Garofalini*, Rutgers University, USA

1:40 PM

(GOMD-SI-002-2011) Group IV Nanoclusters embedded in Silica Glass
P. Kroll*, UT Arlington, USA; J. Du, UNT Denton, USA; K. Seino, F. Bechstedt, U Jena, Germany

2:00 PM

(GOMD-SI-003-2011) Investigation of Ion-Exchange 'Stuffed' Silicate Glass Structures by Molecular Dynamics Simulation
P. K. Kreski*, A. N. Cormack, A. K. Varshneya, Alfred University, USA

2:20 PM

(GOMD-SI-004-2011) Structural Irregularities and Interfacial Features in Network Glasses (Invited)
J. Kieffer*, Y. Yue, K. Becker, University of Michigan, USA

3:00 PM

Break

3:20 PM

(GOMD-SI-005-2011) Atomistic Modelling of the Mechanical Properties of Silicate Glasses (Invited)
A. Cormack*, L. Adkins, Alfred University, USA

4:00 PM

(GOMD-SI-006-2011) Deformation Mechanisms of Densified Silica Glass
L. Huang*, F. Yuan, Rensselaer Polytechnic Institute, USA

4:20 PM

(GOMD-SI-007-2011) A study of silica glass fiber structure using molecular dynamic simulations
L. Adkins*, A. N. Cormack, Alfred University, USA

4:40 PM

(GOMD-SI-008-2011) Cation field strength effect on aluminum coordination in rare earth aluminosilicate glasses: a molecular dynamics study
J. Du*, L. Kokou, University of North Texas, USA

5:00 PM

(GOMD-SI-009-2011) First-principles molecular dynamics simulations of chalcogenides liquids and glasses (Invited)
C. Massobrio*, IPCMS, France

5:40 PM

(GOMD-SI-071-2011) Silica Molecular Dynamic Force Fields: A Practical Assessment
T. F. Soules*, G. H. Gilmer, M. J. Matthews, J. S. Stolken, M. D. Feit, Lawrence Livermore National Laboratory, USA

Symposium II: The Amorphous State

Session D: Medium Range Order

Room: Ossabaw

Session Chair: Paul Voyles, University of Wisconsin, Madison

1:00 PM

(GOMD-SII-040-2011) Fluctuation Electron Microscopy: Observing Subcritical Nuclei in Chalcogenide Glasses (Invited)
J. R. Abelson*, U. Illinois at Urbana-Champaign, USA

1:40 PM

(GOMD-SII-041-2011) Nucleation Mechanisms and Ring Size Distributions in Alkali and Alkaline Earth Disilicate Glasses
M. O. Naylor*, A. N. Cormack, Alfred University, USA

2:00 PM

(GOMD-SII-042-2011) Boson Peak of Lithium and Cesium Borate Glass Studied by Low Temperature Heat Capacity and Raman Scattering
S. Kojima*, Y. Matsuda, M. Kodama, University of Tsukuba, Japan; N. Surovtsev, Russian Academy of Sciences, Russian Federation; H. Kawaji, T. Atake, Tokyo Institute of Technology, Japan

2:20 PM

(GOMD-SII-043-2011) Experimental and Computational Studies of Short- and Medium-Range Order on the Surfaces of Oxides
K. Mueller*, N. Washton, Pacific Northwest National Laboratory, USA

2:40 PM

(GOMD-SII-044-2011) Modeling of Glass Durability through Advances in the Understanding of Medium Range Order (MRO)
C. Jantzen*, J. M. Pareizs, Savannah River National Laboratory, USA

3:00 PM

Break

Session D: Medium Range Order and Amorphous Metals

Room: Ossabaw

Session Chair: Paul Voyles, University of Wisconsin, Madison

3:20 PM

(GOMD-SII-045-2011) Fluctuation Electron Microscopy for studying amorphous materials (Invited)
M. M. Treacy*, Arizona State University, USA

4:00 PM

(GOMD-SII-046-2011) On the stability of carbon nanostructures in silicon oxycarbide materials: Part I
J. Ryan*, Pacific Northwest National Laboratory, USA; P. Kroll, University of Texas at Arlington, USA; C. G. Pantano, The Pennsylvaia State University, USA; K. Alvine, Pacific Northwest National Laboratory, USA

4:20 PM

(GOMD-SII-047-2011) On the stability of carbon nanostructures in silicon oxycarbide materials: Part II
P. Kroll*, University of Texas at Arlington, USA; J. Ryan, Pacific Northwest National Laboratory, USA

4:40 PM

(GOMD-SII-048-2011) Reverse Monte Carlo Modeling of Fluctuation Electron Microscopy Data
J. Hwang, University of Wisconsin, Madison, USA; Y. E. Kalay, METU, Turkey; M. J. Kramer, Ames Laboratory, USA; P. Voyles*, University of Wisconsin, Madison, USA

5:00 PM

(GOMD-SII-049-2011) Abnormal dynamics of metallic glass-forming liquids (Invited)
Y. Yue*, Aalborg University, Denmark; C. Zhang, L. Hu, Shandong University, China; J. C. Mauro, Corning Incorporated, USA

Symposium III: Optical Materials and Devices

Session E: Optical Coatings

Room: Pulaski

Session Chairs: S. Sundaram, NYS College of Ceramics, Alfred University; Norman Anheier, Pacific Northwest National Laboratory

1:00 PM

(GOMD-SIII-033-2011) Self-assembled multifunctional nanostructured coatings (Invited)
H. Fan*, Sandia National Laboratoriess, USA

1:40 PM

(GOMD-SIII-034-2011) Solution Processed Chalcogenide Glass for Integrated Mid-Infrared Optical Elements (Invited)
C. B. Arnold*, Princeton University, USA

2:20 PM

(GOMD-SIII-035-2011) Exploiting intrinsic material properties for improved integrated chalcogenide waveguide resonators for mid-IR sensing (Invited)
K. Richardson*, J. Wilkinson, S. Novak, Clemson University, USA; N. Carlie, Schott North America, USA; J. Musgraves, B. Zdyrko, I. Luzinov, Clemson University, USA; V. Singh, A. Agarwal, L. C. Kimerling, Massachusetts Institute of Technology, USA; J. Hu, University of Delaware, USA; A. Canciamilla, F. Morichetti, A. Melloni, Politecnico di Milano, Italy

3:00 PM

Break

3:20 PM

(GOMD-SIII-036-2011) Nano-Macro Scale Chalcogenide Coatings by Evaporation-Condensation
S. K. Sundaram*, B. J. Riley, B. R. Johnson, Pacific Northwest National Laboratory, USA

3:40 PM

(GOMD-SIII-037-2011) Multilayer Deposition for X-Ray Applications (Invited)
R. Conley*, N. Bouet, Brookhaven National Laboratory, USA

4:20 PM

(GOMD-SIII-038-2011) Spectroscopic Ellipsometry for Optical Coatings (Invited)
J. A. Woollam*, G. K. Pribil, R. A. Synowicki, T. E. Tiwald, J. A. Woollam Co., Inc., USA

5:00 PM

(GOMD-SIII-039-2011) Mid-Infrared Dispersion and dn/dT Analysis using Prism Coupling
N. C. Anheier*, A. H. Qiao, Pacific Northwest National Laboratory, USA

Symposium IV: Glass Technology

Session D: Glass Melting and Processing

Room: Cumberland

Session Chair: Rajiv Tiwary, PPG Industries, inc.

1:00 PM

(GOMD-SIV-019-2011) Mathematical model of cold cap
R. Pokorny*, P. Hrma, D. Kim, Pacific Northwest National Laboratory, USA

1:20 PM

(GOMD-SIV-020-2011) Kinetics of Quartz Particle Dissolution During Glass Melting
J. Marcial*, P. Hrma, S. H. Henager, Pacific Northwest National Laboratory, USA

1:40 PM

(GOMD-SIV-021-2011) Bench-Scale Melt Rate Testing and Modeling
A. Choi*, D. Miller, D. Immel, Savannah River National Lab, USA

2:00 PM

(GOMD-SIV-022-2011) The Benefits of Polyalkylene Carbonate Binders (QPAC®) for Low Temperature Glass Frit or Powdered Glass in Glass Sealing Applications
P. A. Ferraro*, S. Hanggodo, Empower Materials, USA

2:20 PM

(GOMD-SIV-023-2011) The effect of batch makeup and heating rate on the melting behavior of high level waste glass
D. Pierce*, P. Hrma, R. Pokorny, Pacific National Northwest Laboratories, USA

2:40 PM

(GOMD-SIV-024-2011) Microwave synthesis of chalcogenide glasses in Sb-S-I system
P. Gupta*, A. Stone, H. Jain, V. Dierolf, Lehigh University, USA

3:00 PM

Break

Session E: Liquid Synthesis and Sol-gel Derived Materials

Room: Cumberland

Session Chair: Gang Chen, Ohio University

3:20 PM

(GOMD-SIV-025-2011) Sol-gel derived multi-porous glass scaffolds for bone regeneration (Invited)
R. M. Almeida*, Instituto Superior Tecnico, Portugal

4:00 PM

(GOMD-SIV-026-2011) Organically Modified Siloxane Melting Gels (Invited)
L. C. Klein*, Rutgers University, USA; A. Jitianu, Lehman College, City University of New York, USA; M. Jitianu, William Paterson University, USA

4:40 PM

(GOMD-SIV-027-2011) Water Adsorption-induced Deformation of Micro- and Mesoporous Silica
S. Dong, G. Chen*, Ohio University, USA

5:00 PM

(GOMD-SIV-028-2011) Effect of silver incorporation on crystallization and microstructural properties of sol-gel derived TiO2 films
B. Akkopru Akgun*, C. Durucan, Middle East Technical University, Turkey; N. P. Mellott, Alfred University, USA

5:20 PM

(GOMD-SIV-029-2011) Improvement of sol-gel optical stacking
X. Dieudonné*, H. Piombini, K. Vallé, P. Belleville, CEA, France

Thursday, May 19, 2011

Symposium II: The Amorphous State

Session E: Amorphous Metals

Room: Ossabaw

Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

8:00 AM

(GOMD-SII-050-2011) Structure of Zr Bulk Metallic Glasses Constrained at Short and Medium Range (Invited)
J. Hwang, University of Wisconsin, Madison, USA; Y. E. Kalay, METU, Turkey; M. J. Kramer, Ames Laboratory, USA; P. Voyles*, University of Wisconsin, Madison, USA

8:40 AM

(GOMD-SII-051-2011) Phase selection and microstructural dynamics of devitrification in Cu-Zr (Invited)
R. E. Napolitano*, I. Kalay, Iowa State University, USA; E. Kalay, Middle East Technical University, Turkey; T. Cullinan, M. Lamb, Iowa State University, USA

9:20 AM

(GOMD-SII-052-2011) Modeling the mechanical behavior of amorphous metals (Invited)
E. R. Homer*, Sandia National Laboratories, USA; C. A. Schuh, Massachusetts Institute of Technology, USA

10:00 AM

Break

Session F: Spin Glasses

Room: Cumberland

Session Chairs: John McCloy, Pacific Northwest National Laboratory; Kostya Trachenko, Queen Mary University of London

8:00 AM

(GOMD-SII-053-2011) Understanding spin glass transition as a dynamic phenomenon (Invited)
K. Trachenko*, Queen Mary University of London, United Kingdom

8:40 AM

(GOMD-SII-054-2011) Ferroelectric Relaxors: Building Bridges between Theory and Applications (Invited)
E. Furman*, Q. Zhang, C. Randall, M. Lanagan, C. Pantano, Penn State University, USA

9:20 AM

(GOMD-SII-055-2011) Ion Irradiation Induced Property Changes in Granular Magnetite Films (Invited)
W. Jiang*, J. S. McCloy, A. S. Lea, Pacific Northwest National Laboratory, USA; J. A. Sundararajan, Q. Yao, Y. Qiang, University of Idaho, USA

10:00 AM

Break

10:20 AM

(GOMD-SII-056-2011) First Order Reversal Curve Study of Artificially Structured Nanomagnets (Invited)
K. Liu*, University of California, USA

11:00 AM

(GOMD-SII-057-2011) Cluster spin glass behavior in the Li-spinels (Invited)
T. W. Heitmann*, University of Missouri, USA

11:40 AM

(GOMD-SII-058-2011) Glassy magnetic behavior in disordered Ni,Co:CuMn2O4 spinels (Invited)
J. S. McCloy*, Pacific Northwest National Laboratory, USA; C. Leslie, University of Washington, USA; W. Jiang, Pacific Northwest National Laboratory, USA

Symposium IV: Glass Technology

Session A: Glasses for Energy and Environmental Applications

Room: Pulaski

Session Chair: Amanda Billings, Savannah River National Laboratory

8:00 AM

(GOMD-SIV-002-2011) Interactions of Viscous Glass Sealants with SOFC Stack Components
M. O. Naylor*, J. E. Shelby, S. T. Misture, Alfred University, USA

8:20 AM

(GOMD-SIV-003-2011) Near infrared down-conversion in chloro-sulfide glasses for the application on solar cell
B. Fan*, C. Point, J. Adam, X. Zhang, UMR CNRS-Université de Rennes I "Sciences Chimiques de Rennes", Laboratory of glasses and ceramics, France

8:40 AM

(GOMD-SIV-004-2011) Sintered Glass Core/Shell Waste Forms for 129I
T. Garino*, T. Nenoff, J. Krumhansl, D. Rademacher, Sandia National Laboratories, USA

9:00 AM

(GOMD-SIV-005-2011) Immobilization of High and Low Aluminate Waste with Borosilicate Glass
F. C. Johnson*, Savannah River National Laboratory, USA

9:20 AM

(GOMD-SIV-006-2011) Incorporation of High TiO2 Concentrations in High Level Waste Glass
K. M. Fox*, F. C. Johnson, T. B. Edwards, Savannah River National Laboratory, USA

9:40 AM

Break

10:00 AM

(GOMD-SIV-007-2011) Crystal Precipitation in Nuclear Waste Glasses and the Effects on Waste Form Durability
A. L. Billings*, J. W. Amoroso, Savannah River National Laboratory, USA

10:20 AM

(GOMD-SIV-008-2011) Effect of Composition on Vapor Hydration Test Response of Phosphate Glasses for Low Activity Waste Vitrification
W. Lepry*, D. Kim, J. D. Vienna, Pacific Northwest National Laboratory, USA

10:40 AM

(GOMD-SIV-009-2011) Characterization of Iron Phosphate Glasses Containing Simulated Hanford Low Activity Waste
S. T. Reis*, R. K. Brow, C. S. Ray, C. W. Kim, D. E. Day, Missouri University of Science and Technology, USA

Session C: Glasses for Medicine and Biotechnology

Room: Ossabaw

Session Chair: Brad Tischendorf, Medtronic

10:20 AM

(GOMD-SIV-014-2011) Controlling the Formation of Calcium Compounds when Bioactive Glasses React In-vivo
S. Jung, Mo-Sci Corporation, USA; D. E. Day*, Missouri University of Science and Technology, USA

10:40 AM

(GOMD-SIV-015-2011) Effect of Microstructure on the Strength of Glass-infiltrated Ceramic Composite for Artificial Teeth
H. Lim*, C. Kim, Inha University, Republic of Korea

11:00 AM

(GOMD-SIV-016-2011) Kinetic analysis of dissolution behavior of bio-active borate and silicate glasses in aqueous solutions
J. George*, R. Brow, Missouri University of Science and Technology, USA

11:20 AM

(GOMD-SIV-017-2011) Crystallisation of Strontium Bioactive Glasses
M. D. O'Donnell*, RepRegen Ltd, United Kingdom; L. Chapman, National Physics Laboratory, United Kingdom; H. Tang, Imperial College, United Kingdom; P. Tomlins, National Physics Laboratory, United Kingdom; J. Jones, Imperial College, United Kingdom

Monday, May 16, 2011

Symposium I: Glass Science

Session E: Non-Silicate Glasses I

Room: Sapelo
Session Chair: Juejun Hu, University of Delaware

9:20 AM

(GOMD-SI-049-2011) EXAFS analysis of local structure of Ge in amorphous and crystallized Ge(x)Te(1-x) thin films

Y. Choi*, Lehigh University, USA; B. Cheong, Korea Institute of Science and Technology, Republic of Korea; A. Kovalskyy, H. Jain, Lehigh University, USA

The crystal-amorphous phase-change in Ge(x)Te(1-x) thin films depends strongly on composition. We employ Ge K-edge EXAFS analysis to elucidate this experimental observation in terms of the local structural environment of Ge atoms in Ge(x)Te(1-x) thin films, where Ge/Te ratio (as determined by x) is set to be deficient (Ge29Te71 in atomic ratio), exact (Ge50Te50) or rich (Ge65Te35) with respect to the stoichiometric composition. The results show that the first coordination shell of Ge atoms consists of Ge-Ge and Ge-Te pairs in the amorphous phase of Ge50Te50 sample, and the coordination number of Ge is the lowest among the three amorphous phases. In addition, the Ge-Ge subshell shows relatively small EXAFS-type Debye-Waller factor. These structural environments of Ge atoms in the amorphous Ge50Te50 film are suggested to be responsible for the lowest and fastest crystallization temperature and time, respectively, observed for this particular composition.

9:40 AM

(GOMD-SI-050-2011) Structural models of Ag incorporation into As2S3 thin films

A. Kovalskyy, Lehigh University, USA; V. Lyubin, M. Klebanov, Ben-Gurion University of the Negev, Israel; M. Vlcek*, FCHT University of Pardubice, Czech Republic; H. Jain, Lehigh University, USA

Incorporation of Ag into As-based chalcogenide glass (ChG) thin films is a promising technology for novel gray-scale lithography, optical recording, non-volatile memories, etc. However, there are continuing controversies regarding the structural models of how Ag is incorporated in the ChG matrix, which appear to arise from the variation of sample preparation methods. Therefore, in this work we have evaluated the structure of As_2S_3-Ag thin films prepared under different conditions such as coevaporation, photodissolution of Ag in air, and X-ray-induced dissolution in vacuum. Some properties of such films are different, for example, coevaporation leads to strongly non-linear dissolution. Structural information is obtained from high-resolution XPS, XANES, EXAFS and Raman spectroscopy. Electronic and atomic structure, oxidation states for separate elements and bonding information are presented as a function of the preparation conditions. The results are compared with existing structural models for bulk Ag-doped As_2S_3.

10:00 AM

(GOMD-SI-051-2011) Analysis of Constraint Theory in Germanium Arsenic Sulfuide Glasses

P. F. Wachtel*, J. Musgraves, Clemson University, USA; N. Carlie, Schott North America, USA; J. Wilkinson, C. Ostrouchov, K. Richardson, Clemson University, USA

This study examines the properties of glasses across the GexAs30-xS70 and GexAs40-XS60 composition spaces in order to elucidate the atomic-scale mechanisms behind the change in macroscale properties such as density, glass transition temperature, and band gap energy. Raman spectroscopy is used to correlate these property changes to the evolution of the glass structure. Using these structure-property correlations, measured changes in bulk properties will be examined in the context of Phillips-Thorpe constraint theory and through purely stoichiometric considerations. The impact of nanoscale phase separation, seen in the Raman spectra of the glasses, on the resultant properties will be discussed, as well as the driving force behind the phase separation itself.

10:20 AM

(GOMD-SI-052-2011) Structure of S-rich Ge-S glasses by X-ray photoelectron spectroscopy

R. Golovchak, A. Kovalskyy*, H. Jain, Lehigh University, USA

Although the structure of germanium sulfide glasses has been studied intensively by various techniques, some compositional irregularities in short-range ordering of S-rich Ge-S glasses remain unexplained. Moreover, only a little is known about the correlation between electronic and atomic structure of these glasses. In this work the structure of binary Ge_xS_{100-x} chalcogenide glasses ($10 < x < 30$) is studied by high-resolution X-ray photoelectron spectroscopy (XPS), which has become the most promising tool for the characterization of short-range order and electronic structure of disordered solids. On the basis of compositional dependences of fitting parameters for Ge and Se core level spectra, the ratio between edge(ES) - and corner-shared (CS) tetrahedra is determined. It is shown that short-range order of Ge-S glasses includes fragments of high-temperature monoclinic crystalline form of GeS_2, crystal consisting of two ES and four CS tetrahedra.

10:40 AM

(GOMD-SI-053-2011) Tellurium glasses for far infrared applications

C. Boussard-Plédel*, Glasses and Ceramics group - UMR CNRS 6226, France; B. Bureau, Glasses and Ceramics group - UMR CNRS 6226, France; C. Conseil, Glasses and Ceramics group - UMR CNRS 6226, France; X. Zhang, Glasses and Ceramics group - UMR CNRS 6226, France; J. Lucas, Glasses and Ceramics group - UMR CNRS 6226, France

Selenium and tellurium exhibit great differences in their glass forming properties. The tellurium lone pair delocalized electrons make the formation of polymerized covalent bondings more difficult and increase the electrical conductivity. At the same time, due to a higher atomic weight, Te offers the advantage of shifting the IR edge towards longer wavelengths until 20 μm. Several glass forming systems containing only Te as a chalcogen, combined with Ge plus Ga or I, were investigated. Despite the high glass to crystal competition during the glass preparation, monoindex fibers as well as core/clad fibers can be prepared. Glasses with a small amount of Se, increasing the fiber drawing ability were also studied. The fibers are potential candidates for carbon dioxide detection in the frame of the European Space Agency programs, using the strong absorption in the 15 μm region. All these glasses containing a large amount of Te exhibit electrical conductivities which make the transparency depending on temperature.

11:00 AM

(GOMD-SI-054-2011) Structural environments and intra-4f-configurational transitions of trivalent Dy ions in Ge–As–S and Ge–Ga–S glasses

Y. Choi*, Korea Aerospace University, Republic of Korea; H. Jain, Lehigh University, USA

Dy L3-edge EXAFS analysis is employed to compare the local structure of Dy embedded in Ge–As–S and Ge–Ga–S glasses. The Dy–S distance on average is conspicuously longer in Ge–Ga–S glass despite the number of the nearest neighboring S atoms being nearly identical. The enhanced rare-earth solubility of Ge–Ga–S glass is then explained as due to the smaller covalence of Ga–S bonds compared with Ge–S or As–S bonds, and structural correlation between GaS4 tetrahedra and Dy ions. The discrepancy in the local structural environments of trivalent Dy, however, results in no significant changes in the spectral lineshape and the mean energy of its intra-4f-configurational transitions. From a comparison between the oscillator strengths of Dy3+ ions embedded in these glasses, we verify that the real-cavity model, for the local-field corrections, accommodates the observed changes of the oscillator strengths much better than the virtual-cavity model.

11:20 AM

(GOMD-SI-055-2011) New Functionalities in Non-Oxide Glasses (Invited)

S. K. Sundaram*, B. J. Riley, H. Qiao, C. F. Windisch, Jr., M. K. Murphy, J. V. Ryan, J. S. McCloy, B. R. Johnson, Pacific Northwest National Laboratory, USA

New functionalities in non-oxide glasses identified in the past decade of research at Pacific Northwest National Laboratory (PNNL) will be presented. The functionalities are basically derived from either process innovation or an electromagnetic irradiation. Multiscale materials processing technology has demonstrated the ability to process chalcogenide glasses across nano to macro scale in one step. Promise of this process will be highlighted. Exposure to different wavelength electromagnetic radiation has led to advanced functionalities: 1) alpha/gamma-irradiation generating an electrical response in chalcopyrites, 2) gamma-irradation of chalcogenides affecting both their atomic structure and broad-range of optical properties, and 3) visible laser-irradiation inducing changes in the millimeter wavelength optical properties of chalcogenides. These functionalities show promise for applications in nuclear detection, optical sensing, and active/passive photonic materials and devices.

Symposium II: The Amorphous State

Session A: Glass Transition and Relaxation in Glasses and Glassforming Liquids I

Room: Ossabaw
Session Chair: Prabhat Gupta

9:20 AM

(GOMD-SII-001-2011) The Emergence of Solid Behaviour in Amorphous Materials (Invited)

S. Williams*, D. Evans, Australian National University, Australia

An amorphous solid must show dispersion in its constitutive relation for oscillatory shear, otherwise it will not dissipate energy to the thermal reservoir. Furthermore amorphous solids are not in a state of metastable equilibrium, rather they are in a state of quasiequilibrium. Neither viscoelastic or Green-Kubo theory are consistent with both of these requirements. <p> Here we generalise linear response theory for the case of oscillatory shear, for both equilibrium solids and quasi-equilibrium amorphous solids. An important outcome of this theory is that the standard Green-Kubo result, relating a liquid's infinite frequency shear modulus to the variance in its stress, does not hold for a solid. Our theory properly addresses this point which directly leads to a constitutive relation for a solid with dispersion.

10:00 AM

(GOMD-SII-002-2011) The energy landscape of glass formers and beyond (Invited)

A. Heuer*, C. Rehwald, O. Rubner, C. Schroer, Institute of Physical Chemistry, Germany

We explore the potential energy landscape in the supercooled state via computer simulations of small model systems. In this way we understand why silica is a strong glass-former and the Lennard-Jones system displays a more fragile behavior. Then we analyze the information content of the finite-size effects. Interestingly, the diffusion constant shows a very weak and the structural relaxation time a very strong finite-size effect [1]. This result can no longer be fully understood in configuration space but also reflects the coupling of different regions in real space. We formulate a minimum model of the glass transition which can be regarded as a generalization of the kinetically constrained models [2]. Furthermore the non-linear response is discussed in the context of the finite-size effects. [1] C. Rehwald, O. Rubner, A. Heuer, Phys. Rev. Lett. 105, 117801 (2010). [2] Y. J. Jung, J. P. Garrahan, and D. Chandler, Phys. Rev. E 69, 061205 (2004).

10:40 AM

(GOMD-SII-003-2011) The Interplay between Structure and Dynamics in Glass-forming Alloys (Invited)

A. Widmer-Cooper*, University of Sydney, Australia

Despite being described as amorphous, it is now well established that many model glass-forming liquids - from alloys to network formers - have long-lived structural heterogeneities that affect their dynamics. In particular, structural relaxation and large-scale motion appear more likely to occur in regions in which soft modes are concentrated. I will introduce the isoconfigurational ensemble and use it to explain this body of work. I will then discuss the mechanism by which structural relaxation takes places in some glass-forming alloys, how this is influenced by structural heterogeneities in the supercooled liquid, and in turn how structural relaxation changes the spatial distribution of soft regions. In particular, results will be shown from molecular dynamics simulations of several 2D and 3D glass-forming mixtures.

11:20 AM

(GOMD-SII-004-2011) Spatial Correlation of the Dynamic Propensity in a Glass-Forming Binary Alloy (Invited)

M. G. Razul, G. S. Matharoo, P. H. Poole*, St. Francis Xavier University, Canada

We present simulation results on the dynamic propensity (as defined by Harrowell et al.) in a Kob-Andersen binary Lennard-Jones liquid of 8788 particles. We compute the spatial correlation of the dynamic propensity as a function of both temperature T, and the time at which the particle displacements are measured. For T<0.6, we find non-zero correlations at the largest length scale accessible in our system. We also examine the "coordination propensity", the isoconfigurational average of the coordination number of the minority B particles around the majority A particles. We find significant correlations between the spatial fluctuations of the dynamic and coordination propensities. We also find non-zero correlations of the coordination propensity at the largest length scale accessible in our system up to T=1.0. Compared to dynamical length scales previously reported, our results indicate the existence of fluctuations in the KA liquid that are larger than has perhaps been generally appreciated.

Symposium III: Optical Materials and Devices

Session C: Transparent Ceramics I

Room: Pulaski
Session Chair: Adam Stevenson, Ecole Nationale Superieure de chimie de Paris

9:20 AM

(GOMD-SIII-016-2011) The Impact of transparent ceramic materials on future lasers (Invited)

M. Richardson*, University of Central Florida, USA

The presentation attempts to provide a vision for the future for transparent ceramics in the field of high power lasers, from a laser designer's viewpoint. Ever since the birth of the laser age, most high power lasers have been based on crystalline material. There are several reasons for this, including the energy level structures of rare earths in crystalline hosts and their good thermal conductivity. However, as the laser field has matured, especially with the introduction of efficient monochromatic diode-based optical excitation, laser architectures, power capabilities and configurations have outstripped the capabilities of conventional crystal fabrication. The new methods of fabricating amorphous doped transparent ceramic laser materials promises not only to overcome these limitations, but also to lead to a transformation in advanced laser technology. This presentation will give a perspective on this exciting prospect, and the consequences it will have for applications for tomorrows lasers.

10:00 AM

(GOMD-SIII-017-2011) Submicrometer-Grained Transparent Sesquioxide Ceramics

J. Ballato*, K. Serivalsatit, Clemson University, USA

Rare-earth doped transparent sesquioxide ceramics, i.e. Y_2O_3, Sc_2O_3, and Lu_2O_3, are being developed as next generation laser gain media in high energy solid state laser systems. However, a significant challenge remains regarding the reduction of grain size to sufficiently sub-wavelength dimensions in order to minimize light scattering at grain boundaries and enhance thermomechanical properties. In this work, we present the development of submicrometer- grained transparent sesquioxide ceramics using a modified two-step sintering approach. These transparent ceramics exhibited a transparency equivalent to that of single crystals in the near infrared spectral region. The properties of these transparent ceramics will be discussed.

10:20 AM

(GOMD-SIII-018-2011) Microstructural Characterization of Optical Ceramics using Electron Backscatter Diffraction

M. Nowell*, EDAX-TSL, USA

The performance and behavior of polycrystalline optical ceramics depends on the internal microstructure of the material, and the understanding and manipulation of this microstructure is the key for materials properties optimization. Electron Backscatter Diffraction (EBSD) has become a useful and widely used characterization technique for measuring the crystallographic orientation and structure of materials. This technique provides spatially specific orientation data with nanometer scale resolution. With this data, it is then possible to measure texture, grain size, grain shape, grain boundary character, and phase distributions. In this work, the microstructure of polycrystalline magnesium aluminate spinel under different processing conditions has been measured with EBSD, and differences in optical transmission correlated to the resultant data. In addition, some of the sample preparation issues and data sampling strategies for obtaining quality EBSD data will be discussed.

10:40 AM

(GOMD-SIII-019-2011) Scattering in Transparent Materials

C. Brecher, ALEM Associates, USA; S. R. Miller, R. Gurjar*, RMD Incorporated, USA; A. Lempicki, ALEM Associates, USA

Transparent ceramics have received much recent study. From missiles to medicine, ceramics offer major advantages over crystals or glasses. While intuitively obvious, transparency is very difficult to quantify; since it is not merely transmission of light but of a distant image, it is far more sensitive to scattering than to absorption. But while absorption is well grounded in theory and experiment, this is not true for scattering. The most critical issue in transparency is how much of an incident beam can pass through a scattering medium without itself being scattered. We used a Stover scatterometer to measure this quantity in aqueous suspensions of polystyrene microspheres. We find strong dependence on both concentration and size, with interaction becoming weaker as either of these becomes smaller. But the quantitative relationships differ substantially from those found with conventional transmission spectrophotometry. The implications of these results and their application to transparent ceramics will be discussed.

11:00 AM

(GOMD-SIII-020-2011) Crystallization and second harmonic generation surface and bulk responses of lithium niobium silicate glass ceramics

H. Vigouroux*, E. Fargin, A. Fargues, ICMCB-CNRS, France; B. Le Garrec, CEA, France; M. Dussauze, V. Rodriguez, F. Adamietz, ISM, France; G. Mountrichas, E. Kamitsos, NHRF, Greece; S. Lotarev, V. Sigaev, D. Mendeleyev University of Chemical Technology of Russia, Russian Federation

Transparent ferroelectric glass-ceramics are becoming prospective candidates for nonlinear optical materials for high power laser. Transparent glass-ceramics with second order optical non linearity-properties can be obtained through bulk precipitation of non-centrosymmetric submicroscopic crystals. Heat treatments consisting of both nucleation and growth steps, at the appropriate temperatures were realized on the glass sample 35Li2O-25Nb2O5-40SiO2 to perform translucid glass-ceramics. Depending on heat treatments, surface and/or bulk crystallization of the LiNbO3 crystalline phase were observed. The X-Ray Diffraction analysis has revealed a preferred c-axis orientation of LiNbO3 crystallites at the surface, and in the bulk to a less extent. Second Harmonic Generation (SHG) has shown original bulk SHG signal in this glass. The non-linear susceptibility has been estimated larger than the one of KDP crystal. Origin of this bulk SHG signal will be discussed.

11:20 AM

(GOMD-SIII-021-2011) The Quest for Large Optical Components in Multi Petawatt and Fusion Lasers (Invited)

B. J. Le Garrec*, CEA-CESTA, France

The laser challenges and state of the art in high energy, solid-state lasers will be reviewed. While fusion lasers are mostly based on glass materials, a number of new laser systems are currently under construction or being planned that will incorporate new laser materials based on optical ceramics. The quest for large optical components is not restricted to the gain material: there is a need for large crystals to be used as electro-optical switch or frequency converters. Some trends in laser architecture will be detailed through the examples of european programmes: European High Power Energy Research (HiPER) and Extreme Ligth Infrasteucture (ELI).

Session H: Ion Conductors and Energy Storage Materials I

Room: Cumberland

Session Chair: Steve Martin, Iowa State University

9:20 AM

(GOMD-SIII-051-2011) Superionic glass-ceramic electrolytes for all-solid-state batteries (Invited)

M. Tatsumisago*, A. Hayashi, Osaka Prefecture University, Japan

All-solid-state batteries using inorganic solid electrolytes are one of the ultimate goals of rechargeable energy sources for EV and PHEV. Sulfide glass-based materials are one of the most promising candidates for inorganic solid electrolytes. We have developed the Li2S-P2S5 glass-ceramics, which are obtained from mechanochemically prepared glasses and exhibit high lithium ion conductivities of more than 3x10-3 S cm-1. The present paper reviews the preparation and characterization of superionic Li2S-P2S5 glass-ceramics; precursor glass preparation, crystallization conditions, and doping effects of additives are reported. Their application to various all-solid-state lithium secondary batteries using not only typical electrode active materials like LiCoO2 but the materials which are difficult to use in liquid electrolyte batteries is also reported. An excellent battery performance of all-solid-state cells using composite electrodes with S/C and Li2S/C is demonstrated.

10:00 AM

(GOMD-SIII-052-2011) Predicting Glass Former Units and Transport in Ion-Conducting Network Glasses (Invited)

P. Maass*, University of Osnabrueck, Germany

A theoretical approach is presented for relating structural information to long-range transport properties in ion-conducting network glasses. It relies on the types of glass forming units and the charges associated with them. Changes in the concentrations of the network forming units lead to a re-distribution of Coulomb traps for the mobile ions and to a subsequent change in long-range ionic mobilities. It is shown how by this mechanism the variation of conductivity activation energies in single and mixed glass former glasses with the composition can be predicted quantitatively by using just one parameter, which characterizes the spatial fluctuations of trapping energies due to topological disorder effects. The mole fractions of the individual network forming units enter the theory as input variables. Experimentally, these fractions can

be determined most accurately by solid state NMR techniques. In addition we show how they can be successfully predicted by thermodynamic modeling.

10:40 AM

(GOMD-SIII-053-2011) Structures and properties of ion conducting glasses (Invited)

N. Greaves*, University of Cambridge, United Kingdom; E. Flikkema, CNRS-CEMHTI, France; Z. Zhou, University of Cambridge, United Kingdom; Y. Vaills, CNRS- CEMHTI, France

Ion diffusion properties in silicate glasses are related to the local atomic structure obtained from X-ray absorption spectroscopy and long range order obtained from small angle X-ray scattering. Empirical relations are established between the activation energy for alkali transport, the variance in alkali-oxygen distances, and the dimensionality of alkali channels in single and in mixed alkali glasses. In all cases dilute alkali concentrations result in well-defined sites and low ionic conductivity. Moreover, as the modifier concentration increases the silicate fractal dimension of the network deceases from 3. Molecular dynamics combined with surface and volume-based virtual reality methods reveal the architecture of the ionic pathways in silicate glasses and the accessible free volume available for transport within them. Notably this volume falls when more than one alkali is present, offering a simple explanation for the non-linear transport properties associated with the mixed-alkali-effect.

11:00 AM

(GOMD-SIII-054-2011) Structure of amorphous Na2S+P2S5 prepared by melt quenching and mechanical milling

S. S. Berbano*, I. Seo, C. M. Bischoff, K. E. Schuller, S. W. Martin, Iowa State University, USA

$xNa_2S + (1-x)P_2S_5$ was prepared by melt-quenching and mechanical milling. The products were characterized using x-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), and Raman spectroscopy. The x-ray amorphous range was extended to the low-alkali composition of x = 0.33 by using mechanical milling. However, for mechanically milled samples with $x \geq 0.75$, the disordered α-Na_3PS_4 crystal was present in the product. FT-IR and Raman spectroscopy of the melt-quenched and mechanically milled samples showed similar structures.

11:20 AM

(GOMD-SIII-055-2011) Crystalline phase content and ionic conductivity correlation in Li2O-Al2O3-TiO2-P2O5 glass ceramic

S. Soman*, Indian Institute of Technology Bombay, India; Y. Iwai, J. Kawamura, Institute of Multidisciplinary Research for Advanced Materials, Japan; A. Kulkarni, Indian Institute of Technology Bombay, India

Fabrication of Li ion microbatteries for miniature devices is the recent focus in battery research. Li ion conducting glasses/glass ceramics are possible candidates as electrolyte for their high conductivity and breakdown potential, at room temperature. $14Li_2O$-$9Al_2O_3$-$38TiO_2$-$39P_2O_5$ glass was fabricated by melt quenching technique above 1400°C. NMR measurements confirmed presence of Li ions along with Al, P. DTA showed T_g at 296°C, T_{C1} at 536°C and T_{C2} at 635°C. Heat treatment was carried out between 550–950°C for 6h to crystallize this glass. Crystalline phases were identified from powder XRD. The crystalline phase content and conductivity varied with heat treatment temperature. Ionic conductivity was measured using impedance spectroscopy from 10 mHz to 1 MHz and between -50 to 300°C. The highest conductivity of 10^{-4} S/cm at room temperature was observed for sample crystallized at 850°C. Thin films of uniform thickness (0.5 μm) have been fabricated using PLD and characterized.

Symposium I: Glass Science

Session E: Non-Silicate Glasses II

Room: Sapelo
Session Chair: Andriy Kovalskyy, Lehigh University

1:00 PM

(GOMD-SI-056-2011) Infrared Quantum Dot Chalcogenide Films for Integrated Light Sources

N. Patel*, S. Geyer, J. Scherer, M. Bawendi, Massachusetts Institute of Technology, USA; N. Carlie, J. D. Musgraves, K. Richardson, Clemson University, USA; J. Hu, P. Lin, P. Becla, Massachusetts Institute of Technology, USA; C. Dimas, Masdar Institute of Science, United Arab Emirates; L. C. Kimerling, A. Agarwal, Massachusetts Institute of Technology, USA

Infrared (IR) light sources are desired in the field of chem-bio sensing because the IR regime is dubbed the "fingerprint" regime, where most molecules show vibrational absorption. For a sensor-on-chip device, the development of an integrated IR light source is mandatory. Colloidal quantum dots (QDs) which emit near IR light are fabricated with low cost solution processing methods. Incorporation of these QDs into IR transparent chalcogenide glasses, such as GeSbS, for fabrication of an integrated IR light source is investigated. Both solution processed and thermally evaporated glasses are evaluated. For solution-processed films, suitable chemistries for solutions of both QDs and dissolved glass were found and films were produced by spin coating. Layered structures using films of GeSbS and QDs dispersed in PMMA were also fabricated for improved dispersion of QDs. All approaches produced films with near-IR photoluminescence showing promise for the fabrication of an on-chip integrated IR light source.

1:20 PM

(GOMD-SI-057-2011) Novel Methods for the Preparation of High Purity Chalcogenide Glass for Optical Fiber Applications (Invited)

D. W. Hewak*, K. Huang, K. J. Knight, University of Southampton, United Kingdom

Chalcogenide glass is traditionally made by melt quenching of purified elements in a sealed system. Raw materials are weighed and inserted into an ampoule, which is evacuated, sealed and heated to the melting temperature while rockign to ensure homogenization. With this technique, high purity chalcogenides suitable for drawing into low loss fibers can be achieved. In this presentation we describe our work with two alternative methods for chalcogenide glass preparation; open atmosphere melting and chemical vapour deposition. These techniques have the potential to provide higher purity glass and easy scaling of the process. In both methods, a flowing reactive atmosphere allows in situ purification of the melt, something not possible with sealed ampoule methods. We describe these processes, their advantages and disadvantages and provide experimental data on their effectiveness in producing high quality chalcogenide glass

2:00 PM

(GOMD-SI-058-2011) Conductive chalcogenide glasses for sensing applications

P. Lucas*, Z. Yang, K. Reynolds, B. Bureau, University of Arizona, USA; M. Anne, University of Rennes, France

Novel telluride glasses with high electrical conductivity, wide infrared transparency and good resistance to crystallization were developed and used to design an opto-electrophoretic sensor for detection and identification of hazardous microorganisms. The sensor is based on an attenuated total reflectance element made of Ge-As-Te glass that serves as both an optical sensing zone and an electrode for driving the migration of bio-molecules within the evanescent wave of the sensor. An electric field is applied between the optical element and a counter electrode in order to induce the migration of bio-molecules carrying surface charges. This presentation will report on the glass development as well as the sensors design and testing.

2:20 PM

(GOMD-SI-059-2011) Solid Glass Electrolyte Enabled In-situ X-ray Absorption Spectroscopy of Electroactive Elements in Working Li-ion Batteries (Invited)

F. Alamgir*, Georgia Institute of Technology, USA

One of the core issues in Li-ion battery research is its safety against thermal runaway reactions. The presence of oxygen in its near-atomic or molecular state within the battery fuels such reactions. A glassy-electrolyte-enabled packaging-free Li battery design, with a Li_2S-P_2S_5 electrolyte, allowed us to measure changes in the electronic structure at oxygen sites while the battery was being charged. To our knowledge, this is the first reported in-situ measurement of oxygen electronic structure in a lithium-based battery. Oxygen x-ray absorption spectroscopy (XAS) shows empty O states (holes) induced by battery charging. Surface oxygen defect states are also detected. Oxygen indeed plays a direct role in the charge compensation reaction with the unwanted side-effect of creating conditions for oxygen evolution from the cathode material.

Session F: Glass-Ceramics

Room: Cumberland
Session Chair: Amanda Brennecka, Sandia National Laboratories

3:20 PM

(GOMD-SI-060-2011) Crystallization behavior of chromium doped CaO-ZrO2-SiO2 glass-ceramics system

M. Bahman, Imam Khomeini International University, Islamic Republic of Iran; B. Mehdikhani*, Institute of Standards & Industrial Research of Iran, Islamic Republic of Iran

The influence of some nucleating agents on the sintering, crystallization and mechanical properties of CaO– ZrO2– SiO2 glasses were investigated by DTA, XRD, SEM and EDX microanalysis. A well crystallized material of relatively high density (95% of theoretical density) was obtained after sintering at 1000°C for 1h by adding 5mol% Cr2O3. Crystalline phases identified were wollastonite, calcium zirconium silicate and calcium zirconium oxide. The addition of Cr2O3 was shown to reduce the sintering temperature of the base CaO– ZrO2– SiO2 glass-ceramic. Possible applications of the present chromium containing glass-ceramics are the production of coloured glazes and in coatings and enamels with "anti-static" behavior. The glass ceramics obtained from the studied materials is greenish coloured, so it is possible to use the studied glasses as coloured frits for tile glazes.

3:40 PM

(GOMD-SI-061-2011) Crystallisation of powellite phase in aluminoborosilicate glasses

T. Taurines*, B. Boizot, UMR 7642 CEA-CNRS-Ecole Polytechnique, France

The goal of this work is to optimize the SiO2-B2O3-Na2O-CaO-Al2O3-MoO3 system composition and heat treatments to obtain crystallisation of a monodisperse powellite phase (CaMoO4) with controlled size and composition in the glass host matrix. The purpose is to get a two-phase model system to study irradiation effects in these complex materials. The influence of temperature and duration time of heat treatments is studied. Small amounts of rare earth elements are added to the glass-ceramics since it acts as good surrogates for trivalent minor actinides. In this work, the structure of the glass-ceramics is investigated by Raman spectroscopy, X-ray diffraction and SEM. The environment of the spectroscopic probes (Gd3+ and Eu3+ ions) have been determined by EPR and time resolved photoluminescence. This approach has permitted to obtain two-phase model glass-ceramics and brings information on the speciation of actinide ions between the glass and the powellite phase as a function of the different heat treatments.

4:00 PM

(GOMD-SI-062-2011) Critical assessment of DTA/DSC methods to study glass crystallization kinetics

V. M. Fokin, A. A. Cabral, R. M. Reis, E. D. Zanotto*, Fed. University Sao Carlos, Brazil

Several methods based on DTA/DSC experiments have been proposed for quantitative studies of glass crystallization kinetics. Since thermal analysis equipment is handy, these techniques require only a small sample, and it has been frequently claimed that they are much faster than the conventional microscopy methods, such DTA/DSC methods have gained wide acceptance. In the present work we focus on some important problems related to such methods. For this purpose the main assumptions underlying DSC/DTA methods were experimentally tested and crystal nucleation rates were estimated for the same melt by both thermal analyses and optical measurements. We conclude that, if properly employed, some non-isothermal methods may indeed give reliable kinetic information, but they all need previous information about the crystallization process and are as laborious as the traditional microscopy methods.

4:20 PM

(GOMD-SI-063-2011) Fluorescence Properties of Rare-Earth Co-Doped Fluorochlorozirconate Glasses

M. Vu*, University of Tennessee Space Institute, USA; C. Passlick, Martin Luther University of Halle-Wittenberg, Germany; J. A. Johnson, C. E. Johnson, University of Tennessee Space Institute, USA; S. Schweizer, Fraunhofer Center for Silicon Photovoltaics, Germany

Rare-earth (RE) doped fluorochlorozirconate (FCZ)-based glasses and glass ceramics are good candidates for efficient photon conversion mechanisms since their low phonon energy reduces non-radiative losses. The FCZ glasses are based on a mixture of Zr, Ba, La, Al, and Na fluorides, which are additionally doped with chlorine to enable the growth of BaCl2 nanocrystals in the glass matrix upon thermal processing. For medical applications, the glasses are doped with divalent europium, of which some is converted to Eu3+ during heat treatment; Mössbauer spectroscopy was performed to determine the ratio of Eu2+/Eu3+. Eu2+ does not show any fluorescence when embedded in the glass matrix but shows an intense luminescence when incorporated into the nanocrystals upon excitation in the ultraviolet spectral range. Photoluminescence measurements were performed to assess the energy transfer between dopants - the fluorescence behavior of Gd3+, Nd3+, Tb3+,or Yb3+ co-doped with Eu2+ in FCZ glasses is presented.

4:40 PM

(GOMD-SI-064-2011) TeO2-Bi2O3-ZnO glass ceramic with high transparency in NIR region

X. Hu*, D. Musgraves, D. Vanderveer, J. Boerstler, N. Carlie, P. Wachte, Clemson University, USA; S. Raffy, University of Bordeaux, France; R. Stolen, K. Richardson, Clemson University, USA

We report on the fabrication of TeO2-Bi2O3-ZnO glass ceramics with high transmittance in near infrared (NIR) region. Transparent tetragonal bipyramid crystals with sizes on the order of tens of micrometers, and with refractive index closely matched to the glass matrix were formed using a two-step heating method. The crystalline phase present was identified as a function of heat treatment times and temperatures using X-ray diffraction. In addition, optical properties, such as transmittance and refractive index, and mechanical properties including Vickers hardness were measured for both the glass and glass ceramics.

5:00 PM

(GOMD-SI-065-2011) Glass Ceramic Waste Form Development for Combined Fission Products Waste Streams from Used Nuclear Fuel

J. Crum*, Pacific Northwest National Lab, USA; A. Kossoy, Los Alamos National Lab, USA; B. Riley, Pacific Northwest National Lab, USA; M. Tang, Los Alamos National Lab, USA; L. Turo, Pacific Northwest National Lab, USA

In this work, glass ceramics were investigated for immobilization of fission products generated from aqueous separations of used nuclear fuel.

Glass ceramics can provide benefits in two areas that currently limit waste loading in glass waste forms. First, glass has limited solubility of key waste components (e.g. Mo, alkali, alkaline earths, lanthanides) that can be incorporated in large quantities into durable crystalline phases. Second, crystalline structures are more resistant to decay-generated heat (and can thus support higher waste loading) considering the fact that they have a higher temperature stability than glasses limited by the glass transition temperature. For these reasons, multi-phase glass ceramics were developed via a melt process and their structure and properties will be presented.

Symposium II: The Amorphous State

Session A: Glass Transition and Relaxation in Glasses and Glassforming Liquids II

Room: Ossabaw
Session Chairs: Sabyasachi Sen, University of California at Davis; Ulrich Fotheringham, SCHOTT AG

1:00 PM

(GOMD-SII-005-2011) Particle dynamics in dense colloidal suspensions with short-ranged attractive potential

P. Habdas*, A. Latka, Saint Joseph's University, USA; P. Yunker, M. Lohr, A. G. Yodh, University of Pennsylvania, USA

We study colloidal particle dynamics of a model glass system using confocal and fluorescence microscopy as the sample evolves from a hard-sphere glass to a liquid with attractive interparticle interactions. The transition from hard-sphere glass to attractive liquid is induced by short-range depletion forces. The development of liquid-like structure is indicated by particle dynamics. We identify particles which exhibit substantial motional events and characterize the transition using the properties of these motional events. As samples enter the attractive liquid region, particle speed during these motional events increases by about one order of magnitude and the particles move more cooperatively. Interestingly, we find that colloidal particles in the attractive liquid phase do not exhibit significantly larger displacements than particles in the hard-sphere glass. We also report on studies of the particle dynamics in dense regions near the glass-glass transition.

1:20 PM

(GOMD-SII-006-2011) The Predictive Power of Three Parameter Viscosity Models

U. G. Fotheringham*, F. Lentes, SCHOTT AG, Germany; D. B. Dingwell, LMU-University of Munic, Germany

Recent work has challenged the three parameter Vogel-Fulcher-Tammann (VFT) viscosity model. Both in the glass transition and the melting range the VFT curves have been inferred to be too steep. Here, this inference is checked with data obtained on optical glasses in the three regimes where viscosity is commonly measured, i.e. the glass transition range (by beam bending), the softening range (by fibre elongation), and the working range (by concentric cylinder). These data are fit according to VFT and two recent models (Avramov-Milchev, Mauro-Yue-Ellison-Gupta-Allen). The extrapolated fits are compared with special concentric cylinder tests carried out to below 1 Pa*s. An alternative three parameter model is considered which is based on Adam-Gibbs theory and additionally needs specific heat data, to calculate configurational entropy and thus obtain extra information on glass fragility. We will review this approach examining its viscosity predictions both for very high temperatures and temperatures below glass transition.

1:40 PM

(GOMD-SII-007-2011) A discussion of iso-structural viscosity based on trap-dynamics

P. Gupta*, A. Heuer, The Ohio State University, USA

We present a general expression for the non-equilibrium (iso-structural) viscosity based on the trap dynamics in free energy landscapes and discuss its implications. According to this expression, a) thermodynamic and kinetic influences on viscosity are fully separable but do not agree with those given by the Adam-Gibbs model. b) the iso-structural viscosity is, in general, non-Arrhenius with respect to temperature and the iso-structural activation energy increases with decrease in the fictive temperature. c) the temperature dependence of equilibrium viscosity based on our expression disagrees with those of the existing empirical expressions for viscosity.

2:00 PM

(GOMD-SII-008-2011) Universal characteristics of the liquid-liquid critical point (Invited)

N. Greaves*, University of Cambridge, United Kingdom

The universality of critical phenomena is well-known in systems as diverse as molecular fluids and magnetic materials. The anomalous rise in compressibility is accompanied by fluctuations of increasing correlation length and relaxation time as the critical point is approached - critical opalescence. Evidence is now gathering for a new critical point in the supercooled state, separating a single phase liquid from polyamorphic phases sharing the same composition but differing in density and entropy. In situ small angle X-ray scattering experiments on the refractory yttria-alumina liquids will be described where liquid-liquid transitions have been recorded. These experiments map out the anomalous maxima in compressibility and the time-averaged correlation length of density fluctuations in the vicinity of the transition, metrics that follow the universal power law relations predicted by the 3D Ising model and observed in all order-disorder transitions.

2:20 PM

(GOMD-SII-028-2011) Heat capacity at the glass transition

K. Trachenko*, Queen Mary University of London, United Kingdom

A fundamental problem of glass transition is to quantitatively explain the jump of heat capacity at the glass transition temperature Tg without asserting the existence of a distinct solid glass phase. Similar problems are also common to other disordered systems, including spin glasses. We propose that if Tg is defined as the temperature at which the liquid stops relaxing at the experimental time scale, the jump of heat capacity at Tg follows as a necessary consequence due to the change of the liquid's elastic, vibrational and thermal properties. In this picture, we discuss time-dependent effects of glass transition, and identify three distinct regimes of relaxation. Our approach explains widely observed logarithmic increase of Tg with the quench rate and correlation of the heat capacity jump with liquid fragility.

2:40 PM

(GOMD-SII-009-2011) Structural Relaxation Mechanism Associated with Glass Transition in Ge-Se Liquids

T. Edwards*, S. Sen, University of California at Davis, USA

The nature of temperature dependent structural changes in a supercooled germanium selenide liquid of composition Ge20Se80 is investigated using insitu high-temperature Raman spectroscopy. In addition, Raman spectroscopic measurements are also carried out ex-situ on sub-Tg annealed glass samples to obtain the timescale of these structural changes near Tg. The timescale of enthalpy relaxation has been measured on the same samples using DSC. When taken together, the results of these experiments indicate a progressive conversion of the edge-shared GeSe4 tetrahedra in the structure into corner-shared tetrahedra, upon lowering of temperature. Moreover, the timescale and activation energy of this tetrahedral conversion "reaction" correspond well with those of enthalpy and shear relaxation in this glass-forming liquid near glass transition. The implications of these structural changes in controlling the viscous flow in germanium selenide network liquids will be discussed.

3:20 PM

(GOMD-SII-010-2011) Ideal glassformers and glass transition paradigms (Invited)

C. Angell*, V. Kapko, D. Matyushov, Arizona State University, USA

We apply the empirics of industrial age coal briquetting (for maximum trucking efficiency), to the design of model molecular glassformers. We use molecular dynamics on the Gay-Berne model for liquid crystals, with potential- tuning of the aspect ratio, to find the minimum melting point amongst plausible crystals. An aspect ratio range near that of maximum hard ellipsoid packing efficiency, appears to have no stable crystal state. It may be an "ideal glassformer". This system may be well suited for study of static vs dynamic correlations concerning which there is much controversy for fragile liquids. We discuss the breakdown of Stokes-Einstein equation in fragile liquids in relation to the proposed first order transition resolution of the Kauzmann paradox and the Ediger phases found by controlled vapor depositions for fragile liquids, but not intermediate, liquids. Strong liquids will be shown to be opposite in character, with no Stokes-Einstein breakdown and indeed correlation lengths that decrease as Tg is approached.

4:00 PM

(GOMD-SII-011-2011) Revisit of entropy issues in non-equilibrium states

A. Takada*, Asahi Glass Company, Japan

The residual entropy of glasses is still the subject of controversy. There are several different ways to define entropy theoretically. The framework of statistical mechanics and thermodynamics is applied not only to glass problems but also to several mathematical, physical and/or chemical problems in non-equilibrium states where entropy plays an important role in understanding their statistical mechanics and thermodynamics. Regarding such problems comparison between two different viewpoints of entropy, ensemble-counting and time-integration, are discussed.

4:20 PM

(GOMD-SII-012-2011) On the Dependence of the Properties of Glasses on Cooling and Heating Rates (Invited)

J. Schmelzer*, Germany

The glass transition is theoretically described in terms of a generic approach employing De~Donder's structural order parameter method, appropriate expressions for the relaxation behaviour of glass-forming systems and a simplified but qualitative correct model of glass-forming melts with one order parameter related to the free volume of the system. It is shown how – based on thermodynamics of irreversible processes – one can give a straightforward explanation of isothermal relaxation behaviour proportional to the square root of time (~t^(1/2)) and the origin of the Kohlrausch relaxation law. Employing this approach to the description of vitrification and devitrification, the behaviour of a variety of thermodynamic quantities describing glass-forming systems is interpreted theoretically. Particular attention is devoted here to the estimation of these quantities in dependence on the cooling and heating rates, varying latter parameter in a broad interval.

5:00 PM

(GOMD-SII-013-2011) Energy correlations in supercooled states of silicon

X. Mei, W. Mohamed, J. Eapen*, NC State University, USA

Energy dissipation can be closely coupled to stress and density changes in several practical applications. In radiation interactions of ions and neutrons, for example, the target material briefly undergoes phase transformation which is governed, to a large extent, by the rate at which energy is dissipated from the system. Glass formation by supercooling also involves similar processes, albeit at different time scales. In this paper, we investigate equilibrium energy correlations in silicon using molecular dynamics. We show that at high temperatures, the energy and density relaxations are strongly coupled to each with very similar relaxation times for all wave vectors. Upon supercooling, density relaxation becomes progressively slower for short wave vectors with a marked increase in relaxation time (relative to energy relaxation). We correlate this observation with the strengthening of the Brillouin peak and the emergence of a low frequency peak in the density of states.

5:20 PM

(GOMD-SII-014-2011) Experimental and Computer Investigation of Thermal Relaxation in AsxSe1-x Glasses

E. A. King*, R. G. Erdmann, P. Lucas, University of Arizona, USA

Members of the As_xSe_{1-x} family of chalcogenide glasses exhibit a wide range of thermal relaxation behavior as a function of x. DSC data were collected for these glasses ranging in average bond coordination from $\langle r \rangle = 2.10$ to 2.55. These data were modeled and fitted using a robust parametric optimizer coupled to the TNM model of glass relaxation to find the TNM parameters that best fit the experimental data. Several aspects of this study are presented, including an analysis of the sensitivity of the TNM model to details of the DSC curve normalization, the performance of the model with and without optimization of ΔH and the effects of model parameters on the geometry of the simulated DSC curves. A comparison of the best-fit parameters to those obtained by other experimental techniques is also presented. We conclude with a discussion of the varying applicability of the TNM model to different members of the As_xSe_{1-x} family of glasses.

Session G: Water and Glass

Room: Sapelo

Session Chairs: Minoru Tomozawa, Rensselaer Polytechnic Institute; Minoru Tomozawa, Rensselaer Polytechnic Institute

3:20 PM

(GOMD-SII-059-2011) Diffusion and redox reactions of water-related species in silicate melts (Invited)

H. Behrens*, Leipniz University of Hannover, Germany

In this paper an overview is given on our current knowledge of diffusion of water-related species in silicate melts. Hydrogen-bearing species may induce redox reactions in melts, i.e. hydrogen may initiate reduction of polyvalent elements such as iron and sulfur, while H2O may act as an oxidant. In order to improve our understanding of diffusion-controlled redox reactions in glass melts, we have performed experiments in which water diffuses into a dry sulfide-bearing soda lime silicate melt at elevated pressures (1 - 2 kbar) and temperatures (1000 – 1250°C). No oxidation of sulfide was observed in experiments under water-undersaturated conditions (water content was below the solubility of water in the melt) while for the experiments with a free H2O fluid phase XANES spectra show complete transformation of sulfide to sulfate near the melt surface and coexistence of sulfate in sulfide in the centre of the melt.

4:00 PM

(GOMD-SII-060-2011) Effect of Water Penetration on the Strength and Toughness of Silica Glass (Invited)

S. Wiederhorn*, NIST, USA; T. Fett, Karlsruhe Institute of Technology, Germany; J. Guin, University of Rennes, I, France

The effect of water on the strength and static fatigue behavior of silica glass will be discussed. Water can diffuse into newly formed fracture surfaces to generate a zone of swelling around the crack tip and along the surfaces of the crack. Constraint of the swollen material by the surrounding glass generates a zone of compressive stress at the fracture surface, resulting in a negative component of the stress intensity factor at the crack tip. The results are similar to those found for transformation toughening. The effect of surface swelling can explain several significant observations on silica glass: the reported strengthening of silica glass by soaking in water, 88 C; the observation of a static fatigue limit in silica glass at very low values of the applied stress intensity factor; and the observation of crack face displacements made by atomic force microscopy.

4:40 PM

(GOMD-SII-061-2011) Effect of Water on Internal Friction for a SiO2-Al2O3-Na2O-MgO Glass

T. Tsujimura*, M. Nishizawa, A. Koike, Y. Kuroki, Asahi Glass Co., Ltd., Japan

In order to investigate an effect of water on alkali behavior in the glass structure below Tg, the internal friction peaks (Q-1) of SiO2-Al2O3-Na2O-MgO glasses with various water contents were measured from room temperature to 500 °C using the resonance method near 1kHz. For the less polymerized glass (high NBO/T), the low temperature peak (50-150°C) due to alkali ion movement becomes smaller and the high temperature peak (over 300°C) becomes larger with increasing water content, which is consistent with previous works (e.g., Day and Stevels, 1974). For more polymerized glass (low NBO/T), on the other hand, the high temperature peak (probably due to interaction between alkali and alkali-earth ions) disappears and the low temperature peak increases with increasing water content. The effect of water on the internal friction for polymerized glass is more prominent than that for depolymerized glass.

5:00 PM

(GOMD-SII-062-2011) Nanostructure of water-containing glass by MD simulation

S. Ito*, Tokyo Institute of Technology, Japan; T. Taniguchi, Asahi Glass Co., Ltd., Japan

To clarify the effect of water in glass on mechanical behaviors, such as stress relaxation, deformation, cracking, breakage etc., the nanostructure of water-containing glass in the system of (Li, Na, K)2O-Al2O3-SiO2 was investigated by using molecular dynamics simulation. The glasses with various water contents were prepared by adding H2O molecules to the water-free glasses. Some amount of the added H2O reacted with glass network and non-bridging oxygen formed,(≡Si-O-Si≡+ H2O→≡Si-OH + HO-Si≡), depending on kind of alkali, water content and temperature. As a result, the number of network rings decreased and the void in the network increased, and the elastic moduli except Poisson's ratio decreased remarkably. Under stress, the water-containing glasses deformed easily with increasing OH-content. The role of water on mechanical properties will be discussed in terms of glass nano-structure.

5:20 PM

(GOMD-SII-063-2011) Water diffusion in silica glass and wet oxidation of Si: A new interpretation for the high speed of wet oxidation

M. Tomozawa*, Rensselaer Polytechnic Institute, USA

The relationship between water diffusion in silica glass and the oxidation kinetics of silicon was considered. It is suggested that the diffusion of molecular water, which can diffuse faster than oxygen and has not been observed in a normal water diffusion study in silica glass, is responsible for the faster oxidation of silicon in wet oxidation than in dry (oxygen) oxidation.

Symposium III: Optical Materials and Devices

Session C: Transparent Ceramics II

Room: Pulaski

Session Chair: Adam Stevenson, Ecole Nationale Superieure de chimie de Paris

1:00 PM

(GOMD-SIII-022-2011) Ceramic Scintillators for Computed Tomography (Invited)

H. Jiang*, J. Gent, M. Prescott, GE Healthcare, USA; S. Duclos, J. Vartuli, R. Lyons, C. Vess, R. Hagerdon, K. Mcevoy, A. Setlur, GE Global Research, USA

The image quality of Computed Tomography (CT) has been revolutionalized since GE launched the first transparent ceramic scintillator – HiLightTM in 1988. As a result, the application domain of CT has been dramatically expanded. Ceramic scintillator demonstrated many advantages compared to single crystal scintillators: much higher uniformity, flexibility of doping composition and content, better machinability, and lower cost resulted from better manufacturability. There are currently 3 commercial ceramic scintillators for CT: HiLightTM, GOS, and GemstoneTM. This paper will review the development history of the ceramic scintillators, discuss their properties and processes, and outline potential future directions.

1:40 PM

(GOMD-SIII-023-2011) Strength-Size Scaling and Flaw Tolerance in Coarse-Grained Transparent Magnesium Aluminate Spinel Windows

J. Swab, R. Pavlacka*, S. Kilczewski, G. Gilde, US Army Research Laboratory, USA

Transparent ceramics are prime candidates for use as strike face materials in window packages. Transparent spinel ($MgAl_2O_4$) ceramics currently under investigation for use in vehicle window applications are commonly characterized by a very coarse microstructure (~300 μm grain size). As a result, experimentally measured strength values are significantly lower than fine grained spinel. Moreover, strength is independent to surface finish. Evaluations of the fracture mechanics and fractography indicate that the strength limiting flaws may be cleaved grains and, thus, intrinsic in nature. Investigations of the unusual strength size scaling behavior and flaw tolerance that result from this distinctive flaw population, as well as the processing opportunities this affords, will be discussed.

2:00 PM

(GOMD-SIII-024-2011) Forming Transparent Ceramics for Al-rich Formulations of $MgO.nAl_2O_3$ (n>1)

A. Sutorik*, J. Swab, G. Gilde, C. Cooper, R. Gamble, E. Shanholtz, R. Pavlacka, US Army Research Laboratory, USA

Solid solution magnesium aluminate spinel with the alumina rich compositions $MgO.n\ Al_2O_3$ (n>1) has been prepared as polycrystalline ceramic with average in-line transmissions of >80% in the visible spectrum for several compositions of n. Starting powders are prepared from mixtures of high purity $Mg(OH)_2$ and γ-Al_2O_3 thoroughly mixed in an aqueous slurry. Water is removed by rotary evaporation. The solids are collected, dried, calcined, mixed with LiF (as a sintering aid), and sieved. The powders are sintered into dense ceramics by hot pressing at 1600 °C under vacuum and 20 MPa uniaxial load followed by hot isostatic pressing at 1850 °C under 200 MPa Ar. Final grain sizes ranged between 300-1000 μm. The influence of Al content on the optical and physical properties of the ceramics will be discussed.

2:20 PM

(GOMD-SIII-025-2011) Highly transparent Al-rich MgO.nAl2O3 spinel (1 ≤ n ≤ 2.5) by reaction sintering of MgO and Al2O3

K. Waetzig*, A. Krell, A. Michaelis, Fraunhofer Institute for Ceramic Technologies and Systems, Germany

This study investigates transmission and hardness of Al-rich spinel ($MgO{\cdot}nAl_2O_3$, $1 \le n \le 2.5$) produced by reaction sintering of MgO and Al_2O_3 powders. The transmission of light through polycrystalline materials is influenced by scattering on pores or second phase particles and by absorption on defect sides. To eliminate residual porosity deagglomerated powders and high temperatures are needed. With highly pure powders and optimized process parameters concerning deagglomeration, shaping, sintering and hotisostatic pressing in a wide transmission range (250 to 800 nm wavelengths) a near theoretical limit (independent of Al-content) have been realized. The hardness of the spinel decreases with increasing Al-content. In comparison of different synthesis pathways reaction sintering is the method of choice to produce Al-rich highly transparent spinel materials.

2:40 PM

(GOMD-SIII-026-2011) Reversible optical properties of an infrared transparent Y2O3-MgO nanocomposite

D. Jiang*, A. K. Mukherjee, University of California-Davis, USA

A sol-gel processed nanopowder with a grain size below 30nm was used to produce Y2O3-MgO nanocomposite by spark plasma sintering technology. With a grain size below 100nm the fully dense nanocomposite exhibits an excellent transmission (~80%) in the mid-infrared range. The optical property of the nanocomposite is found to be highly reversible by changing annealing atmosphere from vacuum to air. Combined with X-ray diffraction analysis, it is reasoned that that oxygen vacancy has a dramatic influence on the transmittance of oxide ceramics.

Session B: Photosensitivity and Photomodification

Room: Pulaski

Session Chair: Pierre Lucas, University of Arizona

3:20 PM

(GOMD-SIII-010-2011) Optical agility of chalcogenide films using their photosensibility (Invited)

V. Nazabal*, Chemistry Sciences Center of Rennes, UMR 6226, University of Rennes, France; P. Nemec, Faculty of Chemical Technology, University of Pardubice, Czech Republic; M. Cathelinaud, UPS CNRS 2274, France; G. Boudebs, Université d'Angers, France; M. Chauvet, UMR CNRS 6174, Département d'optique, France; F. Charpentier, Chemistry Sciences Center of Rennes, UMR 6226, University of Rennes, France; M. Lequime, UMR6133, CNRS-ECM-UPCAM-UP, France; X. Zhang, Chemistry Sciences Center of Rennes, UMR 6226, University of Rennes, France

An important property differentiates chalcogenide glasses from other materials is their well-known high photo-sensitivity to light exposure, which presents several types of photo-induced changes in the structure and properties. The photoinduced refractive index or band gap energy change of chalcogenide films can be exploited for many kind of applications covering the field of photolithography, light trimming bandpass filters, selective optical writing of Bragg gratings or channels waveguide… On the other hand for many applications in the field of infrared optics, amorphous chalcogenides insensitive to light exposure are required. Within this framework, the photosensitivity properties of sulphide and selenide films elaborated using pulsed laser deposition, evaporation assisted by electron beam, RF magnetron sputtering were studied with the aim of taking advantage of their photosensitivity or conversely to limit its effects following goal for subjects as diverse as bandpass filters or nonlinear optics.

4:00 PM

(GOMD-SIII-011-2011) Atomistic nature and dynamics of optically and thermally induced changes in chalcogenide glass thin films

D. Zhao*, H. Jain, Lehigh University, USA

Chalcogenide glass (ChG) thin films exhibit many intriguing photoinduced effects. For example, band gap light can change their optical absorption, refractive index, chemical reactivity, and volume. As a result, integrated optical devices can be fabricated by direct laser writing or photolithography. The atomistic mechanisms of photosensitivity are investigated by in situ X-ray absorption spectroscopy (XAS). It is found that a photochemical reaction is triggered locally in which the non-equilibrium homopolar bonds (e.g. As-As, S-S) are converted into heteropolar bonds (e.g. As-S). This bond switching process drives the expansion of bond length throughout the network structure of the material. In addition, the state-of-the-art time-resolved XAS provides the first-hand information about the atomistic dynamics of photostructural changes in ChG. Finally, the optically and thermally induced changes of atomic structure are compared as well, and found to be identical.

4:20 PM

(GOMD-SIII-012-2011) Direct Femtosecond Laser Writing in silver-containing glass

T. Cardinal*, K. Bourhis, ICMCB-CNRS, France; A. Royon, CPMOH-CNRS, France; M. Treguer, Y. Petit, J. Videau, ICMCB-CNRS, France; J. Choi, M. Richardson, UCF, USA; L. Canioni, CPMOH-CNRS, France

Direct Laser Writing (DLW) of nanostructures in transparent media is challenging and relies on the control of the local electron/hole trapping, phase separation and diffusion processes. In a silver zinc phosphate glass, 3D fluorescent structures with dimensions below the diffraction limit were obtained using a high repetition rate IR femtosecond laser. By adjusting the laser dose (fluence, number of pulses, and repetition rate), the intense fluorescent structures, composed of silver aggregates, are achieved thanks to oxidation/reduction processes and local heating. The process allows tailoring of the luminescence properties at the nanometer scale (intensity, spectrum, spatial distribution). The repetition rate of the laser and the glass composition are identified as key parameters. Different properties can be implemented such as third harmonic generation and second order non linearity. DLW offers a unique alternative for fabricating 3D photonic structures with new functionalities such as 3D optical data storage.

4:40 PM

(GOMD-SIII-013-2011) Ultrafast Laser Processing of Hybrid Micro- and Nano-Structures in Silicate Glasses

P. Mardilovich*, L. Fletcher, N. Troy, S. Risbud, D. Krol, University of California, USA

We investigated ultrafast laser processing of semiconductor doped glasses with the aim of fabricating hybrid micro-/nanostructures of semiconductor nanocrystals precipitated in micron scale domains defined by laser exposure. We used focused ultrafast laser pulses to locally modify structure in glasses doped with Cd, S and Se. We then subjected thus processed samples to various regimes of heat treatment to precipitate the nanocrystals. The fs-laser processing produced micron-sized regions in the glass with markedly different properties and behavior from the surrounding bulk. The resultant structures were investigated using optical and electron microscopy, as well as confocal fluorescence and Raman microscopy. We will discuss the experimental observations and results, addressing how laser processing parameters affect structural changes in the irradiated glass, and how these changes subsequently influence the semiconductor precipitation dynamics on a local scale.

5:00 PM

(GOMD-SIII-014-2011) Mechanisms of NaF growth in photo-thermo-refractive glass

K. Chamma, J. Lumeau*, L. Glebova, L. B. Glebov, University of Central Florida, USA

PTR glass is a photosensitive silicate glass which provides refractive index change after UV-exposure and thermal development. The origin of photosensitivity is explained by precipitation of NaF crystals inside the glass matrix. While nucleation of NaF in PTR glass has been thoroughly studied, mechanisms of growth of NaF have drawn a limited interest. To study the NaF growth, we combined several techniques: optical spectroscopy, interferometry, DSC and XRD. We have found that size of NaF crystals in UV-exposed PTR glass as determined by broadening of diffraction lines does not exceed ~20 nm. The parameter limiting the growth of the NaF crystals is the exhaustion of Na^+F^- within the glass matrix. XRD analysis of NaF powder allowed us to calculate the crystals volume fraction their average size. We also demonstrated that these parameters can be combined with Rayleigh scattering model to predict scattering at any wavelength and thermal treatment, proving that scattering is determined by single crystals.

5:20 PM

(GOMD-SIII-015-2011) 3D temperature distribution and crystallization mechanisms of ferroelectric LaBGeO5 during femtosecond laser irradiation inside bulk glass

A. Stone*, M. Sakakura, Y. Shimotsuma, Lehigh University, USA; K. Miura, K. Hirao, Kyoto University, Japan; V. Dierolf, H. Jain, Lehigh University, USA

Femtosecond (fs) laser crystallization is a promising method for producing functional crystals in 3D arrangements inside glass for applications like optical switching, integrated photonics, and optical memory. In principle, fs laser crystallization should not be restricted by the focal depth due to intensity-dependent absorption mechanisms, yet we found that crystallization rates in $LaBGeO_5$ glass show a strong dependence on the location of the focal point with respect to the surface. To investigate this issue, we have modeled the time evolution of 3D temperature distribution at varying focal depth. We found that temperature alone was insufficient to explain the crystallization rate depth dependence. In-situ observation of the modification profile clarified other key aspects of crystallization which explain the observed depth dependence and provide a basis for developing strategies to circumvent it and realize full 3D space-selectivity.

Session H: Ion Conductors and Energy Storage Materials II

Room: Cumberland
Session Chair: Steve Martin, Iowa State University

1:00 PM

(GOMD-SIII-056-2011) Understanding the alkali dynamics in silicate systems for small and large electric fields (Invited)

A. Heuer*, H. Lammert, L. Lühning, Institute of Physical Chemistry, Germany

Via molecular dynamics simulations of lithium silicate we characterize the energy landscape, experienced by the lithium ions. It turns out that the dynamics can be very well described by a vacancy mechanism with nearly independent vacancies[1]. Based on these results we formulate a simple model of ion conduction which allows us to go beyond the linear response regime and to characterize the non-linear conductivity. Whereas in 1D analytical results can be obtained, in 3D numerical approaches have to be used. These results can be compared with corresponding experiments. In this way we obtain additional information about the nature of ion conduction. [1] H. Lammert, A. Heuer, Phys. Rev. Lett. 104, 125901 (2010).

1:40 PM

(GOMD-SIII-057-2011) First and second universalities in ion-conducting glasses (Invited)

K. Funke*, University of Muenster, Germany

Glassy electrolytes and other disordered ion-conducting materials have been found to show an unexpected degree of similarity in their broadband conductivity spectra. In particular, two surprising "universalities" have been detected. One of them, the "first universality", is a fingerprint of activated hopping along interconnected sites, while the other, the "second universality", reflects non-activated, strictly localized movements of the ions. The former is observed at sufficiently high temperatures, while the other is found at sufficiently low ones, e.g., in the cryogenic temperature regime. In either case, rate equations have been found that reproduce the relevant time dependence of the ion dynamics as well as the spectra themselves. Therefore, these equations may be regarded as manifestations of the underlying common laws. At the same time, they also form a sound basis for understanding and visualizing the phenomena in terms of simple physical pictures.

2:20 PM

(GOMD-SIII-058-2011) Structure/Property Correlations in the Ionic Conductivity of Mixed Glass Former Glasses in the Na_2S+GeS_2+P_2S_5 Glass System

C. Bischoff*, K. Schuller, S. W. Martin, Iowa State University, USA

A non-linear and non-additive composition dependent change in ionic conductivity is known as the Mixed Glass Former Effect (MGFE). Alkali ion conducting glasses are of particular interest for use in ion conductive batteries. Sulfide amorphous materials show promise as solid-state electrolytes due to their significantly large alkali ion conductivities as compared to their oxide counterparts. Impedance spectroscopy measurements of the $yNa_2S + (1-y)[xGeS_2 + (1-x)PS_{5/2}]$ glass system exhibit a MGFE. Vibrational and MAS-NMR spectra reveal structural changes of the glass formers and unequal sharing of the alkali ion. Structure property relationships will be discussed.

2:40 PM

(GOMD-SIII-059-2011) Structural Studies and Models of Sodium Borophosphate Mixed Glass Former Glasses

R. B. Christensen*, S. W. Martin, G. Olson, Iowa State University, USA

Ion-conducting glasses hold the potential for widespread use in batteries, fuel cells, sensors, and thermionic devices. It has been reported in the literature that the ionic conductivity of ternary alkali glasses can be increased by up to two orders of magnitude at constant alkali concentration by mixing glass forming anions or cations. In order to increase understanding of this Mixed Glass Former Effect (MGFE), a study of the physical properties and structures of multiple ternary glass systems have been undertaken. One of these systems includes (Na2O)y[(B2O3)x (P2O5)(1-x)](1-y) [y = 0.35, 0.50, x =0, 0.1, 0.2…1] glasses. In this system all series, y = 0.35 and y = 0.5 glasses were studied. 31P and 11B Magic Angle Spin-Nuclear Magnetic Resonance studies were used to determine the structural composition trends of these glasses. These results have been compared to Reverse Monte Carlo models generated from X-ray Diffraction studies on the same glasses. The insights these comparisons yield will be discussed.

Poster Session

Room: Madison

(GOMD-SI-P001-2011) Influence of Structural changes on the ESR Spectra of Mn2+ doped Lead Phosphate Glasses

C. Dayanand*, Tirumala Engineering College, India

The lead phosphate glass system exhibit remarkable structural changes with composition. The present work aims at correlating the changes observable in the ESR spectra with structural changes in the Mn2+ doped LP glasses over a wide range of composition. The ESR spectra of these glass samples were recorded on Bruker ER 200D-SRC X-band spectrometer. The ESR spectra of Mn2+ doped Lead Phosphate glasses in

the compositional region, 0.3 - 0.55 revealed an intense hyperfine (hf) sextet with gav =2.00 and with hf coupling constant A =97G. The ESR spectra of Mn2+ doped LP quenched samples in the compositional region (0.6 = 0.75) revealed the central sextet superposed on weak but clearly resolved 30 line spectrum and have been attributed to Mn2+ ions occupying sites both in glassy and crystalline phases. In the spectra of Mn2+ in glasses the maxima are so close to the central transition that they are obscured by the hf structure (sextet).

(GOMD-SI-P002-2011) Laser Aerolevitation Manufacturing of Alkaline Earth Silicates

C. Nie*, W. Trull, P. Dulal, S. Feller, M. Affatigato, Coe College, USA

We report on our work using a laser aero-levitation system to manufacture alkaline earth silicates. These silicates have extremely high melting points, and it is difficult to produce them using the furnace method. The laser levitation system can reach very high temperatures near 2700°C while using a containerless method that inhibits heterogeneous nucleation. The work also addresses compositional accuracy through the use of energy-dispersive X-ray spectroscopy (EDX). We specifically report on the formation of magnesium, calcium, strontium, and barium silicates, and in these systems the glass forming range was extended from that previously given in the literature. In the case of the xBaO-(1-x)SiO2 family, for example, the glassforming range was stretched to $20 < x < 50$ mol%. Preliminary investigations of the structure are also reported from Raman and other spectroscopic measurements. Work supported by the United States National Science Foundation under grant numbers DMR-0904615 and MRI-0922924.

(GOMD-SI-P003-2011) The Production of Cesium Borate Glass for Use in Atomic Clocks

E. Wiese Moore*, Coe College, USA; J. Bernstein, Massachussetts Institute of Technology, USA; A. Ramm, J. North, J. Maldonis, J. Alberts, S. Feller, M. Affatigato, Coe College, USA; M. Mescher, W. Robbins, R. Stoner, B. Timmons, Massachussetts Institute of Technology, USA

The goal of this project was to create cesium borate glasses as the source of Cs ions in the construction of new atomic clocks. These glasses, with solid metal electrodes, were used as a Cs ion source in a high vacuum system. The resulting disc samples were approximately 0.5 mm thick and 1.3 mm in diameter. A silver anode provides an injection source of highly mobile ions which sweep Cs to the cathode surface, from which they evaporate into the vacuum. Cathode metallization with finger patterns was used leaving bare glass for Cs evaporation. Laser absorption measurements show Cs vapor generation synchronous with an applied DC voltage. Work supported by the National Science Foundation under grant DMR 09-04615.

(GOMD-SI-P004-2011) Alumina Effect on Enthalpy of Mixing of Mixed Alkali Silicate Glasses

P. J. Lezzi*, M. Tomozawa, RPI, USA

Enthalpy of mixing of mixed alkali (Na2O and K2O) silicate glasses containing various concentrations of alumina was determined using an ion-exchange equilibrium method. For glasses with constant alkali concentration, enthalpy of mixing was found to become less negative with alumina addition. Reduction of the magnitude of enthalpy of mixing with alumina addition can be attributed to the reduction of non-bridging oxygen and ionic field strength. Combining the present results with results obtained earlier, magnitude of enthalpy of mixing for the mixed alkali silicate glasses with and without alumina was expressed by a function of a modified Tobolsky parameter, which takes into account the alkali concentration and difference in cation-to-effective anion distances. Experimental data on conductivity of aluminosilicate glasses can be understood in terms of the magnitude of the enthalpy of mixing and we can conclude that the mixed alkali effect is closely correlated with the negative enthalpy of mixing.

(GOMD-SI-P005-2011) Glass-Forming Ability of Soda Lime Borate Liquids

Q. Zheng*, Aalborg University, Denmark; J. C. Mauro, Corning Incorporated, USA; M. M. Smedskjaer, Aalborg University, Denmark; M. Potuzak, Corning Incorporated, USA; R. Keding, Max Planck Institute for the Science of Light, Germany; Y. Yue, Aalborg University, Denmark

We investigate the glass-forming ability (GFA) of a series of iron-containing soda lime borate compositions [xNa2O-10CaO-(89-x)B2O3-1Fe2O3 (x=5, 10, 15, 20, 25, 30 and 35 mol%)] by examining their crystallization behavior and fragility. GFA is characterized in terms of Hrubÿ parameter KH and our newly established criterion. In general, the GFA decreases with increasing content of Na2O. Interestingly, we observe that after the first upscan to 1000 °C at 20 K/min and a subsequent downscan at the same rate, two glasses containing 20 and 25 Na2O mol% do not exhibit any crystallization exotherms during the second upscan at 20 K/min to 1000 °C. Even when the upscan rate is lowered to 5 K/min, the same phenomenon is observed. This means that the stability of these glasses against crystallization is dramatically enhanced for these two compositions. This particular behavior is explained in terms of the temperature dependence of the boron speciation.

(GOMD-SI-P006-2011) Spherical bioactive glass particles and their interaction with human mesenchymal stem cells in vitro

S. Labbaf*, O. Tsigkou, M. M. Stevens, A. E. Porter, J. R. Jones, Imperial College London, United Kingdom

Bioactive glasses (BG) possess great potential as porous scaffolds for bone regeneration, however concerns arise on their long term fate in the body as small particles may be released after implantation, which could lead to undesirable reactions to surrounding cells. In addition, BG nanoparticles have the potential to be injected directly into the defect site to allow healing and regeneration of bone tissue. As mesenchymal stem cells (MSCs) are precursors to osteoblasts, the effect of nanoparticles on their behaviour is critical. In this study BG nanoparticles have been synthesised and fully characterised using a range of techniques. In this study, we compare the effect of BG nanoparticle on the uptake and distribution inside MSCs using 3D confocal microscopy and transmission electron microscopy. The effect of the BG nanoparticles on cell viability as a result of particle uptake was also determined.

(GOMD-SI-P007-2011) Aqueous Corrosion of Polyphosphate Glasses

C. Smith*, R. Brow, Missouri University of Science and Technology, USA

Zinc polyphosphate glasses are candidates for a variety of optical applications but phosphate glasses in general are known to have poor chemical durability. In this study, Zn-Mg- and Zn-Al-polyphosphate glasses with a range of phosphate anions, determined from their O/P ratios, have been prepared and their dissolution behavior in aqueous solutions determined. Sample weight losses are related to ion-release rates as determined from ICP analyses of solutions as a function of time and temperature. Changes in solution pH are related to changes in solution chemistry and are explained using a thermochemical model to predict stable species in solution. This information is then used to develop a compositional model to identify chemically stable glasses.

(GOMD-SI-P008-2011) Engineered Corrosion-induced Passivation Layers for Glass Waste Forms

D. C. Skorski*, J. Ryan, Pacific Northwest National Laboratory, USA

Much attention has been paid to modeling the aqueous corrosion of glass waste forms so that their performance in a repository environment can be reliably calculated. One of the major schools of thought on glass corrosion mechanisms is that dissolution results in the formation of alteration products at the surface of the glass and these present a barrier to transport of water and/or other glass components. Interestingly, this occurs without the glass being specifically designed to produce passivating layers. In this work, we are investigating the design of glass compositions to encourage the eventual production of either a barrier layer that decreases the corrosion rate and increases the long-term durability of existing waste forms, or alteration phases that incorporate targeted ra-

dionuclides and significantly delay their release. Geochemical modeling is used to assist in the design of glass compositions that result in alteration phases with the potential to incorporate major dose-contributing elements.

(GOMD-SI-P009-2011) Dissolution Behavior of Na/Ca-Phosphate Glasses In in Aqueous Solutions

L. Ma*, R. K. Brow, M. E. Schlesinger, Missouri University of Science and Technology, USA

Phosphate glasses are being considered for use in a variety of biomedical applications, including tissue engineering, because they exhibit controlled dissolution behavior and are bio-compatible. Several series of xNa2O-xCaO-(100-2x)P2O5 (x=24~31 mol%) glasses were prepared with compositions in the meta- to polyphosphate range. Dissolution rates of corresponding phosphate glasses were determined from weight loss measurements and ion concentrations in solutions, and pH shifts were recorded. The effects of experimental conditions on dissolution rate are investigated, including solution temperature and pH value. The effect of glass structure, defined by the average phosphate anion size and depending on the O/P ratio, on the dissolution behavior will be discussed.

(GOMD-SI-P010-2011) Analytical modeling of thermodynamic iron redox equilibria and aqueous dissolution behavior of iron phosphate glasses

M. L. Schmitt*, R. K. Brow, Missouri S&T, USA

A theoretical model is proposed to predict the thermodynamic equilibrium between Fe(III) and Fe(II) in phosphate glass melts based on nominal compositions and melting conditions. Unlike previously proposed models, this model considers both the redox equilibrium of the iron ions and the structural equilibrium with changing oxygen content. The model also extends beyond binary iron phosphates to make predictions for sodium-, zinc- and lead-iron phosphates. A second model is proposed to predict dissolution rates for phosphate glasses in aqueous solutions using many concepts developed in the redox equilibria model. Reactions between water and individual bonds within the glass structure are described by considering thermodynamic principals, such as free energy of hydration, as well as compositional and structural properties. Comparisons of model predictions to empirical data from both the authors' research and literature results are used to validate both models.

(GOMD-SI-P011-2011) A Raman Spectroscopy Study of the Structure of Iron Phosphate Glasses

L. Zhang*, R. Brow, Missouri University of Science and Technology, USA

The Raman spectra of ten crystalline ferric, ferrous, and mixed ferric-ferrous phosphate compounds were collected, and those results are used to interpret the Raman spectra of iron phosphate glasses with a wide variety of O/P and Fe/P ratios. The systematic changes in Raman peak positions with glass compositions are related to changes in the numbers of bridging and nonbridging oxygens, which lead to changes in the average P-O bond distances. A correlation exists between the average P-O bond distance and the Raman peak frequencies in the crystalline compounds, and this correlation is used to provide information about the structures of the iron phosphate glasses. For example, the average P-O bond distance is estimated to decrease from about 1.57 Å for iron metaphosphate glasses (O/P~3.0) to 1.54 Å for iron orthophosphate glasses (O/P~4.0). These bond distances are in good agreement with those reported from diffraction studies of similar glasses.

(GOMD-SI-P012-2011) Microstructure and physical properties of the GexAsySe1-x-y glasses with the same mean coordination number of 2.5

R. Wang*, A. Smith, D. Choi, S. Madden, B. Luther-Davies, Australian National University, Australia

We prepared and analyzed five pieces of GexAsySe1-x-y glasses with the same mean coordination number (MCN) of 2.5. The density measurements exhibit a maximum in chemically stoichiometric Ge12.5As25Se62.5 sample, suggesting an obviously atomic re-arrangement when one element was placed by another one. Tg measurements show that the glasses have almost same glass transition temperature, indicating that the glass network connectivity has no much change. Although Raman scattering and XPS spectra of the glasses indicate that the percentage of the different structural units could change with the changing chemical compositions, there is no evidence to confirm the existence of the separated structural units that can cut the glass network connectivity. Therefore the glasses with same MCN but different composition have similar glass network connectivity, and the chemical compositions only slightly modify the physical properties of the glasses.

(GOMD-SI-P013-2011) Stabilization of Second Harmonic Generation in Thermally Poled, Alkali Doped Chalcogenide Glasses

T. Shoulders*, K. Richardson, Clemson University, USA; M. Dussauze, University Bordeaux 1, France; D. Musgraves, Clemson University, USA

High second-order non-linear susceptibilities are created in thin windows of thermally poled chalcogenide glasses doped with small amounts of alkali. Thermal poling was carried out at voltages from 200V to 1000V and temperatures just below Tg. A cross-section of the samples was probed with combined micro-SHG and micro-Raman spectroscopy to determine the depth and structure of the non-linear layer. The nature of the second order signals was measured using the Maker fringe technique, which has shown evidence of an electric field induced second harmonic in the glass. It has been proposed that the migration of alkali in the direction of the cathode during thermal poling leads to the creation of the embedded electric field under the anode surface. Maker fringes obtained at regular intervals after the poling treatment showed the stability of the non-linear layer.

(GOMD-SI-P014-2011) Influence of imprinting conditions on the surface morphology of chalcogenide glasses

B. Jin, Y. Choi*, Korea Aerospace University, Republic of Korea; W. Chung, Kongju National University, Republic of Korea; D. Shin, Hanyang University, Republic of Korea; H. Jain, Lehigh University, USA

In an effort to fabricate planar photonic circuits on the surface of chalcogenide glasses via the imprint technique, we have investigated the evolution of surface morphology of some Se-based chalcogenide glasses under various imprinting conditions. Specifically, the surfaces as well as the overall deformed shape of samples have been monitored as function of glass composition, stamp material, uniaxial pressure, temperature and duration. Under optimum conditions the samples deform very well and reflect the shape of stamp up to a few hundred micrometers in depth. Under other conditions, mostly circular-shaped dimples up to several tens of micrometers in diameter appear on the pressed surface of samples. The empirical correlation between the characteristics of the dimpled surfaces and the processing conditions is discussed.

(GOMD-SI-P015-2011) Thermal expansion investigation of iron sodium silicate glass

B. Mirhadi, B. Mehdikhani*, Imam Khomeini International University, Islamic Republic of Iran

In this study, a theoretical procedure was developed with the aim of obtaining an estimation of the crystallization fraction in glass-ceramics by means of thermal expansion measurements. The theoretical model was applied to the crystallization of an iron sodium silicate glass composition FeSi2O6 as crystalline phases. The crystallization mechanism was investigated by means of DTA, XRD, FTIR,SEM and the thermal expansion by Differential Dilatometer. A relationship between the weight fraction of crystal phase and the linear thermal expansion coefficient was obtained. The values of the fraction of crystal phase, evaluated by means of dilatometric measurements, showed a good agreement with the results obtained by means of density variation and XRD analyses.

(GOMD-SI-P016-2011) Optical absorption and Crystallisation of sodium desilicate glasses containing chromium oxide

B. Mehdikhani*, B. Mirhadi, Imam Khomeini International University, Islamic Republic of Iran

The crystallisation of Na2O.3SiO2 glasses doped with Cr2O3 (0-0.12-0.16-0.2–0.8-2-3-7mol%) has been investigated by UV-Vis-FTIR spectroscopy, XRD and SEM microscopy. The results showed that, By in-

creasing content of chromium oxide, Transmission of light through sodium silicate glasses reduced due to ligand field and charge transfer mechanisms, colored glass was developed in some special wavelengths. Transmission of light through sodium silicate glasses with the presence of chromium oxide change and, also lead to formation of crystalline phases. More increasing of chromium oxide caused that light transmission in spectrum of these glasses being reduced, so that increasing chromium oxide up to 3% molar case that light absorbed, in which, by investigation chromium oxide effect on constituent units of glass lattice by means of infrared spectrum at 400-4000 cm-1 region, it was identified that new peak at 640cm-1 has been appeared.

(GOMD-SII-P017-2011) Relaxation dynamics of supercooled silicon using molecular dynamics simulations

X. Mei*, W. Mohamed, J. Eapen, NC State University, USA

Supercooled states of silicon have been investigated in the past with molecular dynamics simulations (MD) using classical Stillinger–Weber (SW) potential. Sastry and Angell [Nature Materials, 2, 739 (2003)] have demonstrated a fragile–to–strong transition near 1060 K. Subsequent hybrid ab initio simulations by Jakse and Pasturel [PRL, 99, 205702 (2007)] confirmed this liquid–liquid transition. In this paper, we investigate the equilibrium density and stress relaxation dynamics in supercooled Si using SW potential. Our simulations show that SW potential gives reasonable liquid state dynamics – evaluated through intermediate scattering and dynamic structure functions – only at temperatures above 2700 K. The liquid state structure however, as noted from several prior investigations, is reasonably well–reproduced at the physical melting point (~1680K). We further delineate the different mechanisms for density and stress relaxations in liquid and supercooled states of silicon.

(GOMD-SII-P018-2011) A low-cost electrometer for measuring conductivity and glass transition in sugar glass

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The glass transition is requisite to any serious discussion of glass science and the phenomena serves as the entry point to understanding relaxation in glass. Yet laboratory methods to explore this phenomenon, such as DSC, are generally not accessible to the undergraduate engineering student, let alone the high school classroom. Recently we have described a low-cost DTA[1] suitable for students to explore the glass transition in candy glass and other low-melting, glassy materials. We present here an alternate and complementary, low-cost conductivity method to determine the glass transition in candy glass, suitable for the undergraduate laboratory. This method is based on conductivity vs. temperature where an inflection points in sugar glass provides a clear signal of the glass transition. The method utilizes a simple, high impedance current amplifier built around a low cost (<$5) OP AMP IC. [1] W. Heffner, GOMD, May 16-19, 2010, Corning, NY.

(GOMD-SII-P019-2011) Electronic Consequences of Electron-Phonon Interaction in Impurity States of Doped Semiconductors

B. Cai*, M. Zhang, D. Drabold, Ohio University, USA

In this work, we introduce Boron and Phosphorous into amorphous Si and hydrogenated amorphous Si models. By analyzing the electronic structure, we attempt to describe the doping mechanism in this system and provide an explanation for the low doping efficiency. We then studied the electron-phonon interaction involving the impurity states in a-Si:P and a-Si:B, and compared to Ga, As and Sb doped amorphous Ge. Large energy variations in the impurity states indicate that the electron-phonon interaction is so strong that any transition involving impurity state(s) require configurational reorganization, suggesting that Miller-Abrahams models for transport may be inadequate.

(GOMD-SIII-P020-2011) Optical spectra of DIVALENT and TRIVALENT iron in sodium silicate glasses

B. Mirhadi, Imam Khomeini International University, Islamic Republic of Iran; B. Mehdikhani*, Institute of Standard and Industrial Research of Iran (ISIRI), Islamic Republic of Iran

Iron commonly exists as an equilibrium mixture of ferrous ions, Fe2+, and ferric ions, Fe3+, in glass. Fe3+ is a strong absorber of ultraviolet light and imparts a yellow color to glass, while Fe2+ has an absorption band in the near-infrared, resulting in a blue coloration. This study synthesized sodium silicate glasses with iron contents (0.5, 1, 2, 3 wt %). One of samples (0.5% mol of iron oxide) has been melted in different temperatures. UV-VIS spectrum of these samples was obtained by spectroscopy. Color variation of glasses due to adding iron oxide and melting temperature was studied by colorimetric. It was determined by wet chemical analysis. Increase amount of ferric ions, in turn, donate green-yellowish color to glasses. In addition, increasing melting temperature of glasses result in ferrous ions increase in glass and its color appears green-bluish. Using iron nano-powder oxide resulted in the formation of less ferrous ions in comparison with using micronized ions.

(GOMD-SIII-P021-2011) Role of manganese as a oxidizing agent in sodium silicate glasses containing iron oxide

B. Mirhadi, B. Mehdikhani*, Imam Khomeini International University, Islamic Republic of Iran

Iron commonly exists as an equilibrium mixture of ferrous ions, Fe2+, and ferric ions, Fe3+, in glass. Fe3+ is a strong absorber of ultraviolet light and imparts a yellow color to glass, this state, glasses absorption ultraviolet light and can be used as a filter of ultraviolet light. While Fe2+ has an absorption band in the near-infrared, resulting in a blue coloration. This study synthesized sodium silicate glasses with high iron contents (1 mol%) in which virtually all the iron was fully oxidized to the ferric redox state, resulting in a UV-absorbing, yellow glass. The effect of increasing manganese oxide(0.25, 0.5, 1, 1.5%mol) by ultraviolet-visible spectroscopy has been investigated and changing of ferrous and ferric ions has been determined by wet chemical analysis.

(GOMD-SIII-P022-2011) UV-Vis spectroscopy of transition metals in sodium silicate glasses

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Optical absorption Fe2O3 ,V2O5, Cr2O3 in sodium silicate glasses has been studied using ultraviolet-visible spectroscopy. Iron commonly exists as an equilibrium mixture of Fe2+, Fe3+, in glasses. Fe3+ is a strong absorber peaks at 380, 420 and 435 nm while iron(II) absorbs at 1050 nm. Enhancement of chromium in glass leads to formation of two absorption bands in 470 and 640 nm wavelengths that indicating optical peak of Cr3+ ion in this glasses. Vanadium is present in sodium silicate glasses in three possible valencies, V5+, V4+ and V3+. Overlapping of charge transfer peak related to V5+ ions and ligand field peak related to V3+ ions in 380 and 420 nm cause that a specified peak appears in this region and overlapping take place. Presented peak of 630 nm is due to V3+ ions. A broad absorption peak at 1000 nm is observed that is associated to V4+ ions.

(GOMD-SIII-P023-2011) Infrared absorption of polyvalent oxides in glass

B. Mirhadi, B. Mehdikhani*, Imam Khomeini International University, Islamic Republic of Iran

In this work effect of addition polyvalent oxide such as V2O5, Cr2O3 has been investigated by FTIR spectroscopy in the region of 4000-400 cm-1. Enhancement vanadium oxide in this glasses case that new peak at 900 cm-1 appeared. Spectrum that ranged from 400 to 1400 cm-1 has absorption for the sake of main silicate groups of the network and different bounding configuration. remain of the spectrum from 1400 to 4000cm-1 consist of vibration of water's atomic bond, hydroxyl (Si-OH) or other similar groups. With increase of vanadium and chromium oxide, absorption peaks of infrared spectrum shift toward smaller wave number region. vanadium vibration peak will appear at 1005-1025 cm-1 region if present ions of composition be V5+ completely. However, the formed peak due to vanadium oxide addition at 900 cm-1 is representative of V4+ ions formation in glass and chromium vibration peak will appear at 640cm-1

(GOMD-SIII-P024-2011) Optical properties of Mn2+ doped Lead phosphate Glasses

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The objective of studying optical absorption spectra of Mn2+ doped LP glass system is to understand (i) the effect of magnetic ion like Mn2+ on the absorption edge and on energy bands of LP glass system. (ii) to study the effect of lead phosphate glass network on the electronic structure and energy levels of Mn2+ ion. Mn2+ is an excellent ion for probing the local site geometry in various glassy matrices even by optical absorption technique the potential value of Mn2+ for structural diagnosis studies in glasses is very high.Therefore the work is takenup. The Mn2+ doped and pure LP glasses were prepared and these samples optical absorption spectra were recorded on a Shimadzu -UV3101PC, UV-VIS-NIR Spectrophotometer. It is observed that the role of Mn2+ impurity in LP glass appears to be limited to promoting the ease of glass formation. It is interesting to note that the detection of a weak but definite absorption band at 261 nm (38,310 cm-1) is attributed to 6A1g -> 4A2g (F) transition.

(GOMD-SIII-P025-2011) Does photoinduced anisotropy in chalcogenide glasses have atomic structure signature?

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Linearly polarized band-gap / sub-bandgap light can produce various anisotropic phenomena in the originally isotropic chalcogenide glasses and thin films, e.g. birefringence, dichroism and anisotropic deformation. Recently, visible giant anisotropic deformation of free-standing As2S3 film illuminated by linearly polarized light was reported by Tanaka. In the present work, in situ EXAFS experiments in which the polarization of band-gap pump laser is altered in relative to that of X-ray probe are carried out on both free-standing and supported chalcogenide thin films. In contrast to the photoinduced anisotropy which is apparent or even significant in the free-standing film, the atomic structure shows no or unresolved polarization dependence. It is concluded that the photoinduced anisotropy may not find its origin from the atomic structural change.

(GOMD-SIII-P026-2011) Laser-induced anomalous plasmonic evolution in silver nanocomposite glass: An in situ optical microspectroscopy study

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Nanocomposite glasses with embedded metal nanoparticles (NPs) possess outstanding potential in photonics. A subject of interest is material modification via laser irradiation. In this work, the optical properties of a laser-irradiated Ag nanocomposite glass are studied during heat treatment (HT) by in situ optical microspectroscopy. The material consists of an Ag NP-doped phosphate glass prepared by melting and HT processes. Irradiation was carried out by linearly polarized laser pulses from a 5 ns Nd:YAG laser at 532 nm (10 Hz). A sample displaying a surface plasmon resonance (SPR) around 462 nm was irradiated for 30 minutes with a fluence of 150 mJ/cm2, resulting in the vanishing of NP resonance modes. HT of such sample lead to the development of an anomalous SPR band for the NPs. The atypical SPR evolution appeared both temperature- and time-dependent. The influence of laser irradiation on the NP transformations likely taking place is discussed.

(GOMD-SIII-P027-2011) Relation between structure and photochemistry of silver-containing phosphate glasses

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The development of optics requires transparent composite materials for many applications (waveguides, data storage…). Recent interest has grown for generating local optical contrast in glass using Direct Laser Writing by high repetition rate fs laser system. Full understanding of the involved photo-chemical processes is needed. Silver zinc phosphate glasses are good candidates for laser structuring by taking advantage of the laser cumulative effects and the material photosensivity. Tailoring the resulting properties relies on the understanding of the glass and its photosensitivity. The glass structure is analyzed using Raman, XPS and NMR spectroscopies. The photosensitivity of the glass is studied using different irradiation ways. Combined EPR and luminescence spectroscopies offer insights on the emitting silver sites. A close relation has been evidenced between the glass composition and its structure (glass matrix, silver concentration), the photosensitivity and the laser characteristics.

(GOMD-SIII-P028-2011) Pulsed Laser Deposited Ga-Ge-Te Amorphous Thin Films

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One of the promising far-infrared transmitting amorphous materials is being represented by Ga-Ge-Te family, which already showed transparency up to 28 μm. In this work, we fabricated Ga-Ge-Te thin films by UV pulsed laser deposition. Prepared layers were characterized in terms of their chemical composition (by energy-dispersive X-ray analysis), morphology (using scanning electron microscopy), structure (employing Raman spectroscopy), optical properties (via analysis of spectroscopic ellipsometry data) as well as photosensitivity applying near band gap irradiation. Observed features are compared with gallium free amorphous Ge-Te thin films. Comparison of properties of the bulk Ga-Ge-Te glass and their films is also presented.

(GOMD-SIII-P029-2011) The effects of sintering aids on defects and densification in transparent Nd:YAG ceramics

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To understand the role of SiO_2 doping in densification and microstructure development of Nd:YAG transparent ceramics, 1 at% Nd:YAG powders were doped with 0.035-0.28 wt% SiO_2 and vacuum sintered between 1484°C and 1750°C. ^{29}Si magic-angle spinning nuclear magnetic resonance showed that Si^{4+} substitutes onto tetrahedrally coordinated Al^{3+} sites at sintering temperatures > 1600°C. Coarsening was limited by a solute drag mechanism as suggested by cubic grain growth kinetics and TEM energy dispersive x-ray spectroscopy observations of increased Nd^{3+} concentration near grain boundaries. Increasing SiO_2 content increased both densification and grain growth rate and led to increasingly coarsening-dominated sintering trajectories. For the first time, the average grain size could be controlled (2.8 μm – 18 μm) in highly transparent ceramics using a combination of SiO_2 content, sintering temperature, and sintering time.

(GOMD-SIII-P030-2011) Phase separation and crystallization mechanism in non linear optical LiNbO3-SiO2 glasses

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Lithium niobate is a ferroelectric material, widely used for applications in optics like nonlinear optical materials. The precipitation of lithium niobate crystalline particles in the glass of composition Li2O/Nb2O5/SiO2 allows a fast, low-cost and massive production of this optical material compared to sintering techniques or Czochralski method. A two-steps heat-treatment consisting of both nucleation and growth on Li2O/Nb2O5/SiO2 glass provides a translucid glass-ceramic with nonlinear optical properties. The μ-Raman mapping is realized on this glass and clearly shows modification of the Nb-O vibration mode around 650 cm-1. This reveals demixtion areas in this glass-ceramics. In the Nb2O5-enriched area, crystallization occurs through the precipitation of different crystal sizes. Depending on crystallites orientation and sizes, the measured Second Harmonic Generation signal is affected. Correlation between the crystallization state and SHG signal will be studied.

(GOMD-SIII-P031-2011) The Effect of Silica on Emission Property of Various Cr4+-Doped Glass Ceramics

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A broadband nature of Cr4+emission in crystals and glass ceramics is attractive to the applications, such as broadband amplified spontaneous

source and amplifier. However, in many cases the Cr4+ doped crystal/glass ceramics has to integrate with silica, i.e. Cr4+-doped optical fiber, resulting in a rapid degradation of optical properties of Cr4+. This consequence severely limits their potential applications. Our first step of study is to investigate the interface between silica and Cr4+-doped glass ceramics, which include Cr:Fosterite, Cr:Zn2SiO4, Cr:Ca2GeO4, Cr:Ca2SiO4, etc., by XPS, XRD, IR spectroscopy, and SEM. Their extents of interaction will be discussed and thereof the best candidate, which is the most inert to silica, will be presented.

(GOMD-SIII-P032-2011) Processing and Mechanical Properties of Transparent Lu2O3 Laser Host Ceramics

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Transparent Lu_2O_3 ceramics are being investigated as potential laser gain media for high energy laser applications due to their ability to accommodate high concentrations of ytterbium without an appreciable decrease in thermal conductivity. This study investigates the processing and mechanical properties of highly transparent Lu_2O_3. The effect of powder synthesis and powder processing methodologies on densification and sintered transparency are evaluated and discussed. The mechanical properties of Lu_2O_3 (including strength, fracture toughness and hardness) are reported here and compared with other sesquioxide ceramics.

(GOMD-SIII-P033-2011) Compositional and structural changes in thermally poled borosilicate glass and their link to non linear optical properties

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Thermally poled glasses have been currently studied because of their non linear optical (NLO) properties interesting for photonic applications. This treatment permits to entrap a strong electric field below the anodic glass surface. This internal electric field is a consequence of a space charge layer induced by a cationic depletion zone. The ionic entities concentrations and the electrode nature will influence the poling mechanisms and the second harmonic generation (SHG) response. In this context, we have investigated polarized sodium borosilicate glasses. By coupling vibrational spectroscopy and SHG techniques, we have characterized the poling effects on both borate and silicate networks and linked these structural rearrangements to the NLO response. These results contribute to a better understanding of the poling mechanisms and their influences on the NLO properties which is necessary to progress towards possible applications in photonic.

(GOMD-SIII-P034-2011) Development of Pr3+-doped ZBLA fluoride waveguide for compact laser source emitting in visible

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The objective of this study is focused on red, orange and green emissions of Pr3+ :ZBLA channel waveguide. The elaboration of channel waveguide including glass sample preparation, photolithography process and ionic exchange experiments will be detailed. Spectroscopic studies will be described which were performed to optimize the rare earth doping level in order to reach the best compromise respecting a good optical quality, a highest lifetime and efficient emission intensity at 635, 605 and 520 nm. Finally, optical characterizations of ion exchanged Pr3+: ZBLA channel waveguides will be presented.

(GOMD-SIII-P035-2011) Size Effects on Properties of Novel High Z Scintillators

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Current radiation detection materials suffer from performance and reliability issues, such as low luminosity, volume restrictions, and chemical instability. Critical to overcoming these restraints is the development of scintillators with well-understood interactions with radiation. We elected to probe the fundamental changes in scintillation behavior based on particle size, activator concentration, and surface chemistries of the W-based materials. The materials studied included bulk and nanomaterials of the standard MWO_4 (M=Pb,Ca,Cd) and the new high-Z WE_x (E =S,Se,Te) materials. The synthesis processes and characterization of these W-based nanomaterials will be presented. In addition, their scintillator behavior was determined using X-ray diffraction, electron microscopy, various luminescence techniques, and luminescence decay times. Scintillation yields are also measured and compared to currently-accepted materials for radiation-detection to determine a better understanding of radiation-material interactions.

(GOMD-SIII-P036-2011) Monitoring of the geological storage of CO2 using chalcogenide waveguides

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Follow-up of CO2 injection and site monitoring are crucial to ensure storage safety. The carbon dioxide shows a characteristic optical absorption spectrum in the Mid-infrared region (MIR region). So, chalcogenide glasses, which can transmit light in the 1-10 μm region, are well adapted for the monitoring of CO2. Several ways of recording the IR absorption of the CO2 were studied. The first one works on the principle of the absorption of light between two chalcogenide fibers. A detection limit down to 500 ppm was observed. The second one consists on using a rare earth doped chalcogenide optical fiber as our own MIR source centered around 4.3 μm. This one offers the advantage to remote the sensing zone over several kilometers. And alternatively to those ways of detection, microfluidic waveguides made of sulphide and selenide thin films were developed and tested using the evanescent wave principle with liquids and gas absorbing in the nIR.

(GOMD-SIII-P037-2011) The Effect of Gold Doping on the Conductivity of Sodium Trisilicate Glass

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The optical properties of gold-doped ruby glass have made it a very attractive subject to study. Most of these studies have tried to characterize the source of the ruby color or the transformation that the gold goes through during heat treatment; however, few if any of these studies have focused on the electrical properties of this material. We varied the state of gold in sodium trisilicate glass either through the addition of tin, as a reducing agent, or through heat treatment. A noticeable increase in the ac conductivity of approximately one order of magnitude was observed when the glass was doped with 0.10% gold. Furthermore, it was observed that this increase in conductivity varied with the optical properties, and therefore the state of the gold nanoparticles.

(GOMD-SIV-P038-2011) Chalcogen-based aerogels as a multifunctional platform for remediation of radioactive waste

B. Riley*, J. Chun, J. Ryan, S. K. Sundaram, D. Strachan, PNNL, USA

Chalcogen-based aerogels, termed chalcogels, are prepared by interlinking between chalcogenido clusters and a catalyst. The wide range of compositional flexibility of precursors involved in producing these materials has been used to create chalcogels with a wide range of mechanical, structural, and chemical properties. We primarily focus on the inherent selective chemical affinity of these chalcogels as a multifunctional platform for the remediation of radioactive wastes, e.g., I-129. The selectivity of these chalcogels can be understood by Pearson's Hard/Soft Acid-Base (HSAB) principle with the soft Lewis acid/soft Lewis base complex formation between the chalcogen and the iodine. We have significantly improved the surface areas of a Ge-Pt-S chalcogel from the literature data and demonstrated a very high affinity for iodine. Further development is being done to reduce the melting temperature of these chalcogels in order to facilitate waste consolidation following immobilization.

(GOMD-SIV-P039-2011) Evaluation of nepheline formation in nuclear waste glasses

C. P. Rodriguez*, M. J. Schweiger, A. E. Winschell, J. S. McCloy, Pacific Northwest National Laboratory, USA

Nepheline crystallization has a large impact on the chemical durability of High level waste glasses. Optical Basicity and the Nepheline Discriminator are two ways of describing a given complex glass composition. They are being studied together in a quadrant system as metrics to explore nepheline crystallization and chemical durability as a function of waste glass composition. These metrics were calculated for glasses with existing data and also for theoretical glasses, to explore nepheline formation at quadrant IV (presumed to be mostly good chemical durability). Several of these compositions were chosen and glasses were made to fill sparse regions at quadrant IV. To evaluate nepheline formation and chemical durability on these glasses, quantitative XRD analysis and PCT test were conducted. This presentation will summarize the theoretical and experimental basis for these models.

(GOMD-SIV-P040-2011) Utilization of a Laboratory-Scale Melter to Determine Melting Rate of Waste Glass Feeds

J. Das Gupta*, D. Kim, M. Schweiger, W. Buchmiller, J. Vienna, Pacific Northwest National Laboratory, USA

The purpose of this study is to evaluate the laboratory-scale melter (LSM) as a tool to determine the processing rate of various slurry feeds for the vitrification of high-level waste (HLW). The LSM uses a fused quartz crucible with 3 or 4 inch diameter. This LSM setup allows cold-cap (similar to batch blanket in commercial glass furnaces) formation above the molten glass to be directly monitored to obtain a steady-state melt rate of the HLW feeds. Simulated HLWs, AZ-101 and C-106/AY-102, with different levels of glass yield at 300 g/L, 400 g/L and 500 g/L (g glass per L of slurry) were processed in the LSM. This paper presents the results of LSM tests compared with the melting rate data obtained from large-scale melter tests. The results of analyses of cold-cap samples collected from LSM runs will also be presented.

(GOMD-SIV-P048-2011) The DHS database for High Performance Materials

G. Fischman*, Future Strategy Solutions, LLC, USA

The National Institute of Building Sciences has developed a database that focuses on materials under development that could be used for the construction, infrastructure and facilities management industries. This database is being developed for the Department of Homeland Security's Infrastructural and Geophysical Division and has the potential of facilitating the development of new materials that can be used for new construction and infrastructure with goals towards increased security, higher energy efficiency and lower cost. This poster will explain the purpose and the process for submitting materials to this database.

(GOMD-SIV-P049-2011) Sorting of glass, plastics and minerals

A. Schnehen*, C. Makari, Binder & Co. AG, Austria

Binder+Co deals with sensor-based separation of transparent and non-transparent bulk materials. Since the beginnings of this technology, Binder+Co has always been a market leader in the processing of waste glass. With CLARITY, Binder+Co brought onto the market the first 3-way- system which simultaneously sorts waste glass on the basis of color (recognition of 16 millions shades) and separates contaminants (such as ceramic, stone, porcelain and metals). The latest generation of CLARITY recognizes heat-resistant and lead glass and thus secures a crucial competitive advantage for its customers. By fusing a UV sensor with a RGB camera, heat-resistant special glasses and lead-containing glasses can be identified and reliably excluded without using X-ray fluorescence. The sensor-based sorting technology of Binder+Co ranges from stand-alone machines to complete turnkey systems. Only an optimum system design and correct conditioning of the input material will give customers in the glass industry an economic and technological edge.

(GOMD-SIV-P041-2011) Soda-lime silicate glass under hydrostatic pressure and indentation: a micro-Raman study

T. Deschamps*, CEA, France; C. Martinet, LPCML, Université Lyon1, France; J. Bruneel, Université Bordeaux1, France; B. Champagnon, LPCML, Université Lyon1, France

Raman micro-spectroscopy is used to analyse the plastic behaviour of window glass (a soda-lime silicate glass) under high hydrostatic pressure and Vickers indentation. We show pressure induced irreversible structural changes, notably an increase of Q2 species at the expense of Q3. For the first time, a very accurate Raman ↔ pressure calibration curve has been established. Local density variations of a Vickers-indented window glass has been characterised by micro-Raman mapping using a high spatial resolution device. The effects of glass depolymerisation on indentation and hydrostatic compression are discussed.

(GOMD-SIV-P042-2011) Borate Based Bioactive Glasses for Soft Tissue Regeneration

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As the average age of the human population increases, the need for improved materials to treat damaged or diseased soft tissue is increasing at an alarming rate. Functional skin and muscle are imperative for everyday living, yet these tissues lack sufficient materials required for effective treatment. Diabetic and elderly people with non-healing wounds often require amputation of their limb as the only effective form of treatment available. Fortunately, a new family of bioactive glasses is showing great promise in the area of soft tissue regeneration as these glasses have been chemically modified to stimulate blood vessel formation (angiogenesis), which is a key component needed in growing soft tissue. These same glasses placed on non-healing diabetic wounds of humans have completely healed the wounds on the order of weeks, with minimal scarring reported. Therefore, this new family of bioactive borate glasses appears to be an effective option in filling the need for new soft tissue regenerating materials.

(GOMD-SIV-P043-2011) Effect of temperature on UV-Vis spectroscopy of sodium silicate glasses contained nanoparticle iron oxide

B. Mirhadi, B. Mehdikhani*, Imam Khomeini International University, Islamic Republic of Iran

The redox state of iron in the sodium silicate glasses was varied by changing the melting conditions, such as melting temperature and particle size of iron oxide. The oxidation states of the iron ion were determined by wet chemical analysis and UV–Vis spectroscopy methods. Iron commonly exists as an equilibrium mixture of ferrous ions, Fe2+ , and ferric ions Fe3+. In this study, sodium silicate glasses contained nanoparticles iron oxide (0.5% mol) were melted in various temperatures. Increase of temperature leads to transformation of ferric ions to ferrous and intensity of ferrous peak in 1050 nm was increased. Nanoparticle iron oxide cause that, less amount of ferrous ions was formed and Fe2+/Fe3+ equilibrium ratio compare with using micronize iron oxide powder was decrease.

(GOMD-SIV-P044-2011) Preparation of CaO-MgO-SiO2 Glass-Ceramic Using Na2SiO3 Waste Solution

C. Yamagata, O. Z. Higa, Instituto de Pesquisas Energeticas e Nucleares, USA; A. D. Rodas, Instituto de Pesquisas Energeticas e Nucleares, Brazil; S. T. Reis*, Missouri University of Science and Technology, USA

In recent years, glass-ceramics of the ternary CaO-MgO-SiO2 system have been studied for biomedical applications because of their good mechanical and chemical properties. CaO-MgO-SiO2 glass-ceramic powder was synthesized by a novel method: Ca and Mg were precipitated on SiO2 gel obtained from Na2SiO3 solution, an effluent derived from the alkaline fusion of zircon. Non-aggregated SiO2 particles were initially prepared by surfactant template sol-gel technique, via acid-catalyzed hydrolysis of Na2SiO3. The CaO-MgO-SiO2 glass-ceramic powders were characterized by Micro-Raman Spectroscopy, SEM, BET, FTIR and XRD. XRD analysis of the sample sintered at 1300 oC confirmed that they were mostly composed of wollstonite (CaSiO3) and

arkemanite (Ca2MgSi2O7) crystalline phases and dicalcium silicate (Ca2SiO4) in minor intensity. The simulate blood fluid (SBF) was used to test the in vitro bioactivity and no toxic effect was found in the cytotoxicity test with CHO (Chinese hamster ovary) cells

(GOMD-SIV-P045-2011) Synthesis and Characterization of Phase-change Nanowires Confined in Periodic Mesoporous Silica
C. Ihalawela*, B. Prasai, G. Rosen, G. Chen, Ohio University, USA

Phase-change memory materials (PCMM) have been used for optical memories (e.g., DVDs) and are a promising candidate for next-generation non-volatile electric memories. To downsize the memory devices, an electrochemical synthesis method has been proposed due to its excellent void-filling capability. In this paper, we report the synthesis of PCMM inside mesoporous silica film using an electrochemical method. The mesoporous silica films are prepared by a sol-gel method using triblock copolymers as a structure-directing agent through an evaporation-induced self-assembly process. Elemental (Se) and binary (Sb-Te) semiconductors are grown inside the periodic mesoporous silica by electrodeposition. The confined semiconductor nanowires are characterized by energy dispersive x-ray spectroscopy, x-ray scattering, x-ray absorption fine structure, and transmission electron microscopy. The structure and phase-transition behavior due to the nanoscale confinement effect will be discussed.

(GOMD-SIV-P046-2011) Nanoparticle-incorporated indium tin oxide (ITO) thin films obtained through sol-gel process
H. Yavas*, M. T. Kesim, C. Durucan, Middle East Technical University, Turkey

Indium tin oxide (ITO) thin films have been used as transparent electrode in many applications such as display panels, solar cells, touch screens and electrochromic devices. Commercial grade ITO thin films are usually produced by sputtering technique. On the other hand, liquid based coating techniques such as sol-gel, which is simple and easily applicable in the economic sense, has the potential for developing ITO thin films. In this study, ITO nanoparticle incorporated hybrid sols prepared from inorganic indium ($InCl_3.4H_2O$) or ($InNO_3.xH_2O$) and tin ($SnCl_4.5H_2O$) precursors were employed to form ITO thin films on soda lime silica float glass substrates. The effects of ITO nanoparticle incorporation, sol aging and post coating heat treatments on the structural, electrical, optical and morphological properties of ITO thin films have been reported.

(GOMD-SIV-P047-2011) Sol-gel derived silver-incorporated hybrid ITO thin films
M. T. Kesim*, H. Yavas, C. Durucan, Middle East Technical University, Turkey

Wet processing techniques such as sol-gel offer several advantages for preparation of indium tin oxide (ITO) thin films. These include simple processing needs, possibility for coating large area substrates and low equipment cost. Herein, sol-gel routes for developing silver-ITO thin films on glass have been established. The aqueous coating sols were prepared from $In(NO_3)_3.xH_2O$, $SnCl_4.5H_2O$, $Ag(NO_3)$ and acetylacetone, 1-propanol, acetonitrile. The electrical and optical properties of the films were determined by 4-point probe method and UV-Vis spectroscopy. The structural properties of ITO films were examined by FESEM and XRD. The effect of silver amount and thermal treatment on microstructure, phase identity and electrical/optical properties of hybrid ITO films have been reported. A correlation between optical film properties, microstructure and chemical/physical state of silver has been established.

Tuesday, May 17, 2011

Symposium I: Glass Science

Session B: Glass Structure and Properties I

Room: Cumberland
Session Chair: Randall Youngman, Corning Incorporated

9:20 AM

(GOMD-SI-010-2011) Perfect glasses with novel mechanical properties (Invited)
N. Greaves*, L. L. Greer, University of Cambridge, United Kingdom; G. Sankar, University College London, United Kingdom

Whilst the formation of low entropy glasses by melt-quenching is precluded by devitrification, amorphisation of microporous crystalline materials offers a practical route by which such "perfect glasses" can be created. MASNMR, inelastic X-ray scattering and nanoindentation methods enable the entropy and mechanical properties to be followed as amorphisation progresses. Topological order in the starting crystals remains constant while the low entropy glass is established, as does the Landau-Placzek ratio and the velocity of sound - pointing to the retention of crystalline entropy, non-ergodicity and mechanical modulii. In particular B/G <1 and Poission's Ratio is close to zero. At the same time Young's modulus is substantial even though the mechanical hardness is low. Compared to the precursor low density crystals, which are generally only available as micro-sized powders, amorphisation enables monolithic low entropy glass specimens to be fabricated with practical dimensions.

10:00 AM

(GOMD-SI-011-2011) Structural characteristics of low- and high-density amorphous phases in yttrium aluminate glasses: results from multinuclear NMR spectroscopy
N. Nasikas, ICEHT/FORTH, Greece; S. Sen*, University of California at Davis, USA; G. Papatheodorou, ICEHT/FORTH, Greece

Rare earth aluminates are important materials regarding their properties and technological applications. Besides the formation of yttrium aluminum garnet (YAG) which is an important host crystal for solid-state lasers, liquids and glasses in the Y2O3 – Al2O3 binary system has received significant research attention in the last two decades in relation to the observation of polyamorphism in the supercooled liquid and glassy state. We will report the results of a multinuclear NMR spectroscopic study of the structure of yttrium aluminate glasses with $24 \leq x \leq 41$ mol% Y2O3 prepared by containerless aerodynamic levitation techniques and CO2 laser melting. These results provide important and unique insight for the first time into the structural characteristics of the low- and high- density amorphous phases (LDA and HDA) associated with the density driven liquid-liquid phase transition in these glass-forming liquids.

10:20 AM

(GOMD-SI-012-2011) Composition dependence of the viscosity and other physical properties in the arsenic selenide glass system
J. Musgraves*, P. Wachtel, S. Novak, J. Wilkinson, K. Richardson, Clemson University, USA

The viscosity of the As(x)Se(100-x) family of glasses has been measured for $10 \leq x \leq 40$, and fit both with the VFT equation and a newer viscosity equation from Mauro et al. which describes the viscosity in terms of other physical functions. This viscosity equation is fully parameterized as a function of composition, permitting the prediction of arbitrary viscosity curves in the composition space studied. Measurement of other physical properties of the glasses, including the density, glass transition temperature, and coefficient of thermal expansion have been performed in order to calculate the viscosity as a function of temperature and glass composition. The variation in kinetic fragility of the glasses is explained in the context of frozen-in configurational entropy in the glasses. The

configurational entropy has an apparent maximum at the composition As(30)Se(70).

10:40 AM

(GOMD-SI-013-2011) Electrical Transport Properties of Bulk Amorphous Semiconductors

B. R. Johnson*, J. S. McCloy, B. J. Riley, J. V. Crum, J. V. Ryan, S. K. Sundaram, Pacific Northwest National Laboratory, USA; D. N. Hebert, A. A. Rocket, University of Illinois, Urbana-Champaign, USA

Amorphous semiconductors have novel properties and applications in electronics and photonics. Examples of such materials include the amorphous chalcogenides (e.g. a-Se, As-Se, As-Se-Te etc.) and chalcopyrites (e.g. Cd-Ge-As). Example applications include optical phase-change memory (Ge-Sb-Te), vidicon tubes (Sb2S3, a-Se), and photovoltaics (a-Si:H). Broader application of these materials depends on a deeper understanding of their charge carrier transport properties and how these properties correlate to their structure and composition. This talk will discus synthesis of a few select bulk amorphous semiconductors, their structure, and characterization of their charge carrier transport properties such as conductivity, mobility, and relative work function.

11:00 AM

(GOMD-SI-014-2011) Raman and X-ray Absorption Studies of the Structure of Alkali Tungstate Glasses

C. W. Ponader*, K. Adib, B. Aitken, Corning Incorporated, USA

Bulk alkali tungstate glasses, with Li, Na and K, are of interest because of the absence of traditional glassforming components. Mixed-alkali tungstate glasses containing 52.5 to 62.5 mole% WO3 have been characterized using Raman spectroscopy and X-ray absorption spectroscopy of tungsten. The Raman and near-edge x-ray spectra show that tungsten occupies both tetrahedral and octahedral sites in these glasses. The site distribution varies with the tungsten content. This is indicated by a 14% decrease in the intensity of the pre-edge peak in the x-ray spectra and a decrease in the intensity of the Raman tetrahedral stretching bands relative to the octahedral bands as the tungsten content increases. Modeling of the EXAFS spectra guided by these results allows the determination of the ratio of octahedral to tetrahedral tungsten sites.

11:20 AM

(GOMD-SI-015-2011) The Structure and Properties of Polyphosphate glasses from the ZnO-MgO-P2O5 and ZnO-Al2O3-P2O5 Systems

C. Smith*, R. Brow, Missouri University of Science and Technology, USA

Zinc polyphosphate glasses are candidates for a variety of optical applications. Polyphosphate glasses have structures that are based on phosphate anions of decreasing average chain lengths with increasing O/P ratios between 3.0 and 3.5. Zn-Mg-phosphate and Zn-Al-phosphate glasses were prepared and properties such as density, refractive index, coefficient of thermal expansion and glass transition temperature, were measured and related to composition. Glass structures were characterized by vibrational spectroscopy and the phosphate anion distributions were determined using high pressure liquid chromatography. This structural information will be related to the compositional trends in glass properties.

11:40 AM

(GOMD-SI-016-2011) Structure-Property Relationships in Cerium Aluminophosphate and Silicophosphate Glasses

J. L. Rygel*, C. G. Pantano, The Pennsylvania State University, USA

Cerium oxide is a common glass additive for optical property modification, particularly to limit the formation of deleterious color centers formed during exposure to high-energy radiation. Phosphate glasses provide a unique opportunity for studying cerium incorporation due to their high rare-earth solubility, ~25 mol%, and the interesting magnetic, acoustic, luminescent, and low-temperature thermal properties often exhibited by rare-earth metaphosphate glasses. Two series of glasses, nominally AlP3O9 - CeP3O9 and CeP3O9 - SiP2O7, have been synthesized to investigate the behavior of this rare-earth cation in a range of compositions near the metaphosphate. Physical properties, as well as chemical stability and radiation damage resistance, of these glasses will be described and correlated to local structure, particularly rare-earth clustering and the presence of octahedrally coordinated Si, as determined by Ce K-edge EXAFS and 29Si, 27Al, and 31P NMR.

Session C: Glass Corrosion I

Room: Sapelo
Session Chair: Stephane Gin, CEA

9:20 AM

(GOMD-SI-028-2011) Development of first-principles-based models for glass dissolution

P. Zapol*, H. He, J. Cunnane, Argonne National Laboratory, USA

Glass waste forms in a repository will eventually contact with water leading to dissolution and release of radionuclides. Long-term predictions based on empirical rate laws for glass dissolution might incur large uncertainties and can be improved using atomistic-informed models. Initial development of such models is based on well-characterized crystalline aluminosilicates that have a well-defined structure, but embody key characteristics of waste form glass, such as compositions of multiple cations, pH dependence and formation of secondary phases. We have performed first-principles-based modeling of surface site distribution on orthoclase surfaces, as well as calculations of barriers for water reactions with neutral, protonated and deprotonated sites. The dissolution rate far from equilibrium is compared to experiments. This can provide insights into the molecular-level mechanisms of glass dissolution.

9:40 AM

(GOMD-SI-029-2011) Filling the Gaps from Atomistic to Continuum Modeling to Better Predict Nuclear Waste Glass Dissolution

L. J. Criscenti*, Sandia National Laboratories, USA

Long-term storage of high-level nuclear waste in glass is dependent upon the rate at which glass dissolves. Research has been done to evaluate the gaps in our understanding of glass dissolution. A major research thrust is to incorporate our increasing knowledge of atomistic processes into continuum-scale models to improve predictions of glass dissolution rates in a repository setting. Gaps exist between both (1) atomistic and mesoscale and (2) mesoscale and continuum models. Also, most computational studies have been performed on simple glasses, rather than multicomponent glasses analogous to those proposed for waste containment. One step in bridging this gap is to develop models for multicomponent glass dissolution. Monte Carlo methods and classical molecular dynamics simulations will be used to systematically create Si-Al-B-Na glass structures and surfaces. These simulated structures will be validated through comparison with experimental data where possible.

10:00 AM

(GOMD-SI-030-2011) Modeling of Glass Dissolution with Transition-State Theory

D. Strachan*, Pacific Northwest National Laboratory, USA

Over the past 20 years, we have used the transition-state theory form of the rate equation for glass as the form of the dissolution rate law. Since many of the experiments and storage environments resulted in aqueous solutions with alkaline pH values, there are many reported results for rate law parameters for what has been reported as the "basic leg" of the dissolution rate as a function of pH. Although we have very few test results from experiments performed at acid pH values ("acid leg"), we have some values for the rate law parameters. These two "legs" of the dissolution rate law are currently treated separately, whereas a rate law that covers the pH range from 0 to 14 is scientifically more useful. In this presentation, I will show the results of modeling efforts to have a single rate expression that covers this pH range.

10:20 AM

(GOMD-SI-031-2011) Why glasses with high dissolution rates may undergo low corrosion? (Invited)

C. Cailleteau*, CEA/DEN, France; F. Devreux, Ecole Polytechnique-CNRS, France; O. Spalla, CEA/DSM, France; F. Angéli, S. Gin, CEA/DEN, France

Two series of borosilicate glasses were prepared for studying the influence of the substitution of (i) CaO for Na2O and (ii) ZrO2 for SiO2 on glass durability. They were corroded in buffered aqueous solution at pH 6.9 and pH 8.0. An inverse correlation was found between the initial dissolution rate and the final degree of corrosion in the saturation regime. It was observed as a function of pH for a given glass as well as a function of glass composition at fixed pH. ToF-SIMS study of the permeation of foreign ions in the corrosion layer, SAXS characterization of the layer reorganization, neutron scattering with index matching by D2O-H2O exchange, and Monte-Carlo simulations of the corrosion provide the key to this paradoxical behavior: glasses with fast dissolution rate undergo a fast restructuring of the corroded layer into a passivating film, which rapidly stops corrosion by porosity closure; on the contrary, the slow restructuring of glasses with slow dissolution rate leads to a higher degree of corrosion.

10:40 AM

(GOMD-SI-032-2011) Evidence for a New Glass Corrosion Mechanism from Isotope Tracer Experiments (Invited)

T. Geisler*, University of Muenster, Germany; A. Janssen, Institute for Transuranium Elements, Germany; R. Denkler, University of Muenster, Germany; M. Kilburn, University of Western Australia, Australia; A. Putnis, University of Muenster, Germany

Established corrosion models are based on diffusion-controlled hydration and ion exchange reactions operating in the solid state and subsequent re-condensation of the hydrolyzed glass network. Here we report the results of Si, Mg, and O isotope tracer experiments with different borosilicate glasses under static conditions (T = 90 to 150°C, pH = 0 to 10) that contradict such view. NanoSIMS and Raman measurements on cross sections of the experimentally altered glasses revealed chemical and structural banding patterns inside silica-based corrosion zones as well as an enrichment of the respective isotope that was enriched in solution. No diffusion profiles were observed. In some experiments ^{18}O was added after some time has passed. Here we found the ^{18}O enrichment to set in somewhere inside the corrosion rims. These observations can be best explained by congruent glass dissolution that is spatially and temporally coupled to the precipitation of amorphous silica at an inwardly moving reaction interface.

11:20 AM

(GOMD-SI-033-2011) Solid-State NMR Investigations of Nuclear Waste Glass Corrosion

K. A. Murphy*, K. T. Mueller, C. G. Pantano, The Pennsylvania State University, USA; J. V. Ryan, N. M. Washton, Pacific Northwest National Laboratory, USA

The observed decrease in the dissolution rate of some nuclear waste glasses is not fully understood. Two models have been used to explain this observation: silicic acid saturation and the formation of a transport barrier. In order to determine the rate controlling mechanism, the function of the alteration layer must be established. Solid-state NMR spectroscopy was utilized to characterize differences between the structure of the bulk glass and the alteration layer. Two waste glasses were chosen for investigation and their bulk structures were probed using Bloch decay magic angle spinning (MAS) NMR experiments. Leaching was carried out and cross-polarization (CP) MAS NMR was used to investigate the structure of the alteration layer. Reactive silanol quantification was also accomplished by functionalization with a chlorosilane onto the glass surface and subsequent analysis by 19F MAS NMR. Other techniques used to support and complement NMR observations including inverse gas chromatography, BET, XPS, and SEM.

11:40 AM

(GOMD-SI-034-2011) Kinetic evaluation of aqueous dissolution of P0798 simulated HLW glass as a function of dissolved silica concentration by using micro-channel flow-through test method

Y. Inagaki*, K. Sakanani, Kyushu University, Japan; S. Mitsui, Japan Atomic Energy Agency, Japan; K. Idemitsu, T. Arima, Kyushu University, Japan; K. Noshita, Hitachi Ltd., Japan

Modeling long-term dissolution of HLW glass in geological disposal needs a consistent evaluation of glass dissolution kinetics under conditions of near silica-saturation. The evaluation of the kinetics also needs reliable and precise data obtained under well-constrained experimental conditions for multiple parameters such as pH, solution concentrations of elements and reactive glass surface area. In the present study, therefore, aqueous dissolution tests were performed for a Japanese type of simulated HLW glass, P0798, by using "Micro-channel flow-through test method" as a function of dissolved silica concentration at several constant pHs. The test results showed that the glass matrix dissolution proceeds at certain rates even under conditions of near silica-saturation, and behavior of aluminum can play an important role in the glass dissolution as well as ion-exchange of alkaline elements.

Symposium II: The Amorphous State

Session A: Glass Transition and Relaxation in Glasses and Glassforming Liquids III

Room: Ossabaw
Session Chair: Prabhat Gupta

9:20 AM

(GOMD-SII-015-2011) What have we learned from experiments about relaxation in silica glass? (Invited)

M. Tomozawa*, Rensselaer Polytechnic Institute, USA

For the past fifteen years, we have investigated relaxation phenomena of silica glasses. Differential Scanning Calorimeter (DSC) has been a favorite experimental tool for the structural relaxation study of many glasses but this technique is not very useful for silica glasses. On the other hand, vibrational spectroscopy, especially Fourier Transform Infrared Spectroscopy (FTIR) turned out to be quite useful tool for the structural relaxation study. Here, our research results on the structural relaxation studies of silica glasses using FTIR will be reviewed. Topics will include Fictive temperature measurement by IR; Memory effect; Relaxation with single relaxation time; Structural relaxation times as a function of fictive temperature and heat-treatment temperature. Some stress relaxation study will also be discussed.

10:00 AM

(GOMD-SII-016-2011) What have we learned about relaxation in glass forming liquids from light scattering experiments? (Invited)

D. Sidebottom*, Creighton University, USA

Shortly after the development lasers nearly 50 years ago, researchers quickly began using these highly coherent light sources to investigate the dynamics of liquids and in particular those dynamics near the glass transition. In this short review, we examine the quasi-elastic scattering of liquids that makes up the Rayleigh-Brillouin spectrum and how relaxations inherent in the liquid can be inferred by light scattering techniques. We review some of the major findings obtained by dynamic light scattering studies and how they have shaped our current understanding of supercooled liquids near the glass transition.

10:40 AM

(GOMD-SII-017-2011) Silicate glasses under pressure (Invited)

B. Champagnon*, T. Deschamps, C. Martinet, C. Sonneville, D. de Ligny, Université Lyon1, France

Silicate glasses submitted to an increasing pressure show first an elastic deformation and then a plastic deformation characterized by a permanent densification. In situ Raman scattering experiments allow to follow these different stages of deformations and to correlate them with structural changes. The rate of the decrease of the inter-tetrahedral angle or of the intensity of the Boson peak in the elastic domain are discussed in connection with the anomaly of the elastic constants of SiO2 or GeO2.This anomaly vanishes in permanently densified glasses or with a change in their composition. These effects are linked with molecular dynamics simulations and with the intrinsic disorder of glasses.

11:20 AM

(GOMD-SII-019-2011) Kinetic and Thermodynamic Effects of Nanoconfinement on Glass Transition in Glycerol

S. Sen*, University of California at Davis, USA

The dynamics of glass-forming liquids under nano-confinement is key to understanding a variety of phenomena in nature and in modern technology. We will report the results of a variable temperature 13C NMR spectroscopic study of supercooled glycerol that directly demonstrates an abrupt change in the activation energy of molecular dynamics upon confinement of the liquid in ~2 nm pores in mesoporous silica. This result implies a fragile-to-strong transition of glycerol under nanoconfinement. We will also present the results of a high-pressure 13C NMR study of glycerol that strongly indicate nanoconfined glycerol to be denser than the bulk liquid. Such change in the density of the liquid is consistent with the variation in its Tg and may be indicative of a fundamental and possibly universal effect of confinement on the thermodynamic properties of a liquid.

Symposium III: Optical Materials and Devices

Session D: Active Optics

Room: Pulaski

Session Chair: David Scrymgeour, Sandia National Laboratories

9:20 AM

(GOMD-SIII-027-2011) Nonlinear photonic crystals utilizing ferroelectric oxide thin films and their application in tunable photonic circuits (Invited)

P. T. Lin*, MIT, USA; B. W. Wessels, Northwestern University, USA

2-D photonic crystals (PhCs) using epitaxial BaTiO3 thin films are investigated. Enhanced optical nonlinearities were achieved by using the photonic band gaps. The increased nonlinearity potentially enables chip-scale optical devices with a much lower operation voltage. To fabricate PhCs ion beam lithography was used. The photonic stop bands are measured by the transmission spectra from which a strong light localization in the optical cavities is observed. The band structures are determined by the PhCs periodicities and symmetries. The optical response is also simulated using the finite difference time domain (FDTD) calculation. Significant enhancement of the intrinsic optical nonlinearities is demonstrated in the BaTiO3 PhC devices. Three topics to be discussed: (1) Enhanced Pockels effects from E-O measurements (2) Demonstration of thermally tunable photonic circuits from diffraction measurements and (3) Enhanced fluorescence from dye covered PhCs.

10:00 AM

(GOMD-SIII-028-2011) Fs-Laser Micro Machining of Waveguide Amplifiers Inside Er-Yb Doped Zinc Polyphosphate Glass

L. B. Fletcher*, J. J. Witcher, N. Troy, University of California Davis, USA; R. K. Brow, Missouri University of Science and Technology, USA; D. M. Krol, University of California Davis, USA

Permanent modification to the glass structure induced by fs-laser pulses can be used inside a variety of glass substrates to fabricate 3-D photonic devices. Zinc phosphate glasses, are excellent glasses for fabricating compact waveguide lasers that operate in the C-band. Previous research with zinc polyphosphate glasses has demonstrated relationships between the initial composition and the structural changes that result from fs-laser modification. We have found that densification of the glass occurs inside the irradiated area for zinc polyphosphate glass compositions with a [O]/[P] ratio close to 3.25. In this study, waveguide amplifiers have been fabricated using a 1 kHz, 180 fs-laser. Fs-laser writing parameters such as the laser fluence and the beam focusing geometries have been studied and optimized. Near field guiding profiles, insertion losses, internal gain, and photo-induced changes using confocal fluorescence and Raman microscopy were measured after waveguides were written.

10:20 AM

(GOMD-SIII-029-2011) Influence of Silver ions injection and SHG by thermal poling on sodium and niobium borophosphate glasses

E. Fargin*, A. Delestre, A. Fargues, M. Lahaye, ICMCB, France; V. Rodriguez, M. Dussauze, F. Adamietz, ISM, France; L. Canioni, A. Royon, M. Bellec, CPMOH, France

Second Harmonic Generation in polarized vitreous materials could permit the development of new electro-optic devices. The high second order optical nonlinearity ($\chi(2)$=5pm/V) obtained on thermally poled sodium and niobium borophophate glasses offers a good potential for this kind of applications. The goal is to obtain a waveguide for electro optical applications. To achieve this objective a thin silver layer is deposited on the surface of a sodium niobium borophosphate glass. A thermal poling realized on this glass allows silvers ions injection and internal electric field creation. A complete characterization of the effects induces by this technique has been done showing thermal poling and silver injection influences on the glass local composition, structure and optical linear/nonlinear properties. Thermal poling voltage influence is observed and a model of some mechanisms induced during this treatment is proposed.

10:40 AM

(GOMD-SIII-030-2011) Thermally poled oxide glasses: correlation between polarization mechanisms and non linear optical properties

D. Marc*, V. Rodriguez, Univ. Bordeaux 1 - CNRS, France; E. Fargin, T. Cardinal, G. Guimbretiere, CNRS, France; T. Cremoux, Univ. Bordeaux 1 - CNRS, France; T. Shoulders, Clemson university, USA; E. Kamitsos, NHRF, Greece; K. Richardson, Clemson university, USA

Poled glasses are promising materials for a large variety of applications such as for photonics or biomaterials. In order to control their physical and chemical properties, one needs to determine and understand the different processes occurring during thermal polarization treatments. To progress in this direction, we have investigated the structural rearrangements induced by poling on different oxide glasses. To determinate the space charge induced by poling, the Maker fringes technique and second harmonic generation imaging have been employed. Structural changes were studied by micro-Raman and infrared vibrational spectroscopy, and have highlighted strong correlations between space charge, non linear optical response and structural modifications. Careful assignments of the vibrational spectra have permitted to describe the polarization processes. This large base of results is of a great interest to progress towards future applications.

11:00 AM

(GOMD-SIII-031-2011) Structure and Optical Properties of Pulsed Laser Deposited Ge-Sb-Te Thin Films by Raman Scattering Spectroscopy and Spectroscopic Ellipsometry

P. Nemec*, University of Pardubice, Czech Republic; V. Nazabal, A. Moreac, Université de Rennes 1, France; J. Gutwirth, M. Frumar, University of Pardubice, Czech Republic

Among phase-change memory materials, Ge-Sb-Te family is of large interest from the point of view of currently used optical discs technology and future electrical based memories as well. In this work, we characterize by Raman scattering spectroscopy pulsed laser deposited (GeTe)1-x(Sb2Te3)x, (x = 0, 0.33, 0.50, 0.66, and 1) layers in terms of the structure in as-deposited state (amorphous phase) as well as in crystalline state induced by thermal annealing (fcc phase). Observed features in amorphous layers are attributed to Sb-Te bonds vibrations in Sb-Te3 units, edge- and corner-sharing GeTe4-nGen (n = 0, 1, 2) tetrahedra modes. Raman spectra measured on crystallized samples are presented and analyzed as well. Applying Cody-Lorentz approach, spectroscopic ellipsometry revealed optical functions of fabricated layers. The parameters of Cody-Lorentz model are discussed in relation with the chemical composition and state of the layers.

11:20 AM

(GOMD-SIII-032-2011) Crystal coherence length effects on the infrared optical response of MgO thin films (Invited)

J. Ihlefeld*, J. C. Ginn, Sandia National Laboratories, USA; D. J. Shelton, University of Central Florida, USA; V. Matias, Los Alamos National Laboratory, USA; P. G. Kotula, M. A. Rodriguez, Sandia National Laboratories, USA; G. D. Boreman, University of Central Florida, USA; P. G. Clem, M. B. Sinclair, Sandia National Laboratories, USA

The role of crystal coherence length on the infrared (IR) optical response of MgO thin films is investigated. Equiaxed random polycrystalline and (001)-oriented textured MgO thin films were prepared by sputtering and ion-beam assisted deposition on (001)-oriented silicon. Film crystalline quality was modified by ex situ anneals in air and film crystalline coherence was characterized by X-ray diffraction line broadening and transmission electron microscopy. The infrared optical and dielectric response investigated via spectroscopic ellispometry revealed a strong dependence of crystalline coherence on the infrared dielectric response. Optical phonon damping constants derived from the infrared optical response scale directly with the crystalline coherence length suggesting that the defects responsible for crystal coherence length limitations, including dislocations, grain boundaries, and small angle tilt boundaries can strongly affect the phonon-polariton response.

Symposium I: Glass Science

Session B: Glass Structure and Properties II

Room: Cumberland
Session Chair: Randall Youngman, Corning Incorporated

1:20 PM

(GOMD-SI-017-2011) Yb3+ doped SiO2-Al2O3-P2O5 fiber performs: the role of Al and P on clusters dissolution

T. Deschamps*, N. Ollier, T. Charpentier, CEA, France; H. Vezin, CNRS, France; C. Gonnet, Draka, France

Yb3+ doped glasses are used for high-power fiber laser in the 1 μm region. Silica host codoped with Al and P reduces Yb3+ clustering and limits the pump-induced loss mechanism (photodarkening). However, the structure of SiO2-Al2O3-P2O5 and the environment of Yb3+ inserted in such glasses are still under debate. Yb3+ doped fiber preforms with different Al and P contents have been analysed by MAS-NMR, pulse EPR and photoluminescence. We show that the local environment of Yb3+ depends on the Al/P ratio. The HYSCORE reveals the existence of interactions between Yb3+ and the 27Al, 31P and 29Si nuclei which change with the Al/P ratio, and the presence of a strong Si-Yb interaction has been clearly connected with a more intense cooperative luminescence signal evidenced the presence of Yb clusters. The best composition which allows the dissolution of Yb3+ ions has been highlighted. Structural changes induced by irradiation and the role of Al and P to prevent photodarkening will be also discussed.

1:40 PM

(GOMD-SI-018-2011) High-temperature ^{11}B Magic Angle Spinning Nuclear Magnetic Resonance Spectroscopy Study of Network Dynamics in Borosilicate and Borate Glass-forming Liquids

J. Wu*, N. Kim, J. F. Stebbins, Stanford University, USA

High-temperature (up to 660°C) ^{11}B MAS NMR line-shape measurements were made on sodium borate ($(Na_2O)_{0.3}(B_2O_3)_{0.7}$) and sodium aluminoborosilicate ($(Na_2O)_{0.2}(B_2O_3)_{0.21}(Al_2O_3)_{0.08}(SiO_2)_{0.51}$) glasses. Temperature calibration, which can be a challenging problem in such experiments, was done by observing phase transitions in CuI, CuBr and $NaNbO_3$ with ^{63}Cu MAS NMR and ^{23}Na MAS NMR. ^{11}B MAS NMR peaks corresponding to $^{[3]}$B and $^{[4]}$B groups are well-resolved in the spectra of glasses at 14.1 T with spinning speed of 5 kHz. Spectra collected in situ at high temperature remained largely unchanged until well above the glass transition temperature. At higher temperature partial peak collapse occurred due to exchange of boron between the two sites. We modeled this exchange using recently measured T effects on boron speciation. The inverse rates of exchange are close to the shear relaxation times calculated from the bulk viscosities.

2:00 PM

(GOMD-SI-019-2011) Diffusion of Sodium in Sodium Boroaluminosilicate Glasses: Impact of Mixed Network Formers and the Influence of Water

X. Wu*, Cornell University, USA; Q. Zheng, J. Mauro, M. Potuzak, A. J. Ellison, Corning Incorporated, USA; R. Dieckmann, Cornell University, USA

To investigate how the diffusion of sodium in sodium boroaluminosilicate glasses is influenced by the network former composition, sodium tracer diffusion measurements using the radioactive isotope sodium-22 have been performed. Two series of glasses were considered, $[(Na_2O)_{0.71}(B_2O_3)_{0.24}(Fe_2O_3)_{0.05}]_{0.2}[(SiO_2)_x(Al_2O_3)_{1-x}]_{0.8}$ and $[(Na_2O)_{0.73}(B_2O_3)_{0.24}(As_2O_3)_{0.03}]_{0.18}[(SiO_2)_x(Al_2O_3)_{1-x}]_{0.82}$ with x varying from 0.8 to 1. Sodium tracer diffusion experiments were performed by diffusion annealing in dry and wet air at atmospheric pressure at different temperatures between 200 and 300 °C. Experimental results will be presented and discussed.

2:20 PM

(GOMD-SI-020-2011) Sodium Environments in Binary and Ternary Oxide Glasses

R. Youngman*, C. Hogue, J. Dickinson, A. Ellison, B. Aitken, Corning Incorporated, USA

Alkali and other glass modifiers have pronounced impact on glass structure and related physical properties. Many of these effects are commonly studied from the vantage point of changes in the coordination environment of the glass-forming cations (e.g. B, Al, Si), as well as resulting changes to Tg, viscosity and other important glass properties. Another approach to understanding these phenomena is to directly study the modifier cation. In particular, Na and Li are well suited for solid state NMR experiments. We have made extensive use of 23Na NMR to study this modifier in a wide variety of simple binary and ternary oxide glasses, including silicates and tellurites. We observe distinct differences depending on the glass composition and charge-balancing role of Na.

2:40 PM

(GOMD-SI-021-2011) Comparison of the Structure and Properties of Normal, Abnormal and Intermediate Glasses

Q. Zhao, L. Huang*, Rensselaer Polytechnic Institute, USA

Normal glasses such as the most common soda-lime (window) glass, have a negative temperature derivative and a positive pressure derivative of elastic moduli, while abnormal glasses like silica and silica-rich glass behave in the opposite way. It would be natural to imagine that there are intermediate glasses with elastic moduli independent of temperature and/or pressure. We demonstrate that such intermediate glasses can be obtained by pressure-quenching or by chemical modifications. We compare the structure and properties of normal, abnormal and intermediate glasses by using Raman and Brillouin light scattering techniques. The deformation and fracture of these three types of glasses are studied in micro-indentation and nano-indentation experiments, by using SEM and AFM to examine the indent cross-section, densification and pile-up.

3:20 PM

(GOMD-SI-022-2011) Structure and bonding in oxide liquids and glasses using in-situ x-ray and neutron diffraction

R. Weber*, MDI, USA; C. J. Benmore, Argonne National Laboratory, USA; J. Neuefeind, L. Santodonato, Oak Ridge National Laboratory, USA; L. Skinner, Stony Brook University, USA; M. Wilding, Aberystwyth University, United Kingdom; S. Tumber, MDI, USA; L. Lazareva, J. B. Parise, Stony Brook University, USA

The application of: x-rays or neutrons, a containerless sample environment, and fast detection enables in-situ studies of structural evolution in metastable liquids as they are cooled towards the glass transition. The complementary use of x-rays and neutrons (with isotopic substitution) enables measurement of local and intermediate range structure. Previous revealed substantial temperature-dependent changes in coordination and bonding in Al2O3-SiO2, CaO-SiO2, and MgO-SiO2 liquids. Oxide liquids were studied using high energy x-rays at the APS and neutrons at the SNS. Measurements were made at temperatures from 500-2500 °C and under highly non-equilibrium conditions. The structural measurements are compared to predictions from mode coupling theory near Tg. The experiments will be briefly described and the results presented and discussed in the broader context of the glass forming behavior of high melting point, relatively fragile oxide liquids.

3:40 PM

(GOMD-SI-023-2011) First experiments at Nanoscale Ordered Materials Diffractometer (NOMAD) at the Spallation Neutron Source (SNS)

J. Neuefeind*, ORNL, USA

In August 2010 the beam shutter opened for the first time for the NOMAD diffractometer. NOMAD is in many respects similar to GLAD diffractometer well known to the glass community that was located at the IPNS. It is an instrument designed to determine by Fourier transform of a structure function pair distribution functions. NOMAD is a relatively short instrument with 19.5 m distance between the moderator and the sample and a direct view of the moderator. With the detector coverage installed at the moment - which represents about half of the designed detector coverage capability - about 2 10^6 neutrons per second are detected form a strongly scattering sample. Count rates that high clearly open up opportunities for parametric studies and/ or small sample sizes. An early experiment includes scattering from a laser heated aerodynamically levitated silicate melts. A report of the status of the instruments and the results of early experiments will be given.

4:00 PM

(GOMD-SI-024-2011) X-ray absorption spectroscopy analysis of formation and structure of Au nanoparticles in sodium trisilicate glass

C. Saiyasombat*, M. Wojciechowski, H. Jain, Lehigh University, USA

Development of color in ruby glass through the precipitation of gold nano-particles is a well known phenomenon. We have investigated its atomistic mechanism by X-ray absorption near edge structure (XANES) analysis at the Au L_3-edge and Sn K-edge in sodium trisilicate glass doped with 0.1mol% $HAuCl_4$; 0.04mol% SnO_2 was added to facilitate the reduction of Au ions. The samples were prepared by conventional melt-quench technique followed by thermal treatment. Development of ruby color was followed with optical spectroscopy, which showed red-shift of gold peak with heat treatment, while XANES indicated transformation of ionic gold to metallic gold. However, the tin remained as Sn^{4+} ions even after heat treatment, indicating that tin was reduced during glass solidification, and gold diffusion is the rate limiting step.

4:20 PM

(GOMD-SI-025-2011) Hydrogen formation observed during high pressure treatment of silica glass

C. Li*, J. Price, M. Tomozawa, E. Watson, Rensselaer Polytechnic Institute, USA

During treatment of silica glass at high pressures and temperatures (1~3 GPa, 1100-1250°C) in a solid-media pressure apparatus, hydroxyl and hydride were observed to form in the silica. The FTIR absorbance signals appeared only when the glass sample was pressurized in the presence of water together with graphite at high temperature, and the hydroxyl signal disappeared completely when the glass was heat-treated at 1000°C in air for one hour. These results indicate that hydrogen diffused into and reacted with the silica glass during the high pressure-temperature treatment. Reduction of H2O by graphite at high pressure/temperature conditions is the probable source of hydrogen.

4:40 PM

(GOMD-SI-026-2011) Generalized thermodynamic approach for determining the fictive temperature of glasses with arbitrary thermal history

X. Guo*, M. Potuzak, J. Mauro, D. Allan, T. Kiczenski, Corning Inc., USA; Y. Yue, Aalborg University, Denmark; R. Stewart, Corning Inc., USA

We propose a generalized approach to calculate fictive temperature as determined by the thermodynamic state of a glass. The technique is validated both experimentally and numerically using a novel approach for modeling of glass relaxation behavior. We demonstrate that a glassy fictive temperature can be determined at any calorimetric scan rate in excellent agreement with modeled values. The technique is universally applicable to glasses of any thermal history, as proved through a series of numerical simulations where the fictive temperature is precisely known within the model.

5:00 PM

(GOMD-SI-027-2011) Network Modeling of Glass Structures

P. Kroll*, M. Mwania, UT Arlington, USA

We developed a network algorithm to model chemically ordered amorphous structures. The approach is based on the classical WWW algorithm and extended to handle different kinds of vertices (chemical identity) and different kind of connectivity (valences). Our field of study comprises Si based glasses and amorphous ceramics, including silica, amorphous SiCO and the quaternary SiBCN. Targeting models that can subsequently be computed using density functional methods, we illustrate the approach and indicate its advantage over standard melt-quench methods. We will highlight recent applications, including segregation of nanoclusters, percolation in ternary glasses, and the inclusion of octahedral vertices in metal oxide glasses.

Session C: Glass Corrosion II

Room: Sapelo
Session Chair: Stephane Gin, CEA

1:00 PM

(GOMD-SI-035-2011) Characteristics of alteration layers formed on simulated HLW glass under silica-saturated solutions

T. Maeda*, Japan Atomic Energy Agency, Japan; K. Hotta, Radiation Application Development Association, Japan

Static corrosion tests were conducted for P0798 type simulated high-level radioactive waste glass in amorphous silica saturated solutions at a

wide range of pH in order to investigate the rate limiting step under near-saturation condition. The depth profiles of elements at the surface of corroded glass were observed by use of SIMS. In each pH condition, alteration layer formed at the glass surface, where soluble elements such as B and Na depleted, while Si and Al remained to an equal degree of that in pristine glass. The thickness of the layer grew with time during the test, and increased with decrease in solution pH. It is consistent with a hypothesis that ion exchange by H+ or H3O+ ions controls the rate under near-saturated condition. (*This study is regulatory support research funded by the Nuclear and Industrial Safety Agency, Ministry of Economy, Trade and Industry, Japan.)

1:20 PM

(GOMD-SI-036-2011) Glass Corrosion in Solution Exchange Tests

W. Ebert*, Argonne National Laboratory, USA

Solution exchange tests are commonly used to quantify the diffusive release rates of contaminants from porous materials, but are only rarely used to study glass corrosion. Coupled with the results of static and continuous flow methods, solution exchange methods can provide insights that are useful for distinguishing the effects of chemical affinity and mass transport processes on glass corrosion. Different test methods can (and should) be used to highlight different aspects of glass dissolution behavior to provide insights into what process controls the dissolution rate under different conditions. New data will be presented to demonstrate the use of solution exchange methods to characterize the dissolution behaviors of two borosilicate glasses being studied as surrogate waste forms for fuel reprocessing wastes. These data and literature data will be used to discuss the effects of testing variables on the test results, interpretation with regard to the controlling process, and limitations for using the solution exchange method.

1:40 PM

(GOMD-SI-037-2011) Water dynamics in nuclear waste glass during corrosion: A quasi-elastic neutron scattering study

K. J. Alvine*, J. V. Ryan, Pacific Northwest National Lab, USA; M. Tyagi, NIST, USA

The long-term corrosion of nuclear waste glass when exposed to ground water is an open area of scientific interest. The motion of water into these glasses and their alteration phases is a critical question for the mechanisms of ion exchange, hydrolysis, and reactive transport. We present here quasi-elastic neutron scattering (QENS) studies measuring the water dynamics in waste glasses modeled after the SON68 French simulant glass. The glass composition and isotopic makeup were engineered to maximize neutron transparency for all components except hydrogen. High-water content glasses were synthesized by melting at 200GPa. Additional samples were subjected to both static and vapor hydration corrosion conditions to introduce water into the alteration phase structures. The observed internal water dynamics was found to vary depending on the glass conditions.

2:00 PM

(GOMD-SI-038-2011) Isotopic tracing to highlight glass dissolution mechanisms

A. Verney-Carron*, LISA, France; S. Gin, CEA, France; G. Libourel, CRPG, France; P. Jollivet, CEA, France

Isotopic (29Si and 18O) tracing during nuclear glass alteration experiments have demonstrated that the gel is formed by hydrolysis/condensation reactions. This mechanism favors a structural and textural reorganization of the gel which acts as a diffusion barrier. However, the diffusion coefficients of alkalis into solution measured for Roman archaeological glass are much higher than for nuclear glass (3 to 4 orders of magnitude). This can be explained by the composition and the polymerization degree. Especially, alkalis in sodo-calco-silicate glass depolymerize the glass network, whereas they play a role of charge compensator in boro-silicate glass. The aim of this study is here to compare the isotopic (29Si and 18O) signatures of the gel formed on archaeological glass in order to determine the influence of the glass composition and structure on the protective role of the gel.

2:20 PM

(GOMD-SI-039-2011) Comparison of Glass Leaching Behavior Using a Variety of Test Methods (Invited)

I. S. Muller*, A. Papathanassiu, A. Barkatt, I. L. Pegg, The Catholic University of America, USA

A wide variety of test methods have been developed to assess the leaching behavior of glasses for the immobilization of nuclear wastes. Many of these methods, specified in regulatory requirements, simply provide standard protocols for comparison between glasses on a common basis. Others seek to accelerate various aspects of the corrosion mechanism in view of the very long time scales that are ultimately of interest with respect to the performance of the waste form in the disposal facility. Yet other methods are designed to probe specific aspects of the overall glass corrosion mechanism with a view to determining values of key parameters in the various rate equations that have been proposed. In this paper we will review many of these methods, focusing on results obtained from their application to high-sodium glasses developed for the immobilization of low-activity wastes (LAW) from the Hanford site, over a wide range of glass compositions, a variety of test methods, and durations extending over ten years.

3:20 PM

(GOMD-SI-040-2011) Reprise of Alteration of the Simulated HLW Glass at High Temperature in Beishan Underground Water (Invited)

Z. Zhang*, China Institute of Atomic Energy, China

Immersed at 150 degree centigrade in Beishan brine underground water with glass-surface-area-to-solution- volume ratio of 6000 m-1, the glass re-alterated rapidly with the sharp release of B, Na, Li, Cs and Mo from the cold HLW glass after a stable period of 180 days. The cold HLW was degraded up to 65.4% for the immersion period of 730days resulting in the release of Mo, Cs and Nd up to 65.4%, 2.7% and 0.7% from the glass respectively. Deferent from the behavior at 150 degree centigrade, the glass was very stable at 90 degree centigrade with limited leaching of Na, B, and Li. With the reprise of alteration underway, new minerals were formed from the quartz, saponite, oknite, dickite, dolomite, tynite, amphibole, nontronite, zeolite to borax.

3:40 PM

(GOMD-SI-041-2011) The dissolution behavior of simple borate glasses in aqueous environments

K. Goetschius*, R. K. Brow, Missouri S&T, USA

The dissolution behavior in aqueous environments of glasses from the system R2O-CaO-B2O3 (R=Li, Na, K) was studied to examine the effects of borate coordination number and modifying ion field strength. Samples were corroded in DI water and a 0.25 M phosphate solution using a single pass flow through test to reduce the effects of changes in solution chemistry on the reaction kinetics. X-ray diffraction and vibrational spectroscopies were used to characterize the formation of surface corrosion products, and ICP-OES was used to determine the concentration of the components in solution as a function of time. In general, the glasses dissolve congruently in deionized water and the corrosion rates decrease as the fraction of tetrahedral borons increase.

4:00 PM

(GOMD-SI-042-2011) A long-term glass leaching experiment in a granitic environment: importance of reactive-transport processes

S. Gin*, C. Guittonneau, J. Mestre, N. Godon, CEA Marcoule, France

We have investigated a 26 years old glass leaching experiment conducted in an open granitic environment in order to improve our understanding of the mechanisms controlling glass dissolution under geological disposal conditions. Despite a constant and low mean dissolution rate, about 1000 times lower than the initial dissolution rate, we show that the alteration layer has neither an uniform thickness, nor a homogeneous morphology. This unexpected behaviour is likely due to local heterogeneities of the solution chemistry. Such conclusions are supported by the observation of the behaviour of Mg. This element precipitates with Si into clay minerals, weakening the passivating properties of the

gel and leading to local rate increases. These investigations highlight the importance of such an experiment to assess the respective role of the solution composition and of the water renewal rate on the glass dissolution kinetics.

4:20 PM

(GOMD-SI-043-2011) Glass corrosion in cement waters

S. Depierre*, F. Angeli, F. Frizon, S. Gin, CEA Marcoule, France

In the French geological repository concept, intermediate-level vitrified wastes would be stored in cement medium. In the present work, the glass corrosion mechanisms and kinetics, expected to strongly depend on chemical composition and alkaline pH of the leaching water, are studied in different cement waters corresponding to different stages of the cement aging. In order to investigate theses effects, static experiments were conducted in water at pHs between 12 and 13.5 and in cement waters at short term and in cement waters at long term. Firstly, we observed that cement waters diminished by a factor around 5 the initial dissolution rate of the glass compared to the reference media in KOH. This effect, not yet clearly understood, could be due to the presence of calcium in cement waters that would limit the Si-O bonds hydrolysis. Secondly, the rate drop was also increased by the calcium brought by the solution. These effects are related to the passivating properties of the alteration layer.

4:40 PM

(GOMD-SI-044-2011) Nuclear waste glass alteration at high pH

K. Ferrand, K. Lemmens, M. Aertsens*, Belgian Nuclear Research Centre, Belgium

In the Belgian Supercontainer design for the geological disposal of vitrified nuclear waste, the waste glass will be surrounded by a carbon steel overpack and an Ordinary Portland Cement buffer. The glass will thus be in contact with pore water of initial pH 13.5. To determine the alteration rate of the reference nuclear waste glasses SON68, SM539 and SM513 in such an environment, and to identify the key mechanisms responsible for the glass alteration in Supercontainer conditions, tests were performed in KOH solutions, and in synthetic cement waters simulating the pore water expected in young, evolved and old concrete. Tests were done with and without hardened cement powder. The results show an acceleration of the glass alteration rate compared to neutral pH conditions. They are interpreted and discussed following a general glass alteration model. The preliminary conclusion is that a low long term glass alteration rate will be reached only if diffusion limitations impose a pH at the glass surface that is much lower than 13.5.

5:00 PM

(GOMD-SI-045-2011) Corrosion of Phosphate-doped Alkali Borosilicate Glasses in Alkaline Solutions

X. Cheng*, R. K. Brow, G. Chen, Missouri University of Science and Technology, USA

Enamel coatings have been applied to provide corrosion protection and enhanced bond strengths for steel reinforcement (rebar) in concrete structures. Understanding how changes in glass composition affect corrosion behavior under alkaline conditions is necessary to optimize the enamels. In this study, Na-borosilicate glasses, modified with up to 7 mole% P2O5, were prepared and their corrosion behavior in an alkaline solution that simulates cement pore water chemistry was determined. Corrosion behavior was studied by weight loss measurements and solution analyses, and surface corrosion products were characterized by x-ray diffraction and micro-Raman spectroscopy. The initial addition of 3mole% P2O5 to a base glass of 25Na2O-25B2O3-50SiO2 (mole%) reduces the corrosion rate by nearly an order of magnitude, whereas subsequent additions of P2O5 up to 7 mole% increase corrosion rates.

Symposium II: The Amorphous State

Session B: Model/Experiment: Links and Limits

Room: Ossabaw
Session Chair: David Drabold, Ohio University

1:00 PM

(GOMD-SII-020-2011) Electric and Magnetic Fields Applied to Materials: Computed Response by First Principles (Invited)

J. Zwanziger*, Dalhousie University, Canada

Density functional theory is an effective and efficient way to compute the electronic structure of materials. When implemented in the projector-augmented wave formalism and a planewave basis, accuracy rivals all-electron methods for much smaller calculations. Here I will discuss recent progress in implementing electric and magnetic field response within this formalism, including first principles calculations of dielectric response, photoelasticity, and magnetic susceptibility.

1:40 PM

(GOMD-SII-021-2011) XAFS Study of Electrodeposited Ge-Sb-Te Phase-change Memory Materials

B. Prasai, D. A. Drabold, G. Chen*, Ohio University, USA

Phase-change memory materials (PCMM) are based on binary or ternary chalcogenides that exhibit rapid crystallization under electrical or optical pulse excitation. Among various methods of synthesizing PCMM, sputtering is employed dominantly for device applications. However, its poor performance in void filling has become a critical issue in downsizing the memory devices. In this paper, we report K-edge x-ray absorption fine structure study of electrodeposited binary (Sb-Te) and ternary (Ge-Sb-Te) PCMM, which exhibit excellent void-filling capability. The purpose is to understand the structural response of the amorphous network to the composition change. Extended x-ray absorption fine structure analysis of the PCMM reveals a composition dependency of the local structure of the PCMM, and x-ray absorption near-edge structure analysis indicates a variation of the electronic structure as a function of the composition. Our study sheds light on the atomic and electronic structures of electrodeposited PCMM.

2:00 PM

(GOMD-SII-022-2011) Resolving the vibrational and configurational contributions to thermal expansion in isobaric glass-forming systems

M. Potuzak*, J. C. Mauro, T. J. Kiczenski, A. J. Ellison, D. C. Allan, Corning Incorporated, USA

A fundamental understanding of isobaric thermal expansion behavior is critical in all areas of glass science and technology. Current models of glass transition and relaxation behavior implicitly assume that the thermal expansion coefficient of glass-forming systems can be expressed as a sum of vibrational and configurational contributions. However, this assumption is made without rigorous theoretical or experimental justification. Here we present a detailed statistical mechanical analysis resolving the vibrational and configurational contributions to isobaric thermal expansion and show experimental proof of the separability of thermal expansion into vibrational and configurational components for Corning Jade® glass.

2:20 PM

(GOMD-SII-023-2011) Thermal conductivity of amorphous ceramics from first principle calculations

B. Kouchmeshky, P. Kroll*, UT Arlington, USA

We calculate thermal conductivity of amorphous materials from ab-initio molecular dynamics simulations. Our approach – an implementation of the Boltzmann-Transport-Equation-phonon-thermal-conductivity-model (BTE for phonons) – is intended to replace its counterparts that use empirical potentials in cases in which a suitable phenomenological force field is unknown or incapable to describe correctly the

amorphous state. In this study, we focus on amorphous structures of silicon dioxide (SiO2), silicon carbide (SiC) and silicon nitride (Si3N4)-based ceramics. We compare results obtained by first principles calculations with those received using classical empirical potentials. Overall, our results are very close to experimental data. We observe an intriguing breakdown of thermal conductivity in amorphous ceramics at high temperatures still below the melting point.

2:40 PM

(GOMD-SII-024-2011) Electronic consequences of B and P in a-Si:H: an ab initio simulation

D. Drabold*, B. Cai, Ohio U, USA

It is known that a-Si:H may be doped either n- or p-type, a fact which is the basis of many of the technological applications of the material. The doping efficiency is extremely low, however, and the reason for this is not altogether clear. With this in mind, we add boron and phosphorous to appropriate computer models of hydrogenated amorphous silicon in an attempt to develop an atomistic understanding of n and p doping in these materials. We include relaxation effects and to the maximum degree possible, explore the range of configurations accessible to the impurities. Previous work[1] has revealed that B in a-Si introduces holes that are trapped in strained parts of the a-Si network. In this talk, we extend this analysis to hydrogenated material and for the first time, undertake simulations of P. [1] I. Santos, P. Castrillo, W. Windl, D. A. Drabold, L. Pelaz and L. A. Marques, Self Trapping in B-doped a-Si: an intrinsic origin of low acceptor efficiency, Phys. Rev. B 81 033203 (2010)

3:20 PM

(GOMD-SII-025-2011) Computing Transport coefficients for amorphous semiconductors using the Microscopic Response Method (Invited)

M. Zhang*, D. A. Drabold, Ohio University, USA

Both localized states and extended states contribute to the conductivity or Hall mobility of amorphous semiconductors. Experiments and simulations show that the e-ph interaction for localized states is much stronger than that of extended states, and a localized carrier induces static displacements of its neighboring atoms: when a carrier enters or leaves a localized state, the nearby atoms adjust their vibrational configurations. We therefore have to adopt different Hamiltonian partitions for localized and extended states and a consequence is that the temperature dependence of transport coefficients in amorphous semiconductors contains a reorganization energy. We suggested a diagrammatic expansion for the transport coefficients based on a microscopic response method. This work is supported by Army Research Office under MURI W91NF-06-2-0026. M.-L. Zhang and D. A. Drabold, Phys. Rev. Lett. 105, 186602 (2010); Eur. Phys. J. B. 77, 7-23, (2010); arXiv: 1008.1067.

4:00 PM

(GOMD-SII-026-2011) Bond Percolation in C- and N-Doped Silica Glass

P. Kroll*, UT Arlington, USA

Adding carbon or nitrogen into the structure of silica glass, thus forming solid solutions of SiC and Si3N4 with silica, is studied using continuous random network models. On increasing the dopant concentration the average network connectivity <r> increases as well. Eventually, Si-C or Si-N bonds form a three-dimensional substructure within the glass phases of a-SiCO and a-SiNO, respectively. We locate this threshold concentration at <r>≈2.9 in both cases. Additional density functional calculations are then used to calculate properties. Associated with the bond percolation threshold is a counterintuitive softening of the network structure. In both materials systems, the bulk modulus exhibits a discontinuity – the structure gets more compliant upon adding the stiffening dopant – right at the bond percolation threshold.

4:20 PM

(GOMD-SII-027-2011) Ab-initio simulation of solid electrolyte glasses

B. K. Prasai*, D. A. Drabold, G. Chen, Ohio University, USA

Chalcogenide glass is of great importance not least of all because it becomes a solid electrolyte when doped with metals like silver, offering very high ionic conductivities. Such electrolytes are getting attention for their technological importance with application in 'Conductive bridge' (flash) memory devices. We use plane-wave density functional methods to model Germanium-Selenide glasses doped with various concentrations of silver and copper. We also carry out thermal simulation at different temperatures on these glasses and analyze the ion trajectories. The optical gap increases with increasing Ag content and decreases with increasing Cu content. Our study shows that the most diffusive ions sample the widest variation in local density. The study of trap centers for Ag rich and Cu rich glasses shows that because of the higher coordination number of Cu, it is more rigidly trapped compared to Ag with its lower coordination number.

4:40 PM

(GOMD-SII-018-2011) Characterization of Shear Stress Relaxation of Glass Using a Parallel Plate Viscometer

V. Y. Blouin*, G. Vallet, H. Kadali, J. Musgraves, K. Richardson, P. Joseph, Clemson University, USA

Numerical modeling of precision glass molding requires material properties of glass at molding temperature. Among these properties, stress relaxation parameters corresponding to the shear behavior must be determined experimentally using a creep recovery test. This paper presents the experimental procedure and numerical treatment of the experimental data for extracting the stress relaxation properties in shear using a parallel plate viscometer. Helical spring glass samples that exhibit pure shear deformation when subjected to compression are used at different temperatures and under various loading schedules. The simplicity of the parallel plate viscometer provides high accuracy in terms of temperature control and displacement measurement. Manufacturing helical spring glass samples, however, brings practical challenges especially when dealing with special optical glasses. Post-processing of the experimental data based on a Prony series formulation is presented and discussed.

5:00 PM

(GOMD-SII-029-2011) Statistical mechanics of glass-forming systems

R. J. Loucks*, Alfred University, USA; J. C. Mauro, Corning Incorporated, USA; S. Sen, University of California-Davis, USA

A common assumption in the glass science community is that the entropy of a glass can be calculated by integration of measured heat capacity curves through the glass transition. Such integration assumes that glass is an equilibrium material and that the glass transition is a reversible process. However, as a nonequilibrium and nonergodic material, the equations from equilibrium thermodynamics are not directly applicable to the glassy state. We show that it is not possible, in general, to calculate the entropy of a glass from heat capacity curves alone, since additional information must be known related to the details of microscopic fluctuations. Our analysis demonstrates that a time-average formalism is essential to account correctly for the experimentally observed dependence of thermodynamic properties on observation time, e.g., in specific heat spectroscopy. This result serves as experimental and theoretical proof for the nonexistence of residual glass entropy at absolute zero temperature.

5:20 PM

(GOMD-SII-030-2011) Universality of the High Temperature Viscosity Limit of Glass-Forming Liquids

Q. Zheng*, Aalborg University, Denmark; J. C. Mauro, A. J. Ellison, M. Potuzak, Corning Incorporated, USA; Y. Yue, Aalborg University, Denmark

We fit viscosity measurements for over one thousand glass-forming liquids to three viscosity models: VFT, AM and MYEGA. Based on these re-

sults, we conclude that the universal viscosity limit of glass-forming liquids at high temperature is 10-2.93 Pa. s, independent of composition. The glass-forming liquids include silicate, borate, metallic, molecular, and ionic liquids, which proves the universality of this value. With knowledge of this universal high temperature viscosity value, the fitting process is simplified since there are only two free parameters in any viscosity model. This value makes physical sense since it is determined by the liquid quasilattice vibration time ($\tau_\infty \approx 10\text{-}14$ s), which is the time between successive assaults on the rearrangement energy barrier.

Symposium III: Optical Materials and Devices

Session A: Optical Absorption

Room: Pulaski
Session Chair: Mark Davis, SCHOTT North America, Inc.

1:00 PM

(GOMD-SIII-001-2011) Suppression of stimulated Brillouin scattering through multi-tone phase modulation

J. Mauro*, S. Raghavan, A. Ruffin, Corning Incoporated, USA

High signal launch powers are often necessary in fiber optic networks to meet signal-to-noise ratio and receiver sensitivity requirements. One of the drawbacks of high launch powers is stimulated Brillouin scattering (SBS). Two standard methods have been proposed to suppress SBS through transmitter design: (i) dithering of the optical frequency of the laser and (ii) imparting a sinusoidal phase modulation to the optical carrier. Essentially both these methods involve broadening the optical spectrum, thereby increasing the SBS threshold power. Whereas these methods have focused on phase modulation using a single sinusoidal drive, here we focus our attention on multi-tone phase modulation and show that the phase relationship among the various tones can impact the resulting SBS threshold by several dB. Incorporation of a phase locking mechanism can provide significant advantage for high-power optical applications.

1:20 PM

(GOMD-SIII-002-2011) Absorption loss management in telluride glass fibers

P. Lucas*, Z. Yang, University of Arizona, USA; S. Jiang, T. Luo, Advalue Photonics, USA

Chalcogenide glasses have great technological importance for applications in the infrared domain. Heavy component elements result in low phonon energy and confer very wide infrared transparencies to these glasses. Among chalcogenides, tellurides glasses exhibit particularly large transmission down to more than 20 microns. However this gain is associated with a decrease in band-gap which result in significant charge carrier absorption. This presentation will report on the design, synthesis and testing of telluride glass fibers with low-losses as well as their intrinsic limitations and temperature dependence.

1:40 PM

(GOMD-SIII-003-2011) Glass-Clad Semiconductor Core Optical Fibers

S. Morris*, J. Ballato, T. Hawkins, P. Foy, C. McMillen, R. Stolen, Clemson University, USA; R. Rice, Northrop Grumman Space Technology, USA

Silicon photonics has become an emerging field over the past few years due to the potential advantages it may provide in optoelectronics and optical sensing applications. Extending silicon photonics from a planar waveguide platform to an optical fiber-based technology would be a significant progression in this emerging field. This talk will discuss a new class of optical fibers: highly crystalline silicon and germanium core optical fibers fabricated using fiber draw techniques. Selection of the appropriate cladding glass composition has been shown to be significant in reducing oxygen diffusion to the core as well as minimizing thermal expansion mismatch between the core and cladding materials. Long lengths of both silicon and germanium core fibers have been fabricated, possessing an approximately 15 micrometer core within a 150 micrometer diameter glass cladding. The core material has been shown to be phase-pure, highly crystalline, and with a nominal amount of oxygen diffused into the core from the cladding.

2:00 PM

(GOMD-SIII-004-2011) Polarized absorption characterization of spheroid-shaped nanoparticles embedded in a mesostructured silica film

D. Vouagner, Université Lyon1, France; L. Bois, UCB LYON I, France; E. Nardou, S. Sirotkin, B. Champagnon*, Université Lyon1, France; F. Chassagneux, UCB LYON I, France

Polarized absorption is used to study the orientation of spheroid-shaped silver nanoparticles (NPs) embedded in mesostructured silica sol gel films. In fact, it is a well-adapted method to characterize elongated NPs in amorphous matrix [1]. Polarization-dependent absorption spectra clearly evidence a common orientation of spheroid-shaped NPs in the silica film. More, their mean aspect ratio can be estimated from polar plots obtained by plotting the maximum value of the plasmon band absorption versus the polarization angle of the polarizer. Comparison is made with the analysis of mesostructured silica sol gel films containing nanospheres. Moreover, low-frequency Raman scattering is employed as a complementary technique to estimate the mean diameter of spherical NPs as well as the size of spheroid-shaped NPs. [1] Y;P. Zhao, S.B. Chaney, S. Shanmukh, R. A. Dluhy, J. Phys. Chem. B, 110 (2006) 3153-3157

2:20 PM

(GOMD-SIII-005-2011) Studying Loss Mechanisms in Chalcogenide Glass Planar Structures

V. Singh*, Massachussetts Institute of Technology, USA; J. Hu, University of Delaware, USA; J. Musgraves, N. Carlie, Clemson University, USA; A. Agarwal, Massachussetts Institute of Technology, USA; K. Richardson, Clemson University, USA; L. C. Kimerling, Massachussetts Institute of Technology, USA

Chalcogenide glasses are an attractive option for infrared photonic devices due to their wide optical transparency window and studying optical losses in these materials is critical to device applications. While loss mechanisms in chalcogenide fibers have been studied in detail, such information is lacking for planar, thin-film devices. To address this deficit, we have conducted studies on As2S3 and Ge23Sb7S70 glasses and found that the main contributions come from impurity absorption losses due to vibrational bonds of oxygen, carbon, and hydrogen and from scattering losses due to sidewall roughness. We have attempted to quantitatively separate these two loss contributions using microdisk resonators pulley-coupled to bus waveguides at 1550 nm wavelength. Through these investigations, we found that scattering loss dominates impurity absorption in our chalcogenide materials. We also quantitatively studied the impact of thin-film processing on impurity incorporation in glasses using secondary ion mass spectroscopy.

3:00 PM

(GOMD-SIII-006-2011) Temperature dependent absorption and Urbach tail scaling in LuAG single crystals

M. Letz*, Schott AG, Germany; A. Gottwald, M. Richter, Physikalisch-Technische Bundesanstalt (PTB), Germany; V. Liberman, Massachusetts Institute of Technology, USA; L. Parthier, Schott Lithotec AG, Germany

Lutetium aluminum garnet (LuAG) is one of the most promising candidates for a high-index lens material for use in micro-lithographic 193.39nm optics. In the deep ultraviolet (DUV) spectral range the transmission of high purity LuAG was measured using monochromatized synchrotron radiation. In the vicinity of the band gap below 7.8 eV, a scaling behavior of the absorption as a function of photon energy was observed. Temperature dependent measurements allow us to distinguish different absorption mechanisms which differ by their ability to couple to phonon excitations. Interpreting the Urbach tails measured at different temperatures, we show that the temperature independent tail is due to defects in the lattice, whereas the temperature dependent part originates from the short term localization of exciton modes coupling to

lattice distortions. These results allow us to extrapolate the maximum transmittance which can be obtained with LuAG crystals at the lithographic wavelength of 193.39 nm.

3:20 PM

(GOMD-SIII-007-2011) Absorption in photo-thermo-refractive glass: metrology, contributions and mitigation

J. Lumeau*, K. Chamma, L. Glebova, L. Glebov, University of Central Florida, USA

PTR glass is a photosensitive silicate glass which provides refractive index change after UV-exposure and thermal development. This glass is used for volume Bragg gratings (VBGs) recording and these elements find many applications in high power laser systems. In this paper, we present the methods that were developed (calorimetry and spectroscopy) in order to reveal the origin of the absorption in pristine PTR glass and in VBGs produced by UV exposure followed by thermal treatment. We show that absorption of silver containing particles is the main source of absorption in volume Bragg gratings while absorption in pristine glass is limited by the level of contamination of the glass melt. Finally, we show that absorption of volume Bragg gratings can be decreased to level close to 10^{-4} cm^{-1} at 1 μm by mitigating the silver containing particles through optical dissipation of these particles. We show that this process is based on a thermal process.

3:40 PM

(GOMD-SIII-008-2011) Optical Properties of Vanadyl doped [VO2+(VS)and VO2+(VS)] Lead Phosphate Glass System

C. Dayanand*, Tirumala Engineering College, India

The detailed investigations of Lead Phosphate glasses employing IR technique[1] and optical absorption technique [2] have revealed that the structure of LP glasses undergoes gradual changes. Thorough knowledge of Optical properties of transparent glasses will enable successful utilization of glasses for optical application such as windows, filters and lasers. The preparation of these samples was described elsewhere [2]. The impurities VOSO4.5H2O and V2O5 were introduced into all the glasses and their optical absorption spectra were recorded on Shimadzu 3000-UV-VIS-NIR spectrophotometer region is 350nm to 900nm. The spectra consists of mainly two absorption bands designated as A and B. A: 22,050cm-1 and B: 14,117cm-1 in LP(VS) and slight variation in LP(VP) glasses. The electronic absorption spectra of both VO2+(VS and VO2+ (VP) could be explained successfully in terms of the energy level diagram developed for VO5 polyhedron treated as distorted trigonal bipyramid.

4:00 PM

(GOMD-SIII-009-2011) Optical absorption and crystallization of Na2O. SiO2.V2O5

B. Mehdikhani*, Institute of Standard and Industrial Research of Iran (ISIRI), Islamic Republic of Iran; B. Mirhadi, Imam Khomeini International University, Islamic Republic of Iran

The crystallization of Na2O.3SiO2 glasses doped with V2O5 (0-3-5-7–11 mol%) has been investigated by UV-Vis-FTIR spectroscopy, XRD and SEM microscopy. The results showed that, By increasing content of vanadium oxide, Transmission of light through sodium silicate glasses reduced due to ligand field and charge transfer mechanisms, colored glass was developed in some special wavelengths. More increasing of vanadium oxide caused that light transmission in spectrum of these glasses being reduced, so that increasing vanadium oxide up to 11 molar percent case that light absorbed, in which, by investigation vanadium oxide effect on constituent units of glass lattice by means of infrared spectrum at 400-4000 cm-1 region, it was identified that new peak at 900 cm-1 has been appeared that this peak has been shifted to 925 cm-1 by heat treatment. XRD investigation showed that by increasing heat treatment temperature of sample up to 900°C strong peaks appeared.

4:20 PM

(GOMD-SIII-060-2011) PbS Quantum Dots Formation in Glasses Controlled by Ag Nanoclusters

K. Xu, J. Heo*, Pohang University of Science and Technology, Republic of Korea

Lead chalcogenide quantum dots (QDs) in glasses have potential applications in photonics due to the strong quantum confinement effect of lead chalcogenide QDs. Glasses containing lead chalcogenide QDs can be used for optical switches and fiber-optic amplifiers for telecommunication. Thermal treatment of the precursor glass is the most common method of precipitating QDs, but this method results in the random and broad size distribution of resultant QDs. Ion implantation and femtosecond laser irradiation have been attempted to control the spatial distribution of QDs in glasses. Ion implantation can induce the formation of QDs within hundreds of nanometers from the surface of glasses, and femtosecond laser irradiation can control the spatial precipitation of QDs inside glasses. Ag nanoclusters are well-known to act as nuclei and promote the formation of oxide nanocrystals in glass matrices. Therefore, use of Ag nanoclusters may be a way to control and promote the formation of QDs in glasses.

Wednesday, May 18, 2011

Symposium I: Glass Science

Session G: Surface and Interfacial Phenomena

Room: Sapelo
Session Chair: Carlo Pantano, Penn State University

8:00 AM

(GOMD-SI-066-2011) Understanding and controlling environmental effects on friction and wear behaviors of silica and glass surfaces (Invited)

S. H. Kim*, C. G. Pantano, L. C. Bradley, Z. R. Dilworth, Pennsylvania State University, USA

Friction and wear behaviors of soda lime and amorphous silica glasses were studied. In ambient conditions, the adsorption of molecular species on solid surfaces is inevitable. Thus, the solid properties alone are not sufficient to fully understand the interfacial properties; mechanochemical interplay between the solid surfaces and the adsorbed molecules becomes important. Under mechanical loads causing a mild mechanical wear of silica surface, it was found that introduction of water vapor facilitates the chemical wear of the surface while alcohol vapor can protect the surface almost completely. The chemical origin of this environmental effect will be discussed. The soda lime glass show a similar behavior in humid conditions, but the effect of alcohol vapor is different from the silica surface. The effects of sodium leaching on the structure of water and alcohol layers adsorbed on glass as well as the wear process of glass will be discussed.

8:40 AM

(GOMD-SI-067-2011) Adsorption Reactions on Multicomponent Silicate Glass Fiber Surfaces

J. Stapleton*, C. Pantano, K. Mueller, The Pennsylvania State University, USA

Multicomponent silicate glasses are pervasive in modern society as evidenced by the diversity in their application ranging from biotechnology to building materials. Often these glasses are one component of a multicomponent system including organic adhesives or other modifiers. Investigating the interfacial phenomena in these systems is important to gain better understanding of the overall performance. Of particular interest in this study is the interface between multicomponent silicate glass fibers and adhesive polymers. These polymeric systems often possess a variety of different organic functional groups. In this study we selected acetic acid as a probe molecule representative of the carboxylic acid functional group found in many adhesives. Methods were developed that enable analyses to be carried out without damaging or altering the pristine as drawn fiber surface.

9:00 AM

(GOMD-SI-068-2011) Effect of glass composition on chemisorption mechanisms of probe molecules on sodium aluminosilicate glasses

K. Adib*, J. E. Dickinson, Corning Incorporated, USA

We have explored chemisorption mechanisms of probe molecules, such as water, on surfaces of sodium-aluminosilicate glasses. X-ray Photoelectron Spectroscopy of oxygen core levels and valence band were used to determine the fraction of non-bridging oxygens (NBO) as well as the binding energies of different oxygen bonding arrangements on ultra-high vacuum fractured surfaces of these glasses. For those glasses where the NBO fraction of the total oxygen was held constant, a 0.2 eV variance was observed in the binding energies of the NBO O1s core levels consistent with substantial changes, as a function of composition, in the ionicity of the bond between the NBO and sodium. Such wide variance is not observed when the silica content in the glass composition is held constant. Exposure of the vacuum fractured surface to low levels of water vapor results in formation of surface hydroxyls and the displacement of sodium by hydrogen on the NBO.

9:20 AM

(GOMD-SI-069-2011) The Effect of the Water-Silica Interface on Enhanced Hydronium Ion Formation and Transport

S. Garofalini*, G. Lockwood, Rutgers University, USA

Electrochemical studies have shown enhanced proton transport in mesoporous silica containing water. Achieving an accurate description of proton transport in such atomistically large and structurally complex systems requires application of dissociative potentials in molecular simulations. A dissociative water potential that matches many properties of bulk water and nanoconfined water and shows the appropriate dissociative chemisorption of the water molecules on the silica surface also showed the enhanced formation of hydronium ions at these surfaces, similar to ab-initio molecular dynamics simulations. In addition to the formation of surface silanol (SiOH) sites, where protons are strongly bound, the simulations also show the location of weakly binding proton adsorption sites on the silica surface that contribute to enhanced proton transport beyond that observed in the nanoconfined water phase alone. The details of these sites and proton transport will be discussed.

9:40 AM

(GOMD-SI-070-2011) The influence of coupling agents at a glass/polymer interface

J. Banerjee*, J. Stapleton, C. Pantano, Pennsylvania State University, USA

Coupling agents are critical for improved wet performance in glass/polymer composite systems such as fiberglass insulation and composites. We have previously shown that the sodium-rich glass/-COOH polymer interfacial region is hydrolytically unstable due to leaching of sodium from the glass surface. The interfacial region for glass/silane/polymer system was investigated via a thin film approach as well as cryogenic fracture near the interface, using surface characterization techniques such as Infrared Reflectance Spectroscopy, Attenuated Total Reflection spectroscopy, and X-ray Photoelectron Spectroscopy. The interfacial hydrolytic stability of the glass/polymer system with inclusion of silane, either with pre-silanized glass or application of polymer/silane blends, was studied using humid aging at elevated temperature. Inclusion of silane in sodium-rich glass and carboxylic acid-based polymer chemistry shows improved interfacial stability upon water and temperature attack.

Session D: Ancient Glasses

Room: Sapelo

Session Chair: Denis Strachan, Pacific Northwest National Laboratory

10:20 AM

(GOMD-SI-046-2011) Pattern Formation during the Alteration of Ancient Glasses: Insights from Static Corrosion Experiments (Invited)

T. Geisler*, R. Denkler, University of Muenster, Germany; A. Janssen, Institute for Transuranium Elements, Germany; M. Kilburn, University of Western Australia, Australia; A. Putnis, University of Muenster, Germany

Altered zones of archaeological glasses often show intriguing banding patterns in BSE images, reflecting non-equilibrium formation conditions. Here we report the results of static glass corrosion experiments that revealed chemical and structural banding patterns inside silica-based corrosion zones that resemble those seen in naturally altered glasses. Such patterns cannot be explained by existing glass corrosion models that are based on diffusion-controlled solid state reactions and on the assumption of an overall equilibrium between the glass or the altered layer and solution. However, they can be explained by a model that assumes congruent glass dissolution coupled to the precipitation of amorphous silica at an inwardly moving reaction interface. The feedback necessary for pattern formation is given by the competition between the kinetics of the transport of chemical species through the silica corrosion layer and the dissolution-reprecipitation reactions at the interface.

11:00 AM

(GOMD-SI-047-2011) Chemico-mineralogical studies on impact glass from Lonar Crater: its suitability as natural analogue for nuclear waste glass (Invited)

N. RANI*, J. P. Shrivastava, University of Delhi, India; R. K. BAJPAI, BARC, India

Glass is an important material used for high-level nuclear waste management, accommodates and immobilizes various constituents. The purpose of the present is to ascertain the chemico-mineralogical attributes of the impact glass-a potential natural analogue for the immobilization. Present experimental work on impact glass from Lonar carter relates to the study of near hydrothermal alteration in Parr Reactor induced surface chemistry and their retention capability. The Lonar Crater (latitude 19°57'54"N-19°59'42"N and longitude76°29'6"E-76°31'30"E located in Buldana district of Maharashtra, India). XRD and SEM-EDS analyses of secondary layers indicate that the alteration of impact glass led to the formation of smectite, nontronite. The retention factors indicate that the secondary layer composition of impact glass specimens contain high order of Si, Al, Fe and found to be retained in the residue, indicating almost total fixation of these elements.

11:20 AM

(GOMD-SI-048-2011) Long term alteration of archaeological slags: An analogue for nuclear waste glasses

A. Michelin*, CEA Marcoule, France; D. Neff, CEA Saclay, France; S. Gin, CEA Marcoule, France; P. Dillmann, CEA Saclay, France

The knowledge of glass alteration mechanisms arouses a great interest over the last decades, particularly in the nuclear field since vitrification is used to confine radioactive wastes. These glasses, which are stored in steel canisters, must ensure the confinement of radionuclides over a million year timescale. That's why models have been developed in order to predict the glass long term corrosion. The study of archaeological analogues plays a large part in their validation. Here we consider 16th century blast furnace slags that present large contact between iron corrosion products and glass matrix. Thus they can help us to understand the effect of iron from the steel containers on the glass alteration kinetics. A first part of this work concerns the characterization of interfacial areas between glass and corrosion products. Secondly, leaching experiments are set up to determine dissolution kinetics. Finally, these data will be combined to test the predictive capacity of geochemical models.

Symposium II: The Amorphous State

Session C: Topology and Rigidity

Room: Ossabaw
Session Chairs: Pierre Lucas, University of Arizona; John Mauro, Corning Incoporated

8:00 AM

(GOMD-SII-031-2011) Understanding Glass Hardness from Constraint Theory (Invited)

M. M. Smedskjaer*, Aalborg University, Denmark; J. C. Mauro, Corning Incorporated, USA; Y. Yue, Aalborg University, Denmark

Understanding the composition dependence of glass properties is of critical importance for the quantitative design of new glassy materials. Hardness is an important mechanical property of glasses, but a theoretical prediction of glass hardness has hitherto been impossible. In this work, we present a topological approach for quantitative prediction of hardness of inorganic glasses, taking the ternary soda-lime-borate glassy system as an example. We show that hardness is governed by the number of network constraints at room temperature and that a critical number of constraints is required for a material to display mechanical resistance. By comparison of the hardness prediction with that of the glass transition temperature, we demonstrate the importance of accounting for the temperature dependence of the network constraints. The predicted values of hardness are in excellent agreement with experimental data, and we are also able to account quantitatively for changes in hardness that occur when the surface composition changes.

8:40 AM

(GOMD-SII-032-2011) Topological constraints in glass from Molecular Dynamics Simulations

M. Micoulaut*, M. Bauchy, UPMC, France

Bond-stretching and bond-bending constraints in glasses can be fairly well established from atomic scale trajectories using Molecular Dynamics Simulations, allowing for a neat evaluation under thermodynamic conditions (pressure, temperature). We describe the algorithms and present results for various chalcogenide and oxide glasses and liquids.

9:00 AM

(GOMD-SII-033-2011) Distribution of temperature dependent topological constraints

B. Mathieu*, M. Micoulaut, UPMC, France

In this talk, we focus on temperature-dependent topological constraints in silicate glasses which can be computed from classical Molecular Dynamics Simulation. Close to the glass transition, a bimodal distribution appears for the standard deviation of the partial bond angle distribution of the bridging oxygen (BO), indicative of intact and broken bond-bending constraints, the latter being induced by the increased thermal activation. We show that these broken bond-bending constraints have a heterogeneous distribution with a characteristic lengthscale.

9:20 AM

(GOMD-SII-034-2011) 2D NMR in germanium-selenium chalcogenide glasses (Invited)

M. Deschamps*, Université d'Orléans, France; C. Roiland, F. Charpentier, G. Yang, B. Bureau, Université de Rennes, France

Characterizing the short to intermediate range structure of chalcogenide glasses is necessary to understand the structure-property relationships. 77Se NMR is a unique probe of the environment of Se atoms, however, 77Se has a low natural abundance (7.76%), and 77Se NMR can only provide one-dimensional spectra with overlapping spectral contributions. Isotopic enrichment to 100% allowed us to obtain two-dimensionnal spectra which correlate the chemical shift of neighbouring Se atoms, allowing us to extract the spectral parameters of each type of Se environment and providing a convenient way to decipher the 77Se NMR spectra in several glasses.

10:20 AM

(GOMD-SII-036-2011) Correlation between topology and physical properties in As-Se glasses

P. Lucas*, University of Arizona, USA; G. Yang, B. Bureau, T. Rouxel, University of Rennes, France; O. Gulbiten, University of Arizona, USA; J. Sangleboeuf, University of Rennes, France

The structure of As(x)Se(1-x) glasses is investigated by Raman spectroscopy and nuclear magnetic resonance. It is shown that the reticulation of the glass structure increases continuously until x=0.4 following the "chain crossing model" and then undergoes a transition towards a lower dimension pyramidal network containing an increasing number of molecular inclusions at $x > 0.4$. These structural features are correlated with low temperature physical properties such as the Young's modulus, shear modulus, bulk modulus, Poisson's ratio and the density but also with high temperature properties such as activation energy for viscous flow, enthalpy relaxation, and fragility. These results are discuss with respect to the temperature dependence of topological constraints.

10:40 AM

(GOMD-SII-037-2011) Effects of Rigidity Percolation on Structural Relaxation in Supercooled Germanium Selenide Liquids

S. Sen*, E. Gjersing, University of California at Davis, USA

High-resolution 77Se NMR spectroscopy is used to investigate the rotational dynamics of Se atoms in GexSe100-x supercooled liquids with $5 \leq x \leq 23$. The Se atoms in Se-Se-Se linkages are found to be significantly more mobile compared to those in Ge-Se-Se/Ge linkages. The timescale of the rotational dynamics of Se-Se-Se linkages and its temperature dependence are nearly identical for liquids with $x \leq 17$ but the timescale displays an abrupt increase for the liquids with x= 20 and 23, at and above the rigidity percolation threshold. Such a dynamical transition is shown to be consistent with a sudden elastic stiffening of the atomic network of GexSe100-x supercooled liquids at the percolation threshold.

11:00 AM

(GOMD-SII-038-2011) Structure and Topology of Na2O-B2O3-Al2O3-SiO2 Mixed Network Glasses

Q. Zheng*, Aalborg University, Denmark; R. E. Youngman, C. L. Hogue, J. C. Mauro, M. Potuzak, A. J. Ellison, Corning Incorporated, USA; M. M. Smedskjaer, Y. Yue, Aalborg University, Denmark

Boroaluminosilicate glasses serve as the basis for a variety of industrial glasses. Hence, it is critical to understand the relationship between physical properties and structure of these mixed network former glasses. Also it is important to model the effects of composition on properties based on structural speciation by applying constraint theory and then to compare the modeled and experimental results. We have designed six Na2O-B2O3-Al2O3-SiO2 glasses with variation of the [Al2O3]/[SiO2] ratio to access different regimes of sodium behavior. We use 11B, 27Al, 29Si, and 23Na MAS NMR to determine changes in both network speciation and modifier cation environment as a function of the composition. We link these structural changes to changes in measured thermal, mechanical, and rheological properties.

11:20 AM

(GOMD-SII-039-2011) Twinkling Fractal Theory of the Glass Transition: Experimental Proof and Applications (Invited)

R. P. Wool*, University of Delaware, USA

A new approach to understanding the glass transition temperature (Tg) of glass forming liquids called the Twinkling Fractal Theory (TFT) has been experimentally verified. As Tg is approached from above, dynamic solid fractal clusters form and percolate rigidity at Tg. The rigidity percolation cluster is a solid fractal and to the observer, appears to "twinkle" as solid and liquid clusters interchange in dynamic equilibrium with a vibrational density of states g(w)~w^df-1. The solid-to-liquid twinkling frequencies wTF are controlled by the Boltzmann population of intermolecular oscillators in excited energy levels of their anharmonic potential energy functions U(x) such that wTF = wo exp -B(T*2-T2)/kT in which T*≈1.2Tg. Time-lapse AFM images reveal that the per-

colated solid fractal clusters have lifetimes tau which are cluster size R dependent as tau ~ R^1.8. Applications to fracture, rate effects, nanoconfinement, non equilibrium states and thermal properties are discussed.

Symposium III: Optical Materials and Devices

Session G: Solar Energy and Photocatalysis

Room: Pulaski
Session Chair: Matthew Lloyd, NREL

8:00 AM

(GOMD-SIII-045-2011) Organic photovoltaic cells: material processing, device structure and light management (Invited)
J. Xue*, University of Florida, USA

Organic photovoltaic (OPV) cells have attracted great interests in recent years due to their potential to offer low cost solar energy conversion. With advances in new materials and new device architectures, power conversion efficiencies exceeding 8% have now been reported for OPV cells. In this talk, I will present our recent work on improving the efficiency and functionality of OPV cells. First, we have demonstrated interdigitated bulk heterojunction structure based on vertically aligned molecular nanorod arrays, which exhibited twice the efficiency of a bilayer heterojunction from the same material system. We have also fabricated efficient OPV cells on flexible substrates by using an inverted structure containing ZnO nanoparticles, which enabled us to demonstrate a prototype "solar palm tree". Finally, we have developed light trapping optical structures based on transparent polymers to enhance light harvesting in OPV cells by 20-80%.

8:40 AM

(GOMD-SIII-046-2011) Interfaces in organic photovoltaic devices (Invited)
B. Kippelen*, Georgia Tech, USA

In this talk, we will discuss the important role played by interfaces in the operation of organic photovoltaic devices. In particular, we will show how the modification of the electronic properties of the transparent electrode can be used to change the geometry of the solar cell and build solar cells with an inverted geometry and better environmental stability.

9:20 AM

(GOMD-SIII-047-2011) Overcoming Degradation in Organic Photovoltaic Devices with Air Stable Electrodes
M. Lloyd*, NREL, USA

Organic photovoltaics (OPVs) recently attained power conversion efficiencies that are of interest for commercial production. Consequently, one of the most important unsolved issues facing a new industry is understanding what governs lifetime in organic devices and discovering solutions to mitigate degradation mechanisms. Historically, the active organic components are considered vulnerable photo-oxidation and represent the primary degradation channel. However, we present several (shelf life and light soaking) studies pointing the relative stability of the active layers and instabilities in commonly used electrode materials. We show that engineering of the hole/electron injection layer at the electrode can lead to environmentally stable devices with even without encapsulation.

9:40 AM

(GOMD-SIII-048-2011) Electrical and optical properties of CdTe-ZnO nanocomposite thin films as tunable optoelectronic materials for photovoltaic energy conversion
B. G. Potter, R. Beal*, G. Shih, C. Swanborg, C. G. Allen, University of Arizona, USA

The use of quantum-scale semiconductor species as spectral absorption sensitizers in photovoltaic device architectures is of significant interest as a means of increasing energy conversion efficiency. In the present work, nanocomposite CdTe-ZnO thin films were produced via a sequential RF-cosputtering technique and their optical absorption and charge transport properties were examined. Spectral absorption strength and absorption onset energy has been correlated with semiconductor loading and controlled variation in the degree of structural connectivity of the CdTe nanocrystal ensemble. Spectrally resolved photoconductivity confirms the successful extraction of photocarriers from the CdTe phase and their transport to external contacts. A unique contribution of the CdTe nanophase to the spectrally resolved external quantum efficiency observed in a P3HT-ZnO-based heterojunction has been demonstrated.

10:20 AM

(GOMD-SIII-049-2011) PbS and PbSe quantum dot Schottky junction and heterojunction solar cells (Invited)
J. Luther*, National Renewable Energy Lab, USA

Multiple exciton generation provides a promise to extend the efficiency of a single junction solar cell beyond the Shockley Queisser limit of ~33% by using a high-energy photon to generate multiple electrons. This effect is most commonly studied in colloidal quantum dots of PbS or PbSe. Recently, lead chalcogenide based solar cells have seen rapid progress, including the highest measured photocurrents under 1-sun conditions for nanostructured solar cells. The Voc of devices have surpassed the bulk bandgap indicating quantum confinement can help create a fascinating thin film with new collective properties. This talk will discuss coupling strategies for creating conductive quantum dot networks, alloying strategies to improve device metrics, as well as various device structures and contacts to collect electrons from the light absorbing quantum dot arrays.

11:00 AM

(GOMD-SIII-050-2011) Oxyfluoride and sulfide based glass ceramics for LED lighting and for improving solar cells' efficiency (Invited)
X. Zhang*, University of Rennes I/CNRS, France; X. Fan, Zhejiang University, China; B. Fan, C. Point, L. Calvez, J. Adam, University of Rennes I/CNRS, France

Transparent glass ceramics are composite materials obtained by controlled crystallization of glasses. Two types of compositions will be presented: the oxyfluoride glass ceramics combine the excellent thermal mechanical properties with the low phonon energy environment of fluoride crystals. The sulfide glass ceramics are interesting for its still lower phonon energy which is very useful for obtaining high quantum efficiency of wavelength conversion. The composition, preparation technique, spectroscopic properties and potential applications for photovoltaic solar cells and general lighting based on LEDs will be presented.

Symposium IV: Glass Technology

Session B: Glass Strength

Room: Cumberland
Session Chair: Elam Leed, Johns Manville

8:00 AM

(GOMD-SIV-010-2011) Factors Affecting the Reliability of Glass (Invited)
S. Freiman*, Freiman Consulting, USA

The failure resistance of glass is governed by three factors. The short term strength is determined by its fracture toughness, i.e. resistance to rapid crack growth, and the severity of the damage to its surface, i.e. the flaw distribution. The other factor, important for reliability under stress for a longer period of time, is the sensitivity of the glass to environmentally enhanced crack growth, i.e., the slope of a stress intensity factor-crack velocity curve. In this presentation I will discuss the phenomena that contribute to each of the above parameters and show some perhaps surprising relationships between the structure and chemistry of glasses and their physical and mechanical properties. I will show how fractographic analysis can lead to interesting relationships between fracture

surface measurements and perhaps fundamental fracture parameters. Finally, I will discuss a new approach to increasing the resistance of glass to crack growth.

8:40 AM

(GOMD-SIV-011-2011) Using the Hertzian Ring Crack Initiation Approach to Measure Surface Flaw Size

R. Tandon*, Sandia National Laboratories, USA

The surface crack size distribution (csd) in brittle materials is an important descriptor of surface quality, and a predictor of crack initiation loads. Here the Hertzian indentation approach is used to measure csd on a glass surface. Using analytical and finite-element approaches, we show that frictional tractions significantly alter the contact stresses for dissimilar elastic contacts. Data comparing crack initiation loads and cracking location for WC-glass, and glass-glass contacts supports the predictions. An approximate analysis for determining csd's from crack initiation loads is described. The crack sizes obtained on a glass surface using the Hertzian approach are significantly lower than ones obtained using a conventional strength test. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract-DE-AC04-94AL85000.

9:00 AM

(GOMD-SIV-012-2011) A Fracture Mechanics View of the Practical Strength of Glass (Invited)

R. Bradt*, The University of Alabama, USA

The failure criterion after Griffith is presented in fracture mechanics format in terms of the fracture toughness,the applied stress and the flaw size (including a geometric constant). Each of these terms is addressed in the manner which they affect the strength. How to increase the practical strength is revealed by this analysis of the controlling factors.

9:40 AM

(GOMD-SIV-013-2011) Two Point Bend Studies of Fatigue Effects in Silicate Glasses

Z. Tang*, R. K. Brow, Missouri S&T, USA; C. R. Kurkjian, University of Southern Maine, USA

Failure of silicate glasses in wet environments has been described by fatigue effects due to the chemical reaction between water and strained bonds at the crack tip. Two-Point Bend (TPB) studies have been performed on freshly-drawn silicate glass fibers under different conditions, including water at different temperatures, air with different relative humidities and liquid nitrogen. The dynamic fatigue effect is observed from TPB experiments at different faceplate velocities. The calculated dynamic fatigue parameter (n_{df}) is 15.5 for a commercial soda-lime silicate glass and 19 for E-glass. These values are similar to those reported values from slow crack growth measurements and other dynamic/static loading experiments. The effect of structure in a series of sodium aluminosilicate glasses on fatigue behavior will also be described.

Symposium III: Optical Materials and Devices

Session F: Sensors and Scintillators

Room: Cumberland
Session Chair: Mary Bliss, Pacific Northwest National Laboratory

10:20 AM

(GOMD-SIII-040-2011) Laser formation of micro to nano-scale 2D and 3D SbSI single crystal ferroelectric features in chalcogenide glass for device integration

P. Gupta*, A. Stone, N. Woodward, Lehigh University, USA; L. Ding, East China University of Science and Technology, China; M. Sakakura, Y. Shimotsuma, K. Miura, K. Hirao, Kyoto University, Japan; V. Dierolf, H. Jain, Lehigh University, USA

Antimony sulpho-iodide (SbSI) is a well known semiconductor ferroelectric chalcogenide that has attracted much interest for application in infrared detectors, ferroelectric memories and integrated photonic devices. However, large differences in the vapor pressure of Sb, S and I present difficulty in forming good quality SbSI thin-film through deposition methods or growing bulk crystals from vapor transport processes. To overcome this material challenge, laser assisted crystallization techniques have been developed. CW laser is employed to produce localized heating profiles, thereby forming SbSI single crystal architecture on the surface of glass. Formation of 3D features in the interior is attempted with femtosecond laser, but with additional challenges. These techniques hold promise for direct integration of optically and electrically active features on microelectronic and photonic chips for detectors and sensors.

10:40 AM

(GOMD-SIII-041-2011) Novel chalcogenide glasses for nano-cavity photothermal chem-bio detection

J. Hu*, University of Delaware, USA; D. J. Musgrave, Massachusetts Institute of Technology, USA; N. Carlie, Clemson University, USA; A. Agarwal, Massachusetts Institute of Technology, USA; K. Richardson, Clemson University, USA; L. Kimerling, Massachusetts Institute of Technology, USA

Nano-cavity photothermal spectroscopy is a novel technique for ultrasensitive chem-bio detection. We illustrate that through simultaneous localization of optical and thermal interactions in a planar nano-cavity, detection sensitivity can be improved by > 1E4 compared to state-of-the-art. Key to the nano-cavity photothermal detection is the use of novel infrared-transparent chalcogenide glass alloys for optical resonant cavity fabrication. Through composition engineering, these glasses feature a photothermal material figure-of-merit more than two orders of magnitude higher compared to conventional photonic materials such as silica and silicon. We show that high-quality chalcogenide glass thin films can be deposited via thermal evaporation over large areas with high uniformity. Record cavity quality factors up to 5E5 have been achieved in planar chalcogenide glass resonant cavities, leading to high photothermal detection sensitivity.

11:00 AM

(GOMD-SIII-042-2011) Fabrication and Scintillation Response of Rare Earth Doped Transparent Ceramics

L. G. Jacobsohn*, K. Serivalsatit, S. A. Roberts, Clemson University, USA; E. G. Yukihara, Oklahoma State University, USA; T. A. DeVol, J. Ballato, Clemson University, USA

Scintillators are materials that luminesce following interaction with ionizing radiation, finding use in a wide range of security, medical, industrial, and research applications. Transparent ceramics are being investigated as low-cost substitutes for single crystals scintillators. The fabrication of transparent ceramics and evaluation of the scintillation response of rare earth doped oxide ceramics, including Y2O3:Eu, was carried out. Precursor nanopowders were prepared by precipitation techniques followed by calcination to convert the precipitates into oxides.

Their structure and morphology were characterized by x-ray diffraction and transmission electron microscopy measurements, respectively. Transparent ceramics were obtained by sintering in vacuum, followed by hot isostatic pressing in argon. The scintillation response was evaluated by differential pulse height distribution measurements, and the luminescence spectra were collected under ultra-violet and x-ray irradiation.

11:20 AM

(GOMD-SIII-043-2011) Synthesis and Properties of Transparent (Gd,Lu)x(Ga,Al)yO12:Ce Ceramic Scintillator

Y. Wang*, G. Baldoni, RMD, USA; C. Brecher, W. Rhodes, ALEM Associates, USA; K. Shah, RMD, USA; N. Cherepy, J. Kuntz, S. Payne, Lawrence Livermore National Laboratory, USA

Mixed garnet ceramics offer excellent optical and scintillation properties such as high light output, high gamma ray stopping power and fast response which make these materials potential candidates for radiation detection applications. The relative low densification temperatures employed for polycrystalline ceramic processing offer an alternative to single crystal growth in obtaining less expensive scintillators for medical imaging applications such as Positron Emission Tomography (PET). In this study, optically transparent (Gd,Lu)x(Ga,Al)yO12:Ce (GLuGAG:Ce) ceramic scintillators were fabricated via a sinter-HIP approach employing nano-sized starting powders. The relationship between compositional variations and processing conditions and the optical and scintillation properties were evaluated. Phase pure and highly transparent bodies were obtained. The scintillation properties and transparency will be discussed.

11:40 AM

(GOMD-SIII-044-2011) Scintillating glasses for slow and fast neutron detection

M. Bliss*, D. A. Haas, S. M. Bowyer, L. Smith, D. S. Barnett, J. A. Stave, Pacific Northwest National Laboratory, USA

Neutron detection is inherently difficult and direct fast neutron detection is nearly impossible in field measurements. Our group has extensive experience in thermal neutron detection with 6Li loaded-glass and is now studying glasses loaded with thorium for use as fast neutron detectors. 232Th (100% natural abundance) is insensitive to thermal neutrons, but 200 MeV of energy is released when higher energy neutrons induce fission. The 6Li fission reaction releases much less energy, but it currently appears that more of this energy is converted to a usable optical signal by the rare earth activator. Signals from both types of glasses are studied in detail to better understand the solid-state energy transfer from the fission products to the glass matrix to the rare earth activator in these systems. Differentiation of the neutron signals from other radiations is key to these materials being successfully applied to a broad range of radiation detection applications.

Symposium I: Glass Science

Session A: Atomistic Modeling of Glass Structures and Interfaces

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

1:00 PM

(GOMD-SI-001-2011) The Role of the Water-Silica Interface on the High Thermal Expansion of Nanoconfined Water (Invited)

S. Garofalini*, Rutgers University, USA

Although recent experiments have shown an anomalously high thermal expansion of water confined in nanopores of silica, the cause of this enhanced expansion has eluded description. Molecular simulations have previously been applied to this problem, but have used rigid (non-reactive) water potentials, missing important behavior occurring at the interface. In order to provide for more realistic simulations of nanoconfined water in silica, we developed a dissociative water potential that matches many experimental properties of bulk water and shows dissociative chemisorption of the water molecules on the silica surface, with hydroxylation consistent with experiment. The simulations uniquely show the high thermal expansion of nanoconfined water in comparison to bulk water, similar to the experimental data. Analysis of the simulations and the role of the interface on behavior will be presented.

1:40 PM

(GOMD-SI-002-2011) Group IV Nanoclusters embedded in Silica Glass

P. Kroll*, UT Arlington, USA; J. Du, UNT Denton, USA; K. Seino, F. Bechstedt, U Jena, Germany

We give a systematic assessment of electronic structure and optical properties of Si, Ge, and SiC nanoclusters (NCs) up to 2 nm in diameter and fully embedded in amorphous SiO2. Complete models comprising 500-1500 atoms are computed using standard periodic density functional methods. Electronic and optical properties of embedded clusters are different from isolated H-terminated clusters. The suboxide interface impacts properties of Si- and Ge-NCs, but less so those of SiC-NCs. In addition, non-planar interfaces provide different influence on NCs as may be expected from planar interfaces. The interfacial energy of embedded Ge-NCs is lower than that of Si-NCs. SiC-NCs compare well with Si. For small SiC-NCs below 1 nm diameter we have indication that segregated amorphous SiC is more favorable than well-ordered NCs. Our results highlight the critical role and the impact of the interface between nanocluster and embedding glass matrix – and how the chemistry of the interface influences electronic and optical properties.

2:00 PM

(GOMD-SI-003-2011) Investigation of Ion-Exchange 'Stuffed' Silicate Glass Structures by Molecular Dynamics Simulation

P. K. Kreski*, A. N. Cormack, A. K. Varshneya, Alfred University, USA

Sodium silicate glasses have been simulated, and, subsequently, have had potassium ions directly substituted for sodium ions. After this ion swapping, the systems were allowed to relax under various boundary conditions: NVT, NPT with zero system pressure, and NPT with system pressure determined from laboratory measurements of potassium 'stuffed' sodium silicate glass. The resulting simulated stuffed glass structures will be compared against those of the end-member sodium and potassium silicate glasses. Analyses will be primarily based on NBO content, radial distribution function, Qn distribution, bond angle distribution, and ring size distribution. Possible stuffing ion accommodation mechanisms will be discussed.

2:20 PM

(GOMD-SI-004-2011) Structural Irregularities and Interfacial Features in Network Glasses (Invited)

J. Kieffer*, Y. Yue, K. Becker, University of Michigan, USA

Given the strong degree of disorder associated with amorphous structures, it is difficult to ascertain what structural feature constitutes a systematic deviation from the molecular configurations associated with the regular bulk glass. In view of establishing a quantitative assessment of what can be considered irregularities in glass structures, we use molecular dynamics simulations based on a reactive force field to generate realistic models of structures that may develop as a result of various types of perturbations, including chemical incompatibilities, atomic collisions, and the presence of interfaces. Structural characteristics of the affected regions, as determined by appropriately adapted spatial correlation functions, are compared with those of bulk glasses that have the same compositions.

3:20 PM

(GOMD-SI-005-2011) Atomistic Modelling of the Mechanical Properties of Silicate Glasses (Invited)

A. Cormack*, L. Adkins, Alfred University, USA

In this talk, we will discuss the application of molecular dynamics simulations to modelling the mechanical properties of silicate glasses. We will first show how well calculated elastic moduli compare with experi-

mental data. Then we will describe the behavior under a tensile load of silicate glasses. In addition to bulk glasses, we will present results on both glass whiskers and glass fibers. Finally, we will comment on some of the technical challenges associated with these simulations.

4:00 PM

(GOMD-SI-006-2011) Deformation Mechanisms of Densified Silica Glass

L. Huang*, F. Yuan, Rensselaer Polytechnic Institute, USA

Molecular dynamics (MD) simulations, based on a charge-transfer three-body potential, have been carried out to study deformation mechanisms of densified silica glass prepared either by pressure-quenching from the liquid state or by hydrostatic compression-decompression in the glassy stage. Large-scale MD simulations of uniaxial tension and compression tests, as well as nano-indentation tests were carried out in normal and densified silica glass. Our simulations indicate that the interplay between densification and shear flow is crucial for the mechanical behavior of silica glass and it can be tuned by adjusting the initial glass density. A reduction of brittleness with increasing density of silica glass is generally observed. In addition, the correlation between densification, shear flow and Poisson's ratio of silica glass is examined and a qualitative explanation is proposed.

4:20 PM

(GOMD-SI-007-2011) A study of silica glass fiber structure using molecular dynamic simulations

L. Adkins*, A. N. Cormack, Alfred University, USA

In this study we have simulated silica fibers in a range of sizes up to experimental scale. We will discuss the surface structure of the fibers, including the presence of unusual species and their population as a function of surface depth for different fiber geometries and sizes. We have also broken the fiber under tensile strain and will discuss the elastic properties and fracture surface structure.

4:40 PM

(GOMD-SI-008-2011) Cation field strength effect on aluminum coordination in rare earth aluminosilicate glasses: a molecular dynamics study

J. Du*, L. Kokou, University of North Texas, USA

Rare earth aluminosilicate glasses find technological applications as laser and amplifier host materials, radiation delivery agent for cancer therapy, and model systems for nuclear wastes. Detailed understanding of the structure of these glasses are of both technological and scientific importance. Solid state NMR studies have found that cation field strength has a strong effect on aluminum coordination speciation in aluminosilicate glasses. In this paper, we use molecular dynamics simulations to understand the effect of the field strength of rare earth ions (e.g. La3+ vs Y3+) on the aluminum coordination number in rare earth aluminosilicate glasses. The general structure features of these complex oxide glasses will be presented based on molecular dynamics simulations. Then we will focus on the explanation of the role of rare earth ion field strength, the effect of silica concentration on aluminum coordination and structure in these aluminosilicate glasses.

5:00 PM

(GOMD-SI-009-2011) First-principles molecular dynamics simulations of chalcogenides liquids and glasses (Invited)

C. Massobrio*, IPCMS, France

This talk will provide a broad overview and a selection of a few, well focused examples in the area of first-principles modelling of chalcogenides disordered materials. Among the issues being considered we can mention: a) the setup of atomic-scale simulations describing along extended time trajectories and for systems of adequate sizes the structural features of a given disordered system, b) the comparative assessment of the performances of plane waves and mixed bases schemes, these latter being more advantageous for very large N (number of atoms), c) the delicate interplay between the details of the electronic structure description (exchange-correlation functional within DFT) and the network organization, d) the correlation between specific structural units and the onset of intermediate range order and e) the interpretation of experimental data as a unique tool to establish the predictive power of first-principles approaches.

5:40 PM

(GOMD-SI-071-2011) Silica Molecular Dynamic Force Fields: A Practical Assessment

T. F. Soules*, G. H. Gilmer, M. J. Matthews, J. S. Stolken, M. D. Feit, Lawrence Livermore National Laboratory, USA

The purpose of this paper is to compare simple and efficient pairwise force fields for silica glass and assess their applicability for use in large scale molecular dynamic (MD) simulations of laser damage mitigation. Pairwise potentials obtained by fitting quantum mechanical results, such as the BKS and CHIK potentials exhibit many of the properties of the liquid such as densification. However while this and other liquid properties of the MD simulation are qualitatively correct they are observed at temperatures much higher than observed experimentally. Softer potentials are constructed that do give liquid properties at experimental temperatures. However in all cases the activation energies for diffusion are lower than the experimental activation energies for viscosity.

Symposium II: The Amorphous State

Session D: Medium Range Order

Room: Ossabaw
Session Chair: Paul Voyles, University of Wisconsin, Madison

1:00 PM

(GOMD-SII-040-2011) Fluctuation Electron Microscopy: Observing Subcritical Nuclei in Chalcogenide Glasses (Invited)

J. R. Abelson*, U. Illinois at Urbana-Champaign, USA

Phase transformation begins with nucleation, in which a small aggregate of atoms organizes into a new symmetry. The thermodynamic driving forces and kinetic rates have been predicted by nucleation theory; however, actual observation of nanometer-scale nuclei in an amorphous matrix has been elusive. Chalcogenide glasses, under investigation for phase-change electronic memories, exhibit crystallization behavior that depends strongly on composition and thermal history. We detect subcritial nuclei embedded in these materials using a statistical technique, fluctuation transmission electron microscopy (FEM), and we determine the crystallization kinetics using pulsed laser experiments. In this talk, we present and discuss evidence for the stochastic nature of nucleation, the time- and temperature-dependence of the distribution of subcritical nuclei, and their effect on the crystallization rate. We also discuss four methods to extract quantitative size and density information from FEM data.

1:40 PM

(GOMD-SII-041-2011) Nucleation Mechanisms and Ring Size Distributions in Alkali and Alkaline Earth Disilicate Glasses

M. O. Naylor*, A. N. Cormack, Alfred University, USA

The relationships between glass structure and devitrification mechanisms are still poorly understood. A better understanding of medium range order, when compared to crystalline counterparts, may inform what determines whether homogeneous or heterogeneous nucleation will occur. To this end, we have used molecular dynamics to model the structures of some alkali and alkaline earth disilicate glasses. Lithium disilicate and barium disilicate compositions were chosen to represent glasses exhibiting homogeneous nucleation, whereas sodium disilicate and potassium disilicate glasses were selected to represent compositions showing heterogeneous nucleation. We will discuss the similarities and differences in the ring size distributions of these glasses, both as a function of modifier, and in relation to that of their crystalline counterparts, with respect to the role that the medium range order may play in the

nucleation mechanisms. Furthermore, a ring breaking mechanism is proposed.

2:00 PM

(GOMD-SII-042-2011) Boson Peak of Lithium and Cesium Borate Glass Studied by Low Temperature Heat Capacity and Raman Scattering

S. Kojima*, Y. Matsuda, M. Kodama, University of Tsukuba, Japan; N. Surovtsev, Russian Academy of Sciences, Russian Federation; H. Kawaji, T. Atake, Tokyo Institute of Technology, Japan

The composition dependence of boson peaks has been studied by low temperature heat capacity and Raman scattering measurements in lithium and cesium borate glass, xM2O-(1-x)B2O3 (M=Li, Cs). The boson peak frequency markedly increases for the increase of the lithium composition, while for the increase of the cesium composition it is nearly constant. The origin of the boson peak of alkali borate binary glass is probably the coupled vibration of the libration of boroxol rings and the rattling like vibration of an alkali ion at a void of borate network. It is also found that the boson peak frequency of lithium and cesium borate glass is correlated with the shear modulus measured by the ultrasonic method.

2:20 PM

(GOMD-SII-043-2011) Experimental and Computational Studies of Short- and Medium-Range Order on the Surfaces of Oxides

K. Mueller*, N. Washton, Pacific Northwest National Laboratory, USA

Local structure and atomic ordering in the bulk of amorphous materials has been studied routinely with solid-state NMR spectroscopy. In these studies, computational chemistry has played a key role in mapping spectral information (i.e. chemical shift tensors and local electric field gradients) onto local short-range order. We have extended such studies in two important areas: the ability to study atomic distributions on surfaces (or within surface layers), and an approach to medium-range structural ordering for molecules that have formed reaction products on a complex oxide surface. As one example, we demonstrate the use of ^{1}H-^{29}Si cross polarization coupled to the Carr-Purcell-Meiboom-Gill acquisition sequence to speciate hydroxyl groups reactive to covalent binding with a chlorosilane probe molecule. Computational methods are then used to calculate chemical shielding tensors, and the results provide structural information out to the fourth nearest-neighbor atoms.

2:40 PM

(GOMD-SII-044-2011) Modeling of Glass Durability through Advances in the Understanding of Medium Range Order (MRO)

C. Jantzen*, J. M. Pareizs, Savannah River National Laboratory, USA

The chemical durability, expressed as a glass dissolution rate, is important for the use of glass as a disposal media for nuclear waste. Advances in the measurement of medium range order (MRO) in glasses has led to the understanding that the molecular structure of a glass controls the distribution of ion exchange sites, hydrolysis sites, and the access of water to those sites. An investigation into the role of glass stoichiometry, in terms of MRO clusters which resemble various mineral species, has shown that the stoichiometry and structure in the parent glass may control the activated surface complexes that form in the leached layers. The stoichiometry and structure, in terms of Q distributions, can be represented by the atomic ratios of the glass. This provides two potential approaches to glass durability modeling: one based on the mineral like clusters and one based on cation ratios.

Session D: Medium Range Order and Amorphous Metals

Room: Ossabaw

Session Chair: Paul Voyles, University of Wisconsin, Madison

3:20 PM

(GOMD-SII-045-2011) Fluctuation Electron Microscopy for studying amorphous materials (Invited)

M. M. Treacy*, Arizona State University, USA

Fluctuation Electron Microscopy, or FEM, is an experimental transmission electron microscopy technique that examines variations in scattering between small volumes in a thin sample. The statistics of the scattering fluctuations between volumes provides a surprisingly sensitive probe of medium-range order (MRO) in amorphous materials. By examining the speckliness of the scattering as a function of scattering angle, a fingerprint of medium-range order emerges. The technique works best when the probe resolution is comparable to the length scale of the medium-range order, about 0.5 nm – 3 nm. FEM is not a high-resolution technique, and in fact fails at high resolution (< 0.5 nm). In this talk I will present an overview of FEM, and will describe recent advances in the technique that promise to make FEM more quantitative.

4:00 PM

(GOMD-SII-046-2011) On the stability of carbon nanostructures in silicon oxycarbide materials: Part I

J. Ryan*, Pacific Northwest National Laboratory, USA; P. Kroll, University of Texas at Arlington, USA; C. G. Pantano, The Pennsylvaia State University, USA; K. Alvine, Pacific Northwest National Laboratory, USA

Silicon oxycarbide is a metastable material that has generated interest because of the great flexibility in properties that is attainable with a change in carbon-to-oxygen ratio. These materials have exhibited a strong propensity to include carbon-carbon – "free carbon" – bonding within the structure regardless of synthesis method, although the relative amounts can be controlled to some degree. While evidence for the presence of this free carbon is overwhelming, its structural role has been a matter of debate. Characterization techniques sensitive to ordered bonding in the length scale of roughly 0.5 to 5nm such as fluctuation electron microscopy (FEM), Raman spectroscopy, and nuclear magnetic resonance have been coupled with compositional studies by x-ray photoelectron spectroscopy and Rutherford backscattering spectroscopy to produce a new view of the structural role of carbon in SiOC materials.

4:20 PM

(GOMD-SII-047-2011) On the stability of carbon nanostructures in silicon oxycarbide materials: Part II

P. Kroll*, University of Texas at Arlington, USA; J. Ryan, Pacific Northwest National Laboratory, USA

Computational results based on correlations between microstructure and the enthalpy of formation of the resulting model confirm the experimental results presented in Part I. A very strong driving force exists to separate glassy SiOC and the free carbon phase. Models without covalently bonded interfaces between the two phases are significantly favored over those with covalent bonds between segregated carbon and the amorphous matrix. The effect prevails even if the graphene segregation achieves nano-sized dimensions. Dangling bonds at the edges of graphene segregations and a separate glass phase appear less penalized than a bonded interface between the two. Within the glassy SiCO matrix, segregation of SiC is favored because the enthalpy of formation of a homogeneous SiCO glass increases linearly with increasing phase content of SiC. The medium-range order of SiCO, thus, is composed of small inclusions of SiC in a random SiCO glass, with carbon/graphene segregations incasing domains of SiCO.

4:40 PM

(GOMD-SII-048-2011) Reverse Monte Carlo Modeling of Fluctuation Electron Microscopy Data

J. Hwang, University of Wisconsin, Madison, USA; Y. E. Kalay, METU, Turkey; M. J. Kramer, Ames Laboratory, USA; P. Voyles*, University of Wisconsin, Madison, USA

Fluctuation electron microscopy (FEM) has been shown to yield information about nanoscale order in glassy materials, but interpreting that data is notoriously difficult. We have developed a hybrid reverse Monte Carlo modeling approach which combines medium-range structural data from FEM with short-range structural data from x-ray, electron, or neutron diffraction or an empirical interatomic potential on an equal footing. Including the FEM data results in changes in the structure of the model without reducing the agreement with the short-range data, within the uncertainty in the data. Models refined only against short-range data are inconsistent with FEM data. The models refined against FEM data contain pseudo-planar structural order which can be identified and visualized from the full three-dimensional reciprocal space of the model.

5:00 PM

(GOMD-SII-049-2011) Abnormal dynamics of metallic glass-forming liquids (Invited)

Y. Yue*, Aalborg University, Denmark; C. Zhang, L. Hu, Shandong University, China; J. C. Mauro, Corning Incorporated, USA

We present some recent findings about abnormal dynamic behaviour of metallic glass-forming liquids (MGFLs), i.e., the fragile-to-strong (F-S) transition. This behaviour is observed not only on the marginal metallic glasses, but also on the bulk metallic glasses. We have proposed a model for the F-S transition that accurately captures the scaling of dynamics across both the fragile and strong regimes. In addition, we demonstrate that the F-S transition is likely associated with a thermodynamic transition, namely, a drastic endothermic change in the isobaric heat capacity over the temperature region of F-S transition. We also discuss the structural origin of the F-S transition. Finally, we illustrate a possible link between the extent of the F-S transition and the glass forming ability.

Symposium III: Optical Materials and Devices

Session E: Optical Coatings

Room: Pulaski

Session Chairs: S. Sundaram, NYS College of Ceramics, Alfred University; Norman Anheier, Pacific Northwest National Laboratory

1:00 PM

(GOMD-SIII-033-2011) Self-assembled multifunctional nanostructured coatings (Invited)

H. Fan*, Sandia National Laboratoriess, USA

Self-assembly techniques are one of the powerful and efficient methods to the synthesis of nanostructured films. In this presentation, I will discuss on our recent progress in development of multifunctional nanostructured coatings that are engineered using self-assembly techniques. First, I will discuss on an interfacial self-assembly process to synthesize multifunctional nanoparticles and to assemble them into ordered, three-dimensional, nanoparticle films. Through control of structural parameters of nanoparticle assemblies, we are able to fabricate uniform reflective optical coatings. Second, I will discuss on the development of a phase separation driven self-assembly process in which 3D nanostructured porous films are synthesized and fabricated into uniform multiple layered films that exhibit a wide anti-reflective optical band.

1:40 PM

(GOMD-SIII-034-2011) Solution Processed Chalcogenide Glass for Integrated Mid-Infrared Optical Elements (Invited)

C. B. Arnold*, Princeton University, USA

Chalcogenide glass materials exhibit a variety of optical properties that make them desirable for communications and sensing applications. However, processing limitations for these materials have made the direct integration of waveguides with sources or detectors challenging. In this presentation, we introduce solution processing of chalcogenide glass materials for producing integrated optical and photonic components. We demonstrate that the solution processing preserves the optical properties of the original glass and discuss the use of traditional printing and soft-lithographic methods to produce integrated optical elements. A few examples will be discussed including multimode As2S3 waveguides coupled with quantum cascade lasers and single mode As2S3 waveguides and splitters produced on flexible and non-planar substrates. These solution-based methods enable a suite of processes that can be applied to chalcogenide solutions in order to create a diverse array of mid-IR optical structures.

2:20 PM

(GOMD-SIII-035-2011) Exploiting intrinsic material properties for improved integrated chalcogenide waveguide resonators for mid-IR sensing (Invited)

K. Richardson*, J. Wilkinson, S. Novak, Clemson University, USA; N. Carlie, Schott North America, USA; J. Musgraves, B. Zdyrko, I. Luzinov, Clemson University, USA; V. Singh, A. Agarwal, L. C. Kimerling, Massachusetts Institute of Technology, USA; J. Hu, University of Delaware, USA; A. Canciamilla, F. Morichetti, A. Melloni, Politecnico di Milano, Italy

Chalcogenide glass (ChG) materials have made in-roads into infrared photonic devices in both thin film and fiber form. Compact, on-chip, planar chalcogenide devices produced by CMOS-compatible processing techniques have been shown to exhibit comparable or superior performance to those of commercially available surface plasmon resonance (SPR)-based systems when evaluated for device sensitivity, component footprint, and/or sensing response. Utilizing attributes of chalcogenide glasses often considered "material limitations" (including low glass transition, limited solvent-specific chemical durability and near-bandgap photosensitivity), we demonstrate enhancements to ChG device performance using thermal reflow, solution-based glass film deposition and near bandgap film illumination. Post-fabrication trimming based on the intrinsic photosensitivity of the chalcogenide glass are exploited to compensate for fabrication imperfections of ring resonators.

3:20 PM

(GOMD-SIII-036-2011) Nano-Macro Scale Chalcogenide Coatings by Evaporation-Condensation

S. K. Sundaram*, B. J. Riley, B. R. Johnson, Pacific Northwest National Laboratory, USA

We have extended our multiscale materials processing technology (2008 R&D100 award winner) to one (Se, Te), two (As2Se3), and three (As24S38Se38) component systems. Starting materials are evaporated and condensed on clean fused silica surface inside a sealed ampoule at specific starting pressure exposed to different temperature gradients. Features spanning across nano to macro scales have been observed. Scanning and transmission electron microscopies have been used to characterize the microstructural features. Energy dispersive spectroscopy has been used to determine chemistry of these multiscale features. Size distribution is correlated to the processing conditions (temperature and ampoule pressure). These results are compared to the results of multiscales of As2S3. A mechanism of multiscale processing will be presented.

3:40 PM

(GOMD-SIII-037-2011) Multilayer Deposition for X-Ray Applications (Invited)

R. Conley*, N. Bouet, Brookhaven National Laboratory, USA

An overview of the basic physics of multilayer growth by sputter deposition and their application as x-ray optical elements will be presented. Multilayer research at the NSLS-II concentrates on development of multilayer Laue lens (MLL), which have the potential to provide an unprecedented level of x-ray nano-focusing. The multilayer deposition system at NSLS-II contains many design features in order to facilitate growth of combined depth-graded and laterally-graded multilayers with precise thickness control and low interfacial roughness over many thousands of layers, providing total film growth in one run of up to 100μm thick or greater. A precision in-vacuum linear motor servo system raster scans a substrate over an array of magnetrons with shaped apertures at well-defined velocities to produce a multilayer coating. The design, commissioning, and performance metrics of the deposition system will be discussed. Latest growth results of MLL, reflective multilayers, and other interesting coatings will be presented.

4:20 PM

(GOMD-SIII-038-2011) Spectroscopic Ellipsometry for Optical Coatings (Invited)

J. A. Woollam*, G. K. Pribil, R. A. Synowicki, T. E. Tiwald, J. A. Woollam Co., Inc., USA

Spectroscopic Ellipsometry (SE) is used for the measurement of optical coatings in a wide variety of research and industrial applications. SE is a non-destructive technique routinely used to characterize substrates and optical coatings from the vacuum ultraviolet to the far infrared. SE allows determination of film thickness and complex refractive index for single and multi-layer optical coatings. An overview of spectroscopic ellipsometry including instrumentation, measurements, and data analysis will be presented. This talk surveys a variety of applications including characterization of float glass, transparent conductive oxides, thin film photovoltaics, displays, optical filters, anti-reflection coatings, and multi-functional coatings. Examples from visible to long-wavelength infrared spectral ranges will be presented. Emerging areas for SE will also be discussed, such as combined SE and spectrophotometric (R/T) measurements, in-line measurements, and large area uniformity measurements for coatings on large glass panels.

5:00 PM

(GOMD-SIII-039-2011) Mid-Infrared Dispersion and dn/dT Analysis using Prism Coupling

N. C. Anheier*, A. H. Qiao, Pacific Northwest National Laboratory, USA

We present a prism coupler that is capable of characterizing optical dispersion and thermal index variations (dn/dT) in bulk and thin film materials at measurement wavelengths extending through the mid-infrared (3 to 12 μm). Most dispersion and dn/dT characterization methods require compromises in accuracy, cost, and timeliness, or cannot access the mid-infrared spectral region where many of the most important sensing and defense applications exist. Prism coupling analysis provides rapid feedback needed to guide future optical materials discovery programs, study glass photosensitivity, provide quality assurance of optical materials acquired from commercial sources, and optimize the designs of optical components used in high performance mid-infrared sensing platforms. The challenges of developing a mid-infrared prism coupler, the calibration steps necessary to achieve the desired measurement accuracy, and dispersion data of mid-infrared optical materials are presented.

Symposium IV: Glass Technology

Session D: Glass Melting and Processing

Room: Cumberland

Session Chair: Rajiv Tiwary, PPG Industries, inc.

1:00 PM

(GOMD-SIV-019-2011) Mathematical model of cold cap

R. Pokorny*, P. Hrma, D. Kim, Pacific Northwest National Laboratory, USA

The ultimate goal of batch-melting studies, laboratory-scale, large-scale, or mathematical modeling is to increase the rate of glass processing in an energy-efficient manner. Mathematical models are not merely an intermediate step between laboratory-scale and large-scale studies, but are also an important tool for processing copious amounts of data and assessing responses of melters to vast combinations of process parameters. In the simplest melting situation considered in this study, a cold cap of uniform thickness rests on a pool of molten glass from which it receives a steady uniform heat flux. Thus, as the feed-to-glass conversion proceeds, the temperature, velocity, and the extent of feed reactions are functions of the position along the vertical coordinate, and these functions do not vary with time. This model is used for the sensitivity analyses on the effects of key parameters on the cold-cap behavior to select the parameters that will be determined for the feeds and to update the model code.

1:20 PM

(GOMD-SIV-020-2011) Kinetics of Quartz Particle Dissolution During Glass Melting

J. Marcial*, P. Hrma, S. H. Henager, Pacific Northwest National Laboratory, USA

During high-level waste (HLW) glass processing, quartz particles usually dissolve last. The rate of dissolution of quartz particles affects melter-feed behavior such as foaming and melt viscosity that are crucial for the rate of melting. Measured data indicate that quartz dissolution in an HLW feed sample heated at 5°C/min proceeds in two stages. First, diffusion boundary layers around quartz particles grow until they impinge on those of neighboring particles. Second, as the concentration of silica in the bulk glass increases, the dissolution continues at a slower rate. These two stages are described using dissolution data and estimated diffusion coefficient of silica in the melt.

1:40 PM

(GOMD-SIV-021-2011) Bench-Scale Melt Rate Testing and Modeling

A. Choi*, D. Miller, D. Immel, Savannah River National Lab, USA

Bench-scale melt rate tests are being conducted at SRNL to help formulate the optimum glass forming frit that will melt well when blended with the high-level wastes of widely varying compositions and still produce high-quality waste glasses. However, such tests are both time-consuming and costly. To help reduce the amount of efforts required for the frit development, SRNL is developing a thermodynamic-based tool that can be used to predict relative melt rates from given feed chemistry; however, its success is critically dependent upon the accuracy of data against which it must be calibrated. To ensure the accuracy of data, SRNL is also developing a new technique for measuring batch-melting rates using x-ray imaging and computed tomography analysis. This paper will present a summary of findings in both modeling and experimental efforts being made at SRNL.

2:00 PM

(GOMD-SIV-022-2011) The Benefits of Polyalkylene Carbonate Binders (QPAC®) for Low Temperature Glass Frit or Powdered Glass in Glass Sealing Applications

P. A. Ferraro*, S. Hanggodo, Empower Materials, USA

QPAC® Polyalkylene Carbonate is an exceptional binder in glass frit because it decomposes at a very low temperature with minimal residue after debind. The binder's low decomposition temperature allows for the binder to be burned off below the melting temperature of the glass.

The low levels of residue and carbon contamination remaining after debind minimizes the formation of unwanted metals such as lead in the final sintered product. Glass pastes using polyalkyene carbonate binders will be studied. The paste viscosity, decomposition profiles and other sealing glass properties will be analyzed and compared to pastes using traditional binders. The advantages can be applied to numerous glass powder applications including glass packaging, glass solder, hermetic seals, solar cell devices and display encapsulation.

2:20 PM

(GOMD-SIV-023-2011) The effect of batch makeup and heating rate on the melting behavior of high level waste glass

D. Pierce*, P. Hrma, R. Pokorny, Pacific National Northwest Laboratories, USA

Batches of a simulated high level waste glass with varying makeup, i.e., different alumina sources, all carbonates, and all nitrates with sucrose addition, were subjected to thermo-gravimetric analysis. Batch samples were heated from ambient temperature to 1200°C at constant heating rates ranging from 2°C/min to 21°C/min. Major gas releasing reactions began after 100°C and were complete by 600°C. Using Kissinger's method, we calculated activation energies for 5 to 9 major reactions, depending on the batch, and then estimated the order of each reaction with a least squares method. No attempt was made at this time to determine the chemistry of these reactions. The overall kinetics of the batch-conversion will be applied to a mathematical model for the melting process.

2:40 PM

(GOMD-SIV-024-2011) Microwave synthesis of chalcogenide glasses in Sb-S-I system

P. Gupta*, A. Stone, H. Jain, V. Dierolf, Lehigh University, USA

Bulk chalcogenide glasses are prepared by quenching well homogenized melts of the desired compositions below the glass transition temperature. This conventional preparation often requires >24 hrs radiative heating and mixing of the batch kept in quartz ampule by rocking action in a furnace. Considerable reduction in preparation time are observed for glasses prepared in microwave ovens where electric and magnetic field of the microwave radiation couple with the chalcogenide batch mix for instant transfer of heat specifically to the batch. Additionally, for glasses in Sb-S-I system, a self mixing of the batch has been observed in a microwave field. Differential scanning calorimetry studies and electron microscopy techniques have been utilized to compare glasses prepared by conventional and microwave routes.

Session E: Liquid Synthesis and Sol-gel Derived Materials

Room: Cumberland
Session Chair: Gang Chen, Ohio University

3:20 PM

(GOMD-SIV-025-2011) Sol-gel derived multi-porous glass scaffolds for bone regeneration (Invited)

R. M. Almeida*, Instituto Superior Tecnico, Portugal

Sol-gel derived SiO2–CaO–P2O5 glasses with a dual pore structure including nanopores and macropores and mimicking the human trabecular bone have been prepared for possible application as scaffolds for bone tissue regeneration. While nanopores are intrinsic to sol-gel processing, interconnected macropores have been achieved through polymer-induced phase separation together with the sol-gel transition, adding a water soluble polymer (PEO) to the precursor sol. An overall pore size distribution including ~ 5–30 nm nanopores and ~ 20-300 micron macropores has been obtained by mercury intrusion porosimetry. Scanning electron microscopy has evidenced the interconnected pore structure of these scaffold materials and in-vitro tests revealed their bioactivity, confirmed by FTIR and X-ray diffraction. In-vivo experiments have also been conducted on New Zealand rabbits, showing significant osteoconductivity and bone regeneration. The prepared materials have potential use as scaffolds for bone tissue regeneration.

4:00 PM

(GOMD-SIV-026-2011) Organically Modified Siloxane Melting Gels (Invited)

L. C. Klein*, Rutgers University, USA; A. Jitianu, Lehman College, City University of New York, USA; M. Jitianu, William Paterson University, USA

Silica-based organic–inorganic hybrid nanocomposites contain an inorganic framework combined with a variety of organo-functional groups. Siloxane precursors can have between 1 and 4 reactive groups. One class of nanocomposites results from reactions between siloxanes with organic modifiers that are stable towards chemical reaction, e.g., methyl or phenyl. A combination of a siloxane with one hydrolytically stable group with a siloxane with two groups leads to gels with so-called melting gel behavior. For example, methyl triethoxysilane (MTES) with dimethyl diethoxysilane (DMDES) react to form a melting gel. By using hydrolysis and condensation polymerization, it is possible to prepare transparent hybrids that are rigid at room temperature, but soften and flow around 150°C. However, these so-called melting gels can be prevented from further softening by consolidating at around 160°C. This and other examples of the use of the sol-gel process will be reviewed.

4:40 PM

(GOMD-SIV-027-2011) Water Adsorption-induced Deformation of Micro- and Mesoporous Silica

S. Dong, G. Chen*, Ohio University, USA

Capillary action is a phenomenon where water spontaneously enters a narrow tube driven by capillary force. The resulting capillary pressure depends on the size of the tube and could reach hundreds of Mpa. This phenomenon becomes very important for tubes of nm size. To understand the interaction of confined water with nanotubes, we select microporous and periodic mesoporous silica as the model materials, which are synthesized by a sol-gel method using surfactants as the structure-directing agents. These materials have an amorphous atomic structure coupled with distinctive nanostructures and thus can be characterized by small- and wide-angle x-ray scattering (S/WAXS). By measuring both the nanostructure and the medium-range structure of the porous silica simultaneously during water adsorption using in situ S/WAXS, we observe both reversible and irreversible structural changes induced by the capillary action. Our study has implications for the structure and mechanical property of future nanodevices.

5:00 PM

(GOMD-SIV-028-2011) Effect of silver incorporation on crystallization and microstructural properties of sol-gel derived TiO2 films

B. Akkopru Akgun*, C. Durucan, Middle East Technical University, Turkey; N. P. Mellott, Alfred University, USA

Titanium dioxide (TiO2) has been known as an effective photocatalyst under irradiation with ultra-bandgap light for over 30 years. Recently, it has been found that, TiO2 also behaves as bactericidal agent as well. However, the efficiency of TiO2 is limited due to the short life time of e—h+ species, but can be improved through doping with metallic silver (Ag) nanoparticles. The objectives of this work are to establish sol-gel processing parameters for achieving complete and uniform thin film and to investigate the effect of Ag concentration and calcination temperature on microstructural and chemical properties of Ag-TiO2 thin films. Special emphasis is given to understand the chemical interaction between Ag particles and TiO2 matrix upon calcination treatment. The structural and chemical properties of the Ag-TiO2 films have been investigated using analytical techniques including GIXRD, UV-vis, XPS and Raman spectroscopy.

5:20 PM

(GOMD-SIV-029-2011) Improvement of sol-gel optical stacking

X. Dieudonné*, H. Piombini, K. Vallé, P. Belleville, CEA, France

Highly reflective coatings (HR) can be made by the sol-gel process. The materials used are alternating layers of colloidal SiO2 and colloidal ZrO2. During HR multilayer deposition, one can routinely observed

that many defects appear (crack, scattering) limiting the ability to homogeneously stack up to several micrometers in thickness. In order to understand the origin of these limitations, we have studied colloidal-type stacks made of single materials or multimaterials films. This study permitted to define which process and suspensions parameters play a major role on the stacking ability. These results are characterized by the so-called critical thickness which is the achievable stack thickness before the defects appearance. These results are completed using specifically developed optical and mechanical characterizations (ultra-nanoindentation, laser surface acoustic wave, spectroscopy M-lines). These characterizations will help to find a link between the multilayer microstructure and the optical and mechanical film properties.

Thursday, May 19, 2011

Symposium II: The Amorphous State

Session E: Amorphous Metals

Room: Ossabaw
Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

8:00 AM

(GOMD-SII-050-2011) Structure of Zr Bulk Metallic Glasses Constrained at Short and Medium Range (Invited)

J. Hwang, University of Wisconsin, Madison, USA; Y. E. Kalay, METU, Turkey; M. J. Kramer, Ames Laboratory, USA; P. Voyles*, University of Wisconsin, Madison, USA

We have combined short-range structural data from high-energy x-ray diffraction and an empirical interatomic potential with medium-range structural data from fluctuation electron microscopy (FEM) in a reverse Monte Carlo (RMC) structural model of Zr50Cu45Al5 bulk metallic glass (BMG). The RMC models are supplemented by highly coherent variable-resolution FEM measurements. The RMC model shows that the currently popular description of BMG structure based on interlocking quasi-icosehedral nearest-neighbor clusters is incomplete; real BMGs contain nanometer-diameter regions of nearly planar atomic order, possibly of variable composition. A model consisting entirely of icosehedral clusters is inconsistent with the FEM data.

8:40 AM

(GOMD-SII-051-2011) Phase selection and microstructural dynamics of devitrification in Cu-Zr (Invited)

R. E. Napolitano*, I. Kalay, Iowa State University, USA; E. Kalay, Middle East Technical University, Turkey; T. Cullinan, M. Lamb, Iowa State University, USA

Devitrification dynamics and phase selection mechanisms in melt-spun amorphous Cu-Zr alloys are investigated using in-situ high-energy synchrotron X-ray diffraction (HEXRD), conventional/high resolution transmission electron microscopy (TEM/HRTEM), and differential scanning calorimetry (DSC). Crystallization sequences and mechanisms of nano-scale structural dynamics are analyzed and discussed in terms of binary system thermodynamics, nucleation and growth kinetics, crystal-orientation relationships, solute partitioning, and chemical diffusion. Controlled devitrification structures are also examined. This research is supported by U.S. DOE-OS, Ames Laboratory contract No.DE-AC02-07CH11358.

9:20 AM

(GOMD-SII-052-2011) Modeling the mechanical behavior of amorphous metals (Invited)

E. R. Homer*, Sandia National Laboratories, USA; C. A. Schuh, Massachusetts Institute of Technology, USA

Amorphous metals exhibit some impressive mechanical properties and two very disparate mechanical behaviors: glass-like flow at high temperatures and strain localization at low temperatures. However, the time and length scales associated with the microscopic plasticity are so disparate to those associated with the bulk response of these metals that a fundamental understanding of their behavior remains unresolved. We detail our efforts to bridge these time and length scales with a coarse-grained model based on the collective motion of several dozen atoms, known as the shear transformation zone (STZ). The stresses and strains associated with the shearing of the STZs are solved on a finite element mesh and the evolution of the model is governed by the kinetic Monte Carlo algorithm. The model captures glass-like flow and strain localization under the appropriate conditions in both 2D and 3D. Additionally, we have studied the complex behaviors of shear band propagation and microplasticity surrounding stress concentrations.

Session F: Spin Glasses

Room: Cumberland
Session Chairs: John McCloy, Pacific Northwest National Laboratory; Kostya Trachenko, Queen Mary University of London

8:00 AM

(GOMD-SII-053-2011) Understanding spin glass transition as a dynamic phenomenon (Invited)

K. Trachenko*, Queen Mary University of London, United Kingdom

Existing theories explain spin glass transition in terms of a phase transition and order parameters, by assuming the existence of a distinct thermodynamic spin glass phase. In addition to problems related to clarifying the nature of this phase, the common challenge is to explain profound dynamic effects. Here, we propose that spin glass transition can be understood as an entirely dynamic effect, without a reference to a distinct spin glass phase, phase transition and order parameters. In this theory, the susceptibility cusp at the glass transition temperature is due to the dynamic crossover between the high-temperature relaxational and low-temperature spin wave, or elastic, regime. The crossover takes place when t = [l#28#l]tau, where t is observation time and [l#28#l]tau is relaxation time. In our discussion, we explore the parallels between the structural and spin glass transition, and propose that both phenomena can be understood in the same approach based on the dynamic crossover.

8:40 AM

(GOMD-SII-054-2011) Ferroelectric Relaxors: Building Bridges between Theory and Applications (Invited)

E. Furman*, Q. Zhang, C. Randall, M. Lanagan, C. Pantano, Penn State University, USA

Ferroelectric relaxors present new opportunities in applications and continued challenges in theoretical understanding. We will review 3 areas of research on disordered materials that the authors currently engage in. Improvements in electrocaloric effect in inorganic and organic ferroelectric relaxors benefits from high and sustainable polarizability of relaxors. Novel ferroelectric relaxors are being developed for high-temperature capacitor applications. The requirements for such capacitors and recent progress in obtaining high-temperature inorganic relaxors will be outlined. Conventional glasses recently studied at Penn State have excellent electrical energy storage capability comparable to that of ferroelectric relaxors.

9:20 AM

(GOMD-SII-055-2011) Ion Irradiation Induced Property Changes in Granular Magnetite Films (Invited)

W. Jiang*, J. S. McCloy, A. S. Lea, Pacific Northwest National Laboratory, USA; J. A. Sundararajan, Q. Yao, Y. Qiang, University of Idaho, USA

Collections of magnetic particles can exhibit glassy behavior describable by viscosity models. This presentation will report our recent experimental results on the ion radiation induced property changes in granular magnetite films near room temperature. In contrast to single- or multi-layered nanostructures, very few irradiation studies have been performed to date on granular magnetic films. The study films, composed of loosely interconnected nanoparticles with average grain size of ~3 nm, were synthesized using a state-of-the-art nanocluster deposition system. The films are superparamagnetic but become magnetized fol-

lowing MeV Si2+ ion irradiation that leads to a transition to ferromagnetism. A significant increase in the grain size and a dramatic change in the microstructure are observed. Real-time particle clustering and structural evolution in the film under He+ ion irradiation will be shown. Interesting and unusual behavior of the ac and dc magnetic susceptibilities will be reported and discussed.

10:20 AM

(GOMD-SII-056-2011) First Order Reversal Curve Study of Artificially Structured Nanomagnets (Invited)

K. Liu*, University of California, USA

Realistic systems of nanomagnets inevitably have disorders and inhomogeneities, which can be "fingerprinted" by the first order reversal curve (FORC) method. Here we present recent FORC studies on a few technologically important systems. In prototype magnetic recording media, FORC captures irreversible switching due to residual domains pinned by defects/impurities; this leads to a microscopic magnetic memory effect that is also shown in spin glasses. In perovskite oxides, FORC yields quantitative information about the phase separation. In arrays of nanodisks, FORC reveals a crossover from single domain to vortex state, and illustrates the evolution of phase fractions with temperature. In patterned arrays of nanoellipses, FORC extracts quantitatively the interaction within the array. These results demonstrate that FORC is very sensitive to the presence of any disorders and heterogeneities in a system that exhibits hysteresis. Supported by NSF (ECCS-0725902, ECCS-0925626, DMR-1008791) and CITRIS.

11:00 AM

(GOMD-SII-057-2011) Cluster spin glass behavior in the Li-spinels (Invited)

T. W. Heitmann*, University of Missouri, USA

Percolation effects in magnetic systems have become increasingly important in recent years. Stripe formation in the cuprate superconductors and dynamical scaling in disordered quantum critical point materials are but two examples where magnetic spin clusters have emerged as drivers of the underlying physics. I will discuss our efforts to understand the magnetic cluster dynamics and the formation of a cluster spin glass state in a series of model systems. We study the LiM_2O_4 spinels, where M represents transition metal ions. I will focus on the series $Li_x[Mn_{1.96}Li_{0.04}]O_4$, with a particular emphasis on the mapping of its magnetic phase diagram as it pertains to magnetic clusters. This Li-spinel series is a particularly good test-bed for cluster spin dynamics studies owing to the ability to effectively tune the morphology of the clusters through extraction of Li from the host matrix. I will further discuss magnetic susceptibility and neutron scattering studies of these and the related compounds $LiMVO_4$, where M=Co, Ni, Fe.

11:40 AM

(GOMD-SII-058-2011) Glassy magnetic behavior in disordered Ni,Co:CuMn2O4 spinels (Invited)

J. S. McCloy*, Pacific Northwest National Laboratory, USA; C. Leslie, University of Washington, USA; W. Jiang, Pacific Northwest National Laboratory, USA

Spinels have long been known to exhibit considerable flexibility in incorporating various ions into their crystal structure, and magnetic spinel ferrites have been commercially important for inductors and microwave devices. We have studied some disordered spinels in the Ni,Co:CuMn2O4 system exhibiting complex re-entrant spin glass properties. Several compositions were investigated as a function of sintering temperature to study the effects of Cu and Mn valence on site preference and resulting magnetic properties. Helium ion microscopy shows porous structures, and AC magnetic susceptibility shows multiple magnetic transitions which depend on doping level and heat treatment. XPS data suggest that higher sintering temperatures produce Cu2+ rather than Cu+ and Mn3+ rather than Mn4+ in agreement with the literature. Spin glass transitions are noted around 25 K, 70 K, 90 K, and/or 110 K depending on composition and heat treatment.

Symposium IV: Glass Technology

Session A: Glasses for Energy and Environmental Applications

Room: Pulaski

Session Chair: Amanda Billings, Savannah River National Laboratory

8:00 AM

(GOMD-SIV-002-2011) Interactions of Viscous Glass Sealants with SOFC Stack Components

M. O. Naylor*, J. E. Shelby, S. T. Misture, Alfred University, USA

Silicate glasses were developed for viscous sealing of yttria stabilized zirconia (YSZ) electrolytes and aluminized stainless steel (SS) interconnects in intermediate temperature solid oxide fuel cells (SOFC). Many compositions form seals below 850°C and exhibit glass transition temperatures near 600°C even after partial crystallization. Powdered samples were heat treated for up to 1500 hours at 850°C to understand crystallization and thermal stability of evolved microstructures and interfaces. Select compositions were also heat treated at 650°C for long times. Partially crystallized sealants remain approximately 60% amorphous after long heat treatment times. Dissolution of alumina, yttria, and zirconia into the glass tends to inhibit crystallization for many compositions. A subset of the glasses have close CTE matches and survive thermal cycling in YSZ/SS test vehicles.

8:20 AM

(GOMD-SIV-003-2011) Near infrared down-conversion in chloro-sulfide glasses for the application on solar cell

B. Fan*, C. Point, J. Adam, X. Zhang, UMR CNRS-Université de Rennes I "Sciences Chimiques de Rennes", Laboratory of glasses and ceramics, France

A mismatch between sunlight spectrum and the spectral response of Si-based solar cells limits its conversion efficiency which can be improved by modification of the solar spectrum with down-conversion from UV/VIS to near infrared. Yb doped GeS_2-Ga_2S_3-CsCl glasses have been used for this purpose. Two types of down-conversion are observed. In the first case, the charge transfer state of Yb^{3+} provides a broad excitation band (>3000cm^{-1}) in visible with a strong emission around 1000nm. The position of this band can be evidently tuned by the composition of CsCl. In the second case where Yb^{3+} ion is co-doped with another RE^{3+} ion, quantum cutting from VIS to near infrared is achieved by energy transfer between the two ions. In addition, the RE^{3+} ions have much stronger absorption in sulfide glasses than in oxide or fluoride glasses. In conclusion, Yb^{3+} doped chloro-sulfide glass is promising for efficient near infrared down-conversion with broad and strong absorption.

8:40 AM

(GOMD-SIV-004-2011) Sintered Glass Core/Shell Waste Forms for 129I

T. Garino*, T. Nenoff, J. Krumhansl, D. Rademacher, Sandia National Laboratories, USA

A durable waste form for ^{129}I, present in spent nuclear fuel, has been developed using a low-temperature sintering glass and a core/shell structure where the ^{129}I-containing core is encased in a glass shell to protect it from the environment. In fuel reprocessing, $^{129}I_2$ vapor is passed over Ag-exchanged mordenite, a zeolite, to form insoluble AgI. AgI-mordenite is ground and mixed with a low temperature sintering Bi-Si-Zn-Al oxide glass powder to form the core. The core is then surrounded by pressed glass powder parts of the shell and the structure is then sintered at 550°C to form a non-porous monolith. Aqueous leaching studies show a high degree of durability. To avoid CTE-mismatch cracking, silica powder is added to the glass comprising the shell. In conclusion, a new type of durable waste form has been developed for the safe storage of ^{129}I. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:00 AM

(GOMD-SIV-005-2011) Immobilization of High and Low Aluminate Waste with Borosilicate Glass

F. C. Johnson*, Savannah River National Laboratory, USA

A near tank treatment system (NTTS) is currently being considered to treat Hanford S and SX high-level waste (HWL). This system includes a Continuous Sludge Leaching (CSL) process that will remove approximately 90% of the aluminum from the HLW sludge thereby facilitating HLW vitrification. The resulting leachate is then decontaminated by a near tank cesium ion exchange process so that it may be disposed of as low activity waste (LAW). NaOH is recovered from the leachate for re-use in the leaching process, while solidified CSL product is sent to the Integrated Disposal Facility (IDF). As part of a current DOE-EM task, borosilicate glass was selected as a potential waste form for the CSL product. Two levels of aluminate in the waste stream were studied. Formulation of these glass waste forms along with durability results will be discussed.

9:20 AM

(GOMD-SIV-006-2011) Incorporation of High TiO2 Concentrations in High Level Waste Glass

K. M. Fox*, F. C. Johnson, T. B. Edwards, Savannah River National Laboratory, USA

In 2014, Modular Salt Processing (MSP) will be used to disposition radioactive salt solution in the Savannah River Site Tank Farm. MSP will remove Cs-137 from salt solution using Crystalline Silicotitanate (CST) resin in a small column ion exchange (SCIX) apparatus. The salt solution will be struck with Mono Sodium Titanate (MST) to remove key actinides from the salt solution prior to being processed in the SCIX. The Cs-137 laden CST resin, MST and insoluble salt solids will be added to the high level sludge vitrified at the Defense Waste Processing Facility. These additional streams have the potential to impact the glass durability and processing constraints. In particular, the titanium concentration limit must be increased and higher concentrations of niobium and zirconium must be incorporated. This paper will present the results of experimental investigations into improved solubility of these components, as well as impacts to process control models.

10:00 AM

(GOMD-SIV-007-2011) Crystal Precipitation in Nuclear Waste Glasses and the Effects on Waste Form Durability

A. L. Billings*, J. W. Amoroso, Savannah River National Laboratory, USA

Borosilicate glass has been the waste form of choice for vitrifying high-level radioactive waste (HLW) in the US. As waste loadings increase, refractory components such as Al2O3 and Fe2O3 also increase, and crystal precipitation becomes more likely. Crystallization behavior of high waste loading glasses has been examined using isothermal heat treatments, various slow cooling profiles, SEM and quantitative XRD phase analysis. Typically, transition metal ferrite based spinel, nepheline, and lithium silicate crystalline phases are precipitated. The precipitation of these phases and the effects on glass durability using static durability tests (Product Consistency Testing) will be discussed.

10:20 AM

(GOMD-SIV-008-2011) Effect of Composition on Vapor Hydration Test Response of Phosphate Glasses for Low Activity Waste Vitrification

W. Lepry*, D. Kim, J. D. Vienna, Pacific Northwest National Laboratory, USA

The current baseline for immobilizing Hanford's low activity waste (LAW) is a borosilicate glass whose waste loading is limited by allowable concentrations of Na2O and SO3 that dictate the chemical durability and sulfate salt segregation. Phosphate based glasses offer significant increase in loading of wastes that are high in SO3. This study investigated the effect of glass composition on glass corrosion based on vapor hydration test (VHT). One-component-at-a-time change was used to vary glass compositions. Each glass underwent two extreme heat treatments: rapid cooling (quenching) and canister centerline cooling (CCC). For VHT, monolithic samples of 10×10×1.5 mm were exposed to water vapor at 200°C in a sealed stainless steel vessel. The corrosion rate was determined either by measuring the remaining glass thickness or by measuring alteration layer thickness. The paper discusses the effects of glass composition and heat treatment on VHT corrosion rate.

10:40 AM

(GOMD-SIV-009-2011) Characterization of Iron Phosphate Glasses Containing Simulated Hanford Low Activity Waste

S. T. Reis*, R. K. Brow, C. S. Ray, C. W. Kim, D. E. Day, Missouri University of Science and Technology, USA

The DOE intends to immobilize the Hanford low activity waste (LAW) using the vitrification technology. The DOE currently approves only borosilicate type glasses for such purposes. However, these wastes have complex and diverse chemical compositions, including components that are poorly soluble in borosilicate melts. Compared to borosilicate glasses, phosphate glasses can readily dissolve larger amounts of many of these problematic components including S, Al, P, Na, halides, and heavy metals and so it offers one solution to reducing the overall volume of waste glasses required to immobilize LAW. In the present work, the properties and phase distributions of iron phosphate glasses containing up to 35 wt% of Hanford LAW AZ-102 simulant were characterized. Compositions that exceed the DOE corrosion standards were identified. The solubility of sulfate species was characterized by micro-Raman spectroscopy and will be discussed in relation to glass composition and melting conditions.

Session C: Glasses for Medicine and Biotechnology

Room: Ossabaw
Session Chair: Brad Tischendorf, Medtronic

10:20 AM

(GOMD-SIV-014-2011) Controlling the Formation of Calcium Compounds when Bioactive Glasses React In-vivo

S. Jung, Mo-Sci Corporation, USA; D. E. Day*, Missouri University of Science and Technology, USA

The present work focused on controlling the formation of calcium containing compounds formed in-vivo by adding dopants to bioactive borate glasses. Scaffolds composed of randomly oriented borate glass fibers progressively doped with copper (Cu), strontium (Sr), zinc (Zn), and iron (Fe) were implanted in the subcutaneous tissue of rats for up to six weeks. Scanning electron microscopy (SEM) and x-ray diffraction (XRD) showed that the un-doped fibers had fully converted to hydroxyapatite (HA) in four weeks. The Cu-doped scaffold converted to HA, but at a slower rate than the un-doped borate glass. The progressive additions of Sr, Zn, and Fe to the Cu-doped borate glass decreased the amount of HA and increased the amount of calcium carbonate (calcite) in the reacted fibers until only calcite was detected by XRD. It is concluded that dopants such as those used in this study can control the type of reaction products formed when borate glass fibers react with body fluids.

10:40 AM

(GOMD-SIV-015-2011) Effect of Microstructure on the Strength of Glass-infiltrated Ceramic Composite for Artificial Teeth

H. Lim*, C. Kim, Inha University, Republic of Korea

Glass-infiltrated ceramic composite, which can be used for a dental restoration, was prepared by infiltrating glasses into a pre-sintered ceramics, such as alumina, sapphire, and zirconia. The effects of pre-sintering temperature and infiltration temperature on the microstructures of the preform and the glass-infiltrated ceramics were studied. The biaxial strengths of the composites were discussed in terms of microstructures obtained. The infiltrated glass corroded ceramic preforms, and the dissolved ceramics re-precipitated on the ceramic grains during the heat-treatment for infiltration. The higher biaxial strength was obtained in the samples with smaller and tabular shape of grains because crack propagation was deflected around ceramic particles. The highest strength of 590 MPa was observed for the glass-alumina composite. Glass-infiltrated sapphire showed the better translucency than other glass-ceramic composites.

11:00 AM

(GOMD-SIV-016-2011) Kinetic analysis of dissolution behavior of bio-active borate and silicate glasses in aqueous solutions

J. George*, R. Brow, Missouri University of Science and Technology, USA

Bioactive 13-93 glass, along with borosilicate and borate analogues, have been studied for use in scaffolds for bone tissue repair. The present work provides a kinetic analysis of the dissolution behavior of such glasses in buffered potassium phosphate solutions and deionized water. Glass powders were reacted at temperatures between 25 and 60 °C. The release of Si- and B-ions into all solutions were measured by ICP and Ca- and P- ion concentrations were also measured for samples reacted in deionized water. Reaction end-products, including hydroxyapatite, were characterized by x-ray diffraction, micro-Raman spectroscopy, and analytical SEM. The borate-based glasses react faster than 13-93 under all conditions and follow a reaction-controlled kinetic model. In contrast, the silicate glass reaction kinetics are better described by a diffusion controlled model.

11:20 AM

(GOMD-SIV-017-2011) Crystallisation of Strontium Bioactive Glasses

M. D. O'Donnell*, RepRegen Ltd, United Kingdom; L. Chapman, National Physics Laboratory, United Kingdom; H. Tang, Imperial College, United Kingdom; P. Tomlins, National Physics Laboratory, United Kingdom; J. Jones, Imperial College, United Kingdom

Bioactive glasses (BGs) have been used for hard tissue regeneration for over 30 years and clinically since 1993 in orthopedic, spinal, CMF and periodontal applications (e.g. StronBone and NovaBone). Strontium is an attractive addition to BGs due to its up-regulation of osteoblasts and down-regulation of osteoclasts [1]. Bioglass (45S5) is unsuitable for sintering above the glass transition temperature (Tg) as it crystallizes to wollastonite and combeite; this reduces bioactivity which limits usage in applications such as porous granules, scaffolds, coatings and fibres. Here we have developed a series of strontium-substituted glasses with enhanced thermal stability above Tg enabling the production of fully amorphous porous structures. ACKNOWLEDGMENTS: Technology Strategy Board (TSB) grant number BY106G

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