2010 GLASS & OPTICAL MATERIALS DIVISION ANNUAL MEETING

May 16-20, 2010

Corning, NY

Radisson Hotel Corning

FINAL PROGRAM

The American Ceramic Society
www.ceramics.org

Welcome

Greetings and welcome to the 2010 Glass & Optical Materials Division Meeting (GOMD 2010). This exciting Spring program will examine all aspects of the glassy state, from the initial melting and forming processes to glass structure-property relationships and cutting-edge applications. Four concurrent symposia are planned, along with a special symposium to honor the memory of Prof. Robert H. Doremus. Sessions organized by technical leaders from industry, government laboratories, and academia will highlight a wide range of topics in glass science and technology, with emphasis on interdisciplinary studies incorporating physics, chemistry, materials science, mathematics, and engineering.

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 focusing on careers in glass will not want to miss the "Unwritten Rules for Career Success" session planned for Monday during lunch time. Don't miss out on the opportunity to continue your learning experience by attending the Poster Session on Monday evening and be sure to check out the posters entered in the student poster contest.

In addition to 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), don't miss the Otto Schott Research Award and Reception on Tuesday evening. Also, plan to be our guest for the conference dinner on Tuesday evening after the Otto Schott Research Award reception concludes.

Two events will take place after the GOMD conference concludes where you can continue your glass education and knowledge exchange.

- The Usable Glass Strength - Forming a Research Coalition Workshop sponsored by GMIC and DOE will cover significant improvement of the usable strength of commercial glass products and will establish a research coalition to support a multi-year glass strength research agenda. Full GOMD 2010 registration includes this Workshop, but space is limited. Please sign up to attend the Workshop.
- The Fundamentals of Glass Science and Technology Short Course will take place after the GOMD meeting concludes. This course will cover basic glass science and technology in order to broaden or improve one's foundation in the understanding of glass as a material of choice. Separate registration is required for participation in this course.

We extend special thanks to our award sponsors: PPG Industries, Inc. for the George W. Morey Award, Coe College and Corning Incorporated for the Stookey Lecture of Discovery Award, SCHOTT North America for sponsoring lunch for the Norbert J. Kreidl Award for Young Scholars and the Otto Schott Research Award, and Corning Incorporated for the Student Poster Contest.

While in Corning, you will enjoy visiting the Corning Museum of Glass, which includes the world's best collection of art and historical glass, hands-on exhibits, and a fully equipped glass-working studio. Corning is home to dozens of award-winning wineries. Visitors are also encouraged to take this opportunity to visit Alfred University (about 45 miles west), home of the world-recognized education and research program in glass science and engineering.

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 in Corning.

John Mauro
2010 ACerS Glass & Optical Materials Division Program Chair
Corning Incorporated

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Glass & Optical Materials Division Officers

Chair
Mark Davis
SCHOTT North America, Inc.

Vice Chair
John Ballato
Clemson Research Park AMRL

Chair-Elect
Steve W. Martin
Iowa State University

Secretary
Kelly Simmons-Potter
University of Arizona

Special Thanks to Our Sponsors For Their Generosity:

PPG Industries Inc.
Sponsor of the George W. Morey Award

Corning Incorporated & Coe College
Sponsors of the Stookey Lecture of Discovery Award

Corning Incorporated
Sponsor of the Student Poster Competition

SCHOTT North America
Sponsor of the Norbert J. Kreidl Award for Young Scholars Lunch and
Otto Schott Research Award

Program Schedule-At-A-Glance

3 – 7 pm Registration in the Ballroom Foyer

7 am – 7 pm Registration in the Ballroom Foyer

7:30 am – 7 pm Registration in the Ballroom Foyer

7:30 am – 5:30 pm Registration in the Ballroom Foyer

Sunday, May 16

Time	Cayuga	Keuka	Seneca	Carder
5:00 - 7:00 pm		Welcome Reception		

Monday, May 17

8:00 - 9:00 am		Stookey Award Lecture		
9:30 am - Noon	Atomistic Modeling of Glass I: Techniques	Robert H. Doremus Memorial Session I	Glass-Ceramics	
Noon - 1:00 pm			"Unwritten Rules of Career Success" Student Activity	
1:15 - 5:00 pm	Atomistic Modeling of Glass II: Applications	Robert H. Doremus Memorial Session II	High-Strength Glasses	
5:00 - 6:00 pm			GOMD Business Meeting	
6:00 - 8:00 pm				Poster Session

Tuesday, May 18

8:00 - 9:00 am		Morey Award Lecture		
9:15 - Noon	Topology and Rigidity I	Glass Structure and Properties I: Silicates	Glasses for Medicine and Biotechnology	
Noon - 1:00 pm		Kreidl Award Lecture*		
1:00 - 5:00 pm	Rheology	Glass Structure and Properties II: Simulations and Chalcogenides	Glasses for Energy and Environmental Applications	Short-term Corrosion Issues I
		Glass Structure and Properties III: Phosphates		Short-term Corrosion Issues II
5:00 - 6:00 pm				Otto Schott Research Award**
7:00 - 10:00 pm		Conference Dinner		

Wednesday, May 19

8:00 am - Noon	Topology and Rigidity II	Photoinduced Structural Changes in Glass	Melting & Process Modeling	Ancient and Analogue Glasses
	Glass Transition and Relaxation I		Optical Materials I	Modelings
1:15 - 5:15 pm	Glass Transition and Relaxation II	Glass Structure and Properties IV: More Fun with the Vitreous State	Optical Materials II	Long-term Corrosion Testing
	Glass Transition and Relaxation III			

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

**Otto Schott Research Award reception in hotel lobby immediately following award ceremony.

"Unwritten Rules of Career Success" – Student Activity

Monday, May 17th – Noon to 1 pm – Seneca

Gary Pease, Corning Incorporated

Students, do you wonder how you will navigate your career? Come to this insightful session given by Gary Pease, Director of Human Resources at Corning, and learn about critical career success rules that are not normally documented. The session will focus on building skills, knowledge, experiences and relationships that prepare you for those organizational expectations that are not always communicated. Learn the importance of gaining perspective from people with different experience levels and cultural backgrounds.

Lunch will be provided to students participating in this session on a first come, first served basis.

Usable Glass Strength - Forming a Research Coalition Workshop

Sponsored by

The Workshop covers significant improvement of the usable strength of commercial glass products and will establish a research coalition to support a multi-year glass strength research agenda.

Wednesday, May 19th - 1 to 9 PM

- Tour of World Kitchen
- Dinner with Keynote Speaker: David L. Morse, Corning Incorporated, Senior Vice President - Science and Technology, and Director Corporate Research - Topic: "Thin Strong Glass"

Thursday, May 20th - 8 AM to 4 PM

- Morning Session: Presentation by Strategic Strength Team of Strawman proposal identifying challenges, requirements, and opportunities for developing strong glass
- Luncheon: Keynote Speaker from Owens Corning Speaker (TBD), "Open Innovation - The Radical Future of R&D - across Corporate and National Boundaries"
- Afternoon Session: The Core Research Team will present a review of the key research areas and their proposals for 3 key research initiatives in each of 6 focus areas

Fundamentals of Glass Science and Technology Short Course

May 20-21, 2010 ~ 1 p.m. to 5:30 p.m./8 a.m. to 5 p.m.

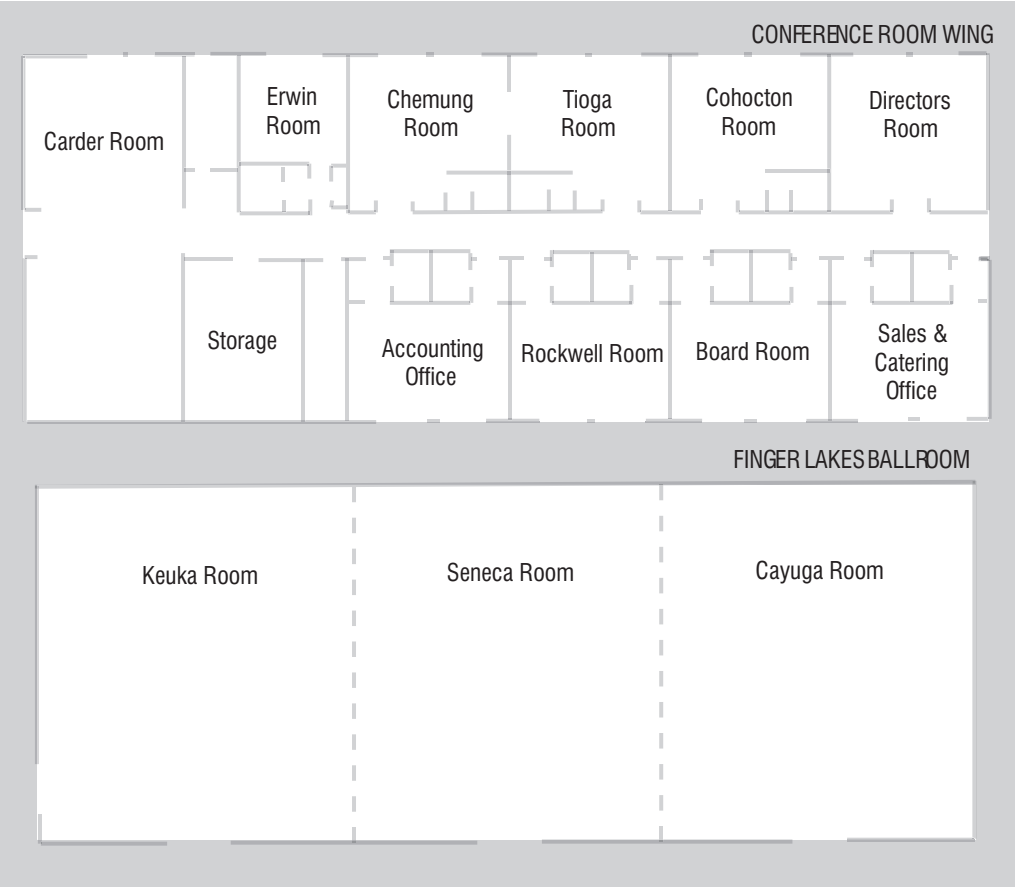
Instructor: Arun K. Varshneya, Alfred University

Course covers basic glass science and technology in order to broaden or improve one's foundation in the understanding of glass as a material of choice. This one and a half day course covers following topics:

- Glass science (commercial glass families, glassy state, nucleation and crystallization, phase separation, glass structure)
- Glass technology, batch calculations
- Glass melting and forming
- Glass properties and engineering principles
- Elementary fracture analysis

Please note that separate registration is required to participate in the Fundamentals of Glass Science and Technology Short Course.

Radisson Hotel Corning Floor Plan



Special Events

Welcome Reception
Sunday, May 16th
5 to 7 pm
Keuka

"Unwritten Rules of Career Success"
Student Activity
Monday, May 17th
Noon to 1pm
Seneca

Poster Session
Monday, May 17th
6 to 8 pm
Carder, Tioga, and Chemung

Otto Schott Research Award Reception
Tuesday, May 18th
6 to 7 pm
Hotel Lobby

Conference Dinner (included with registration fee)
featuring Gregory A. Merkel
"The History, Technology, and Artistry of Iridescent Glassware"
Tuesday, May 18th
7 to 9 pm
The Finger Lakes Ballroom

The creation of iridescent glassware "at the furnace" represents one of the more recent decorative techniques developed in glassmaking over the past 4000 years. Followed by the development of "in situ" metallic lusters on copper- and silver-containing glasses, these two innovations were combined and brought to their artistic pinnacle by Tiffany Furnaces in the 1890s, and were further popularized by Steuben Glass Works in the early 20th century. The technological history behind these exquisite objects spans 1500 years of invention, discovery, happenstance, and lost art, and the unique visual impressions conveyed by these objects rely upon the application of nanotechnologies that were developed long before the advent of electron microscopy.

Award Lectures

The Stookey Lecture of Discovery
Monday, May 17 at 8 am – Keuka/Seneca

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.

Tetsuro Izumitani, Title, Affiliation
Location
Title of Talk
Sponsored by Corning Incorporated and Coe College

The George W. Morey Award
Tuesday, May 18 at 8 am – Keuka/Seneca

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: Minoru Tomozawa, Professor, Rensselaer Polytechnic Institute
Troy, New York, USA
Presentation Title: "Glass and Water"
Sponsored by PPG Industries Inc.

The Norbert J. Kreidl Award for Young Scholars
Tuesday, May 18 at 12 pm – Keuka

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: Morten M. Smedskjaer, Aalborg University,
Aalborg, Denmark
Presentation Title: "Inward Diffusion of Modifying Ions in Glasses and Glass-Ceramics"
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.

The Otto Schott Research Award
Tuesday, May 18 at 5 pm – Carder

The ***Otto Schott Research Award*** recognizes outstanding achievements in basic research, technology, and applications within the field of materials, especially glasses, glass ceramics, and other optical materials or components made thereof.

Award Winner: Prof. Dr. Tanguy Rouxel, LARMAUR (Applied Mechanics Laboratory),
University of Rennes 1, Rennes, France
Presentation Title: "The Brittle to Ductile Transition in Glass: Fundamental and Technological Challenges"
Sponsored by SCHOTT North America Inc.

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Registration Requirements: Attendance at any meeting of the Society shall be limited to duly registered persons.

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Monday, May 17, 2010

Stookey Lecture of Discovery Award

Room: Keuka

8:00 AM

TBA

Symposium I: Robert H. Doremus Memorial Symposium

Robert H. Doremus Memorial Session I

Room: Keuka

Session Chairs: Mark Davis, Schott North America, Inc.; Minoru Tomozawa, RPI

9:30 AM

Opening Remarks
Mark Davis, Schott North America, Inc.; Minoru Tomozawa, Rensselaer Polytechnic Institute

9:45 AM

(GOMD-SI-001-2010) Dr. Doremus - Professor of Liberal Arts (Invited)
A. G. Chan*, Shore Chan Bragalone LLP, United States

10:00 AM

(GOMD-SI-002-2010) Gases in Glasses: The Doremus Perspective (Invited)
J. E. Shelby*, Alfred University, United States

10:30 AM

(GOMD-SI-003-2010) Gas Solubility in Glasses - The Doremus Contributions
J. F. Shackelford*, University of California - Davis, United States

10:45 AM

(GOMD-SI-004-2010) Water diffusion in silica glass (Invited)
M. Tomozawa*, RPI, United States

11:15 AM

(GOMD-SI-005-2010) Diffusion of Water in Quartz: Application to Crystal Growth Kinetics (Invited)
P. D. Ihinger*, University Wisconsin-Eau Claire, United States

11:45 AM

(GOMD-SI-006-2010) Diffusion of Alkali and Alkaline Earth Ions in Silicate Glasses and its Correlation with Liquid Fragility
M. M. Smedskjaer*, Aalborg University, Denmark; J. C. Mauro, Corning Incorporated, United States; J. Deubener, Clausthal University of Technology, Germany; Y. Yue, Aalborg University, Denmark

Symposium II: Glass Science

Atomistic Modeling of Glass I. Techniques

Room: Cayuga

Session Chair: Ulrich Fotheringham, Schott AG

9:30 AM

(GOMD-SII-001-2010) Developing effective potentials from ab initio simulations of amorphous systems (Invited)
W. Kob*, Universite Montpellier II, France; A. Carré, Deutsches Zentrum fur Luft und Raumfahrt (DLR), Germany; J. Horbach, Universite Montpellier II, France; S. Ispas, Deutsches Zentrum fur Luft und Raumfahrt (DLR), Germany

10:00 AM

(GOMD-SII-002-2010) Energy Landscapes and Beyond: A Systematic Approach to Understand the Properties of Supercooled Liquids (Invited)
A. Heuer*, O. Rubner, C. Rehwald, Institut für Physikalische Chemie, Germany

10:30 AM

(GOMD-SII-003-2010) Achieving Long Time Scales in Energy Landscape Simulations using Metabasin Partitioning
R. J. Loucks*, Alfred University, United States; J. C. Mauro, Corning Incorporated, United States; P. K. Gupta, Ohio State University, United States

10:45 AM

(GOMD-SII-004-2010) Simulations of Network Glasses with Multiple Coordination States using a Reactive Force Field
L. Huang*, F. Yuan, Rensselaer Polytechnic Institute, United States

11:00 AM

(GOMD-SII-005-2010) Parallel Atomistic Monte Carlo Computations
A. Zakharian*, D. Vargheese, P. Diep, Corning Incorporated, United States

11:15 AM

(GOMD-SII-006-2010) Reverse Monte Carlo Structures: Evaluation by Molecular Dynamics Simulations
C. R. Mueller*, Technische Universität Ilmenau, Germany; M. Schuch, P. Maass, Universität Osnabrück, Germany; V. Petkov, Central Michigan University, United States

11:30 AM

(GOMD-SII-007-2010) Electronic structure based material design: application to a-Si
D. A. Drabold, B. Cai*, Ohio University, United States; A. Goodwin, Oxford University, United Kingdom

11:45 AM

(GOMD-SII-008-2010) Origin of Dynamical Heterogeneities in Calcium Aluminosilicate Liquids
K. D. Vargheese*, A. Tandia, J. C. Mauro, D. Phong, A. Rovelstad, Corning Inc, United States

Symposium III: Glass Technology

Glass-Ceramics

Room: Seneca

Session Chairs: Robert Schaut, Corning Incoporated; Linda Pinckney, Corning Incorporated (ret.)

9:30 AM

(GOMD-SIII-001-2010) Controlled nucleation and crystallization of glass-ceramics (Invited)
W. Hoeland*, V. Rheinberger, C. Ritzberger, E. Apel, Ivoclar vivadent AG, Liechtenstein

10:00 AM

(GOMD-SIII-002-2010) The early stages of glass ceramics devitrification
W. Bras*, Netherlands Organization for Scientific reserach (NWO), France; N. Greaves, Aberystwyth University, United Kingdom; S. Clark, M. Kunz, Lawrence Berkeley National Laboratory, United States; S. Nikitenko, Netherlands Organization for Scientific reserach (NWO), France; G. Bruno, Corning SAS, France; V. Radmilovic, Lawrence Berkeley National Laboratory, United States

10:15 AM

(GOMD-SIII-003-2010) Crystallization of Lithium silicate Glass-ceramics for artificial teeth
C. Kim*, C. Kim, Inha Univ., Republic of Korea

10:30 AM

(GOMD-SIII-004-2010) A secondary ion mass spectroscopy (SIMS) and Mössbauer study of modified ZBLAN glasses
M. Vu*, A. Terekhov, G. Murray, University of Tennessee Space Institute, United States; S. Schweizer, Fraunhofer Institute, Germany; R. Weber, Materials Development Inc., United States; C. Johnson, J. Johnson, University of Tennessee Space Institute, United States

10:45 AM

(GOMD-SIII-005-2010) Nucleation and growth of glass-ceramics by in-situ High-Temperature X-ray diffraction and Small Angle Neutron Scattering
C. Fernandez-Martin, G. Bruno*, P. Pradeau, M. Comte, Corning SAS- CETC, France

11:00 AM

(GOMD-SIII-006-2010) WITHDRAWN

*Denotes Presenter

11:15 AM

(GOMD-SIII-007-2010) Influence of zirconium and titanium on the crystallization of a calcium aluminosilicate melt
E. Strukelj, Corning SAS, France; M. Roskosz, Université Lille 1, France; M. Comte*, Corning SAS, France; P. Richet, IPGP, France

11:30 AM

(GOMD-SIII-008-2010) Second harmonic generation and giant dielectric response in $BaTi_2O_5$ glass-ceramics
A. Masuno*, Y. Kikuchi, H. Inoue, Y. Watanabe, The University of Tokyo, Japan; J. Yu, Japan Aerospace Exploration Agency, Japan

11:45 AM

(GOMD-SIII-009-2010) Fluoride Nanoscintillators
L. G. Jacobsohn*, K. Sprinkle, C. J. Kucera, T. L. James, T. A. DeVol, J. Ballato, Clemson University, United States

12:00 PM

(GOMD-SIII-010-2010) Preparation of Apatite-Wollastonite-Phlogopite glass-ceramic composites by powder sintering method
A. Faeghi Nia*, Tabriz university, Islamic Republic of Iran

Symposium I: Robert H. Doremus Memorial Symposium

Robert H. Doremus Memorial Session II

Room: Keuka

Session Chairs: Mark Davis, Schott North America, Inc.; Minoru Tomozawa, RPI

1:30 PM

(GOMD-SI-007-2010) Gold in glass: A new state of conduction? (Invited)
H. Jain*, Lehigh University, United States; R. Böhmer, O. Kanert, R. Kuechler, Technical University of Dortmund, Germany

2:00 PM

(GOMD-SI-008-2010) Morphology and Optical Properties of Laser-Patterned Crystals in Glasses (Invited)
T. Komatsu*, T. Honma, Nagaoka University of Technology, Japan

2:30 PM

(GOMD-SI-009-2010) An investigation of microstructure, mechanical and biocompatibility characteristics of yttrium and fluoride doped nano hydroxyapatite
Z. Evis*, S. Toker, A. Tezcaner, D. Keskin, Middle East Technical University, Turkey

2:45 PM

(GOMD-SI-010-2010) Contributions of Robert H. Doremus in the Field of Crystallization Kinetics
M. Davis*, SCHOTT North America, Inc., United States

3:00 PM

Break

3:15 PM

(GOMD-SI-011-2010) MeV Ion Beam Analysis of Glass and Ceramic Surfaces (Invited)
W. A. Lanford*, University at Albany SUNY, United States

3:45 PM

(GOMD-SI-012-2010) Novel Glasses for On-Chip Microelectronic Applications (Invited)
V. J. McGahay*, IBM Corporation, United States

4:15 PM

(GOMD-SI-013-2010) Viscosity of Germania-Doped High Purity Fused Silica Glass
E. M. DeLiso*, Stanton Advanced Ceramics, Inc., United States

4:30 PM

(GOMD-SI-014-2010) Extrusion of Tellurite Glass for Optical Fiber Preforms (Invited)
A. A. Belwalkar*, W. Z. Misiolek, J. Toulouse, Lehigh University, United States

4:45 PM

Closing Remarks
Mark Davis, Schott North America, Inc.; Minoru Tomozawa, Rensselaer Polytechnic Institute

Symposium II: Glass Science

Atomistic Modeling of Glass II. Applications

Room: Cayuga

Session Chair: Jincheng Du, University of North Texas

1:15 PM

(GOMD-SII-009-2010) Spatial and dynamic correlations in alkali transport in silicate glasses by atomic simulation and virtual reality modelling (Invited)
N. Greaves*, Aberystwyth University, United Kingdom

1:45 PM

(GOMD-SII-010-2010) A Molecular Dynamics Study of the Structure and Elastic Properties of Sodium Silicate and Sodium Aluminosilicate Glasses
L. Adkins*, A. N. Cormack, Alfred University, United States

2:00 PM

(GOMD-SII-011-2010) Local structure around Eu(III) ions in aluminate glasses
H. Inoue*, K. Ohno, Y. Watanabe, A. Masuno, The University of Tokyo, Japan

2:15 PM

(GOMD-SII-012-2010) Ab initio calculation of mixed ion dynamics in Silver/Copper doped chalcogenide glass
B. K. Prasai*, B. Cai, D. A. Drabold, Ohio University, United States

2:30 PM

(GOMD-SII-013-2010) The environments of cerium ions in cerium-doped aluminophosphate and phosphosilicate glasses: combining molecular dynamics simulations and ab initio DFT calculations
J. Du*, L. Kokou, University of North Texas, United States

2:45 PM

(GOMD-SII-014-2010) Influence of the Modifier Cation Type on the Infrared Spectral Response of Multi-Component Glasses
A. K. Upadhyay*, K. Becker, J. Kieffer, University of Michigan, United States

3:00 PM

Break

3:15 PM

(GOMD-SII-015-2010) First-principles simulations of glasses: Establishing the rings statistics in B_2O_3 and B_2S_3 (Invited)
G. Ferlat*, Université Paris VI, France

3:45 PM

(GOMD-SII-016-2010) Monte Carlo Simulations of Inert Gas Solubility in Silicate Glasses and Melts
A. Zakharian*, A. Tandia, D. Vargheese, P. Diep, Corning Incorporated, United States

4:00 PM

(GOMD-SII-017-2010) Glass-like dislocation dynamics of degenerate 2D dimer crystals
U. Agarwal*, S. J. Gerbode, I. Cohen, F. A. Escobedo, Cornell University, United States

4:15 PM

(GOMD-SII-018-2010) MD simulations of soda lime silicate glasses with increasing calcia content
A. Cormack, A. Collier*, Alfred University, United States

4:30 PM

(GOMD-SII-019-2010) Molecular Scale Characterization of Mechanical and Structural Properties of xAl2O3–(1-x)SiO2
A. Tandia*, K. Vargheese, Corning Incorporated, United States

4:45 PM

(GOMD-SII-020-2010) Molecular simulations to explore the energy landscape of surface wetting transitions of an oily fluid on a rough surface
E. Savoy*, Corning, Inc, United States; F. Escobedo, Cornell University, United States

Symposium III: Glass Technology

High-Strength Glasses

Room: Seneca

Session Chairs: Arun Varshneya, Alfred University; William LaCourse, Alfred University; Murli Manghnani, University of Hawaii; Tanguy Rouxel, Universite De Rennes 1

1:15 PM

(GOMD-SIII-011-2010) Edge-on Impact Investigations of Stress and Damage Propagation in Monolithic and Novel Laminate Glass and Glass Ceramics (Invited)
E. Strassburger, Ernst-Mach-Institut (EMI),, Germany; P. Patel, Army Research Laboratory, United States; A. Varshneya, Alfred University, United States; J. W. McCauley*, Army Research Laboratory, United States

1:45 PM

(GOMD-SIII-012-2010) Strength of chemically strengthened glass
T. Komai*, Nippon Electric Glass Co.,Ltd, Japan

2:00 PM

(GOMD-SIII-013-2010) Environmentally Friendly Chemically Strengthened Glasses
M. Dejneka*, Corning, United States; C. Chapman, Corning, United States; S. Gomez, Corning, United States; K. Rossington, Corning, United States

2:15 PM

(GOMD-SIII-014-2010) Influence of Edge Preparation on Impact Resistance of Thin Chemically Strengthened Glass
P. K. Kreski*, Alfred University, United States; A. K. Varshneya, Saxon Glass Technologies, Inc., United States

2:30 PM

(GOMD-SIII-015-2010) Effect of different alkalis on the ion-exchange ability of high strength glasses
S. Gomez*, M. J. Dejneka, R. M. Morena, L. A. Lamberson, Corning Incorporated, United States

2:45 PM

General discussion

3:00 PM

Break

3:15 PM

(GOMD-SIII-016-2010) Damage propagation in high strength glasses rods due to high velocity ball impact (Invited)
G. Subhash*, University of Florida, United States

3:45 PM

(GOMD-SIII-017-2010) On the Measurement of Design-Relevant Fracture Properties of Structural Glasses and Ceramics
K. Iyer*, Exponent, Inc., United States

4:00 PM

(GOMD-SIII-018-2010) Using two-point bend technique to predict failure strength of glass fibers
Z. Tang*, R. K. Brow, Missouri S&T, United States; C. R. Kurkjian, University of Southern Maine, United States; N. P. Lower, Rockwell Collins, Inc., United States

4:15 PM

(GOMD-SIII-019-2010) Flaw Distribution Measurements in High Strength Glass via the Hertzian Cone Crack Test
I. Reimanis*, J. A. Jones, Colorado School of Mines, United States; R. A. Schaut, Corning Incorporated, United States

4:30 PM

(GOMD-SIII-020-2010) Crack Propagation in a Soda-Lime Phosphosilicate Glass in Relation to Devitrification
J. Erb*, A. Kovalskiy, H. Moawad, B. Koel, H. Jain, Lehigh University, United States

4:45 PM

(GOMD-SIII-021-2010) What's New in Thermal Tempering of Silicate Glasses?
S. Gulati*, B. Suman, Corning Inc., United States

Posters

Room: Carder

6:00 PM

(GOMD-SII-P001-2010) The Application of Constraint Theory to Self-Organization of Naturally-Occurring Molecules
B. D. Esham*, Alfred University, United States; J. C. Mauro, Corning Incorporated, United States; R. J. Loucks, G. J. McGowan, Alfred University, United States

(GOMD-SII-P002-2010) Electronic Structure Evolution of Phase Change Memory Materials: Ge2Sb2Te5
D. A. Drabold, B. Cai*, Ohio University, United States; S. R. Elliott, Cambridge University, United Kingdom

(GOMD-SII-P003-2010) Qn Speciation in Binary Alkali Silicate Glasses
C. L. Hogue*, A. J. Ellison, S. E. Koval, R. E. Youngman, Corning Incorporated, United States

(GOMD-SII-P004-2010) Intermediate glass prepared by high pressure and temperature treatment of silica glass
C. Li*, M. Tomozawa, J. D. Price, E. Watson, Rensselaer Polytechnic Institute, United States

(GOMD-SII-P005-2010) Thermally Darkening Photochromic Glasses for Visible Polarizers
C. Chapman*, T. Seward, N. Borrelli, M. Dejneka, Corning Incorporated, United States

(GOMD-SII-P006-2010) Photothermal Effects in Chalcogenide Glasses
D. Zhao*, Lehigh University, United States; P. R. Pedreira, L. C. Malacarne, M. L. Baesso, Maringá State University, Brazil; H. Jain, Lehigh University, United States

(GOMD-SII-P007-2010) Conductivity of Sodium Borophosphate Glasses
G. Olson*, R. Christensen, S. W. Martin, Iowa State University, United States

(GOMD-SII-P008-2010) A New 2D MAS approach for quantifying Q(n) species in oxide glass
K. K. Dey*, D. Kaseman, M. Davis, P. J. Grandinetti, The Ohio State University, United States

(GOMD-SII-P009-2010) Fabrication of novel SbSI-based IR-transparent ferroelectric glass-ceramic
L. Ding*, H. Jain, Lehigh University, United States; G. Chen, East China University of Science and Technology, China

(GOMD-SII-P010-2010) Properties of high density silica glass prepared by high pressure quenching routes
L. Huang, F. Yuan*, Rensselaer Polytechnic Institute, United States

(GOMD-SII-P011-2010) Glasses with temperature and/or pressure independent elastic moduli
L. Huang, Q. Zhao*, Rensselaer Polytechnic Institute, United States

(GOMD-SII-P012-2010) Colloidal Behavior of Alkali Borosilicate Glasses
L. Lamberson*, Corning Incorporated, United States

(GOMD-SII-P013-2010) Understanding Oxide-Polymer Interfaces Using Solid-State NMR and Inverse Gas Chromatography
L. Ortiz Rivera*, D. L. Suchy, K. T. Mueller, Penn State University, United States

(GOMD-SII-P014-2010) Analytical thermodynamic modeling of the iron redox ratio in phosphate glasses
M. L. Schmitt*, R. K. Brow, Missouri S&T, United States

(GOMD-SII-P015-2010) Quantifying Q(n)-species in a potassium disilicate glass by 29Si magic angle flipping nuclear magnetic resonance
M. Davis*, K. Sanders, D. Kaseman, S. Parvani, K. K. Dey, P. J. Grandinetti, Ohio State University, United States

(GOMD-SII-P016-2010) EPR study of Ti3+ ions formed under ionizing irradiation in oxide glasses
P. Lombard, N. Ollier*, B. Boizot, CEA, France

(GOMD-SII-P017-2010) Enthalpy of Mixing of Mixed Alkali Glasses
P. J. Lezzi*, M. Tomozawa, RPI, United States

(GOMD-SII-P018-2010) An analysis of borate glasses and crystals using 10B quadrupolar NMR obtained from a field swept magnet
M. McConnell*, K. Tholen, J. Berkowitz, M. Affatigato, S. Feller, Coe College, United States; T. Kemp, D. Holland, M. Smith, University of Warwick, United Kingdom

(GOMD-SII-P019-2010) Physical Properties and Structure of Alkali Borovanadate Glasses
S. Feller, J. North*, A. Ramm, H. Feller, J. Maldonis, Coe College, United States; J. McKnight, B. Baker, P. Bunton, William Jewell College, United States; V. Michaelis, S. Kroeker, University of Manitoba, Canada; M. Vu, M. Affatigato, Coe College, United States

(GOMD-SII-P020-2010) An Al-27 MAS NMR study of the Ca-Al binary metallic glass forming system and related alloys
T. Mullenbach*, Coe College, United States; M. Pierson-Stull, R. Youngman, T. Kiczenski, Corning Incorporated, United States

(GOMD-SII-P021-2010) Crystallization in Sugar Glass and Its Melts - Low Cost Experiments in Glass
W. R. Heffner, S. A. Horst*, Lehigh University, United States

(GOMD-SII-P022-2010) A Low-Cost Student Built DTA for Exploring the Glass Transition
W. R. Heffner*, Lehigh University, United States

(GOMD-SII-P023-2010) Low-cost, hands-on activities in glass science
W. R. Heffner, H. Jain*, Lehigh University, United States

(GOMD-SIII-P024-2010) Lattice orientation analysis of single crystal architecture created in LaBGeO5 glass by femtosecond laser
A. Stone*, H. Jain, V. Dierolf, Lehigh University, United States; K. Miura, K. Hirao, Kyoto University, Japan

(GOMD-SIII-P025-2010) Effect of flour source on sintering and crystallization of Fluoro-Phlogopite glass-ceramic
A. Faeghi Nia*, Tabriz University, Islamic Republic of Iran; M. Vafaeifard, Mining Investment Insurance Corporation, Islamic Republic of Iran

(GOMD-SIII-P026-2010) Zinc and Silver Glass Polyalkenoate Cements: An Evaluation of their Antibacterial Nature
A. Coughlan*, M. Towler, Alfred University, United States

(GOMD-SIII-P027-2010) The Antibacterial Properties and Ion Release Profiles of a novel Zinc based Glass Polyalkenoate Cement
A. W. Wren*, M. R. Towler, Alfred University, United States

(GOMD-SIII-P028-2010) Fluorescent glass patterning on a sheet window glass by screen printing and low temperature heat treatment
Y. Ishikawa*, Y. Ohara, T. Kishi, A. Yasumori, Tokyo University of science, Japan

(GOMD-SIII-P029-2010) Preparation of gold nanoparticles supported on a super-hemispherical lens by using a surface-tension mold technique for chemical sensing
S. Furusawa*, T. Nakagawa, T. Kishi, A. Yasumori, Tokyo University of science, Japan

(GOMD-SIII-P030-2010) Transition Metal Oxide Coatings on Glass
B. M. Adams*, N. P. Mellott, Alfred University, United States

(GOMD-SIII-P031-2010) Dependence of osteoblast cell response on the surface roughness of 45S bioactive glass
R. H. Jain*, S. Wang, H. M. Moawad, M. M. Falk, H. Jain, Lehigh University, United States

(GOMD-SIII-P032-2010) Simulation of Fluid Flow and Temperature on the Glass Sheet Forming for Overflow Fusion Process
H. Wu, Ming Chi University of Technology, Taiwan; H. Lin*, National United University, Taiwan

(GOMD-SIII-P033-2010) Conversion of europium and lanthanum doped lithium borate glass to rare earth phosphate compounds
J. George*, R. Brow, Missouri University of Science and Technology, United States

(GOMD-SIII-P034-2010) Chromium-doped transparent calcium germinate glass-ceramics toward nano-Ca2GeO4 in fiber
J. Wang*, Z. Huang, National Sun Yat-Sen University, Taiwan

(GOMD-SIII-P035-2010) Mechanism of the removal of phosphate ion from an aqueous solution by borosilicate glass
J. Nam*, C. Kim, Inha university, Republic of Korea

(GOMD-SIII-P036-2010) Rare-Earth-Doped Amorphous Nancomposite Polymers for Optoelectronic Applications
K. G. Gipson*, B. Ellerbrock, K. Stevens, P. Brown, J. Ballato, Clemson University, United States

(GOMD-SIII-P037-2010) Barium Vanadate Microspheres
S. Yosinski, L. Tweeton, S. Feller, M. Affatigato*, Coe College, United States

(GOMD-SIII-P038-2010) Antibacterial Properties of Silver and Zinc doped 45S Bioactive Glass
M. J. Michel*, Lehigh University, United States

(GOMD-SIII-P039-2010) Glassy particles as an active component in cementitious materials for the future
M. Moesgaard*, Aalborg University, Denmark; L. Kirkegaard, D. Herfort, Aalborg Portland, Denmark; Y. Yue, Aalborg University, Denmark

(GOMD-SIII-P040-2010) Formation of SiO_2-Rich Surface Layer on Glass Fibers
M. M. Smedskjaer*, Aalborg University, Denmark; J. Deubener, Clausthal University of Technology, Germany; S. Mørup, Technical University of Denmark, Denmark; Y. Yue, Aalborg University, Denmark

(GOMD-SIII-P041-2010) Analysis of Interactions between Glass and Mold Tool in Precision Optical Molding
J. Jackson, P. F. Wachtel*, D. Musgraves, K. Richardson, Clemson University, United States

(GOMD-SIII-P042-2010) Structural and thermal studies of $70Li_2S+(30-x)P_2S_5+xAl_2S_3$ with x=1 or 3 mol%
S. Berbano*, Iowa State University, United States; K. Minami, A. Hayashi, M. Tatsumisago, Osaka Prefecture University, Japan

(GOMD-SIII-P043-2010) Cell response to nano-macro porous bioactive glass scaffolds prepared by the sol-gel method
S. Wang*, M. M. Falk, H. Jain, Lehigh University, United States

(GOMD-SIII-P044-2010) Tailoring and Characterization of Nanopores Networks of Nano/Macro Dual Porous Sol-Gel Bioactive Glasses
S. Wang*, Lehigh University, United States; A. C. Marques, R. M. Almeida, ICEMS, Instituto Superior AU1 Tecnico/TULisbon, Portugal; H. Jain, Lehigh University, United States

(GOMD-SIII-P045-2010) Processing of S520 glass for nano-macro porous bioactive fibers
U. Thamma*, H. M. Moawad, H. Jain, Lehigh University, United States

(GOMD-SIII-P046-2010) Single-mode waveguide of chalcogenide glasses by burying a fiber in substrates
Z. Shaoqian*, X. Zhang, university of Rennes1, France

(GOMD-SIV-P047-2010) Transition Metal Oxide (TMO) Silicate Glasses: Processing and Materials Properties
B. Akkopru*, Alfred University, United States; C. Durucan, Middle East Technical University, Turkey; N. P. Mellott, Alfred University, United States

(GOMD-SIV-P048-2010) The relationship between phosphate glass dissolution and experimentally determined dissolution enthalpies for phosphate compounds
L. Ma*, M. L. Schmitt, R. K. Brow, Missouri University of Science and Technology, United States

(GOMD-SIV-P049-2010) Corrosion Behavior of Ti-Based Bulk Metallic Glass Composites Containing Carbon Nanotubes
P. Lee*, National Taiwan Ocean University, Taiwan

(GOMD-SIV-P050-2010) Corrosion of ancient glass bead samples excavated from prehistoric sites in southern Thailand
P. Dararutana*, The Royal Thai Army Chemical Department, Thailand; Y. Thongkam, Silpakorn University, Thailand; K. Won-in, Kasetsart University, Thailand

Tuesday, May 18, 2010

George W. Morey Award Lecture

Room: Keuka

8:00 AM

Glass and Water
Minoru Tomozawa, Rensselaer Polytechnic Institue, United States

Symposium II: Glass Science

Topology and Rigidity I

Room: Cayuga

Session Chair: Normand Mousseau, Universite de Montreal

9:30 AM

(GOMD-SII-021-2010) Intermediate Phases in Solid Electrolyte glasses (Invited)
P. Boolchand*, D. I. Novita, M. Malki, M. Micoulaut, B. Goodman, Univ of Cincinnati, United States

10:00 AM

(GOMD-SII-022-2010) Intermediate phases in simple models of elastic network self-organization (Invited)
M. V. Chubynsky*, University of Ottawa, Canada

10:30 AM

(GOMD-SII-023-2010) Elastic behavior and fast-ion conduction in glasses
M. Micoulaut*, Université Pierre et Marie Curie, France; M. Malki, Université Pierre et Marie Curie, France, Université Pierre et Marie Curie, FranceCNRS Orléans, France

10:45 AM

(GOMD-SII-024-2010) Electronic Signature of the Intermediate Phase in GexSe1-x Glasses
K. Li, G. Chen*, F. Inam, D. Drabold, Ohio University, United States

11:00 AM

(GOMD-SII-025-2010) Bimodal phase percolation model for the structure of Ge-Se glasses by Raman and NMR
P. Lucas*, E. King, University of Arizona, United States; B. Bureau, Universite de Rennes I, France; O. Gulbiten, University of Arizona, United States

11:15 AM

(GOMD-SII-026-2010) Intermediate phase in sodium borate glasses
P. Boolchand, V. Kandasamy*, Univ of Cincinnati, United States

11:30 AM

(GOMD-SII-027-2010) Constraints, Iso-Tg Regimes, and Phase Separation
P. Gupta*, The Ohio State University, United States

11:45 AM

(GOMD-SII-028-2010) Transition features in GexAsySe1-x-y Glasses
R. Wang*, The Australian National University, Australia

Symposium III: Glass Technology

Glasses for Medicine and Biotechnology

Room: Seneca

Session Chair: Matthew Hall, Alfred University

9:15 AM

(GOMD-SIII-022-2010) Bioactive, Antibacterial Cements for Skeletal Applications (Invited)
M. Towler*, Alfred University, United States

9:45 AM

(GOMD-SIII-023-2010) Effect of strontium on the atomic structure and ion diffusion of bioactive glasses: a molecular dynamics simulation
J. Du*, Y. Xiang, University of North Texas, United States

10:00 AM

(GOMD-SIII-024-2010) Novel Bioactive and Biodegradable 13-93 Glass Scaffolds for Bone Tissue Engineering
Q. Fu*, M. N. Rahaman, Missouri University of Science and Technology, United States

10:15 AM

(GOMD-SIII-025-2010) Direct Write Assembly of Bioactive Glass Scaffolds for Bone Tissue Engineering
Q. Fu*, E. Saiz, A. P. Tomsia, Lawrence Berkeley National Laboratory, United States

10:30 AM

(GOMD-SIII-026-2010) Multifunctional, TiO2-based Coatings on Glass
B. Akkopru*, Alfred University, United States; C. Durucan, Middle East Technical University, Turkey; N. P. Mellott, Alfred University, United States

10:45 AM

(GOMD-SIII-027-2010) Systems and Interfaces: Controlling Bio Processes (Invited)
G. D. Stucky*, UCSB, United States

11:15 AM

(GOMD-SIII-028-2010) Electropolymerization of aniline within redox-mediated organically modified silicate
P. C. Pandey*, Banaras Hindu UNiversity, Institute of Technology, India

11:30 AM

(GOMD-SIII-029-2010) Glass as an Electronic Package Substrate for Consumer and Biomedical Applications
V. Sukumaran*, Q. Chen, N. Kumbhat, F. Liu, S. Min, V. Sundaram, R. Tummala, Georgia Institute of Technology, United States

Symposium V: Glass Structure and Properties

Glass Structure and Properties I: Silicates

Room: Keuka

Session Chair: Sabyasachi Sen, University of California - Davis

9:30 AM

(GOMD-SV-001-2010) Determination of Structural Distributions in Densified Silica Using O–17 NMR (Invited)
P. Grandinetti*, N. Trease, Ohio State University, United States; J. Stebbins, Stanford University, United States; S. Sen, University of California, Davis, United States

10:00 AM

(GOMD-SV-002-2010) Structure and bonding in CaO-SiO2 liquids and glasses
R. J. Weber*, Materials Development, Inc., United States; C. J. Benmore, Argonne National Laboratory, United States; J. B. Parise, Stony Brook University, United States; M. C. Wilding, Aberystwyth University, United Kingdom; J. Du, University of North Texas, United States

10:15 AM

(GOMD-SV-003-2010) Structural heterogeneity in calcium aluminosilicate glasses
M. Moesgaard*, R. Keding, Aalborg University, Denmark; J. Skibsted, Aarhus University, Denmark; Y. Yue, Aalborg University, Denmark

10:30 AM

(GOMD-SV-004-2010) Temperature dependent structural changes in aluminoborosilicate melts
J. Wu*, J. Stebbins, Stanford University, United States

10:45 AM

(GOMD-SV-005-2010) Counting Non-Bridging Oxygens in Calcium and Potassium Aluminosilicate Glasses with Oxygen-17 NMR
L. M. Thompson*, J. F. Stebbins, Stanford University, United States

11:00 AM

(GOMD-SV-006-2010) A Multispectroscopic Study of Lead Silicate Glass Atomic Structure
A. Vitale*, M. Affatigato, S. Feller, Coe College, United States; G. Lehr, Monmouth College, United States; D. Holland, M. Smith, University of Warwick, United Kingdom; A. Hannon, E. Barney, Rutherford Appleton Lab, United Kingdom

11:15 AM

(GOMD-SV-007-2010) Tracer Diffusion of Sodium in Sodium Borosilicate Glasses
X. Wu*, R. Dieckmann, Cornell University, United States

11:30 AM

(GOMD-SV-008-2010) Mechanical properties in pseudo-binary system of Pyrex and soda-lime-silica glass
A. Koike*, S. Ito, Asahi Glass Co., Ltd., Japan

11:45 AM

(GOMD-SV-009-2010) Short-range Structure of Invert Glasses Along the Join MgSiO3-Mg2SiO4
S. Sen*, University of California - Davis, United States; H. Maekawa, Tohoku University, Japan; G. Papatheodorou, ICEHT-FORTH, Greece

Norbert J. Kreidl Award Lecture

Room: Keuka

12:00 PM

Inward Diffusion of Modifying Ions in Glasses and Glass-Ceramics
Morten M. Smedskjaer, Aalborg University, Denmark

Symposium II: Glass Science

Rheology

Room: Cayuga

Session Chair: Lothar Wondraczek, Universitat Erlangen-Nurnberg

1:15 PM

(GOMD-SII-029-2010) Rheology of heterogeneous liquids (Invited)
J. Deubener*, Clausthal University of Technology, Germany

1:45 PM

(GOMD-SII-030-2010) Viscosity of Glass-Forming Liquids
J. C. Mauro*, Corning Incorporated, United States; Y. Yue, Aalborg University, Denmark; A. J. Ellison, Corning Incorporated, United States; P. K. Gupta, The Ohio State University, United States; D. C. Allan, Corning Incorporated, United States

2:00 PM

(GOMD-SII-031-2010) Modeling the Nonequilibrium Viscosity of Glass
D. C. Allan*, J. C. Mauro, M. Potuzak, Corning Incorporated, United States

2:15 PM

(GOMD-SII-032-2010) Viscosity and softening behaviour of alkali zinc phosphosulphate glasses
N. Da*, L. Wondraczek, Universitat Erlangen-Nurnberg, Germany

2:30 PM

(GOMD-SII-033-2010) Progress in the Rheology of Inorganic Glass-Forming Melts (Invited)
Y. Yue*, Aalborg University, Denmark

3:00 PM

Break

3:15 PM

(GOMD-SII-034-2010) Boson peak, inhomogeneity and pressure experiments in SiO2 and GeO2 glasses (Invited)
B. Champagnon*, D. Thierry, M. Christine, Université Lyon1-CNRS, France

3:45 PM

(GOMD-SII-035-2010) Pressure-assisted flow of glass melts in narrow capillaries (Invited)
M. Schmidt*, L. Wondraczek, P. Russell, Max Planck Insitute for the Science of Light, Germany

4:15 PM

(GOMD-SII-036-2010) On the Origin of the Mixed Glass Former Effect: Varying Coulomb Traps of Network Forming Units
P. Maass, Universität Osnabrück, Germany; C. R. Müller*, Technische Universität Ilmenau, Germany; M. Schuch, Universität Osnabrück, Germany

4:30 PM

(GOMD-SII-037-2010) Viscosity of Tellurite Glass: 75TeO2-20ZnO-5Na2O
A. A. Belwalkar*, W. Z. Misiolek, J. Toulouse, Lehigh University, United States

Symposium III: Glass Technology

Glasses for Energy and Environmental Applications

Room: Seneca

Session Chairs: Joachim Deubener, Clausthal University of Technology; Dean Thelen, Corning Incorporated

1:15 PM

(GOMD-SIII-030-2010) Specialty Glass for Thin Film Solar Cell Applications (Invited)
D. Hall*, Corning Incorporated, United States

1:45 PM

(GOMD-SIII-031-2010) Specialty Thin Glass for PV Modules: Mechanical Reliability Considerations
J. Webb*, Corning Incorporated, United States

2:00 PM

(GOMD-SIII-032-2010) Sintering of nanoporous anti-reflective coatings for concentrated solar power applications
A. Mös, G. Helsch, J. Deubener*, Clausthal University of Technology, Germany

2:15 PM

(GOMD-SIII-033-2010) Viscous Sealants for Solid Oxide Fuel Cell Application
M. Naylor*, J. Shelby, S. Misture, Alfred University, United States

2:30 PM

(GOMD-SIII-034-2010) Vanadium phosphate glasses as frits for laser-sealing
R. Morena*, L. A. Lamberson, CORNING Incorporated, United States

2:45 PM

(GOMD-SIII-035-2010) Sealing Glasses for Applications below 200°C
L. Gambino, Rutgers University, United States; A. Jitianu, Lehman College-CUNY, United States; L. C. Klein*, Rutgers University, United States

3:00 PM

Break

3:15 PM

(GOMD-SIII-036-2010) Lithium ion diffusion in silicon-Lithium battery materials
M. Zhang*, D. A. Drabold, Ohio University, United States

3:30 PM

(GOMD-SIII-037-2010) Development of LiFePO4 glass-ceramic for cathode material of lithium ion battery
T. Nagakane*, H. Yamauchi, K. Yuki, A. Sakamoto, Nippon Electric Glass Co.,Ltd., Japan; T. Honma, T. Komatsu, Nagaoka University of Technology, Japan; M. Zou, Y. Okumura, T. Sakai, National Institute of Advanced Industrial Science and Technology, Japan

3:45 PM

(GOMD-SIII-038-2010) Proton Conduction of Sol-Gel Derived Monolithic Electrolytes for use in Mid-Temperature Proton Exchange Fuel Cells
A. Feldman*, J. Kieffer, University of Michigan, United States

4:00 PM

(GOMD-SIII-039-2010) Dielectric Breakdown of Alkali-Free Boroaluminosilicate Glass Thin Films
J. Serra*, M. Lanagan, C. Pantano, Penn State University, United States

4:15 PM

(GOMD-SIII-040-2010) Transition- and Post-Transition Metal doped Glasses and Glass Ceramics for Energy Efficient Lighting (Invited)
L. Wondraczek*, M. Peng, Universitat Erlangen-Nurnberg, Germany

4:45 PM

(GOMD-SIII-041-2010) Removal of Chromium(VI) Ion from a Solution by Barium Borosilicate Glass
I. Baek*, C. Kim, Inha University, Republic of Korea

Symposium IV: Glass Corrosion

Short-term Corrosion Issues I

Room: Carder

Session Chair: Nathan Mellott, Alfred University

1:00 PM

(GOMD-SIV-001-2010) Glass Corrosion 101 (Invited)
C. Pantano*, Pennsylvania State University, United States

2:00 PM

(GOMD-SIV-002-2010) Practical Aspects of Corrosion in Glass Fiber (Invited)
J. F. Bauer*, J Bauer Consulting, United States

2:30 PM

(GOMD-SIV-003-2010) Effects of leaching at glass/polymer interfaces
J. Banerjee*, Pennsylvania State University, United States; J. Hamilton, Johns Manville, United States; C. Pantano, Pennsylvania State University, United States

2:45 PM

Break

Short-term Corrosion Issues II

Room: Carder

Session Chair: Nathan Mellott, Alfred University

3:15 PM

(GOMD-SIV-004-2010) On the Mechanisms of Corrosion Induced Roughening of Silicate Glass Surfaces
N. P. Mellott*, K. Kalac, Alfred University, United States; C. G. Pantano, The Pennsylvania State University, United States

3:30 PM

(GOMD-SIV-005-2010) Acid-induced alteration of Alkali Borosilicate frit
P. Marques*, R. M. Morena, Corning Sas, France

3:45 PM

(GOMD-SIV-006-2010) Aqueous corrosion of the GeSe4 chalcogenide glass:surface properties and corrosion mechanism
Y. Niu, J. Guin*, T. Rouxel, CNRS-Université de Rennes 1, France; A. Abdelouas, Ecole des mines de Nantes, France; J. Troles, Université de Rennes 1, France; F. Smektala, Université de Bourgogne, France

4:00 PM

(GOMD-SIV-007-2010) Analytical modeling of the aqueous dissolution behavior of phosphate glasses
M. L. Schmitt*, L. Ma, R. Brow, Missouri S&T, United States

Symposium V: Glass Structure and Properties

Glass Structure and Properties II: Simulations and Chalcogenides

Room: Keuka

Session Chair: Randall Youngman, Corning Incorporated

1:15 PM

(GOMD-SV-010-2010) Understanding the structures and properties of silicate and aluminosilicate glasses from classical and ab initio molecular dynamics simulations (Invited)
J. Du*, University of North Texas, United States

1:45 PM

(GOMD-SV-011-2010) Mechanical Behavior of Water-Containing Glass by MD simulation
S. Ito*, T. Taniguchi, Asahi Glass Co., Ltd, Japan

2:00 PM

(GOMD-SV-012-2010) Structural Association of Ga and P in Selenide Glass
B. Aitken*, S. Currie, R. Youngman, C. Ponader, Corning Inc., United States

2:15 PM

(GOMD-SV-013-2010) Influence of iso-structural substitutions on physical properties in Ge(As,Sb)(S,Se) glasses
G. Guery*, D. Musgraves, K. Richardson, L. Petit, clemson university, United States; E. Fargin, University of Bordeaux, France

2:30 PM

(GOMD-SV-014-2010) High-resolution 77Se NMR investigation of the structure of GexSe100-x glasses
E. L. Gjersing, S. Sen*, University of California Davis, United States; B. Aitken, Corning Inc., United States

2:45 PM

(GOMD-SV-015-2010) Impact of Chalcogen Deficiency in GeAsPS and GeGaPS Glasses
R. Youngman*, B. Aitken, S. Currie, Corning Incorporated, United States

3:00 PM

Break

Glass Structure and Properties III: Phosphates

Room: Keuka

Session Chair: Randall Youngman, Corning Incorporated

3:15 PM

(GOMD-SV-016-2010) Properties and Structures of Tin Phosphate Glasses modified with Ga2O3 and Sb2O3
J. Lim*, R. K. Brow, Missouri S&T, United States; H. Yang, National United University, Taiwan

3:30 PM

(GOMD-SV-017-2010) Structure-Property Relationships in Cerium Aluminophosphate and Silicophosphate Glasses
J. L. Rygel*, C. G. Pantano, The Pennsylvania State University, United States

3:45 PM

(GOMD-SV-018-2010) Raman Spectra and the Structure of Iron-Phosphate Compounds and Glasses
L. Zhang*, J. Lim, R. K. Brow, M. E. Schlesinger, Missouri S&T, United States

4:00 PM

(GOMD-SV-019-2010) Structural and Dispersive Aspects of the Photoelasticity of Glass
V. Martin*, S. Thomas, V. Dickinson, B. Chen, U. Werner-Zwanziger, R. Dunlap, J. Zwanziger, Dalhousie University, Canada

4:15 PM

(GOMD-SV-020-2010) WITHDRAWN

4:30 PM

(GOMD-SV-021-2010) Structure of Sodium Borophosphate Glasses
R. Christensen*, G. Olson, Iowa State University, United States; A. Matic, Chalmers University of Technology, Sweden; V. Petkov, Central Michigan University, United States; S. W. Martin, Iowa State University, United States

Otto Schott Research Award

Room: Carder

5:00 PM

The Brittle to Ductile Transition in Glass: Fundamental and Technological Challenges
Tanguy Rouxel, University of Rennes 1, France

Wednesday, May 19, 2010

Symposium II: Glass Science

Topology and Rigidity II

Room: Cayuga

Session Chair: Matthieu Micoulaut, Universite Pierre-et-Marie Curie

8:00 AM

(GOMD-SII-038-2010) Spatial correlations in amorphous networks and their electronic consequences: an emerging theory of the Urbach tail (Invited)
D. Drabold*, Ohio University, United States; F. Inam, International Center for Theoretical Physics, Italy; Y. Li, Ohio University, United States

8:30 AM

(GOMD-SII-039-2010) The non-trivial structure of disordered network-forming materials unraveled by first-principles molecular dynamics (Invited)
C. Massobrio*, IPCMS, France

9:00 AM

(GOMD-SII-040-2010) Evolution of the potential-energy surface of amorphous silicon
H. Kallel, N. Mousseau*, F. Schiettekatte, Universite de Montréal, Canada

9:15 AM

(GOMD-SII-041-2010) Characterizing the sodium environnement in amorphous silicates
M. Bauchy*, M. Micoulaut, Université Pierre et Marie Curie, France

9:30 AM

(GOMD-SII-042-2010) Molecular structure of ideal chalcohalide glasses
P. Boolchand, S. Bhosle*, Univ of Cincinnati, United States

9:45 AM

(GOMD-SII-043-2010) Hidden structure in amorphous and glassy materials Y Li, S. Chakraborty and D A Drabold
Y. Li*, S. Chakraborty, D. Drabold, Ohio University, United States

10:00 AM

(GOMD-SII-044-2010) Intermediate phase in ternary GexSbxSe100-2x bulk alloy glasses
P. Boolchand, K. Gunasekera*, P. Chen, Univ of Cincinnati, United States

10:15 AM

Break

Glass Transition and Relaxation I

Room: Cayuga

Session Chair: Prabhat Gupta, The Ohio State University

10:30 AM

(GOMD-SII-045-2010) Structural Relaxation in the Glassy State: Further Evidence for the Path Dependence of the Relaxation Time (Invited)
F. Begum, S. Simon*, Texas Tech University, United States

11:00 AM

(GOMD-SII-046-2010) Microscopic Aspects of Stretched Exponential Relaxation (SER) (Invited)
J. C. Phillips*, Rutgers, United States

11:30 AM

(GOMD-SII-047-2010) Logarithmic Relaxation of Stress Correlator in Supercooled Liquids
J. Eapen*, North Carolina State University, United States

11:45 AM

(GOMD-SII-048-2010) Modeling the enthalpy relaxation of glasses far from equilibrium
X. Guo*, Aalborg University, Denmark; J. Mauro, Corning Incorporated, United States; Y. Yue, Aalborg University, Denmark

Symposium III: Glass Technology

Melting & Process Modeling

Room: Seneca

Session Chairs: Olus Boratav, Corning Incorporated; Li Yang, Corning Incorporated

8:15 AM

(GOMD-SIII-042-2010) The batch-to-melt conversion - mineralogical, caloric and kinetic aspects (Invited)
R. Conradt*, RWTH Aachen University, Germany

8:45 AM

(GOMD-SIII-043-2010) Full conversion of glass furnace to oxygen-fuel combustion
X. He*, M. J. Watson, M. E. Habel, Air Products and Chemicals, Inc., United States; J. Rossi, Fiberglass Industries, Inc., United States

9:00 AM

(GOMD-SIII-044-2010) Bubble Concentration Model
W. W. Johnson*, Corning Incorporated, United States

9:15 AM

(GOMD-SIII-045-2010) Draw Resonance in Viscous Sheets
O. Boratav*, Z. Zheng, Corning Incorporated, United States; A. Amosov, Corning Incorporated, Russian Federation

9:30 AM

(GOMD-SIII-046-2010) The Liquidus Temperature; its Critical Role in Glass Manufacturing (Invited)
F. T. Wallenberger*, A. Smrček, Consultant, United States

10:00 AM

Break

Optical Materials I

Room: Seneca

Session Chairs: Hong Li, Schott North America, Inc.; Amanda Young, Sandia National Laboratories

10:15 AM

(GOMD-SIII-047-2010) Optical Materials for Harsh Ionizing-Radiation Environments (Invited)
K. Simmons-Potter*, University of Arizona, United States

10:45 AM

(GOMD-SIII-048-2010) Use of Gadolinium Oxide for Neutron Detection in Glasses
K. Goetschius*, J. Shelby, Alfred University, United States; A. Huston, S. Rychnovsky, B. Wright, Naval Research Laboratory, United States

11:00 AM

(GOMD-SIII-049-2010) Yb-doped oxide glasses under ionizing irradiation: a relaxation processes study
N. Ollier*, V. Puhkhaya, LSI, France; J. Doualan, R. Moncorgé, CIMAP, France

11:15 AM

(GOMD-SIII-052-2010) Crystalline Semiconductor Core Optical Fibers
S. Morris*, J. Ballato, T. Hawkins, P. Foy, C. McMillen, R. Stolen, Clemson University, United States; R. Rice, Northrop Grumman Space Technology, United States

11:30 AM

(GOMD-SIII-051-2010) Sub-Micron Grained Highly Transparent Y_2O_3 Ceramics: Synthesis, Processing, and Properties
K. Serivalsatit*, B. Kokuoz, B. Yazgan Kokouz, M. Kennedy, J. Ballato, Clemson University, United States

11:45 AM

(GOMD-SIII-050-2010) Effect of Bromine on NaF Crystallization in Photo-Thermo-Refractive Glass
G. P. Souza, V. Fokin, C. Baptista, E. D. Zanotto, Federal University of San Carlos, Brazil; J. Lumeau*, L. Glebova, L. B. Glebov, University of Central Florida, United States

Symposium IV: Glass Corrosion

Ancient and Analogue Glasses

Room: Carder

Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

8:15 AM

(GOMD-SIV-008-2010) The Morphology of Weathering on Ancient Glasses (Invited)
R. H. Brill*, Corning Museum of Glass, United States

9:00 AM

(GOMD-SIV-009-2010) Some thoughts on the use of ancient glasses in performance assessment of nuclear waste glass disposal (Invited)
D. Strachan*, Pacific Northwest National Laboratory, United States; R. Brill, Corning Museum of Glass, United States

9:30 AM

(GOMD-SIV-010-2010) The use of Roman glass to predict the long-term behavior of HLW (Invited)
S. Gin, CEA, France; A. Verney-Carron, CNRS, France; P. Frugier*, CEA, France

10:00 AM

(GOMD-SIV-011-2010) The surface and beyond: new insights in old glass
H. Roemich*, New York University, United States

10:15 AM

Break

Modeling

Room: Carder

Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

10:30 AM

(GOMD-SIV-012-2010) Interaction of Water with Multi-Component Silicate Glass Surfaces (Invited)
A. Cormack*, Alfred University, United States; A. Tilocca, University College London, United Kingdom

11:00 AM

(GOMD-SIV-013-2010) Delayed failure of oxide glasses (Invited)
M. Tomozawa*, RPI, United States

11:30 AM

(GOMD-SIV-014-2010) DFT MD Simulations of Proton Attack on a Silica Surface (Invited)
J. D. Kubicki*, The Pennsylvania State University, United States

Symposium V: Glass Structure and Properties

Photoinduced Structural Changes in Glass

Room: Keuka

Session Chair: Pierre Lucas, University of Arizona

8:00 AM

(GOMD-SV-022-2010) Determination of structural defects in chalcogenide glasses by high-resolution XPS (Invited)
H. Jain*, A. Kovalskiy, R. Golovchak, Lehigh University, United States

8:30 AM

(GOMD-SV-023-2010) In situ Observation of the Photoinduced Atomistic Changes in Chalcogenide Glasses
D. Zhao*, H. Jain, Lehigh University, United States

8:45 AM

(GOMD-SV-024-2010) Photosensitivity in As-S-Se mixed chalcogen glasses: the relative role of selenium versus sulfur
P. Lucas*, F. Lin, Z. Yang, University of Arizona, United States

9:00 AM

(GOMD-SV-025-2010) Dynamic equilibrium under light irradiation shown through photoinduced fluidity
Y. Gueguen*, J. Sangleboeuf, V. Keryvin, T. Rouxel, Université de Rennes 1, France; C. Boussard-Plédel, B. Bureau, J. Troles, UMR CNRS 6226, France; P. Lucas, University of Arizona, United States

9:15 AM

(GOMD-SV-026-2010) Photofluidity and Optical Microfrabrication of Tapers in Low-Loss Chalcogenide Fibers
P. Lucas*, E. Lepine, Z. Yang, University of Arizona, United States; Y. Gueguen, J. Sangleboeuf, B. Bureau, X. Zhang, University of Rennes I, France

9:30 AM

(GOMD-SV-027-2010) Dynamics of femtosecond laser modification in glass
J. J. Witcher*, L. Fletcher, N. Troy, D. Krol, UC Davis, United States

9:45 AM

(GOMD-SV-028-2010) Mechanisms of Laser Induced Modification of Lead and Barium Vanadate Glasses
M. Affatigato*, R. Dongol, L. Tweeton, C. Faris, S. Feller, Coe College, United States

10:00 AM

(GOMD-SV-029-2010) Photoinduced Molecular Assembly in Dip-Coated Films via In-Situ Illuminations
Z. Schneider*, K. Simmons-Potter, B. G. Potter, University of Arizona, United States; T. Boyle, Sandia National Laboratories, United States

10:15 AM

Break

10:30 AM

(GOMD-SV-030-2010) Polarized infrared studies of silica glass exposed to polarized excimer laser irradiation (Invited)
C. M. Smith*, N. F. Borrelli, J. E. Tingley, Corning Incorporated, United States

11:00 AM

(GOMD-SV-031-2010) Study of ionization of cerium in multicomponent silicate glasses
K. Chamma, J. Lumeau*, L. Glebova, L. B. Glebov, University of Central Florida, United States

11:15 AM

(GOMD-SV-032-2010) Femtosecond Laser Waveguide Writing in Erbium Doped Phosphate Glass
L. B. Fletcher*, J. J. Witcher, D. M. Krol, University of California Davis, United States; R. K. Brow, Missouri University of Science and Technology, United States

11:30 AM

(GOMD-SV-033-2010) Analysis of Radiation-Induced Darkening in Ce-doped Phosphate Glasses
R. Woodman*, J. Belcher, C. Ferreira, L. Gonzalez, Infoscitex Corporation, United States; C. Pantano, J. Rygel, The Pennsylvania State University, United States; J. Du, L. Kokou, University of North Texas, United States

Symposium II: Glass Science

Glass Transition and Relaxation II

Room: Cayuga

Session Chair: Prabhat Gupta, The Ohio State University

1:15 PM

(GOMD-SII-049-2010) Structural Aspects of Relaxation in Oxide Glasses (Invited)
J. F. Stebbins*, Stanford University, United States

1:45 PM

(GOMD-SII-050-2010) Understanding liquids and glass transition on the basis of elastic waves (Invited)
K. Trachenko*, University of Cambridge, United Kingdom

2:15 PM

(GOMD-SII-051-2010) Viscoelastic dynamics of network-forming sodium ultraphosphate liquids: a dynamic light scattering study
D. Sidebottom*, R. Fabian, Creighton University, United States

2:30 PM

(GOMD-SII-052-2010) The Glass Transition at the Nanoscale
Y. P. Koh, S. Simon*, Texas Tech University, United States

2:45 PM

(GOMD-SII-053-2010) Universality of Boson Peaks in Lithium Borate Glasses
S. Kojima*, Y. Matsuda, M. Kawashima, S. Aramomi, University of Tsukuba, Japan; M. Kodama, Sojo University, Japan

3:00 PM

Break

Glass Transition and Relaxation III

Room: Cayuga

Session Chair: Roger Loucks, Alfred University

3:15 PM

(GOMD-SII-054-2010) Landscape View of Sub-Tg Relaxation (Invited)
P. Gupta*, J. Mauro, The Ohio State University, United States

3:45 PM

(GOMD-SII-055-2010) Cadmium manganese telluride: optical & magnetic properties
J. McCloy*, T. Droubay, B. Riley, J. Ryan, Pacific Northwest National Laboratory, United States

4:00 PM

(GOMD-SII-056-2010) Nonmonotonic Evolution of Density Fluctuations During Glass Relaxation
J. C. Mauro*, Corning Incorporated, United States; S. Soyer Uzun, University of California—Davis, United States; W. Bras, Netherlands Organization for Scientific Research (NWO), France; S. Sen, University of California—Davis, United States

4:15 PM

(GOMD-SII-057-2010) Fictive Temperature and the Glassy State
R. J. Loucks*, Alfred University, United States; J. C. Mauro, Corning Incorporated, United States; P. K. Gupta, The Ohio State University, United States

4:30 PM

(GOMD-SII-058-2010) The Thermodynamic Significance of Order Parameters
R. J. Araujo*, J. C. Mauro, Corning Incorporated, United States

4:45 PM

(GOMD-SII-059-2010) Heat Capacity, Enthalpy Fluctuations, and Configurational Entropy in Broken Ergodic Systems
B. D. Esham*, Alfred University, United States; J. C. Mauro, Corning Incorporated, United States; S. Sen, University of California—Davis, United States; R. J. Loucks, G. J. McGowan, Alfred University, United States

5:00 PM

(GOMD-SII-060-2010) Residual entropy : harmonization of statistical mechanics and thermodynamics
A. Takada*, Asahi Glass Company, Japan

Symposium III: Glass Technology

Optical Materials II

Room: Seneca

Session Chairs: Hong Li, Schott North America, Inc.; Amanda Young, Sandia National Laboratories

1:15 PM

(GOMD-SIII-053-2010) Low losses highly non linear As2S3 suspended core microstructured optical fibers (Invited)
F. Smektala*, M. El Amraoui, J. Jules, G. Gadret, J. Fatome, Université de Bourgogne, France; C. Polacchini, I. Skrypatchev, Y. Messadeq, Instituto de Quimica, Brazil; G. Renversez, Institut Fresnel, France; M. Szpulak, Institute Of Physics, Poland; J. Troles, Sciences Chimiques de Rennes, France; L. Brilland, Perfos, France

1:45 PM

(GOMD-SIII-054-2010) Towards low loss, high-index-contrast chalcogenide glass photonics: thermal reflow and overlayer spin-coating
J. Hu*, Massachusetts Institute of Technology, United States; N. Carlie, L. Petit, Clemson University, United States; A. Agarwal, L. C. Kimerling, Massachusetts Institute of Technology, United States; K. Richardson, Clemson University, United States

2:00 PM

(GOMD-SIII-055-2010) Grayscale Lithography Using Chalcogenide Glass Resists
A. Kovalskiy*, Lehigh University, United States; M. Vlcek, University of Pardubice, Czech Republic; J. Cech, H. Jain, Lehigh University, United States

2:15 PM

(GOMD-SIII-056-2010) Optimization of spin-coating parameters for optical quality chalcogenide thin films in the As-Ge(Sb)-System
N. Carlie*, L. Petit, J. D. Musgrave, K. Richardson, Clemson University, United States

2:30 PM

(GOMD-SIII-057-2010) Effects of deposition parameters on the optical properties and stability of thermally evaporated Ge-As-Se thin films
D. Bulla*, R. Wang, S. Prasad, A. V. Rode, S. J. Madden, B. Luther-Davies, Australian National University, Australia

2:45 PM

(GOMD-SIII-058-2010) Structure-Optical Property Correlations for Arsenic-Sulfide Glasses in the Visible, Infrared, and Sub-millimeter Regions
J. McCloy, B. J. Riley, S. K. Sundaram, A. Qiao, J. V. Crum, B. R. Johnson*, Pacific Northwest National Lab, United States

3:00 PM

Break

3:15 PM

(GOMD-SIII-059-2010) Chalcogenide optical fibers used for CO2 detection
F. Charpentier*, S. Maurugeon, J. Troles, V. Nazabal, L. Brilland, Universite de Rennes 1- CNRS, France; P. Camy, J. L. Doualan, CIMAP, France; C. Boussard-Pledel, X. H. Zhang, P. Lucas, B. Bureau, Universite de Rennes 1- CNRS, France

3:30 PM

(GOMD-SIII-060-2010) Chalcogenide waveguides integrated microfluidic sensor device
M. L. Brandily-Anne*, Universite de Rennes, France; F. Charpentier, Universite de Rennes 1, France; H. Lhermitte, Universite de Rennes, France; J. Charrier, FOTON, France; B. Bureau, V. Nazabal, Universite de Rennes 1, France

3:45 PM

(GOMD-SIII-061-2010) Utilizing Rare Earth Doped Nanoparticles to Tailor Emission Spectrum of Optical Fiber
T. L. James, C. Kucera, B. Kokuoz, E. Garber, D. Edmonson, Clemson university, United States; D. Griese, M. Miller, E. Chasteen, M. Goodson, Furman University, United States; A. James, Clemson university, United States; W. Baker, Furman University, United States; J. Ballato*, Clemson university, United States

4:00 PM

(GOMD-SIII-062-2010) Structural and Compositional Modification of Glass Surfaces by Thermal Poling
N. J. Smith*, C. G. Pantano, Pennsylvania State University, United States

4:15 PM

(GOMD-SIII-063-2010) Fabrication and Applications of Thin, Free-Standing Borophosphosilicate Glass (BPSG) Films
C. L. Trivelpiece*, J. S. Brenizer, C. G. Pantano, The Pennsylvania State University, United States

4:30 PM

(GOMD-SIII-064-2010) Nanophase semiconductor-transparent conductive oxide composite thin films for photovoltaic applications
G. H. Shih*, C. G. Allen, B. G. Potter, University of Arizona, United States

4:45 PM

(GOMD-SIII-065-2010) Development of an original process for the realization of multi-materials optical fibres
S. Leparmentier, J. Auguste*, G. Humbert, F. Gérôme, C. Restoin, J. Blondy, XLIM, France; B. Desruelle, DGA, France

5:00 PM

(GOMD-SIII-066-2010) Photo luminescence properties of copper ion doped alkali borosilicate glasses in metastable immiscibility region
A. Yasumori*, F. Tada, D. Takemoto, N. Matsui, T. Kishi, Tokyo University of Science, Japan

Symposium IV: Glass Corrosion

Long-term Corrosion Testing

Room: Carder

Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

1:15 PM

(GOMD-SIV-015-2010) Modeling Alteration of Borosilicate High-Level Waste Glass Networks in a Radiation Environment (Invited)
L. Dewan, L. Hobbs*, Massachusetts Institute of Technology, United States; R. Cherifi, Université Pierre et Marie Curie, France; J. Delaye, CEA Valrhô-Marcoule, France

1:45 PM

(GOMD-SIV-016-2010) Initial dissolution rate of P0798 simulated HLW glass as a function of pH and temperature measured by using micro-reactor flow-through test (Invited)
Y. Inagaki*, H. Makigaki, Kyushu University, Japan; S. Mitsui, JAEA, Japan; K. Idemitsu, T. Arima, Kyushu University, Japan; K. Noshita, Hitachi, Ltd, Japan

2:15 PM

(GOMD-SIV-017-2010) Isotopic Enrichment Studies to Determine Elemental Diffusion Profiles Through an Established Alteration Layer
J. V. Ryan*, A. Mitroshkov, D. M. Strachan, Pacific Northwest National Laboratory, United States

2:30 PM

(GOMD-SIV-018-2010) Long-Term Durability Testing of Glasses for the Stabilization of Closed Nuclear Fuel Cycle Waste Streams
A. L. Billings*, J. C. Marra, C. C. Crawford, Savannah River National Laboratory, United States

2:45 PM

(GOMD-SIV-019-2010) Evaluating the long-term weathering of minerals and engineered materials across a range of spatial and temporal-scales
E. M. Pierce*, Pacific Northwest National Lab, United States

3:00 PM

(GOMD-SIV-020-2010) Molecular Modeling of Aluminosilicate Glass Dissolution for High-Level Nuclear Waste Repository Science
L. J. Criscenti*, Sandia National Laboratories, United States; J. D. Kubicki, S. L. Brantley, Pennsylvania State University, United States

Panel Discussion

Room: Carder

Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

3:30 PM

Panel Discussion
with specialists on waste glass, modeling, geochemistry, and ancient glass

Symposium V: Glass Structure and Properties

Glass Structure and Properties IV: More Fun with the Vitreous State

Room: Keuka

Session Chair: Morten Smedskjaer, Aalborg University

1:15 PM

(GOMD-SV-034-2010) Elasticity, Compression Behavior, and Vibrational Properties of Silicate Glasses under High Pressures: A Review (Invited)
M. H. Manghnani*, University of Hawaii, United States

1:30 PM

(GOMD-SV-035-2010) A chemical probe for measuring glass densification under sharp contact?
J. Guin*, Y. Niu, T. Rouxel, CNRS-Université de Rennes 1, France; A. Abdelouas, Ecole des mines de Nantes, France

1:45 PM

(GOMD-SV-036-2010) High frequency sound and boson peak in glasses
B. Rufflé*, University Montpellier II, France

2:00 PM

(GOMD-SV-037-2010) Optical basicity revisited: theory and application to optical properties and crystallization (Invited)
J. McCloy*, Pacific Northwest National Laboratory, United States

2:15 PM

(GOMD-SV-038-2010) Correlation of Network Structure with Devitrification Mechanism in Lithium and Sodium Diborate Glasses
B. Chen, U. Werner-Zwanziger, J. Zwanziger*, Dalhousie University, Canada; M. Nascimento, L. Ghussn, E. Zanotto, Federal University of Sao Carlos, Brazil

2:30 PM

(GOMD-SV-039-2010) Structural Studies of Alkali Tungstate and Molybdate Glasses by X-ray Absorption Spectroscopy
C. W. Ponader*, K. Adib, B. G. Aitken, Corning Incorporated, United States

2:45 PM

(GOMD-SV-040-2010) Vanadium-51 and Boron-11 NMR Study of Ionically Conducting Alkali Borovanadate Glasses
V. K. Michaelis*, University of Manitoba, Canada; J. North, A. Ramm, S. Feller, Coe College, United States; S. Kroeker, University of Manitoba, Canada

3:00 PM

Break

3:15 PM

(GOMD-SV-041-2010) Intermediate-range Order in Nanostructured Silica
G. Chen*, C. Wan, B. Prasai, D. A. Drabold, Ohio University, United States

3:30 PM

(GOMD-SV-042-2010) Interactions of Small Molecules with Oxide Surfaces: Models for Polymer Binding on Glass Fibers
K. T. Mueller*, L. Ortiz-Rivera, D. L. Suchy, J. Stapleton, C. G. Pantano, Penn State University, United States

Monday, May 17, 2010

Symposium I: Robert H. Doremus Memorial Symposium

Robert H. Doremus Memorial Session I

Room: Keuka
Session Chairs: Mark Davis, Schott North America, Inc.; Minoru Tomozawa, RPI

9:45 AM

(GOMD-SI-001-2010) Dr. Doremus - Professor of Liberal Arts (Invited)
A. G. Chan*, Shore Chan Bragalone LLP, United States

Many remember Dr. Robert H. Doremus for his world renowned expertise in ceramics. But few realize that Dr. Doremus was a devoted instructor in the liberal arts. He made it a point to include in his Crystallography and Electrons in Solids courses instruction on technical writing and contemporary literature. My presentation will focus on how and why Dr. Doremus interweaved liberal arts with engineering. My presentation will also explore the impact of this aspect of Dr. Doremus' legacy on his student practitioners of ceramics and materials engineering.

10:00 AM

(GOMD-SI-002-2010) Gases in Glasses: The Doremus Perspective (Invited)
J. E. Shelby*, Alfred University, United States

Much of our current understanding of the solubility and diffusion of gases in glasses and melts is based on the work of Robert Doremus. This presentation will review the literature in this area from the perspective of the Doremus concepts.

10:30 AM

(GOMD-SI-003-2010) Gas Solubility in Glasses - The Doremus Contributions
J. F. Shackelford*, University of California - Davis, United States

I had the privilege of working with Bob Doremus on one of his last professional publications, co-editing Glass and Ceramic Materials (Springer, New York, 2008) for which he provided a review article on "Alumina." Our professional paths intersected nearly 40 years earlier while working on the subject of gas solubility in glasses. He proved to be an excellent mentor as we worked on somewhat parallel treatments of this topic. The current paper will review the overall subject of gas solubility in glasses, emphasizing the seminal contributions made by Doremus over more than four decades. The paper will also emphasize that the phenomenon of gas solubility provides substantial insight to the atomic-scale structure of the solvent glass.

10:45 AM

(GOMD-SI-004-2010) Water diffusion in silica glass (Invited)
M. Tomozawa*, RPI, United States

A small quantity of water in silica glass has large influence on glass properties. Water can enter into silica glass during melting and during heat-treatment. Additionally water can promote the oxidation of silicon, an important process in microelectronic device production. Water in silica glass was found to be hydroxyl water, Si-OH and it was not clear at first exactly how water diffuses in silica glass and various different diffusing species have been proposed. In a conference proceedings published in 1969, Doremus proposed water diffuses as molecular H2O and quickly react to form immobile Si-OH by ≡SiOSi≡ + H2O = 2≡SiOH He further suggested that equilibrium of the above reaction with the equilibrium constant, K = [SiOH]2/[H2O], is established local and obtained the effective diffusion coefficient of water. Subsequent works confirmed that his model is essentially correct.

11:15 AM

(GOMD-SI-005-2010) Diffusion of Water in Quartz: Application to Crystal Growth Kinetics (Invited)
P. D. Ihinger*, University Wisconsin-Eau Claire, United States

Hydrous impurities are found in every quartz crystal. They are incorporated into the crystal lattice during growth, and variations in their abundance reflect changing environmental conditions (P, T, fluid composition). Impurity uptake in quartz is a non-equilibrium process, and contaminants diffuse out of the crystal even with continued crystal growth. Natural hydrothermal crystals preserve well-defined diffusion profiles of hydrous species from core to rim. Identical patterns are observed in crystals grown in the same vein: diffusion profiles at bases show pronounced diffusion profiles reflecting longer times of thermal soaking, whereas diffusion profiles at successively higher elevations show progressively less diffusive loss reflecting shorter thermal exposure times. Diffusive loss at each terminus is minimal suggesting the hydrothermal vein was quenched to lower T shortly after cessation of crystal growth. The profiles quantify the growth time of each crystal in the natural hydrothermal environment.

11:45 AM

(GOMD-SI-006-2010) Diffusion of Alkali and Alkaline Earth Ions in Silicate Glasses and its Correlation with Liquid Fragility
M. M. Smedskjaer*, Aalborg University, Denmark; J. C. Mauro, Corning Incorporated, United States; J. Deubener, Clausthal University of Technology, Germany; Y. Yue, Aalborg University, Denmark

A physical understanding of diffusion processes in glasses is of great scientific and technological importance. In this work, we study the influence of the type of alkali and alkaline earth ions on the ionic diffusivity and fragility of iron-bearing silicate glasses. The modifying-ionic inward diffusion occurs in the glasses when Fe^{3+} is reduced to Fe^{2+}. In the SiO_2-Na_2O-Fe_2O_3-RO (R = Mg, Ca, Sr, Ba) glass series, the extent of diffusion decreases in the sequence Mg^{2+}, Ca^{2+}, Sr^{2+} and Ba^{2+}. In the SiO_2-A_2O-Fe_2O_3-CaO (A = Na, K, Rb, or Cs) glass series, the Ca^{2+} ions diffuse faster than alkali ions and the activation energy of the Ca^{2+} diffusion decreases with alkali size. In both series, the inward diffusion increases with a decrease in the fragility (m) of the glass systems. In this work, we have discussed the origin of this relation. In addition, we have proposed a simple model to explain the correlation between m and T_g of the glasses.

Symposium II: Glass Science

Atomistic Modeling of Glass I. Techniques

Room: Cayuga
Session Chair: Ulrich Fotheringham, Schott AG

9:30 AM

(GOMD-SII-001-2010) Developing effective potentials from ab initio simulations of amorphous systems (Invited)
W. Kob*, Universite Montpellier II, France; A. Carré, Deutsches Zentrum fur Luft und Raumfahrt (DLR), Germany; J. Horbach, Universite Montpellier II, France; S. Ispas, Deutsches Zentrum fur Luft und Raumfahrt (DLR), Germany

Computer simulations of glassforming systems have allowed to increase significantly our understanding of these complex materials. The quality of such simulations depends, however, crucially on the reliability of the used force field between the atoms. Unfortunately present day ab initio simulations do not allow to reach time scales beyond 100 ps, and system sizes are restricted to a few hundred particles. Therefore one often uses effective ("classical") potentials to carry out simulations. However, the problem in these simulations is that the used potentials are often postulated in an ad hoc manner and therefore the predictive power of such simulations is limited. In this talk I will present a recent approach in which we use the results of ab initio simulations in order to develop reliable classical potentials. Although the system considered is SiO2, the

method is very general and hence can also be applied to other glass-forming systems.

10:00 AM

(GOMD-SII-002-2010) Energy Landscapes and Beyond: A Systematic Approach to Understand the Properties of Supercooled Liquids (Invited)

A. Heuer*, O. Rubner, C. Rehwald, Institut für Physikalische Chemie, Germany

We analyze the dynamics of the binary Lennard-Jones system via computer simulations for largely different system sizes (65 <= N <= 2000). For the smallest system size it has been shown in previous work that the dynamics between metabasins can be described as a continuous time random walk (CTRW) when defining waitime times in terms of metabasin residence times. However, in the large N limit one has to consider the system as a superposition of coupled elementary subsystems, each representing CRR-type systems (cooperatively rearranging regions). This requires an alternative way of defining waiting times. Based on these results we can answer several important questions. (1) What is the origin of the different finite-size behavior for small and large q? (2) What do the finite-size effects teach us about the coupling between the CRRs? (3) How does this coupling influence the effective dynamic heterogeneities of the total (ideally macroscopic) system? (4) How does a temperature-dependent dynamic length scale emerge from this scenario? (5) What is the microscopic origin of the coupling between CRRs?

10:30 AM

(GOMD-SII-003-2010) Achieving Long Time Scales in Energy Landscape Simulations using Metabasin Partitioning

R. J. Loucks*, Alfred University, United States; J. C. Mauro, Corning Incorporated, United States; P. K. Gupta, Ohio State University, United States

We propose a technique for computing the master equation dynamics of systems with broken ergodicity. The technique involves a partitioning of the system into components, or metabasins, where the relaxation times within a metabasin are short compared to an observation time scale. In this manner, equilibrium statistical mechanics is assumed within each metabasin, and the intermetabasin dynamics are computed using a reduced set of master equations. The number of metabasins depends upon both the temperature of the system and its derivative with respect to time. With this technique, the integration time step of the master equations is governed by the observation time scale rather than the fastest transition time between basins.

10:45 AM

(GOMD-SII-004-2010) Simulations of Network Glasses with Multiple Coordination States using a Reactive Force Field

L. Huang*, F. Yuan, Rensselaer Polytechnic Institute, United States

Using molecular dynamics (MD) simulations, we uncovered the structural origins of the anomalous thermo-mechanical behaviors in silica glass, e.g., its elastic moduli decrease upon compression and increase upon heating. Moreover, we showed that these anomalies are universal in network glasses, and can be explained by similar mechanisms, whether the network structures are formed from tetrahedral or trigonal building blocks (as demonstrated for silica and boron oxide). Essential for the success of such simulations is the use of a new type of reactive interaction potential that realistically accounts for the charge redistribution associated with changes in bonding structure, and accommodates multiple coordination states during the MD simulations.

11:00 AM

(GOMD-SII-005-2010) Parallel Atomistic Monte Carlo Computations

A. Zakharian*, D. Vargheese, P. Diep, Corning Incorporated, United States

Equilibration of glass structures in atomistic Monte Carlo (MC) simulations can be computationally expensive when large number of trial steps is required. Due to the serial nature of the underlying Markov-chain process, parallel computations are not always straightforward to implement to improve MC simulation efficiency. We describe an algorithm for parallel NPT ensemble Monte Carlo simulations on shared-memory multi-processor systems. Each thread computes its portion of the random particle position displacement sequence, synchronized to preserve the serial chain of updates, while the computationally expensive neighbor-list updates and volume changes are implemented using concurrent loop processing. A speed-up by a factor of ~7 and parallel computation efficiency of ~80% is obtained in the simulations of glasses with 5000 particles on 8 processor systems.

11:15 AM

(GOMD-SII-006-2010) Reverse Monte Carlo Structures: Evaluation by Molecular Dynamics Simulations

C. R. Mueller*, Technische Universität Ilmenau, Germany; M. Schuch, P. Maass, Universität Osnabrück, Germany; V. Petkov, Central Michigan University, United States

The quality of structural models generated by the Reverse Monte Carlo (RMC) method in a typical application to amorphous systems is investigated. To this end diffraction data from a molecular dynamics (MD) simulation of a lithium silicate glass are calculated and used to generate RMC models with different protocols and starting configurations. It is found that partial distribution functions and properties on small lengths scales are well reproduced by the RMC modeling. However, properties in the medium-range order, as, for example, ring size distributions are not well captured. We further show that certain medium-range order features of the RMC models can be a mere consequence of the chosen starting configuration when using commonly applied RMC protocols. Due care herefore has to be exercised when extracting structural features from RMC models in the medium-range order regime and when using corresponding information as a basis for subsequent studies of ion transport properties.

11:30 AM

(GOMD-SII-007-2010) Electronic structure based material design: application to a-Si

D. A. Drabold, B. Cai*, Ohio University, United States; A. Goodwin, Oxford University, United Kingdom

Information-based model design requires building prior information, typically experimental information, into the atomic model. Algorithms, such as Reverse Monte Carlo (RMC) and Experimentally Constrained Molecular Relaxation (ECMR), are promising ways to realize this goal. However, these algorithms usually employ only structural information for creating the model. Electronic structure provides complementary information. In this work, by modeling amorphous silicon, we developed a RMC scheme in which the electronic structure guides the structural optimization. We show that the constraint that a disordered network has a significant optical gap is sufficient to create local tetrahedral order.

11:45 AM

(GOMD-SII-008-2010) Origin of Dynamical Heterogeneities in Calcium Aluminosilicate Liquids

K. D. Vargheese*, A. Tandia, J. C. Mauro, D. Phong, A. Rovelstad, Corning Inc, United States

We investigate the heterogeneous dynamics of calcium aluminosilicate liquids across both the peraluminous and peralkaline regimes. Using the isoconfigurational ensemble method we find a clear correlation between dynamical heterogeneities and concentration fluctuations. Regions of high dynamic propensity have higher concentrations of both calcium and aluminum, whereas low propensity regions are silica-rich. The isoconfigurational ensemble is found to be a powerful tool for studying the origin of heterogeneous dynamics of industrially relevant glass-forming liquids.

Symposium III: Glass Technology

Glass-Ceramics

Room: Seneca
Session Chairs: Robert Schaut, Corning Incoporated; Linda Pinckney, Corning Incorporated (ret.)

9:30 AM

(GOMD-SIII-001-2010) Controlled nucleation and crystallization of glass-ceramics (Invited)

W. Hoeland*, V. Rheinberger, C. Ritzberger, E. Apel, Ivoclar vivadent AG, Liechtenstein

Surface and internal nucleation and crystallization mechanisms were used to develop of glass-ceramics. Fluoroapatite was precipitated in glass-ceramics via internal crystallization of base glasses. Two mechanisms were indedtifyed: precipitation via a disordered primary apatite crystal and a second mechanism in the form of a solid state parallel reaction to rhenanit precipitation. Surface crystallization was induced to precipitate a phosphate-free oxyapatite. Internal nucleation and crystallization has shown to be a very useful tool for developing high-strength lithium disilicate glass-ceramics. A very controlled process was conducted to transform the lithium metasilicate glass-ceramic precursor material into the final product. An amorphous phosphate primary phase was discovered in the process. Nucleation started at the interface between the amorphous phosphate phase and the glass matrix.

10:00 AM

(GOMD-SIII-002-2010) The early stages of glass ceramics devitrification

W. Bras*, Netherlands Organization for Scientific reserach (NWO), France; N. Greaves, Aberystwyth University, United Kingdom; S. Clark, M. Kunz, Lawrence Berkeley National Laboratory, United States; S. Nikitenko, Netherlands Organization for Scientific reserach (NWO), France; G. Bruno, Corning SAS, France; V. Radmilovic, Lawrence Berkeley National Laboratory, United States

The very early stages during the onset of crystallization is difficult to examine. Combined time-resolved Small and Wide Angle X-ray scattering is a rather useful tool when studying the initial stages of crystallization and density fluctuations. Counter intuitive SAXS is much more sensitive to detect the early stages of crystallization then conventional powder diffraction since SAXS is dependent on electron density differences and not on the presence of well ordered structures which can render diffraction. We have applied this technique to Cr doped cordierite glass (Mg2Al4Si5O18). This material was subjected to a two step heat treatment. At the higher temperature two crystalline phases appeared. These grew independently and we could distinguish between bulk and surface crystallization. We determined that the bulk crystals growth was a diffusion limited process. Crystalline lattice size changes were observed allowing the determination of the internal pressures from the matrix material onto the crystals.

10:15 AM

(GOMD-SIII-003-2010) Crystallization of Lithium silicate Glass-ceramics for artificial teeth

C. Kim*, C. Kim, Inha Univ., Korea, Republic of

Glass-ceramics based on lithium disilicate($Li_2Si_2O_5$) are commonly used for dental materials. In this study, various glass-ceramics were prepared with different molar ratio of SiO_2/Li_2O in a glass system of SiO_2-Li_2O-K_2O-Al_2O_3. The glasses were heat-treated in the temperature range of 800-900 degree, and the obtained crystalline phases were analyzed by XRD and SEM. The crystallinity of the glass-ceramics was calculated by Benedetti method, and Vickers hardness and bending strength were measured. The surface crystallization was observed in the glass without nucleation agent. The glasses crystallized into lithium metasilicate and lithium disilicate crystals depending on the SiO_2/Li_2O ratio. The bulk crystallization was induced by adding nucleation agents. P_2O_5 was most effective to get lithium disilicate crystalline phases with small needle-like morphology. The microhardness and bending strength of the glass enhanced with crystallization.

10:30 AM

(GOMD-SIII-004-2010) A secondary ion mass spectroscopy (SIMS) and Mössbauer study of modified ZBLAN glasses

M. Vu*, A. Terekhov, G. Murray, University of Tennessee Space Institute, United States; S. Schweizer, Fraunhofer Institute, Germany; R. Weber, Materials Development Inc., United States; C. Johnson, J. Johnson, University of Tennessee Space Institute, United States

A class of glass-ceramic materials has been developed as a computed radiography imaging plate. The materials are based on ZBLAN doped with europium and chlorine. Upon heat treatment barium chloride nanoparticles containing optically active europium (II) form within the glass matrix. The materials are (semi-)transparent and act as x-ray storage phosphors. The modified ZBLAN glasses studied have been synthesized by different routes resulting in slightly different properties. The process route is crucial to creating the "storage effect". A study using secondary ion mass spectroscopy (SIMS) was carried out to examine the effects of trace oxygen on the material structure/property relationships and Mössbauer spectroscopy was performed to determine the ratio of Eu(II)/Eu(III) in the glass ceramics; these results will be presented and discussed in the context of optimizing the performance of the image plates.

10:45 AM

(GOMD-SIII-005-2010) Nucleation and growth of glass-ceramics by in-situ High-Temperature X-ray diffraction and Small Angle Neutron Scattering

C. Fernandez-Martin, G. Bruno*, P. Pradeau, M. Comte, Corning SAS- CETC, France

High temperature X-ray diffraction (XRD) and small angle neutron scattering (SANS) have been performed to study the crystal nucleation and growth in Li-Al-SiO2 (LAS) glasses. SANS and XRD yield complementary information. SANS provides insights on the nucleation process, while XRD gives information on the growth and element partitioning. XRD shows the presence of coherent domains only above 820C, and a rapid crystallinity increase between 830C and 870C. SANS reveals the existence of particles already at 750C. The SANS signal in a given particle size range displays a maximum, implying that particles grow, leaving the region under investigation. XRD shows that crystallite size increase occurs only during the growth heat treatment (above 900C). In parallel, the b-quartz lattice parameter evolution implies that the SiO2 content increases with temperature and time during hold. This study will be complemented with the comparison to other glass-ceramic systems.

11:00 AM

(GOMD-SIII-006-2010) WITHDRAWN

11:15 AM

(GOMD-SIII-007-2010) Influence of zirconium and titanium on the crystallization of a calcium aluminosilicate melt

E. Strukelj, Corning SAS, France; M. Roskosz, Université Lille 1, France; M. Comte*, Corning SAS, France; P. Richet, IPGP, France

We present an experimental study of the influence of zirconium and titanium on the crystallization of a calcium aluminosilicate melt. Crystallization has been studied at high degrees of supercooling. Because crystallization depends on the structure and properties of the melts, the influence of the nucleating agents on vibrational mode, viscosity and molar volume has also been investigated. As previously described for related compositions, heterogeneous, congruent crystallization of metastable yoshiokaite is observed at the surface of the starting melt after a few hours near 960°C. Zr and Ti strongly affect this crystallization: if Zr effectively allows the formation of yoshokaite in the bulk of the glass, Ti leads first to the formation of an Al2O3 polymorph in the bulk followed by CaTiO3 crystallization. The structural implications of

the results will be discussed along with the crystallization mechanisms operating in these melts.

11:30 AM

(GOMD-SIII-008-2010) Second harmonic generation and giant dielectric response in $BaTi_2O_5$ glass-ceramics

A. Masuno*, Y. Kikuchi, H. Inoue, Y. Watanabe, The University of Tokyo, Japan; J. Yu, Japan Aerospace Exploration Agency, Japan

Two metastable phases of α- and β-$BaTi_2O_5$ were successively obtained during heating process of $BaTi_2O_5$ glass prepared by containerless processing. Optical nonlinearity and dielectric properties of these metastable $BaTi_2O_5$ glass-ceramics were investigated. Second harmonic generation and giant dielectric response were observed at the crystallization temperature of α-$BaTi_2O_5$, while they were disappeared after paraelectric β-$BaTi_2O_5$ was formed. Although the crystal structure of α-$BaTi_2O_5$ has not been determined, these experimental results suggest that α-$BaTi_2O_5$ has a polar crystal structure and then has responsibility for the giant dielectric response. α-$BaTi_2O_5$ also showed larger second harmonic generation at room temperature than stable ferroelectric γ-$BaTi_2O_5$.

11:45 AM

(GOMD-SIII-009-2010) Fluoride Nanoscintillators

L. G. Jacobsohn*, K. Sprinkle, C. J. Kucera, T. L. James, T. A. DeVol, J. Ballato, Clemson University, United States

Present concerns about the illicit importation of radioactive materials across national borders impose the need of low-cost radiation detection systems that can be widely deployed, and challenge the long-standing technology of scintillators based on single-crystals. The objective of this research is to investigate the use of fluoride luminescent nanoparticles for radiation detection. Rare earth doped nanoparticles of CaF2, BaF2, PbF2 and LaF3 were prepared by a modified co-precipitation method using metal nitrates as precursors and ammonium di-n-octadecyldithiophosphate (ADDP) as ligand that allows the growth of solid shells onto nanoparticles. Nanoparticle characterization was carried out by means of XRD, TEM, and photoluminescence measurements. The scintillation response under 241Am excitation was characterized by pulse height distribution measurements. CaF2:Eu/CaF2 core/shell nanoparticles presented significant brightness enhancement due to the addition of shells; the mechanisms underpinning this enhancement are discussed.

12:00 PM

(GOMD-SIII-010-2010) Preparation of Apatite-Wollastonite-Phlogopite glass-ceramic composites by powder sintering method

A. Faeghi Nia*, Tabriz university, Iran, Islamic Republic of

An Apatite-Wollastonite-Phlogopite glass-ceramic composite, was developed by sintering and crystallization of the powdered glass. The non-isothermal and isothermal sintering kinetics were studied for this glass-ceramic. Hot-stage microscopy (HSM) measurements demonstrated that it is possible to sinter and crystallize this glass-ceramic with 80% relative density. The activation energy of sintering was analyzed using previously reported model of sintering and it was obtained :Q=193.83 K.j.mol.K-1. Also it was shown that the microstructure of sample is a function of particle size distribution.

Symposium I: Robert H. Doremus Memorial Symposium

Robert H. Doremus Memorial Session II

Room: Keuka
Session Chairs: Mark Davis, Schott North America, Inc.; Minoru Tomozawa, RPI

1:30 PM

(GOMD-SI-007-2010) Gold in glass: A new state of conduction? (Invited)

H. Jain*, Lehigh University, United States; R. Böhmer, O. Kanert, R. Kuechler, Technical University of Dortmund, Germany

Doping of glass with gold dates back to Roman times when it was used to introduce ruby color. Over the years scientists have focused on the origin of ruby color, including the Nobel laureate Richard Adolf Zsigmondy in late 19th century, who established its origin in gold colloids, and Robert Doremus in the late last century, who focused on the growth of such colloids in relation to optical absorption. Recently, we started investigating electrical properties of metal-glass nanocomposites containing 0.01-0.06 at% gold, and discovered a new high-conductivity state. For the case of both alkali conducting lithium borate and alkali-free lanthanum borogermanate glasses, this state is recognized via a thermally activated process with ~ 0.3 eV activation energy, suggesting its origin in electron hopping between partially ionized gold atoms. In the backdrop of the long history of optical properties of gold in glass, possible mechanisms of the new conduction state and its potential novel applications will be discussed.

2:00 PM

(GOMD-SI-008-2010) Morphology and Optical Properties of Laser-Patterned Crystals in Glasses (Invited)

T. Komatsu*, T. Honma, Nagaoka University of Technology, Japan

The laser-induced crystallization technique is applied to glasses for the patterning of functional crystals such as ferroelectric LiNbO3, ferroelastic β'-Gd2(MoO4)3, and Er3+-doped CaF2, in which continuous wave lasers such as Yb:YVO4 (wavelength: 1080 nm) are irradiated onto glasses containing rare-earth or transition metal ions. The morphology and optical properties of laser-patterned crystals are examined from confocal laser scanning microscope observations, second harmonic (SH) generations, and micro-Raman scattering spectra. In the patterning of β'-Gd2(MoO4)3 crystal lines, self-organized periodic domain structures with periodic SH intensities are patterned along the crystal line growth direction due to the presence of spontaneous strains. In Er3+-doped oxyfluoride glasses, laser irradiation induces the pattering of CaF2 nanocrystals and Er3+ fluorescence intensity is largely enhanced. The mechanism and features of laser-induced crystallization have been discussed.

2:30 PM

(GOMD-SI-009-2010) An investigation of microstructure, mechanical and biocompatibility characteristics of yttrium and fluoride doped nano hydroxyapatite

Z. Evis*, S. Toker, A. Tezcaner, D. Keskin, Middle East Technical University, Turkey

Nano hydroxyapatite (HA) was synthesized by precipitation method and doped with (Y3+) and fluoride (F-) ions at varying compositions. After sintering at 1100oC for 1 hour, the structural properties of pure and doped HAs were investigated by density measurement, X-Ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). High relative densities were achieved in both pure and doped samples. No secondary phases were observed in XRD studies upon doping with Y3+ and F- ions. Lattice parameters decreased due to substitutions of doping ions. Characteristic

absorption bands of HA and additional bands due to F- ion substitutions were observed in FTIR patterns. SEM results revealed that addition of doping ions resulted in smaller grains. Micro-hardness values of HAs were found to be correlated with the amount of dopings. In biocompatibility analysis, cell attachment and proliferation on HA discs were observed by SEM. Both pure and doped HA discs provided a favorable environment for cell attachment and proliferation.

2:45 PM

(GOMD-SI-010-2010) Contributions of Robert H. Doremus in the Field of Crystallization Kinetics

M. Davis*, SCHOTT North America, Inc., United States

Among the many significant contributions that Prof. Robert H. Doremus and his colleagues made in the broad field of glass and related materials, several in the field of crystallization kinetics have emerged as important works. These include papers on crystallization in heavy-metal fluoride glasses, including ZBLAN and related compositions, and the clarification and refinement of methods used to extract kinetic data from thermal analysis studies. More recent research on susceptibility of crystalline materials to ion beam-induced amorphization and its comparison with glass stability has emerged as highly cited work in this field. This presentation will review these papers in light of Prof. Doremus' long and distinguished career.

3:15 PM

(GOMD-SI-011-2010) MeV Ion Beam Analysis of Glass and Ceramic Surfaces (Invited)

W. A. Lanford*, University at Albany SUNY, United States

Thirty five years ago a young Assistant Professor working on ion beam analysis started applying the 15N nuclear reaction method for measuring hydrogen concentration vs depth. One of the problems addressed was: "what happens when ordinary glass is in contact with water." The experiments were easy: heat glass in water and then measure the resulting hydrogen concentration vs. depth. While the data looking interesting, we had no knowledge of glass science much less how water interacts with sodalime glass. The literature led us to Bob Doremus who we visited at RPI. Bob had a remarkable ability to communicate with a contagious enthusiasm, always at an appropriate technical level. This meeting led to collaborations over the intervening decades, including work on diffusion of Br in NaCl done in the last weeks of Bob's life. This paper will review MeV ion beam analysis. These techniques will be illustrated by application to the study of glass and ceramics with emphasis on studies done in collaboration the Bob Doremus.

3:45 PM

(GOMD-SI-012-2010) Novel Glasses for On-Chip Microelectronic Applications (Invited)

V. J. McGahay*, IBM Corporation, United States

Amorphous silica and related films have been used extensively in microelectronic devices since the beginning of the semiconductor industry. Applications include capacitor dielectrics for field effect transistors, mobile ion and moisture diffusion barriers, and electrical isolation. The last category has undergone considerable expansion in recent semiconductor technology generations with respect to film composition and preparation technique. Novel fluorine-doped, carbon-doped, and porous carbon-doped oxide glasses with low dielectric constants have been developed to improve signal delay and power consumption by reducing the parasitic capacitance associated with insulation of microelectronic wires. Structurally, these materials can be viewed as modifications of amorphous silicon dioxide in which bridging oxygens are removed to produce less constrained, lower density materials.

4:15 PM

(GOMD-SI-013-2010) Viscosity of Germania-Doped High Purity Fused Silica Glass

E. M. DeLiso*, Stanton Advanced Ceramics, Inc., United States

The viscosity of high purity fused silica made with the Corning outside deposition process and doped with germania at levels upto 24 mol% GeO2 is compared to the viscosity data reported by R. H. Doremus for Type I silica. A discontinuity in viscosity is seen at low levels of germania addition for the germania-doped high purity fused silica. Borrelli and Kolesova predicted a non-linear behavior in viscosity for GeO2-doped silica as a function of the molar composition of the glass. This non-linear behavior will be shown from the experimental data. Glass structure responsible for this nonlinear behavior was attributed to the presence of Si-O-Ge bonds in the binary mixture.

4:30 PM

(GOMD-SI-014-2010) Extrusion of Tellurite Glass for Optical Fiber Preforms (Invited)

A. A. Belwalkar*, W. Z. Misiolek, J. Toulouse, Lehigh University, United States

Tellurite glass, a low temperature forming glass, is of great interest in holey fiber (HF) fabrication for supercontinuum generation and other nonlinear optical applications, along with other key attributes of good thermal and chemical stability, higher infrared transmission and nonlinear refractive indices and relatively low phonon energies. Extrusion is most suited to produce HF preforms with complex geometry to give better control over light propagation providing wide range of optical functionality. Various tube and HF performs with excellent surface quality were extruded from tellurite glass 75TeO2-20ZnO-5Na2O on lab press. Flow lines were observed within extrudate cross-sections believed to be caused by viscosity variations and inhomogeneous glass flow. A more uniform glass flow was achieved by optimizing the extrusion parameters, viscosity and shear rate, thus eliminating the flow lines within the extrudates. Preforms with improved optical homogeneity yielded fibers with a much reduced optical transmission loss.

Symposium II: Glass Science

Atomistic Modeling of Glass II. Applications

Room: Cayuga

Session Chair: Jincheng Du, University of North Texas

1:15 PM

(GOMD-SII-009-2010) Spatial and dynamic correlations in alkali transport in silicate glasses by atomic simulation and virtual reality modelling (Invited)

N. Greaves*, Aberystwyth University, United Kingdom

By studying ion transport in alkali silicate glasses by atomic simulation we show how surface and volume-based visualisation techniques can be used to depict the spatial relationships between network and mobile ions together with the cooperative relationships between them. Network isosurfaces coupled with immersive viewing clearly reveal ion channels penetrating the whole structure and also depict the free volume accessible for ion transport. Vibrations of individual ions within cooperative subgroups reveal network and rattling movements, as well as frequencies in the vicinity of the Boson Peak. The free volume available to moving alkalis is not distributed homogeneously but intimately associated with co-operative hopping events. Different alkalis are randomly packed and visualisation shows how the accessible free volume is reduced, mirroring the reduction in ionic diffusion, and offering a simple explanation for the well-know mixed alkali effect.

1:45 PM

(GOMD-SII-010-2010) A Molecular Dynamics Study of the Structure and Elastic Properties of Sodium Silicate and Sodium Aluminosilicate Glasses

L. Adkins*, A. N. Cormack, Alfred University, United States

Improving the mechanical properties of glass requires an understanding of how they depend on the structure and composition. In this study, we have used molecular dynamics simulations to examine the structural and corresponding elastic property changes that occur in glass under an applied stress, in a range of sodium silicate and sodium aluminosilicate glasses. The glasses were formed and fractured under a tensile load. We will discuss the particular role of non-bridging oxygens as well as the consequence of increasing the alumina content in the glass on the structural changes which occur as the glass is fracturing.

2:00 PM

(GOMD-SII-011-2010) Local structure around Eu(III) ions in aluminate glasses

H. Inoue*, K. Ohno, Y. Watanabe, A. Masuno, The University of Tokyo, Japan

Europium(III)-doped Y2O3-Al2O3 and La2O3-Al2O3 glasses were prepared using a containerless processing with an aerodynamic levitation furnace. Emission spectra of the Eu(III) ions in the glasses were measured as function of the excitation wavelength by means of the techniques of laser-induced fluorescence line narrowing. The structural models with Eu(III) ions were prepared and the relation between the splitting of the energy levels and the local structure around the Eu(III) ions was evaluated. A structural model have been proposed for the first coordination shell of the Eu(III) ion in the oxide glass by C. Brecher and L. A. Riseberg. It was found that the local structure around the Eu(III) ions in the glasses was different from the model proposed by C. Brecher and L. A. Riseberg. Another first coordination shell is proposed for the Eu(III) ions in the glasses.

2:15 PM

(GOMD-SII-012-2010) Ab initio calculation of mixed ion dynamics in Silver/Copper doped chalcogenide glass

B. K. Prasai*, B. Cai, D. A. Drabold, Ohio University, United States

The problem of mixed-ion conduction in glasses has been an area of intense study. In this talk, we describe recent simulations of mixed-ion conduction in chalcogenide materials. We use plane-wave density function method (VASP) to carry out thermal simulations at several temperatures on Germanium-Selenide glasses doped with various concentrations of Copper and Silver. The trajectories of Cu+ and Ag+ ions will be analyzed, and particular attention will be focused on the dynamical consequences of the simultaneous existence of Cu and Ag in the model.

2:30 PM

(GOMD-SII-013-2010) The environments of cerium ions in cerium-doped aluminophosphate and phosphosilicate glasses: combining molecular dynamics simulations and ab initio DFT calculations

J. Du*, L. Kokou, University of North Texas, United States

Cerium doping finds wide applications in optical glasses. Both Ce3+ and Ce4+ can be present in oxide glasses and their environments are important to the optical absorption and emission properties. In this paper, we present molecular dynamic simulations of cerium-containing aluminosilicate and phosphosilicate glasses using newly developed potential models containing cerium ions. The local environments around Ce3+ and Ce4+ are studied, and the bond length and coordination of cerium ions are determined. Small samples of the glasses are simulated using MD and then further relaxed with DFT calculations. Comparison of the structure of glasses from MD and after DFT relaxation is made. It is found that Ce3+ has a longer bond distance and higher coordination number of oxygen. Most interestingly, cerium ions are found to be preferentially coordinated by phosphorus ions in the second coordination shell in the glasses.

2:45 PM

(GOMD-SII-014-2010) Influence of the Modifier Cation Type on the Infrared Spectral Response of Multi-Component Glasses

A. K. Upadhyay*, K. Becker, J. Kieffer, University of Michigan, United States

The size and field strength of modifying cations has a strong influence on the topology of the glassy network and, consequently, on the properties of the material.Using molecular dynamics simulations based on a reactive force field we systematically investigate the roles of Na2O and CaO in the composition-dependent structural evolution of multi-component silicates and boro-silicates. Our force field allows for multiple coordination states and accounts for the charge transfer upon scission or formation of network bonds. We correlate the various structural features that develop with the network's IR vibrational response, which is commonly used as an experimental structural characterization technique. This analysis is accomplished by using Fourier filtering of atomic trajectories (FFAT) to assign spectral bands to the vibrational modes of structural moieties, yielding unexpected mode identifications and a strong dependence of IR spectra on network constraints.

3:15 PM

(GOMD-SII-015-2010) First-principles simulations of glasses: Establishing the rings statistics in B_2O_3 and B_2S_3 (Invited)

G. Ferlat*, Université Paris VI, France

First-principles molecular dynamics (FPMD) simulations are powerful tools for modeling disorded systems. However care must be given to possible arte-facts which may arise either from the small system sizes and/or from the much too high numerical quenching rates used. We shall present how this problem has been circumvented in our recent studies of the B_2O_3 and B_2S_3 glasses [1,2]. Using FPMD to generate different models, a wide range of observables were then calculated, allowing us to assess in an unambiguous way the fraction of small rings such as the so-called boroxol rings. This study clearly evidences to which extent these observables are sensitive to the medium range-order and solves the apparent contradictions in the literature. From the exploration of the energetics, we shall propose a scenario for the glass transition in these systems. [1] G. Ferlat et al., Phys. Rev. Lett., 101, 065504 (2008). [2] G. Ferlat and M. Micoulaut, Phys. Chem. Glasses, 50, 284 (2009).

3:45 PM

(GOMD-SII-016-2010) Monte Carlo Simulations of Inert Gas Solubility in Silicate Glasses and Melts

A. Zakharian*, A. Tandia, D. Vargheese, P. Diep, Corning Incorporated, United States

Detailed knowledge of non-reactive gas solubility can be used to explore the atomistic structure of amorphous materials. We computed helium and neon solubility dependence on the temperature and composition of silicate melts via atomistic Monte Carlo simulations. To improve computation efficiency, the chemical potential of the solvent-solute system was evaluated using Excluded Volume Map Sampling technique. Deviation of 20-30% from the nominal values of the particle pair-potential interaction parameters was found to be sufficient to achieve consistency with known solubility values. Good agreement was found between the computed and experimentally measured variation of solubility reported in literature for helium and neon, as a function of temperature and composition of host silica and sodium silicate glasses and melts.

4:00 PM

(GOMD-SII-017-2010) Glass-like dislocation dynamics of degenerate 2D dimer crystals

U. Agarwal*, S. J. Gerbode, I. Cohen, F. A. Escobedo, Cornell University, United States

The effect of shape anisotropy on the dynamics of self-assembled mesophases is investigated via simulations of simple models involving densely packed monolayer crystals of spheres and doubly-lobed particles (dimers). Their dynamical behavior was probed by both using a microrheological probe (particle dragging) and imposing a uniform shear

field via non-equilibrium molecular dynamics. It is observed that particle anisotropy introduces stark differences in the dislocation dynamics, which plays a key role in the relaxation mechanism and hence the rheological properties. While dislocations relax freely in the spherical particles, their motion is highly restricted for the dimers. For the latter, the relaxation mechanism can be broken in two-stages wherein the dislocations have a fast local glide response and a slower long range relaxation involving hops from caged configurations. This mechanism of dislocation transport leads to inhomogeneities in stress distributions and may also lead to unusual melting behavior.

4:15 PM

(GOMD-SII-018-2010) MD simulations of soda lime silicate glasses with increasing calcia content

A. Cormack, A. Collier*, Alfred University, United States

The development of new glass compositions requires understanding of glass properties and how they are influenced by compositional (and hence, structural) changes. In this presentation we discuss the impact on sodium migration of changing the calcia to silica ratio in a series of soda-lime-magnesia-silicate glasses. We have used molecular dynamics to model the four glass compositions, obtaining the mean square displacement at 300K over a 2 ns run time. For one composition, we also ran at a number of different temperatures, to obtain an activation energy, which will be compared with that obtained from experimental conductivity data.

4:30 PM

(GOMD-SII-019-2010) Molecular Scale Characterization of Mechanical and Structural Properties of xAl2O3–(1-x)SiO2

A. Tandia*, K. Vargheese, Corning Incorporated, United States

For the design of glass composition with optimal properties, detailed understanding of the correlation between composition, structure and properties is critical. In this study we investigate, by means of molecular scale modeling, the influence of Al2O3 addition on v-SiO2 on key aspects such as ring statistics, elastic properties, network polymerization, atomic coordination, fraction of free volume, compressibility at room temperature. Further more, we have added detailed probing of Qn speciation, linkages around the glass formers, and Oxygen tri-coordinated. We have also carried out an analysis of the atomic coordination variation with respect to temperature. As we cool down a melt from temperature above glass transition regime, we observe different thermal responses of the Si and Al network. Our analysis covers a temperature range around Tg for all compositions.

4:45 PM

(GOMD-SII-020-2010) Molecular simulations to explore the energy landscape of surface wetting transitions of an oily fluid on a rough surface

E. Savoy*, Corning, Inc, United States; F. Escobedo, Cornell University, United States

Molecular simulations to characterize the wetting behavior of an oily fluid on a topologically nano-patterned surface will be discussed. The low surface tension of the fluid results in a rugged energy landscape that tends to trap the simulated nanodrop in metastable states. Using a generalized Hamiltonian replica exchange method, in which neighboring configurations have different surface affinity, we allow the droplet to more efficiently explore the phase space to find the true equilibrium wetting state for multiple intrinsic surface chemistries simultaneously. Resulting contact angles are much closer to those predicted by the theoretical Wenzel equation. It is also found that the energy due to interaction of drop and surface particles correlates well with the series of observed wetted states. Other techniques such as umbrella sampling and forward-flux sampling methods are used to better characterize the underlying transition states.

Symposium III: Glass Technology

High-Strength Glasses

Room: Seneca

Session Chairs: Arun Varshneya, Alfred University; William LaCourse, Alfred University; Murli Manghnani, University of Hawaii; Tanguy Rouxel, Universite De Rennes 1

1:15 PM

(GOMD-SIII-011-2010) Edge-on Impact Investigations of Stress and Damage Propagation in Monolithic and Novel Laminate Glass and Glass Ceramics (Invited)

E. Strassburger, Ernst-Mach-Institut (EMI),, Germany; P. Patel, Army Research Laboratory, United States; A. Varshneya, Alfred University, United States; J. W. McCauley*, Army Research Laboratory, United States

This paper will review work carried out over the last several years using a unique, fully instrumented Edge-on Impact (EOI) facility at EMI, using a Cranz-Schardin high speed camera, modified for dynamic photoelasticity, to quantify stress wave propagation, damage nucleation and propagation during high velocity impacts. This experimental technique has been used to examine monolithic plates (100x100x10 mm) of fused silica, Borofloat™ and Starphire™ glass. More recently, the same methods have been used to study TRANSARM™ and ZERODUR™ glass ceramics and a variety of novel laminates with polyurethane bonding interlayers in the range from 0.64 mm to 5.08 mm thick. This work has now been extended to investigate a variety of interface geometries including saw tooth, corrugated and wave shaped. In addition, Saxon Glass Technologies Ion-Armor™ strengthened glass mounted on Starphire® monolithic plates have also been tested.

1:45 PM

(GOMD-SIII-012-2010) Strength of chemically strengthened glass

T. Komai*, Nippon Electric Glass Co.,Ltd, Japan

Chemical strengthening is one of the methods used to enhance the mechanical strength of glass. It is important to comprehend the effect of ion-exchange characteristics on mechanical strength, such as compressive stress (CS) and depth of compressive stress layer (DL). Several glass samples were prepared under various ion-exchange conditions. Well annealed glass has higher CS and deeper DL than rapidly cooled glass. This implies ion-exchange characteristics are affected by glass composition and annealing profile. In our experiment the strength of each sample was measured by 3 point bending test (3PB) and ring on ring test (ROR). Glass with higher CS and deeper DL had higher strength in both tests. Glass with deeper DL, however, showed larger Weibull coefficients in 3PB than in ROR. In 3PB, it is thought that deeper DL prevents cracks at sample edges and prevents glass strength deterioration.

2:00 PM

(GOMD-SIII-013-2010) Environmentally Friendly Chemically Strengthened Glasses

M. Dejneka*, Corning, United States; C. Chapman, Corning, United States; S. Gomez, Corning, United States; K. Rossington, Corning, United States

Chemically tempered glasses are strong, lightweight and scratch resistant so they are widely used to protect displays in mobile devices such as cell phones, digital music players, and especially touch screen devices. Unlike soda lime silicates, ion exchangeable aluminosilicate glasses capable of deep protective compressive layers and high compressive stresses are challenging to melt and refine, so toxic fining agents such as As_2O_3 and Sb_2O_3 are used. This talk will describe the development of new environmentally green compositions that can be ion exchanged to 50 microns depth with compressive stresses in excess of 700 MPa. Thus, these new glasses provide the same level of protection and strength as their predecessors, but do not contain any hazardous ingredients.

2:15 PM

(GOMD-SIII-014-2010) Influence of Edge Preparation on Impact Resistance of Thin Chemically Strengthened Glass

P. K. Kreski*, Alfred University, United States; A. K. Varshneya, Saxon Glass Technologies, Inc., United States

Thin chemically strengthened glass is one of the materials used as protective windows in personal electronic devices. Center and edge impact resistance of this glass is obtained, using the ball drop method, as a function of varied edge preparation conditions. Among the preparation parameters examined, edge flaw distribution is found to be more important than edge geometry. Dynamic finite element simulations are used to identify stress concentrations during impact.

2:30 PM

(GOMD-SIII-015-2010) Effect of different alkalis on the ion-exchange ability of high strength glasses

S. Gomez*, M. J. Dejneka, R. M. Morena, L. A. Lamberson, Corning Incorporated, United States

Strong glasses can be obtained by exposing a glass containing alkalis to molten salt baths that contain alkali ions which are typically larger than those ions initially in the glass, creating a compressive layer. This compressive layer imparts strength to the glass. Chemical potential differences between the glass and salt bath drive the replacement of some ions in the glass by some ions in the salt bath. Smaller ions diffuse faster in some glasses than larger ions, thus larger depths of compression can be achieved. The rate of diffusion can be strongly influenced by the nature of the alkali ions present in the glass as well as in the salt bath. For example, when replacing Li+ for Na+ the rate of diffusion can be ~10x faster than substituting K+ for Na+. The effect of alkalis on the extent of the diffusion layer in the glass will be studied by electron microprobe analysis. The resulting strength of the studied glasses will also be discussed.

3:15 PM

(GOMD-SIII-016-2010) Damage propagation in high strength glasses rods due to high velocity ball impact (Invited)

G. Subhash*, University of Florida, United States

Chemically strengthened glasses are subjected to high velocity steel ball impact to investigate the damage propagation characteristics. Both long-rod cylindrical geometry and Edge-on-Impact (EOI) geometry have been used. For ball-on-rod impact, the damage propagates in one dimension up to certain depth depending on the velocity of the ball and then is temporarily halted. The stress wave reflected back from the rear surface initiates damage from the rear surface. A detailed study on the nature of cracks induced during early stage of impact, influence of surface defects, effect of surface residual stresses and the influence of velocity on induced stress field will be presented.

3:45 PM

(GOMD-SIII-017-2010) On the Measurement of Design-Relevant Fracture Properties of Structural Glasses and Ceramics

K. Iyer*, Exponent, Inc., United States

Novel test methods are presented for direct laboratory measurement of technologically-relevant fracture modes/systems in flat glasses and ceramic tile. The approach holds promise for providing immediate screening of the structural performance of different grades of a glass or ceramic. Three practical fracture modes/systems that result in complete failure of flat glass specimens are demonstrated: (i) a single conoid macrocrack system, (ii) a back face radial macrocrack system, or (iii) a combination of (i) and (ii). The failure modes are induced by using variations of a ball-on-ring configuration and a ball-on-flat configuration. The approach is novel as fracture is induced deliberately under contact loading conditions similar to those present in several in-field structural failures, and because full specimen failure is achieved.

4:00 PM

(GOMD-SIII-018-2010) Using two-point bend technique to predict failure strength of glass fibers

Z. Tang*, R. K. Brow, Missouri S&T, United States; C. R. Kurkjian, University of Southern Maine, United States; N. P. Lower, Rockwell Collins, Inc., United States

The two-point bend (tpb) technique is used to measure the failure strains of pristine glass fibers under liquid nitrogen (ε_{LN}) and ambient conditions. Compared to failure strain, failure strength is considered more fundamental to materials and also more applicable in industry. The values for (ε_{LN}) for several types of glasses were determined using the two-point bend technique, and failure strengths were calculated based on reported higher order terms for the elastic modulus. Failure strengths predicted using tpb are comparable to reported tensile strengths of similar glasses. For example, 13.8 GPa is calculated from the tpb analysis of fused silica, compared to 12.5 to 15 GPa from inert tensile tests. For E-glass, tpb estimates an inert strength of 6.2 GPa compared to 6.5 GPa for tensile tests. Strength predictions done at room temperature are dependent on relative humidity and testing rate, and will be compared with reported tensile tests.

4:15 PM

(GOMD-SIII-019-2010) Flaw Distribution Measurements in High Strength Glass via the Hertzian Cone Crack Test

I. Reimanis*, J. A. Jones, Colorado School of Mines, United States; R. A. Schaut, Corning Incorporated, United States

Hertzian cone-crack testing has been used to measure flaw distributions in glasses for several decades. Typically, an empirical approach is used in which a surface is indented many times with a hard sphere, and the peak load to fracture is utilized in a statistical analysis. A less common, but direct method developed by Poloniecki and Wilshaw is particularly relevant for very small flaws (e.g., sub-micron). This latter method is used to test four high strength, borosilicate-based glasses. Sensitivity to a variety of variables, including loading rate, environment, and Hertzian sphere diameter are examined systematically. Applicability of this method of Poloniecki and Wilshaw to the determination of flaw distributions in modern, very high strength glasses is discussed.

4:30 PM

(GOMD-SIII-020-2010) Crack Propagation in a Soda-Lime Phosphosilicate Glass in Relation to Devitrification

J. Erb*, A. Kovalskiy, H. Moawad, B. Koel, H. Jain, Lehigh University, United States

As a glass devitrifies, often the strength of resulting glass-ceramic increases and structure becomes chemically and structurally inhomogeneous. We have investigated the impact of such devitrification on crack propagation in soda-lime phosphosilicate 45S bioactive glass. The samples are broken within the ultrahigh vacuum, and the composition/structure of its fractured surface is determining by high-resolution XPS and EDAX. The glass is subjected to a special heat treatment needed for its use as a bone scaffold. Three crystalline phases are identified by XRD. Angle-resolved XPS provides evidence that fracture in as prepared glass occurs along sodium rich and mechanically weak path. However, in partially devitrified samples, fracture occurs through crystallites that are poorer in Na than the glass.

4:45 PM

(GOMD-SIII-021-2010) What's New in Thermal Tempering of Silicate Glasses?

S. Gulati*, B. Suman, Corning Inc., United States

Commercial tempering involves cooling of both surfaces of glass article with a uniform cooling rate. We examine the case when the cooling rates are different on the two surfaces. The solution of heat transfer equation provides the resulting temperature distribution through glass thickness. The temperature distribution is used to obtain residual stress distribution, depth of compression layer for each surface, and warp in flat glass with unconstrained edges. The solution is developed in both Cartesian

and polar coordinates. Examples of flat glass and circular tube are used to illustrate the application of theoretical solutions. Some interesting results are obtained with respect to strength of tempered surfaces and their ability to resist field damage.

Poster Session

Room: Carder

(GOMD-SII-P001-2010) The Application of Constraint Theory to Self-Organization of Naturally-Occurring Molecules

B. D. Esham*, Alfred University, United States; J. C. Mauro, Corning Incorporated, United States; R. J. Loucks, G. J. McGowan, Alfred University, United States

Building upon the ideas presented by Phillips in [1], we develop a model for the number of constraints placed upon a molecule as a function of the number of constituent atoms and the nature of the bonds between them. Examination of common organic molecules reveals that nature favors isostatic or slightly underconstrained structures, with no overconstrained molecules having been encountered in the survey.

(GOMD-SII-P002-2010) Electronic Structure Evolution of Phase Change Memory Materials: Ge2Sb2Te5

D. A. Drabold, B. Cai*, Ohio University, United States; S. R. Elliott, Cambridge University, United Kingdom

For Ge-Te-Sb alloys, there exists a rapid and reversible transition between crystalline and amorphous states. The change in conductivity associated with such a transition is the basis of promising novel FLASH memory devices. Though much experimental and theoretical work has been conducted to understand the phase change mechanism, the relationship between transition in phase and change in conductivity is still poorly understood. In this work, we apply ab-initio molecular dynamic simulations on Ge2Sb2Te5 and tracked both the transition of network and evolution of electronic structure, especially the gap, at the same time. By doing this, we attempt to make experimentally credible model, reproduce the phase transition cycle and correlate the topological "irregularity" with particular state in electronic structure.

(GOMD-SII-P003-2010) Qn Speciation in Binary Alkali Silicate Glasses

C. L. Hogue*, A. J. Ellison, S. E. Koval, R. E. Youngman, Corning Incorporated, United States

A systematic 29Si NMR study of binary alkali silicate glasses has been conducted from 5 to 30 mol% alkali, for each of the various alkali oxides (Li, Na, K, Rb and Cs). 29Si NMR spectroscopy is a highly sensitive method for characterizing the local environment of silicate polyhedra and was used to identify and quantify the Qn species in these glasses, where n is equal to the number of bridging oxygens bonded to silicon. The 29Si NMR data indicate that Qn speciation is sensitive to both the identity and amount of modifier alkali, with comparatively depolymerized species forming for the lighter alkalis than for heavier alkalis at equivalent modifier content. The disproportionation of Qn silicate groups, as well as sensitivity to thermal history, will be discussed in light of these findings.

(GOMD-SII-P004-2010) Intermediate glass prepared by high pressure and temperature treatment of silica glass

C. Li*, M. Tomozawa, J. D. Price, E. Watson, Rensselaer Polytechnic Institute, United States

Structure and properties of glasses change with their cooling rate (or fictive temperature). Normal glasses such as soda-lime glass exhibit lower density when cooled more rapidly while anomalous glasses such as silica glass exhibit the opposite trend. Between these two types of glasses, there are intermediate glasses which do not exhibit density change with cooling rate. These intermediate glasses were found to exhibit unique mechanical properties such as the absence of indentation size effect and high crack initiation load. Anomalous silica glasses were found to become intermediate glasses when heat-treated under high pressure. IR peak wavenumber of silica structural bands exhibits reverse correlation with silica glass density. Under 2 GPa pressure, the silica glass exhibited nearly fictive temperature-independent IR peak wavenumber of silica structural bands, indicating that the density of the silica glass prepared under the high pressure is independent of heat-treatment temperature.

(GOMD-SII-P005-2010) Thermally Darkening Photochromic Glasses for Visible Polarizers

C. Chapman*, T. Seward, N. Borrelli, M. Dejneka, Corning Incorporated, United States

A series of thermally darkening photochromic (TDPC) glasses containing silver, copper, and halogens as the active species in a borosilicate host were fabricated and characterized for their physical and optical properties. Samples of these glasses were stretched near their softening point using a process known as "redraw", in an attempt to induce polarization by elongation of particles of the active species. The glasses evaluated in this work showed similar thermal and optical properties to those from the Araujo et al patent, but polarization measurements showed no significant difference in transmission along the stretching axis.

(GOMD-SII-P006-2010) Photothermal Effects in Chalcogenide Glasses

D. Zhao*, Lehigh University, United States; P. R. Pedreira, L. C. Malacarne, M. L. Baesso, Maringá State University, Brazil; H. Jain, Lehigh University, United States

We have investigated photothermal effects in chalcogenide glasses (ChGs) by thermal lens spectroscopy in which a pump laser raises the temperature of sample thus producing a refractive index gradient, while a probe laser with negligible intensity monitors the time evolution of the thermal diffusion process during laser irradiation. The thermal diffusion coefficients of the investigated ChGs are extracted from the time-resolved spectra, and the temperature profile across the laser spot is obtained from this data. It is shown that the temperature rise from commonly used laser irradiation is too small to produce any measurable volume change or induce any fluidity in the samples. The results provide a direct proof that photoinduced phenomena such as photoexpansion and photofluidity in ChGs arise from the atomic structure rearrangement induced by electronic processes, and not from temperature rise from laser irradiation.

(GOMD-SII-P007-2010) Conductivity of Sodium Borophosphate Glasses

G. Olson*, R. Christensen, S. W. Martin, Iowa State University, United States

Ion-conducting glasses hold the potential for widespread use in batteries, fuel cells, sensors, and thermionic devices. It has been found 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. To better understand this Mixed Glass Former Effect (MGFE), a study on the mixed glass former yNa_2O-$(1-y)[xB_2O_3$–$(1-x)P_2O_5]$ glasses when y= 0.35, 0.50, 0.68, and x= 0.0, 0.1, 0.2… 1.0 has been undertaken. The first step in this study was to confirm the presence of the MGFE in the glasses of interest. Conductivity of this mixed glass former has been studied with the use of a dielectric spectrometer. The effect of changing glass former concentrations and the effect of changing alkali concentrations on conductivity were studied. As expected the glasses showed the MGFE with changing glass former concentrations. Increased conductivity was observed with increasing alkali concentration.

(GOMD-SII-P008-2010) A New 2D MAS approach for quantifying Q(n) species in oxide glass

K. K. Dey*, D. Kaseman, M. Davis, P. J. Grandinetti, The Ohio State University, United States

The magic-angle flipping (MAF) NMR experiment, which produces a two dimensional spectrum correlating isotropic and anisotropic nuclear shielding contributions to the solid-state NMR spectrum, can give over an order of magnitude improvement in quantifying Q(n) species compared to conventional 29Si MAS deconvolutions. Also, MAF does not assume of a Gaussian distribution of isotropic 29Si chemical shifts for

different Q(n) species. Since MAF requires specialized NMR probe which reorient the sample rotation axis, we have investigated 2D PASS (Phase Adjusted Spinning Sideband) NMR for obtaining the same 2D correlation as MAF using a conventional solid-state MAS NMR probe. Additionally, we have increased the sensitivity of 2D PASS by employing CPMG acquisition, which recovers sensitivity lost to inhomogeneous broadenings, a common problem in NMR measurements in glasses. Here we will give examples of this new approach for quantifying Q(n) species in a series of model alkali silicate glasses.

(GOMD-SII-P009-2010) Fabrication of novel SbSI-based IR-transparent ferroelectric glass-ceramic

L. Ding*, H. Jain, Lehigh University, United States; G. Chen, East China University of Science and Technology, China

There is increasing interest in active glass-ceramics that transmit in the infrared. In this work, we report our results on the development of novel IR-transparent, active glass-ceramics containing crystallites of ferroelectric SbSI phase within the GeS2-SbSI and As2S3-SbSI glass systems. Glasses with the composition (GeS2)1-x-(SbSI)x and (As2S3)1-x-(SbSI)x (x=0.5-0.9) have been chosen from the glass-forming domain of these two series for their potential for forming the desired ferroelectric phase. The infrared transmission spectra and X-ray diffraction patterns confirm the amorphous nature of as-prepared samples, whereas Raman spectroscopy demonstrates the structural changes as the glasses of various compositions gradually denitrify. The glass transition temperature and the temperatures for the onset and peak crystallization rate are obtained by differential thermal analysis. The microstructure and phases of crystallites are determined using scanning electronic microscopy and X-ray diffraction (XRD).

(GOMD-SII-P010-2010) Properties of high density silica glass prepared by high pressure quenching routes

L. Huang, F. Yuan*, Rensselaer Polytechnic Institute, United States

Molecular dynamics simulations, based on a charge-transfer three-body potential, have been carried out to study the properties of vitreous silica samples prepared by specific high pressure quenching routes. Our study shows that the anomalous thermo-mechanical properties, such as the minimum in the bulk modulus at ~2-3 GPa gradually diminishes with the increase of silica glass density. Furthermore, the anomalous thermo-mechanical properties of silica glass are inherently connected to the ability of the glass to undergo irreversible densification. By preparing silica glass in ways that eliminates anomalous thermo-mechanical behaviors, e.g., by quenching a melt under pressure, the propensity of the glass to undergo irreversible densification can be eradicated. By controlling the pressure under which the initial glass was quenched, we can obtain silica glass with zero pressure/temperature dependent mechanical properties. Such glass shows very interesting behaviors in contact mechanics.

(GOMD-SII-P011-2010) Glasses with temperature and/or pressure independent elastic moduli

L. Huang, Q. Zhao*, Rensselaer Polytechnic Institute, United States

The most pronounced elastic anomalies that appear in silica-rich glasses are the positive temperature derivative and negative pressure derivative of bulk modulus, as compared with normal glasses, such as window glass (soda-lime-silica) containing more network modifiers. It would be natural to imagine that there are intermediate glasses with elastic moduli that are independent of temperature and/or pressure. Such glasses will be ideal materials of choice for any device that may experience thermal and mechanical shocks during service, especially in systems made of different materials where strain mismatch can develop across the interfaces after such huge thermo-mechanical impact. We demonstrate that such intermediate glasses can be obtained by pressure-quenching or chemical modifications. We will compare the properties of normal, abnormal and intermediate glasses, and explore the potential applications for such intermediate glasses.

(GOMD-SII-P012-2010) Colloidal Behavior of Alkali Borosilicate Glasses

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Several alkali borosilicate glasses were melted and ground into particles of 10-15um size to determine the effect of alkali ion size and concentration on the point of zero charge (PZC). The PZC of all of the glass powders was measured by titration and pH drift experiments. The presence of nano-scale phase separation in some of the alkali-borosilicate glasses resulted in a higher or lower PZC than expected. The overall results suggest that the PZC for alkali-borosilicate glasses, no matter the alkali concentration, is at pH5 except in cases of phase separation.

(GOMD-SII-P013-2010) Understanding Oxide-Polymer Interfaces Using Solid-State NMR and Inverse Gas Chromatography

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Chemical knowledge obtained from simple oxide materials is often applied to multicomponent oxides even though it is widely recognized that unique reaction sites exist at the surface of the more complex systems. The increased complexity of multicomponent surfaces and the resulting implications for polymer binding are being studied through analysis of chemical interactions with model oxide materials and aluminoborosilicate glass fibers. Interactions of small organic molecules and polymer precursors are being probed using a combination of inverse gas chromatography (IGC) and solid-state nuclear magnetic resonance (NMR). The results to be discussed here include changes in ^{13}C chemical shift values for carboxylate species in adsorbed organic acids after deposition onto a surface. Additional results using IGC to study surface reactivity using alcohols and carboxylic acids as probe molecules will also be presented and correlated to structural information obtained from NMR.

(GOMD-SII-P014-2010) Analytical thermodynamic modeling of the iron redox ratio in phosphate glasses

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The iron redox ratio ($Fe^{2+}/\Sigma Fe$) for iron phosphate glasses directly affects the structure and properties of the glass and is a function of nominal composition and melting conditions. A theoretical model has been developed to predict the iron redox ratio for phosphate glass and is based on thermodynamic equilibria of the melt components in given melt environments. The model accounts for the redox equilibrium of the iron ions in the melt in addition to the equilibrium associated with the polymerization and structural changes within the melt with changing oxygen content. Validity of the model is supported by the comparison of predicted redox ratios with experimental Mössbauer and wet chemistry results for various phosphate glass systems, including binary iron phosphates, sodium iron phosphates, zinc iron phosphates and lead iron phosphates.

(GOMD-SII-P015-2010) Quantifying Q(n)-species in a potassium disilicate glass by 29Si magic angle flipping nuclear magnetic resonance

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The distribution of Q(n)-species (n equal to the number of bridging oxygens) in silicate melts dictate their thermodynamic and physical properties. Here, we have employed 2D magic angle flipping (MAF) NMR to measure the Q(n) distribution in a 29Si enriched potassium disilicate glass whose 29Si MAS spectrum is completely unresolved. Relative concentrations of [Q(4)] = 7.23 %, [Q(3)] = 82.97 %, [Q(2)] = 9.80 % were measured. Using the thermodynamic disproportionation model, an equilibrium constant K(3) =0.01029 was calculated, indicating a binary distribution. A Gaussian distribution for each Q(n) species was observed with mean values of -82.74, -91.32, and -101.67 ppm, and standard deviations of 3.27, 4.194, and 5.09 ppm for Q(2), Q(3), and Q(4), respectively. Additionally, nuclear shielding anisotropy values of zeta = -85.0 ppm and eta = 0.46 for Q(2), zeta = -74.9 ppm and eta = 0.06 for Q(3), and zeta = 0.0 ppm and eta = 0.0 for Q(4) were observed.

(GOMD-SII-P016-2010) EPR study of Ti3+ ions formed under ionizing irradiation in oxide glasses

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Ti4+ ions exist in silicate glasses into three different environments: [IV]Ti4+, [V]Ti4+ in a square pyramid geometry and [Vi]Ti4+ [1]. We observed previously under ionizing irradiation a reduction of Ti4+ ions to Ti3+ ions [2]. In the present work, we studied by EPR spectroscopy and simulation the environment of Ti3+ ions formed under ionizing irradiation in SiO2 - Na2O glasses doped with 0 to 5% mol of TiO2. We demonstrate the existence of three different Ti3+ sites (sI, sII and sIII) and an increase of the Ti3+ amount with the dose. We show that the proportion each Ti3+ site depends on the [Na]/[Ti] ratio of the glass and on the total integrated dose. Based on three main assumptions that will be presented, we propose to associate the Ti3+ in site sI with [VI]Ti3+, the site sIII with [V]Ti3+ in a square pyramid geometry. [1] F. Farges. American Mineralogist, 82: 36-43, 1997 [2] N. Ollier, P. Lombard, F. Farges, B. Boizot, J. Non-Cryst. Solids, 354, 480 2008

(GOMD-SII-P017-2010) Enthalpy of Mixing of Mixed Alkali Glasses

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The enthalpy of mixing was determined for alkali silicate glasses using an ion-exchange equilibrium method, where alkali species were Li, Na, and K with total alkali contents of 25 mol% and 33 mol %. It was found that the enthalpy of mixing is negative for all the systems and the magnitude of the enthalpy of mixing was found to increase with total alkali content for the Na2O-K2O-SiO2 glass system and with the size difference of two alkali species for a given alkali concentration. Furthermore, for all the systems investigated, the magnitude of enthalpy of mixing was found to be proportional to the difference of molar volumes of the corresponding single alkali glasses. In interpreting these results, they were considered to be the probable cause of the large activation energy of D.C. electric conductivity and the large elastic relaxation loss of mixed alkali glasses.

(GOMD-SII-P018-2010) An analysis of borate glasses and crystals using 10B quadrupolar NMR obtained from a field swept magnet

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We have analyzed several 10B NMR spectra obtained from a field step magnet system at the University of Warwick (UK). Among the samples analyzed were vitreous borate (R=0), vitreous and crystalline cesium triborate (R=1/3), and vitreous cesium diborate (R=1/2). Here R is the molar ratio of cesium oxide to boron oxide. Vitreous cesium enneaborate (R=1/9) was also fitted using a rudimentary approximation of the superstructural proportions. The spectra were analyzed using a curve simulating Java program known as QuadFit, which employs the Aldermann-Grant interpolation. The anlyses yielded the quarupoleparameters to a high precision as well as the gaussian distribution of their values.

(GOMD-SII-P019-2010) Physical Properties and Structure of Alkali Borovanadate Glasses

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We report on the physical properties of two alkali borovanadate glass systems. We determined the glass transition temperature (Tg), density, and glass forming limits. The systems studied include lithium and cesium borovanadates across a very wide range of alkali-to-boron ratios (R), for several fixed vanadate to boron oxide ratios (K). To obtain structural information we performed ESR and NMR experiments. A structural model is proposed that relates these properties to the atomic arrangements. Work supported by the National Science Foundation under grant number DMR 0904615.

(GOMD-SII-P020-2010) An Al-27 MAS NMR study of the Ca-Al binary metallic glass forming system and related alloys

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Using Al-27 MAS NMR, we have studied the short-range structure of the binary Ca-Al metallic glass forming system. We clearly demonstrate an increase in the amorphous nature of the spectra near the eutectic in the system, as well as a shift to higher frequencies as Al content is increased. Additionally, comparisons to various crystalline model compounds have been made in order to help interpret the spectra of these binary alloys.

(GOMD-SII-P021-2010) Crystallization in Sugar Glass and Its Melts - Low Cost Experiments in Glass

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Hard candy glass provides a perfect paradigm to explore many aspects of glass science, from synthesis to properties and performance. Here we present experiments on nucleation and growth of crystallites during devitrification. They demonstrate surface crystallization at room temperature, the significant influence of moisture in mediating this process, as well as bulk crystal nucleation and growth at elevated temperatures. The experiments are designed to be carried out in a high school laboratory, or even in a home setting with minimal cost, and yet would also be appropriate for inclusion in an undergraduate materials lab. All apparatus including the humidity chamber and the temperature controlled sample chamber were constructed from commonly available items, none costing more than $20. Quantitative results on surface crystallization rates of sugar glass at room temperature and bulk crystallization rates in sugar melts are shown. The maximum growth rate for our sugar glass occurs near 120°C.

(GOMD-SII-P022-2010) A Low-Cost Student Built DTA for Exploring the Glass Transition

W. R. Heffner*, Lehigh University, United States

As part of a series of low-cost experiments for students to explore glass science, we have developed a simple student-assembled apparatus for measuring the glass transition (Tg). While DSC is the common technique for measuring Tg, such apparatus is expensive and generally unavailable outside of the research laboratory. Differential thermal analysis (DTA) is somewhat simpler to implement and provides essentially the same information. We describe a simple DTA apparatus which can be constructed from items available in most high school laboratories. Our DTA consists of measuring the temperature difference between test tubes with sample and reference materials, while both test tubes are heated in an oil bath. It provides excellent resolution of the Tg of sugar glass and other low temperature glasses, and would be suitable for an undergraduate material science laboratory. The strong effect of thermal history, including the effect of quenching and anneal times are examined.

(GOMD-SII-P023-2010) Low-cost, hands-on activities in glass science

W. R. Heffner, H. Jain*, Lehigh University, United States

We have developed a collection of experiments for learning glass science through hands-on activities with sucrose based glass (a.k.a. hard candy). This very accessible material exhibits many aspects of glass science, from synthesis to properties, characterization and engineering applications. Some of the activities described in this paper include: synthesis, phase diagram, density, refractive index measurement, and even a fiber drawing tower. Our priority is to keep all experiments within the resources of a typical high school student, while incorporating quantitative science content. Most of the experiments can be assembled in a high school lab with minimal cost, and yet would also be appropriate for inclusion in an undergraduate materials lab. The scientific content of these experiments progresses systematically, providing an environment to develop an understanding of glassy materials within a framework of active prolonged engagement.

(GOMD-SIII-P024-2010) Lattice orientation analysis of single crystal architecture created in LaBGeO5 glass by femtosecond laser

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Femtosecond laser induced structural modification is a promising method for constructing three-dimensional optical architecture. Toward this goal we have fabricated ferroelectric single-crystal lines inside LaBGeO5 glass using a high repetition rate femtosecond laser and determined their crystallinity and lattice orientation. Scanning Raman microscopy suggests that the lines are highly oriented and that a characteristic orientation is consistently aligned along the direction of line writing, resulting in a gradual reorientation of the lattice when lines are bent by changing writing direction. Scanning electron microscopy with electron backscatter diffraction is used to further clarify the internal structure of the lines at higher magnification and confirm whether or not grain boundaries are present, especially at bends where the lattice orientation changes to match the change in writing direction.

(GOMD-SIII-P025-2010) Effect of flour source on sintering and crystallization of Fluoro-Phlogopite glass-ceramic

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Phlogopite glass-ceramic composition based on MgO-SiO2-Al2O3-B2O3-K2O-F with different Fluorine source(ph(AlF3),ph(MgF2)) prepared. Crystallization and sintering behaviour of giving Phlogopite glass-ceramic as a function of Fluorine source was studied. According to XRD results, Ph(MgF2), crystallized faster than Ph (AlF3) and sintering of Ph(AlF3) started at low temperature . Crystallization of Ph(MgF2) has been observed to be very dependent on the particle size of the glass employed, indicating a strong dependence on surface crystallization, the activation energy of fine Ph(MgF2) was 89.5 K.j/mol while for coarse , is 164.20 K.j/mol .

(GOMD-SIII-P026-2010) Zinc and Silver Glass Polyalkenoate Cements: An Evaluation of their Antibacterial Nature

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The objective of this study is to evaluate whether it is possible to produce silver and zinc containing glass polyalkenoate cement (GPC) coatings for medical devices that have antibacterial activity and which may therefore inhibit biofilm formation on a surface. Two silver and zinc-containing glasses (A: 56.04SiO2 32.98ZnO 0.11Ag2O 10.87Na2O and B: 56.04SiO2 32.76ZnO 0.33Ag2O 10.87Na2O) were synthesized. The GPC coatings were developed by mixing the glass (0.5g) with polyacrylic acid (PAA) (0.2g) and water (0.25g). The coatings were then applied onto Ti6Al4V discs. The GPCs were characterized and their antibacterial properties evaluated against different bacteria using an agar diffusion assay method. Both coatings produced zones of inhibition with each of the bacteria, with B showing greater inhibition zones. This indicates that GPC coatings can adhere to surgical metals and can release zinc and silver ions which retard bacterial growth and thereby should inhibit biofilm formation.

(GOMD-SIII-P027-2010) The Antibacterial Properties and Ion Release Profiles of a novel Zinc based Glass Polyalkenoate Cement

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A 0.48SiO2-0.36ZnO-0.12CaO-0.04SrO glass was produced and mixed with E9 polyacrylic acid (PAA) at a P:L ratio of 2:1.5 to form cements. Cement discs were made mixing 1g glass, 0.37g PAA, 0.37ml H2O with 5, 10 & 15wt% TSC additions (0.037g) and filling a 15mmϕ x2mm mould. Cements were then tested against E. coli, S. epidermidis and B. fragilis. It was found that the Zn-GPC exhibited inhibition at each time frame in E. coli (t-0, 1, 7 and 14 days) with a maximum of 13mm. Cements also produced inhibition in B. Fragilis but only at t-0 days (11mm), and showed bacteriostatic properties when tested in S. epidermidis. Ion release profiles were determined for the cement. It was found that there was no calcium release. Strontium release was low (25mg/L) when compared to zinc (310mg/L) and sodium (320mg/L). It was also found that the antibacterial properties and ion release rates were further improved by the addition of tri-sodium citrate.

(GOMD-SIII-P028-2010) Fluorescent glass patterning on a sheet window glass by screen printing and low temperature heat treatment

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Fluorescent glasses have attracted much attention because of their various applications such as indicators and display devices. Especially, designed displays require large surface patterning of multi-colored fluorescent glasses having both sunlight and weathering durability. A fluorescent silicate glass containing some phosphor ions or fine particles has advantages due to its thermal and chemical durability. In this study, a fluorescent glass patterning was made on a sheet window glass. Alkaline borosilicate based glass frits, which contain rare earth ions or phosphor fine particles such as Eu^{3+}, Tb^{3+} and $ZnSiO_4$:Mn^{2+}, were prepared by a conventional melting method. The obtained frits were coated on a sheet window glass by screen printing and subsequent heat treatment at 650°C for 10min. The coated glasses layer had no cracks and very few bubbles, and showed appropriate fluorescent properties.

(GOMD-SIII-P029-2010) Preparation of gold nanoparticles supported on a super-hemispherical lens by using a surface-tension mold technique for chemical sensing

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The super-hemispherical lenses with gold nanoparticles, which were used as a localized surface plasmon resonance (LSPR)-based chemical sensor, were prepared by using a surface-tension mold technique. Soda-lime-borosilicate glasses were heat-treated on a gold-coated glassy-carbon substrate up to 800°C. The obtained glasses showed super-hemispherical shape, and the gold nanoprticles were supported on the bottom surface of the lens. The lenses showed absorption peak at around 550 nm due to LSPR of the gold nanoparticles. When various organic solvents were supported on the bottom of the lens, the peak wavelength of LSPR was shifted depending on the refractive index of the solvent. The sensitivity as the sensor was strongly affected by both the size distribution of the gold nanoparticle and the surface morphology of the bottom of lens. These results indicate that the gold supported super-hemispherical lens can act as LSPR-based chemical sensor.

(GOMD-SIII-P030-2010) Transition Metal Oxide Coatings on Glass

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Transition metal oxide semiconducting materials have a wide variety of applications, ranging from energy conversion and photochromism to catalytic and antimicrobial surface coatings. Many of these properties are a function of their overall composition and structure. In this study mixed oxide nanocomposites were processed and fully characterized to determine the effect of composition and structure on a variety of light induced properties. The nanocomposite coatings were processed via sol-gel and characterized with X-ray Photoelectron Spectroscopy (XPS), Glancing Incidence X-ray Diffraction (GIXRD), Raman Spectroscopy (RAMAN), and Ultraviolet-Visible Spectroscopy (UV-Vis). Photocatalytic measurements were performed as a function of various excitation wavelengths (UV only, UV-VIS, and VIS only) through monitoring the breakdown of a model organic.

(GOMD-SIII-P031-2010) Dependence of osteoblast cell response on the surface roughness of 45S bioactive glass

R. H. Jain*, S. Wang, H. M. Moawad, M. M. Falk, H. Jain, Lehigh University, United States

Adhesion of bone cells to Ti is significantly affected by its surface roughness. Much less is known about the role of surface roughness of bioglass on its use as an implant. So we systematically investigated the effect of surface roughness on cell response of 45S bioactive glass. Cell proliferation and initial adhesion of MG63 osteosarcoma or MC3T3 pre-osteoblast cells were determined by counting fluorescent stained cells. Morphology and focal adhesion sites were observed after staining for vinculin, the F-actin cytoskeleton, and the nucleus. In contrast to Ti, the proliferation rate was the highest on smoothest surfaces. Cells showed

alignment on samples polished on a SiC paper with grain size ~ cell size. Cells spread, forming long extensions, on smoother samples, indicating better adhesion, while cells on rougher surfaces were rounded. A lack of connection between vinculin and the actin cytoskeleton revealed the effect of surface roughness on cell-glass interaction and adhesion.

(GOMD-SIII-P032-2010) Simulation of Fluid Flow and Temperature on the Glass Sheet Forming for Overflow Fusion Process

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The overflow fusion process was an important method for the manufacture of glass sheet that is currently used for the production of TFT/LCD display devices. The design of forming apparatus was critical for very high surface quality of glass to allow the successful application of semiconductor type material. However, there is only a little of researches had been presented in the literatures, because of difficulties and expansions in experiments. In this study, a numerical model for simulation of molten glass flow through the isopipe during overflow fusion process was carried out. The effect of temperature of forming apparatus, flow rate and viscosity of molten glass on the flow patterns during overflow was investigated. It was found that the stability and flatness of sheet glass was influenced by the temperature of forming apparatus, and the flow rate and viscosity of molten glass flow.

(GOMD-SIII-P033-2010) Conversion of europium and lanthanum doped lithium borate glass to rare earth phosphate compounds

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Europium and lanthanum doped lithium borate glass microspheres, ranging in sizes from 100 to 150 μm, were reacted in 0.25 M K_2HPO_4 to form rare earth phosphate compounds by precipitation reactions. Weight loss and pH change over time were measured for different glass compositions, initial solution pH and reaction temperature. The initially x-ray amorphous precipitated rare earth phosphate materials were heat-treated at temperatures ranging from 673 K to 1273 K for 2 hours to form crystalline compounds. The structures of the heat treated rare earth phosphates were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy, and Fourier-transformed infrared spectroscopy (FTIR). It was determined that a solid solution of $LaPO_4$ and $EuPO_4$ formed after heat treatment at 973 K. The effects of preparation conditions on the fluorescence intensity from Eu-doped samples will be discussed.

(GOMD-SIII-P034-2010) Chromium-doped transparent calcium germinate glass-ceramics toward nano-Ca2GeO4 in fiber

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A higher nonradiative decay and excited state absorptions in a transition-metal doped host are major detrimental factors affecting its active performance. To aim the resolution, a nanocrystal-embedded new glass system maybe worthy to investigate. In this study, nanocrystals of Cr:Ca2GeO4 were selected to be formed in the optical fiber because only Cr4+ centers are possible in this crystal. Glass compositions that are feasible to the nanocrystalline formation of Cr:Ga2GeO4 in a single mode fiber are being investigated, with further emphasizing on the extent of crystalline purity and size distribution of crystal. Particular interests are to investigate the effect of nano size of Cr:Ca2GeO4 on fiber loss, electron-phonon coupling and both pump and signal excited state absorption, and laser/amplification properties . The ultimate goal is to have a better performance of coherent and incoherent fiber light source emitting in the range of 1100 to 1600nm.

(GOMD-SIII-P035-2010) Mechanism of the removal of phosphate ion from an aqueous solution by borosilicate glass

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When a glass in a Na_2O-CaO-B_2O_3-SiO_2 system is reacted in a solution containing phosphate ions, a silica-rich layer is first formed on the glass surface by leaching Na^+ and Ca^{2+} ions from the glass, and then the Ca^{2+} and PO_4^{3-} ions in the solution are uptaken on the silica-rich layer to precipitate hydroxyapatite crystals. In this manner, the phosphate ions can be removed. In this study glasses with different amounts of B_2O_3 have been prepared, and reacted with a solution containing phosphate ions. The effects of B_2O_3, pH, reaction time and amount of glass on the phosphate ion removal were studied. The mechanism of phosphate ion removal by borosilicate glass was discussed after examining of the glass surface by using XRD, SEM, FT-IR and EDS. The thermodynamic parameters, $\Delta G°$, $\Delta H°$ and $\Delta S°$, were calculated. Experimental data were also examined using kinetic models. The removal mechanism of phosphate ions from a solution fit well to a pseudo-second-order kinetics.

(GOMD-SIII-P036-2010) Rare-Earth-Doped Amorphous Nancomposite Polymers for Optoelectronic Applications

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Greater functionality and performance is expected from optical materials that comprise photonic devices and components. Most polymer based optical materials utilize amorphous hydrocarbon polymers. In the specific case of polymer optical fibers, most consist of polymethyl methacrylate, PMMA. The inherent high vibrational energies of PMMA promote the quenching of emission from rare-earth dopants. One solution to this issue is to increase the likelihood for light emission by incorporating nanoparticles into the transparent polymer matrix . The purpose of this work is to develop PMMA optical fibers that contain rare-earth doped fluoride nanocrystals such that the radiative emissions are maximized and the fiber could operate as a more efficient polymer optical fiber amplifier. This work will review the thermal and rheological properties of PMMA nanocomposites and the subsequent production and characterization of the physical and optical properties of the fiber.

(GOMD-SIII-P037-2010) Barium Vanadate Microspheres

S. Yosinski, L. Tweeton, S. Feller, M. Affatigato*, Coe College, United States

It has been found that many glass powders can form micro- or nanospheres when heated in a flame or by a laser. Much of the research in this area of microspheres has concentrated on making hollow spheres, called microballoons, of silica and borosilicate glasses. Our aim was to create highly porous barium vanadate microspheres for possible future applications in material storage. The surface area of porous spheres would provide a greater amount of bonding surface area for dopants than hollow spheres. Barium vanadate glass with a molar fraction of 0.4 to 0.6 barium oxide was used because this glass is stable and has a low Tg. Size distributions of the spheres were quantified and the extent of sphere formation and porosity was examined using a scanning electron microscope. The size of spheres formed is affected by powder size, dropping method, and flame position. The porosity of the microspheres is affected by flame temperature, time spent in flame, and the material onto which the spheres fall. The greatest porosity was achieved by first heating the glass powder at a low temperature and then immediately sending it through the flames of two MAPP gas torches at approximately 2100 °C onto a metal sheet. This research was supported by the National Science Foundation under grant Nos. DMR-RUI-0904615, DMR-MRI-0722682, DMR-MRI-0420539, and DMR-MRI-0320861. Coe College is also thanked for its financial support.

(GOMD-SIII-P038-2010) Antibacterial Properties of Silver and Zinc doped 45S Bioactive Glass

M. J. Michel*, Lehigh University, United States

Bioactive sodium-calcium-phosphosilicate glasses (e.g. 45S), have many biomedical applications as orthopedic and dental graft materials and most recently also as tissue engineering scaffold. In this study we explore the antibacterial properties of 45S bioactive glass (BG), Ag2O doped 45S (AgBG) and Ag2O-ZnO doped 45S bioactive glasses (AgZnBG) in the presence of Escherichia coli K12. The study is carried out with 45S glass doped with 0.1-5 mol% Ag2O, or 0.1-1.0 mol% Ag2O + 3 ZnO,mol%. The antibacterial property of the BG, AgBG, AgZnBG is assessed using a LIVE/DEAD BacLight Bacterial Viability assay. We find that BG has no effect on bacterial growth or viability. However, AgBG and AgZnBG show antibacterial action that is attributed to the leaching of Ag ion from the glass matrix. Additionally, the samples containing Zn had the greatest bactericidal effect. The synergistic antibacterial property of

AgZnBG could provide significant advantages as a bioactive scaffold for dental and maxillofacial applications.

(GOMD-SIII-P039-2010) Glassy particles as an active component in cementitious materials for the future

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5% of the global CO_2 emissions from human activity come from the production of Portland cement clinker (PCC), the major constituent in Portland cement. This work focuses on reducing this CO_2 emission by replacing PCC with suitably reactive glass particles. We attempt to find the optimum composition of the particles with respect to e.g. limestone consumption and melting temperature. In this work, we investigate pozzolanic reactivity of the glass, i.e., the ability of the glass to participate in the strength developing reactions taking place during cement hydration. The pozzolanic reactivity is tested as the reactivity of the glass in a saturated $Ca(OH)_2$ solution which reproduces the conditions in a cement paste. Compressive strength is tested for mortars with 30 wt% substitution of cement with glass particles or with a mixture of glass and limestone. In general, promising strengths are observed for these blended cements. Mortars containing both glass and limestone exhibit the highest strengths.

(GOMD-SIII-P040-2010) Formation of SiO_2-Rich Surface Layer on Glass Fibers

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Man-made amorphous stone wool fibers are widely used for thermal and sound insulation and as a fire barrier. The applications of the glass fibers are influenced by their chemical and mechanical properties and high temperature stability (HTS). In this work, we study the surface modification of iron-bearing aluminosilicate glass fibers by using an internal diffusion process to change the chemical composition of the fiber surface. It is found that reduction of Fe^{3+} to Fe^{2+} results in diffusion of network-modifying cations from the surface toward the interior of the fibers. Consequently, a silica-rich surface layer is created. The extent of the inward diffusion increases with the degree of Fe^{3+} reduction, and the latter can be varied by changing the duration and temperature of the heat-treatment. We demonstrate the impact of the surface modification on the crystallization behavior, HTS, and chemical durability of the fibers.

(GOMD-SIII-P041-2010) Analysis of Interactions between Glass and Mold Tool in Precision Optical Molding

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In production glass molding, it is important to use a glass/mold tool combinations where the glass releases from the mold tool and produces the necessary surface quality for a finished precision optic. This behavior is directly affected by the physical and chemical interaction between the two materials. This study attempts to evaluate the physical interaction between the mold tool material and the glass using a modified Sessile drop technique. The contact angle between the glass and substrate has been measured as a function of glass type, mold tool material, temperature and time. Variation in contact angle is related to the work of adhesion between the glass and the substrate. In addition to contact angle measurements, the mold tool/glass interaction is characterized via white light interferometry and electron microscopy in order to compare the surface roughness and chemical composition of the mold material before and after interaction with the glass at elevated temperatures.

(GOMD-SIII-P042-2010) Structural and thermal studies of $70Li_2S+(30-x)P_2S_5+xAl_2S_3$ with x=1 or 3 mol%

S. Berbano*, Iowa State University, United States; K. Minami, A. Hayashi, M. Tatsumisago, Osaka Prefecture University, Japan

Lithium-ion batteries are widely used. Most, however, contain a flammable polymer–gel electrolyte. A safer alternative to this technology is a solid electrolyte. In this study, the stability of solid electrolytes prepared by mechanical milling was investigated. The $70Li_2S + 30P_2S_5$ (mol%) system was selected because of its high ionic conductivity. In order to investigate structural changes and thermal stability in this system, small compositional substitutions of Al_2S_3 were made for P_2S_5. X-ray diffraction and differential thermal analysis (DTA) studies were performed on these amorphous materials. Milled materials with substitutions of Al_2S_3 were x-ray amorphous after mechanical milling for 20 hours. DTA scans of the amorphous materials showed crystallization peaks assigned to a crystal analogous to $Li_{4-x}Ge_{1-x}P_xS_4$ ($0.6< x <0.8$), $Li_7P_3S_{11}$ and $Li_4P_2S_6$. The substitution of Al_2S_3 was found to decrease the thermal stability of $70Li_2S + 30P_2S_5$, making it less suitable for use as an electrolyte.

(GOMD-SIII-P043-2010) Cell response to nano-macro porous bioactive glass scaffolds prepared by the sol-gel method

S. Wang*, M. M. Falk, H. Jain, Lehigh University, United States

Three-dimensional (3D) bioscaffolds hold promise to meet the increasing demand of bone tissue replacement. Recently, we produced 3D nano-macro dual porous 30%CaO-70%SiO2 bioactive glass scaffolds by a novel sol-gel-cum-spinodal-decomposition method. The aim of this study is to observe in vitro bone cells' response to these scaffolds. MG 63 and MC3T3 osteoblast-like cells were seeded on porous glass and observed by fluorescence microscopy, confocal microscopy and scanning electron microscopy. Two days post-seeding, cells migrate and penetrate >500 μm deep into the bioscaffold. A well-spread, flattened cell morphology indicates good cell attachment on the bioscaffold. Qualitative live/dead cell viability staining shows high proliferation rate, and that the bioscaffold exhibits no cytotoxic effects, with greater than 95% viability. Thus, our new nano-macro dual-porous glass is a promising bioscaffold candidate for use in regenerative medicine and tissue engineering for bone regeneration.

(GOMD-SIII-P044-2010) Tailoring and Characterization of Nanopores Networks of Nano/Macro Dual Porous Sol-Gel Bioactive Glasses

S. Wang*, Lehigh University, United States; A. C. Marques, R. M. Almeida, ICEMS, Instituto Superior AU1 Tecnico/TULisbon, Portugal; H. Jain, Lehigh University, United States

Recently, three-dimensional (3D) nano-macroporous bioactive glass scaffolds with molar composition 30%CaO-70%SiO2 have been prepared by a sol-gel-cum-spinodal decomposition method. These 3D structures are potential bioscaffold candidates to be used in regenerative medicine and tissue engineering for bone regeneration. Since surface nano-topography is known to affect cell functions, it is important to optimize the glass scaffold surface with controlled nanopore sizes. In this work, we demonstrate that the size of nanopores can be tailored continuously and uniformly by solvent exchange in ammonia performed on the wet gel, before the drying step. Using TEM, Hg porosimetry and nitrogen adsorption techniques, we show that the porous sol-gel glass networks develop intra-domains through Ostwald ripening process and thus make inter-domain spaces as nanopores. With increasing ammonia concentration and soaking temperature, the domain size increases, leading to larger nanopores.

(GOMD-SIII-P045-2010) Processing of S520 glass for nano-macro porous bioactive fibers

U. Thamma*, H. M. Moawad, H. Jain, Lehigh University, United States

Recently, a heat+chemical treatment method was developed in our laboratory for introducing multi-modal nano-macro porosity in 45S based biocompatible compositions, which are, unfortunately, unsuitable for fiber drawing. Now we report on the development of this process for 20.9Na2O-7.1K2O-18CaO-2P2O5-52SiO2 (S520) composition, thus introducing the possibility of nano-macro porous fibers for bioactive applications. Polished glass disks were heat treated at 600°C to 950°C and leached by 1M and 3M HCl at 80°C. Porosimetry shows a wide range of pore size from ~8 nm to ~6 μm by single-step heat treatment at 950°C + leaching in 3M HCl at 80°C. A two-step heat treatment (750°C for 1 hour followed by 950°C for 1 hour) + chemical treatment in 3M-HCl yields a higher density and interconnectivity of pores than that of

single-step heat treatment. These processing protocols demonstrate the novel potential of S520 glass-ceramics for bone scaffold applications.

(GOMD-SIII-P046-2010) Single-mode waveguide of chalcogenide glasses by burying a fiber in substrates

Z. Shaoqian*, X. Zhang, university of Rennes1, France

Modal filtering in nulling interferometer is based on the capability of single-mode waveguides to transmit only one complex amplitude function to eliminate virtually any perturbation of the interfering wavefronts. In this recherche , we focus on realizing single-mode waveguide of chalcogenide glasses in the thermal infrared range [6-16μm] by burying a GASIR(Ge-As-Se) fiber core in the substrates of As-Se-S glasses system. To match the single-mode operation, GASIR fiber core of 15μm diameter was drawn, the fiber core was buried into As-Se-S substrates by heating two kinds of glasses to a suitable temperature. The propagation mode was tested by guiding a CO2 laser emitting at 9.3μm into the waveguide. Signal was obtained by an infrared camera. Single-mode components involving a slightly modification of substrates materials are in preparation.

(GOMD-SIV-P047-2010) Transition Metal Oxide (TMO) Silicate Glasses: Processing and Materials Properties

B. Akkopru*, Alfred University, United States; C. Durucan, Middle East Technical University, Turkey; N. P. Mellott, Alfred University, United States

Synthesis of TMO-silicate glasses have gained continuously growing interest due to their optical, electrical, and chemical properties; and their resultant potential for applications in renewable energy, optoelectronics, biosensors, catalyst and the encapsulation of nuclear and hazardous wastes. The performance related properties of the TMO-silicate glasses is strongly dependent upon the overall structure of the glass. Of particular interest here is the structural role of the transition metal ion in the glass; as a network forming, intermediate or modifier ion and the resultant effect on material properties. The aim of this work is to develop different TMO-silicate glasses via sol-gel processing and investigate the effect of processing parameters on the glass structure via XRD, TGA, UV-VIS, and XPS analyses.

(GOMD-SIV-P048-2010) The relationship between phosphate glass dissolution and experimentally determined dissolution enthalpies for phosphate compounds

L. Ma*, M. L. Schmitt, R. K. Brow, Missouri University of Science and Technology, United States

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 alkali-alkaline earth phosphate glasses were prepared with compositions in the meta- to pyrophosphate range. The dissolution enthalpies of phosphate compounds were measured using a solution calorimeter and used to calculate the free energies of hydration, ΔGhyd. Dissolution rates of corresponding phosphate glasses were determined from weight loss measurements, and pH shifts were recorded. The effects of experimental conditions on dissolution rate are investigated, including solution temperature and pH value as well as concentrations of ions in solution. The relationships between the Gibbs free energy of hydration and dissolution rates with varying glass composition and experimental conditions are discussed.

(GOMD-SIV-P049-2010) Corrosion Behavior of Ti-Based Bulk Metallic Glass Composites Containing Carbon Nanotubes

P. Lee*, National Taiwan Ocean University, Taiwan

The corrosion behavior of the Ti50Cu28Ni15Sn7 bulk metallic glass as well as composites modified by the addition of CNT was investigated by electrochemical measurements. Electrochemical characterization was performed in Hanks' solution at 37°C with physiologically relevant dissolved oxygen content. The results of potentiodynamic polarization measurements revealed that the Ti-based bulk metallic glass composites examined showed spontaneously passivity by anodic polarization with a passive current density of about 10-5 A/cm2. The higher corrosion resistance of the Ti-based bulk metallic glass composites was attributed to stable and protective passive films enriched with titanium containing certain amounts of additional elements.

(GOMD-SIV-P050-2010) Corrosion of ancient glass bead samples excavated from prehistoric sites in southern Thailand

P. Dararutana*, The Royal Thai Army Chemical Department, Thailand; Y. Thongkam, Silpakorn University, Thailand; K. Won-in, Kasetsart University, Thailand

The archaeological resources showed that the ancient glass beads excavated in southern Thailand were made more than 1000 years ago. Initial findings suggested that there were number of difference in shade between the glass beads of difference colors. In this work, scanning electron microscope with energy dispersive X-ray fluorescence spectroscopy (SEM/EDS)was used to study their corrosions. SEM micrographs showed more corroded and flaked microstructures. These patterns were produced by the interaction of both ground water and its dissolved chemical compounds with the glass surface.

Tuesday, May 18, 2010

Symposium II: Glass Science

Topology and Rigidity I

Room: Cayuga
Session Chair: Normand Mousseau, Universite de Montreal

9:30 AM

(GOMD-SII-021-2010) Intermediate Phases in Solid Electrolyte glasses (Invited)

P. Boolchand*, D. I. Novita, M. Malki, M. Micoulaut, B. Goodman, Univ of Cincinnati, United States

Intermediate Phases (IPs) were first reported in covalent (chalcogenide) and then in modified oxide (alkali-silicates and –germanates) glasses. We now observe these phases in fast-ion conducting glasses1. We have examined bulk [AgPO3](100-x) [AgI]x glasses over a wide composition 0< x < 60% range, in thermal (modulated DSC), optical (Raman and IR), electrical (AC conductivity) and molar volume experiments. Results on dry samples slow cooled from Tg show the existence of a deep, sharp, and square-well like reversibility window in the 9.5% < x < 37.8% range, which fixes the IP with glass compositions at x < 9.5% as stressed-rigid, and those at x > 37.8% as flexible. Variations in Raman frequency of the symmetric vibration of P-Ot, dc electrical conductivity, and electric permittivity, each are found to display three regimes of behavior with thresholds at the stress (9.5%) and rigidity (37.8%) transitions. 1J.Phys:Cond. Matter 21,205106 (2009).

10:00 AM

(GOMD-SII-022-2010) Intermediate phases in simple models of elastic network self-organization (Invited)

M. V. Chubynsky*, University of Ottawa, Canada

As the composition of network glasses is varied across the transition from floppy to stressed-rigid networks, an intermediate phase is observed, which is attributed to network self-organization. I discuss how a similar intermediate phase arises in very simple models that are physically motivated, yet rely entirely on network topology and counting of constraints, never dealing with the details of the network geometry, interaction potentials, etc. The idea is minimizing the number of "redundant" constraints causing stress. However, one needs to be careful interpreting the results, as a physically negligible insertion or deletion of a single bond in an infinite rigid but unstressed (isostatic) network can make it formally completely stressed or completely flexible. In particular, in one variant of the model, there seem to be two intermediate phases, one fluctuating between isostatic and flexible and one between isostatic and stressed, but in reality this is a single phase that is always nearly isostatic.

10:30 AM

(GOMD-SII-023-2010) Elastic behavior and fast-ion conduction in glasses

M. Micoulaut*, Université Pierre et Marie Curie, France; M. Malki, Université Pierre et Marie Curie, France, Université Pierre et Marie Curie, FranceCNRS Orléans, France

We present a Self-organized Ion Hopping Model (SIHM) that connects ion- conduction with elastic behavior of glasses. The topological model builds on size increasing clusters of typical local structural units, identifies Intermediate Phases, and permits calculating the compositional variation of ionic conductivity. Our results show three régimes of ion-conduction which are correlated with those in elastic behavior. In the stressed-rigid phase, a combination of low carrier rates and low count of isostatic hopping sites leads to low conductivities. In the intermediate phase conductivity builds up as flexible sites appear. In the flexible phase, a logarithmic increase of conductivity is obtained when strain energy is reduced by local deformation due to floppy modes. The SIHM description provides a sound physical basis to understand the recent conductivity data1 on modified oxides and solid electrolyte glasses. 1 M. Micoulaut, M. Malki, D.I. Novita, P. Boolchand, PRB 80 (2009) in press

10:45 AM

(GOMD-SII-024-2010) Electronic Signature of the Intermediate Phase in GexSe1-x Glasses

K. Li, G. Chen*, F. Inam, D. Drabold, Ohio University, United States

We have conducted x-ray absorption near-edge structure (XANES) analyses on binary germanium selenide glasses, in search of electronic signature of the intermediate phase. It has been observed that the white-line of Se K-edge absorption spectra, which is an indication of the lowest unoccupied electronic states, depends on the composition with abrupt changes occurring at the compositional boundaries of the intermediate phase. Molecular dynamic (MD) simulations of the germanium selenide glasses were performed to help understand the atomistic origin of the intermediate phase. Direct simulations of the XANES patterns using the FEFF program and the MD models were also conducted, and the results will be discussed. Existence of the electronic signature of the intermediate phase is confirmed by the MD simulations, which suggest that the intermediate phase originates from competition between Ge-rich and Se-rich clusters.

11:00 AM

(GOMD-SII-025-2010) Bimodal phase percolation model for the structure of Ge-Se glasses by Raman and NMR

P. Lucas*, E. King, University of Arizona, United States; B. Bureau, Universite de Rennes I, France; O. Gulbiten, University of Arizona, United States

High temperature NMR data provide a unique method for investigating the structure of selenide glasses. An extended study of Ge-Se glasses reveal that the structure is very distinct from most previously suggested models for this system. It is shown that the structure is instead based on the percolation of two distinct nanophase of nominal composition GeSe2 and Se. Both Raman and NMR data corroborate this model which is consistent with the original Phillips and Thorpe percolation threshold model but contradicts the intermediate phase model.

11:15 AM

(GOMD-SII-026-2010) Intermediate phase in sodium borate glasses

P. Boolchand, V. Kandasamy*, Univ of Cincinnati, United States

Alkali Borates are essential components of industrial glasses and offer interesting possibilities for applications. We have synthesized dry (Na2O)x(B2O3)100-x glasses over a wide composition range, $0 < x <$ 70%, and have examined them in modulated-DSC, Raman scattering, FTIR, and molar volume experiments. Our results reveal a deep, sharp, and square-well like reversibility window in the $20\% < x < 40\%$ range. In Raman scattering a mode is observed near 775 cm-1 once x increases to 10% and it steadily red-shifts with increasing soda concentration displaying evidence of thresholds. The optical elasticity associated with this network mode1 is being studied. FTIR measurements reveal the fraction of 4-fold to 3-fold coordinated B to steadily increase with x also displaying thresholds. These data will be discussed in the context of the elastic behavior of these glasses. 1 Jour. Mol. Structure 247, 1 (1991).

11:30 AM

(GOMD-SII-027-2010) Constraints, Iso-Tg Regimes, and Phase Separation

P. Gupta*, The Ohio State University, United States

Previously, we have, by considering the temperature dependence of bond-constraints, rationalized the experimentally observed composition dependencies of the glass transition temperature and of fragilities in binary Ge-Se and in alkali-borate systems in terms of the configurational entropy theory of viscosity. This work showed that iso-Tg regimes (composition ranges having constant Tg values) appear in some (e.g., alkali-borates) but not all (e.g., Ge-Se) systems. In this presentation, we argue that iso-Tg regimes are signatures of phase separation and arise as a consequence of simultaneous occurrence of a reducing set of constraints due to change in composition and an increasing set of constraints due to weak constraints that become intact at low temperatures.

11:45 AM

(GOMD-SII-028-2010) Transition features in GexAsySe1-x-y Glasses

R. Wang*, The Australian National University, Australia

We prepared GexAsySe1-x-y glasses with mean coordination numbers (MCN) from 2.2 to 2.86. Tg was found to generally increase with increasing MCN whilst the glass density showed a maximum at MCN≈2.45 and a minimum at MCN≈2.65. The elastic moduli of the glasses were estimated from the shear and compressional wave velocities measured by ultrasonic pulse interferometry. For the first time we simultaneously observed two elastic transition thresholds the first at MCN≈2.45 and the second at MCN≈2.65, which appear closely correlated with changes in the glass microstructure. On the other hand, measurements of the samples with same MCN but different chemical compositions shows that the variance of Tg and elastic moduli is around 5-10% but the density shows a maximum in the chemically stoichiometric sample.

Symposium III: Glass Technology

Glasses for Medicine and Biotechnology

Room: Seneca
Session Chair: Matthew Hall, Alfred University

9:15 AM

(GOMD-SIII-022-2010) Bioactive, Antibacterial Cements for Skeletal Applications (Invited)

M. Towler*, Alfred University, United States

It is accepted that Glass Polyalkenoate Cements (GPCs), currently used in dentistry as both luting cements and as colour matched alternatives to amalgam fillings, have potential in restorative medicine as alternatives to acrylic cements and calcium phosphate filling materials. However, the presence of toxic constituents, such as aluminium, has, to date, inhibited their use. The work presented here will consider the development of new GPCs, based on a strontium calcium zinc silicate acid-degradable glass mixed with aqueous polyacrylic acid, for use across a range of medical applications. These materials have been fully characterised and tested both mechanically (compressive and flexural strength, fracture toughness) and biologically (in vitro and in vivo evaluation) to confirm their suitability for spinal and maxillofacial augmentation.

9:45 AM

(GOMD-SIII-023-2010) Effect of strontium on the atomic structure and ion diffusion of bioactive glasses: a molecular dynamics simulation

J. Du*, Y. Xiang, University of North Texas, United States

Strontium doping has been found to be beneficial to tissue growth due to the effect of Sr2+ ions to prevent bone absorption and maintain bone formation. The atomic structure information of the local environment of strontium ions, how they distribute in multicomponent bioactive glasses and their effect on ion diffusion is crucial to the understanding of the enhanced bioactivities and design of new strontium containing glass compositions for biomedical applications. In this talk, we present our recent results obtained from classical molecular dynamics simulations to understand the structure of strontium doped 45S5 bioactive glasses, where the calcium oxide is gradually replaced by strontium oxide. The coordination environment of strontium ions, their distribution and correlation with other modifier cations, and the effect of strontium concentration on sodium and calcium diffusivity in the bioactive glasses will be presented.

10:00 AM

(GOMD-SIII-024-2010) Novel Bioactive and Biodegradable 13-93 Glass Scaffolds for Bone Tissue Engineering

Q. Fu*, M. N. Rahaman, Missouri University of Science and Technology, United States

Bioactive glass scaffolds (porosity = 75–85%; pore size = 100–500 μm), with a trabecular microstructure but with different compositions, were prepared and evaluated for potential bone repair applications. The glasses consisted of a silicate (13-93) composition, a borosilicate composition (designated 13-93B1) with 1/3 the SiO2 replaced with B2O3, and a borate composition (13-93B3) all SiO2 replaced with B2O3. The degradation of the scaffolds in a simulated body fluid was dependent on the B2O3 content of the glass. In vitro cell culture showed that the 13-93 and 13-93B1 scaffolds provided more favorable substrates than 13-93B3 for supporting the proliferation and function of osteogenic MLO-A5 cells. Subcutaneous implantation in rats showed that all three scaffolds supported tissue infiltration. The results indicate that the combination of scaffold bioactivity and biodegradability can be achieved by replacing an appropriate amount of SiO2 in silicate bioactive glass with B2O3.

10:15 AM

(GOMD-SIII-025-2010) Direct Write Assembly of Bioactive Glass Scaffolds for Bone Tissue Engineering

Q. Fu*, E. Saiz, A. P. Tomsia, Lawrence Berkeley National Laboratory, United States

The objective of this study was to prepare, characterize and evaluate bioactive glass 6P53B scaffolds for potential application in bone tissue engineering. Glass scaffolds were prepared by a direct write assembly technique through a layer-by-layer printing of glass ink. The effects of glass strut thickness and pore size (the gap between the printed "lines") on the mechanical strength were evaluated. In vitro evaluation of the scaffolds in simulated body fluid (SBF) indicated excellent bioactivity of the glass scaffolds. In vivo subcutaneous implantation of the scaffolds in rats showed their ability to support new bone formation when seeded with human bone marrow stromal cells (hMSCs). All these results demonstrate that bioactive glass scaffolds fabricated by the direct write assembly technique may serve as good substrates for repair and regeneration of bone defects.

10:30 AM

(GOMD-SIII-026-2010) Multifunctional, TiO2-based Coatings on Glass

B. Akkopru*, Alfred University, United States; C. Durucan, Middle East Technical University, Turkey; N. P. Mellott, Alfred University, United States

When irradiated with ultra-bandgap light, titanium dioxide (TiO2) behaves not only as an effective photocatalyst but a bactericidal agent as well. Furthermore, it has been shown that through doping, the photocatalytic and bactericidal activity can be modified. The overall objective of this work is to investigate the effect of sol-gel processing parameters on the structural evolution of silver containing TiO2 (Ag-TiO2) coatings on glass. Therefore, different test platforms are investigated in which the physical and chemical properties of Ag nanoparticles as well as the overall structure of the TiO2 matrix are varied in a controlled manner. The effect of processing parameters on material properties are established through application of a wide range of characterization techniques. Furthermore, the effect of composition and material properties of Ag-TiO2 films on multifunctionality is discussed.

10:45 AM

(GOMD-SIII-027-2010) Systems and Interfaces: Controlling Bio Processes (Invited)

G. D. Stucky*, UCSB, United States

This talk will focus on recent research on the use of interface chemistry to control the bioprocesses associated with hemostasis. The target of this research is development of a protocol to accelerate or inhibit blood coagulation by using a nanostructured inorganic-blood interface that controls the blood clotting cascade with high efficacy. Methods for optimizing the hemostasis response to nanostructured materials, as well as incorporating antibacterial activity and using composite systems as enzyme delivery agents will be described. By monitoring both the hemostatic and bone-forming activity of mesostructured hemostatic bioactive glasses that have different compositions, an interesting inverse relationship for this class of materials has been determined. The relationship between in vitro research and in vivo testing, and their ultimate practical commercial evaluation and application, will also be summarized.

11:15 AM

(GOMD-SIII-028-2010) Electropolymerization of aniline within redox-mediated organically modified silicate

P. C. Pandey*, Banaras Hindu UNiversity, Institute of Technology, India

Electropolymerization of aniline is studied within nano-structured network of organically modified sol-gel glass modulated by the presence of tetracyanoquinodimethane (TCNQ), to understand the contribution of redox mediation/electrocatalysis on aniline electropolymerization. In order to study the effect of electrocatalyst together the role of redox-mediator during the electropolymerization of aniline, palladium was also introduced within nano-structured network of ormosils. The polyaniline electrosynthesized within these matrixes yielded very valuable information on the interaction of TCNQ with polyaniline and justified the existence of TCNQ-polyaniline composite.The application of the composite material has been investigated on the development of solid-state ion-selective electrode. The new composite provide a stable dipolar layer with excellent contact with conventional ion sensing membrane.

11:30 AM

(GOMD-SIII-029-2010) Glass as an Electronic Package Substrate for Consumer and Biomedical Applications

V. Sukumaran*, Q. Chen, N. Kumbhat, F. Liu, S. Min, V. Sundaram, R. Tummala, Georgia Institute of Technology, United States

Packaging technology was dominated by High-temperature Co-fired Ceramics (HTCC) in 1980s and Low-temperature Co-fired Ceramics (LTCC) in the 1990s. Subsequently, technology has evolved to organic build-up substrates. However, there are three major shortcomings with present-day organic approach: 1) difficulty in achieving high I/Os at fine pitch, 2) resulting warpage with increased layers, and 3) high cost. This paper focuses on the pioneering exploration of glass interposer technology to overcome the shortcomings of organic and silicon packages with an emphasis on: 1) electrical and mechanical design TPVs, 2) small diameter with fine-pitch through-via formation, and 3) subsequent metallization of vias and on-surface wiring for very high I/Os. Glass, as a package substrate material, provides excellent electrical properties, Si-matched CTE, dimensional stability, bio-compatibility and most importantly, a large area to process large panels that result in highly efficient low-cost packages.

Symposium V: Glass Structure and Properties

Glass Structure and Properties I: Silicates

Room: Keuka
Session Chair: Sabyasachi Sen, University of California - Davis

9:30 AM

(GOMD-SV-001-2010) Determination of Structural Distributions in Densified Silica Using O–17 NMR (Invited)

P. Grandinetti*, N. Trease, Ohio State University, United States; J. Stebbins, Stanford University, United States; S. Sen, University of California, Davis, United States

Details about structural changes occurring in densified silicas have been subject to debate, as it has been suggested that amorphous materials may undergo discontinuous structural transitions with pressure. We have measured the two–dimensional O-17 dynamic-angle spinning solid-state nuclear magnetic resonance spectrum of silica glasses produced from the melt and densified in a multi-anvil device at pressures up to 15 GPa at ambient temperature. From our spectra we have obtained three dimensional histograms correlating O–17 chemical shift, quadrupolar coupling constant and asymmetry parameter for the bridging oxygen were obtained. Using existing correlations between NMR parameters and local structure, the distribution in quadrupolar coupling parameters has been mapped into two dimensional histograms correlating Si–O–Si angle with Si–O distance, Si–O–Si angle with Si–Si distance, and Si–O distance with Si-Si distance. The effect of densification on the silica structure will discussed.

10:00 AM

(GOMD-SV-002-2010) Structure and bonding in CaO-SiO2 liquids and glasses

R. J. Weber*, Materials Development, Inc., United States; C. J. Benmore, Argonne National Laboratory, United States; J. B. Parise, Stony Brook University, United States; M. C. Wilding, Aberystwyth University, United Kingdom; J. Du, University of North Texas, United States

The application of high energy x-rays, a containerless sample environment, and fast detection of scattered x-rays provides a means to study structural evolution in liquids as they are cooled towards the glass transition. Previous studies have revealed substantial temperature-dependent changes in coordination and bonding in Al2O3-SiO2 and MgO-SiO2 melts. In the present work, CaO-SiO2 binary liquids were investigated over a range of temperatures from 20-2000°C. As the liquids cool, large changes in polymerization are observed as the concentration of edge-shared CaO6 polyhedra increases with decreasing temperature. The implementation of the experiments will be briefly described and the results of measurements will be presented and discussed in the broader context of the glass forming behavior of high melting point, relatively fragile oxide liquids.

10:15 AM

(GOMD-SV-003-2010) Structural heterogeneity in calcium aluminosilicate glasses

M. Moesgaard*, R. Keding, Aalborg University, Denmark; J. Skibsted, Aarhus University, Denmark; Y. Yue, Aalborg University, Denmark

The physical and chemical properties of glasses are determined largely by their microstructure in both short- and intermediate-range. Despite numerous studies on the intermediate-range order (IRO), some key questions still remain unanswered. In this work, we investigate the IRO of peralkaline glasses within the calcium aluminosilicate system. This is performed by structural modeling and solid-state ^{29}Si and ^{27}Al nuclear magnetic resonance (NMR) spectroscopy. Two structural modeling approaches are proposed to describe the IRO. One model assumes a random spatial arrangement of Al, whereas the other allows clustering of regions rich in highly polymerized AlO_4 and SiO_4 units and other regions rich in highly depolymerized SiO_4 units. The clustering is described as IRO heterogeneity and this modeling approach provides a good description of the NMR spectra for all glasses. In contrast, the first approach can not convincingly model the NMR data. Thus, structural heterogeneities in the IRO do exist in the studied glasses.

10:30 AM

(GOMD-SV-004-2010) Temperature dependent structural changes in aluminoborosilicate melts

J. Wu*, J. Stebbins, Stanford University, United States

Borosilicate glasses and melts are critical in technology because of the ease of transition among 3- and 4-coordinated boron with composition, temperature (T), and pressure. The effect of T on the structure of aluminoborosilicate liquids has been studied by ^{11}B and ^{27}Al MAS NMR spectroscopy using glass samples prepared with different cooling rates and thus different fictive temperatures (T_f). The abundances of BO_3 group and of non-bridging oxygens (NBO) increase with increasing T_f, indicating that the reaction $BO_4 \leftrightarrow BO_3$ + NBO shifts to the right at a higher T. The observed T dependence of BO_4 species abundance allows us to estimate the ΔH of this reaction to be 20 to 40 kJ/mol in different glass compositions. Heat capacities (C_p) has been measured by differential scanning calorimetry (DSC), and configurational C_p were approximated as $C_{p(conf)} = C_{p,liquid} - C_{p,glass(Tg)}$. The redistribution of boron species contributes a varying fraction of the $C_{p(conf)}$, from 20% to 50%, with different glass compositions.

10:45 AM

(GOMD-SV-005-2010) Counting Non-Bridging Oxygens in Calcium and Potassium Aluminosilicate Glasses with Oxygen-17 NMR

L. M. Thompson*, J. F. Stebbins, Stanford University, United States

Non-bridging oxygens (NBO) are understood to have a significant influence on thermodynamic and transport properties in aluminosilicate melts and glasses. Standard network models assume that NBO are absent along metaluminous joins (e.g. $CaAl_2O_4$-SiO_2 or $K_2Al_2O_4$-SiO_2). However, nuclear magnetic resonance (NMR) on metaluminous (Ca=2Al) Ca-aluminosilicate glasses has shown up to 7% NBO, as well as significant fractions of AlO_5. Using O-17 NMR, this study directly measures NBO contents in two series of Ca aluminosilicate glasses from peralkaline-earth (Ca>2Al) to peraluminous (Ca<2Al) and a similar K-aluminosilicate series. NBO are clearly observed at the metaluminous join in both Ca glass series, persisting well into the peraluminous region. In contrast, NBO in the K-aluminosilicates become undetectable (<1%) when K=Al, correlating with low AlO_5 contents and more in line with conventional approximations.

11:00 AM

(GOMD-SV-006-2010) A Multispectroscopic Study of Lead Silicate Glass Atomic Structure

A. Vitale*, M. Affatigato, S. Feller, Coe College, United States; G. Lehr, Monmouth College, United States; D. Holland, M. Smith, University of Warwick, United Kingdom; A. Hannon, E. Barney, Rutherford Appleton Lab, United Kingdom

Although many structural experiments have been performed on the binary lead silicate glass system, the compositional sequence of the glass is not fully understood in reference to the formation of two glass forming networks, PbO and SiO2. A series of binary lead silicate glasses, spanning a range of lead oxide to silica ratios, J, of 0.5 through 5.0, were prepared for number of spectroscopic techniques including elastic neutron scattering, FTIR, Raman, 29SiMAS NMR, and laser desorption TOF mass spectroscopy. These samples also were characterized by their glass transition temperature. A quantitative structural model, composed of separate lead oxide and silicate tetrahedral was created that is consistent with these varied data. Work performed under grant NSF DMR-0904615

11:15 AM

(GOMD-SV-007-2010) Tracer Diffusion of Sodium in Sodium Borosilicate Glasses

X. Wu*, R. Dieckmann, Cornell University, United States

Sodium tracer diffusion measurements using the radioactive isotope sodium-22 have been performed in sodium borosilicate glasses with the composition $(Na_2O)_{0.2}[(BO_{1.5})_x(SiO_2)_{1-x}]_{0.8}$ with x varying between 0 and 1. At all temperatures investigated between 208 and 503 °C, the logarithm of the sodium tracer diffusion coefficient was found to vary non-linearly with the composition parameter x. Minima were observed at x close to 0.7. A similar trend was also observed for the electrical conductivity studied by collaborators at Iowa State University using the same type of samples as used for the tracer diffusion experiments denoted above. Experimental results will be presented as well as data for pre-exponential factors, activation energies and Haven-ratios. The observed composition dependencies will be discussed in conjunction with findings reported in the literature.

11:30 AM

(GOMD-SV-008-2010) Mechanical properties in pseudo-binary system of Pyrex and soda-lime-silica glass

A. Koike*, S. Ito, Asahi Glass Co., Ltd., Japan

Cracking behavior is different between anomalous glass, where elastic constant shows positive temperature coefficient, and normal glass, where that shows positive one. In this study, mechanical properties and cracking behaviors in pseudo-binary system of Pyrex-type borosilicate glass and window glass; soda-lime-silica glass, which are known to be, respectively, anomalous and normal glass, was investigated. Density and photoelastic constant linearly changed with composition. However, at the intermediate composition, Young's modulus and hardness were maximized and Poisson's ratio was minimized. Measurement results of NMR implied that the glass structure reflects the changes of mechanical properties at the transition region between anomalous and normal. In addition, fracture toughness and crack initiation load were maximized at the intermediate composition, too. From these results, the relationship between cracking behavior and mechanical properties or glass structure will be discussed.

11:45 AM

(GOMD-SV-009-2010) Short-range Structure of Invert Glasses Along the Join MgSiO3-Mg2SiO4

S. Sen*, University of California - Davis, United States; H. Maekawa, Tohoku University, Japan; G. Papatheodorou, ICEHT-FORTH, Greece

The short-range structure of "invert" glasses along the join MgSiO3-Mg2SiO4 have been studied using 29Si and 25Mg MAS NMR spectroscopy. The results indicate a progressive compositional evolution in Q-speciation that approximately follows a statistical distribution. The Mg2SiO4 glass shows an abrupt deviation from this trend with the presence of nearly 40% of the Si atoms as Q1 species. Mg2+ ions are present in predominantly octahedral coordination in all glasses. When taken together, these results indicate that glasses with MgO contents between 50 and 60 mol% are characterized by a structure consisting primarily of at least 3 types of Q-species and MgO6 octahedra. On the other hand, the structure of glasses with > 60 mol% MgO appears to consist of Q0 and Q1 species with structural connectivity being primarily provided by the MgO6 octahedra. The possible consequences of such compositional evolution of structure on the ability of glass formation in this system are discussed.

Symposium II: Glass Science

Rheology

Room: Cayuga

Session Chair: Lothar Wondraczek, Universitat Erlangen-Nurnberg

1:15 PM

(GOMD-SII-029-2010) Rheology of heterogeneous liquids (Invited)

J. Deubener*, Clausthal University of Technology, Germany

Processing of multi-phase systems such as glass-ceramics, enamels, and glass matrix composites are affected by the flow of particulate dispersions. In ideal systems these dispersions are defined as insoluble particles (solid, liquid, or gas) distributed throughout a continuous liquid phase, while in real systems as a consequence of fast dissolution, crystallization, and degassing processes these particle fractions are of temporary nature only. In this study experimental evidence is presented for the complex influences of transient particle fractions on effective (global) viscosity, which results from simultaneous variations of particle fractions and chemical composition of the residual liquid phase. By contrast, the transformation kinetics of the particles is mainly influenced by the local viscosity of interfacial areas. The knowledge of the rheological properties can help to control sintering, ceramization, and desired evolution of microstructure of these materials, e.g. minimize deviation from designed shapes and functions.

1:45 PM

(GOMD-SII-030-2010) Viscosity of Glass-Forming Liquids

J. C. Mauro*, Corning Incorporated, United States; Y. Yue, Aalborg University, Denmark; A. J. Ellison, Corning Incorporated, United States; P. K. Gupta, The Ohio State University, United States; D. C. Allan, Corning Incorporated, United States

The low temperature dynamics of ultraviscous liquids hold the key to understanding the nature of glass transition and relaxation phenomena, including the potential existence of an ideal thermodynamic glass transition. Unfortunately, existing viscosity models such as the Vogel-Fulcher-Tammann (VFT) and Avramov-Milchev (AM) equations exhibit systematic error when extrapolating to low temperatures, despite their relative success at higher temperatures. We present a model offering an improved description of the viscosity-temperature relationship for both inorganic and organic liquids, using the same number of parameters as VFT and AM. The new model has a clear physical foundation based on the temperature dependence of configurational entropy, and it offers accurate prediction of low temperature isokoms without any singularity at finite temperature. Our results cast doubt on the existence of a Kauzmann entropy catastrophe and associated ideal glass transition.

2:00 PM

(GOMD-SII-031-2010) Modeling the Nonequilibrium Viscosity of Glass

D. C. Allan*, J. C. Mauro, M. Potuzak, Corning Incorporated, United States

The nonequilibrium viscosity of a glass is typically lower than that of the equilibrium supercooled liquid. Likewise, a glass formed using a faster cooling rate generally has a lower viscosity than that prepared with a slower cooling rate. In this presentation, we propose a new phenomenological model of nonequilibrium glass viscosity based on enthalpy landscape simulations of selenium glass prepared using cooling rates covering twenty-five orders of magnitude. These computations are performed based on the framework of continuously broken ergodicity. The computations have suggested a new functional form for nonequilibrium viscosity that contains a few phenomenological fitting parameters. These parameters can be fit to data measured on complex glasses that remain beyond the scope of ab initio calculations. We show that the new model of nonequilibrium viscosity provides a significant advantage over previous phenomenological models of glass viscosity.

2:15 PM

(GOMD-SII-032-2010) Viscosity and softening behaviour of alkali zinc phosphosulphate glasses

N. Da*, L. Wondraczek, Universitat Erlangen-Nurnberg, Germany

We report on softening properties and viscosity of glasses from the system ZnO-Na2O-SO3-P2O5 for low-temperature sealing applications. Up to a ratio of network forming ions PO43-:SO42- of about 2:1, gradual substitution of P2O5 by SO3 results in decreasing glass transition and softening temperatures. At the same time, decreasing kinetic fragility is observed, noteworthy even for decreasing total amount of network former from 51 mol.% to 46 mol.%. Thermomechanical and calorimetric analyses reveal a distinct SO42—promoted relaxation phenomenon at temperatures significantly below the macroscopic glass transition temperature what is interpreted as a result of the formation of an increasingly interconnected assembly of SO42- and PO43—units with increasing SO3-content.

2:30 PM

(GOMD-SII-033-2010) Progress in the Rheology of Inorganic Glass-Forming Melts (Invited)

Y. Yue*, Aalborg University, Denmark

In recent years, substantial progress has been made in understanding rheology of glass-forming melts. In my presentation, I focus on some of crucial developments in studies of the viscous behavior of inorganic melts. I describe the new insights into the correlations among the liquid dynamics, thermodynamics, equilibrium viscosity, non-equilibrium viscosity, and non-Newtonian viscosity. I address the role of the new knowledge about the melt rheology in influencing the glass technology by giving several examples. Furthermore, I attempt to establish the link between the melt fragility and the technological aspects such as the melt workability, fiber spinnability, and glass forming ability. I also briefly mention which of the current viscosity models has both physical foundation and highest accuracy in describing the temperature and deformation dependences of viscosity. The impact of the glass structural anisotropy due to tension on mechanical strength has been demonstrated and elucidated.

3:15 PM

(GOMD-SII-034-2010) Boson peak, inhomogeneity and pressure experiments in SiO2 and GeO2 glasses (Invited)

B. Champagnon*, D. Thierry, M. Christine, Université Lyon1-CNRS, France

The origin of the Boson peak is still a controversial topic. Application of an external hydrostatic pressure is a way to test if a single component glass behaves a continuous medium. Decrease of the intensity of the Boson peak of SiO2 and GeO2 glasses in the elastic domain demonstrates its non continuous behaviour and is associated with the intrinsic inhomogeneity of these glasses.

3:45 PM

(GOMD-SII-035-2010) Pressure-assisted flow of glass melts in narrow capillaries (Invited)

M. Schmidt*, L. Wondraczek, P. Russell, Max Planck Insitute for the Science of Light, Germany

We report on an alternative technique for the production of all-solid PCF devices by pressure-assisted infiltration of silica sub-μm capillaries. It is demonstrated that with proper knowledge of the flow behaviour of the considered glasses in highly confined conditions, waveguides with low optical loss can be generated. Exemplarily, the application of such waveguides for broadband supercontinuum generation will be shown.

4:15 PM

(GOMD-SII-036-2010) On the Origin of the Mixed Glass Former Effect: Varying Coulomb Traps of Network Forming Units

P. Maass, Universität Osnabrück, Germany; C. R. Müller*, Technische Universität Ilmenau, Germany; M. Schuch, Universität Osnabrück, Germany

Mixing of two types of glass formers in ion conducting glasses can lead to strong enhancements of ionic conductivities, a phenomenon commonly referred to as the Mixed Glass Former Effect (MGFE). A theory for the MGFE is presented which allows one to describe the change of concentrations of network forming units upon mixing and associated changes in Coulomb trapping energies. Using this structural information the change of the conductivity activation energies is calculated by means of percolation theory and Monte Carlo simulations. Fits of the theory to experiments on a borophosphate system yield good agreement with the measured data both for the concentration variation of the units and the variation of the activation energy.

4:30 PM

(GOMD-SII-037-2010) Viscosity of Tellurite Glass: 75TeO2-20ZnO-5Na2O

A. A. Belwalkar*, W. Z. Misiolek, J. Toulouse, Lehigh University, United States

The steady state shear viscosity of the tellurite glass 75TeO2-20ZnO-5Na2O has been measured as a function of shear rate and temperature using parallel plate rheometry. The data indicate a marked shear thinning behavior in which viscosity is constant for lower shear rates but decreases rapidly above a critical shear rate and then asymptotically approaches to zero. This relaxation behavior of the normalized viscosity is well approximated by a shear rate dependent equation in the temperature range between 609 and 663 K. The relaxation time τ, obtained from a fit of the data to the Cross relation is found to follow an Arrhenius law in the temperature range investigated and the cohesive shear strength of the glass in the same range is calculated to be approximately equal to 1.1 MPa. The viscosity plotted on the Angell-type plot provides a measure of the glass fragility and is compared to that of the other glasses.

Symposium III: Glass Technology

Glasses for Energy and Environmental Applications

Room: Seneca

Session Chairs: Joachim Deubener, Clausthal University of Technology; Dean Thelen, Corning Incorporated

1:15 PM

(GOMD-SIII-030-2010) Specialty Glass for Thin Film Solar Cell Applications (Invited)

D. Hall*, Corning Incorporated, United States

Lower cost is a major requirement for large scale deployment of photovoltaic (PV) power generation. Thin-film technology PV offers a path to cost parity with fossil fuel-based systems in the near-term. Historically it has been assumed that the use of standard Na-lime glass formed by the float process was a prerequisite for low system cost. Recently work on thin specialty glass has shown significant improvement in thin-film PV module solar-to-electric conversion efficiency when compared to Na-lime that results in overall lower system cost. Research at Corning will be reviewed demonstrating that higher efficiency and the necessary reliability can be obtained from thin specialty glass relative to Na-lime float glass.

1:45 PM

(GOMD-SIII-031-2010) Specialty Thin Glass for PV Modules: Mechanical Reliability Considerations

J. Webb*, Corning Incorporated, United States

Typical solar modules use float glass that is standard or low-iron soda-lime-silica with thickness greater than or equal to 3.2 mm. This presentation considers a specialty thin glass as either the substrate or superstrate of a dual-glass laminated TF PV module with a standard tempered 3.2 mm soda lime-silica glass to complete the dual-glass package. Thin specialty glasses are shown to be an attractive option for thin-film photovoltaic module substrates and superstrates. They are able to withstand wind and snow loads along with hail impact. Their fatigue resistance is significantly better than that of soda-lime-silica glass. Thicknesses ranging from 0.7 to 1.5 mm are shown to be suitable for thin film

photovoltaic applications. As with any glass selection, support structure design is a key factor for limiting mechanical stresses to a safe level, thereby ensuring long term reliability of PV modules.

2:00 PM

(GOMD-SIII-032-2010) Sintering of nanoporous anti-reflective coatings for concentrated solar power applications

A. Mös, G. Helsch, J. Deubener*, Clausthal University of Technology, Germany

Broad band quarter-wave anti-reflective (AR) coatings on soda-lime-silica and borosilicate glasses are frequently used in solar technology. An effective refractive index between glass (1.5) and air (1.0) can be achieved by nano-porous SiO2. In tower receivers, which are exposed to the concentrated solar radiation of the heliostats, temperature can reach more than 1000°C. To compensate for reflectance losses of window materials AR-coatings are a part of recent receiver designs. In particular, we studied the sintering of these thin films on silica glass to predict thermal stability under operating conditions. The shrinkage rate of nano-porous films after heat treatment was determined from the gain of transmittance using UV/VIS/NIR spectroscopy and from the decrease of layer thickness by profilometry. The results show that sintering of 20-50 nm sized SiO2 particles proceeds via viscous flow of energy comparable to viscosity of silica glasses in the glass transition range.

2:15 PM

(GOMD-SIII-033-2010) Viscous Sealants for Solid Oxide Fuel Cell Application

M. Naylor*, J. Shelby, S. Misture, Alfred University, United States

Viscous sealants do not fracture like rigid sealants and may enhance SOFC performance during operation. Several silicate based glasses were studied for application as viscous sealants for SOFCs. Gallium and germanium containing silicates with strontium additions were prepared and studied. Several compositions retain a high amorphous content after 1400h at 850 °C in air. Thermal expansion coefficients and glass transition temperatures of annealed and crystallized samples have been measured. Powdered samples of the glasses have been heat treated up to 504h at 850 °C in air to evaluate crystallization. Interactions between the glasses and substrates of alumina, 8YSZ, and stainless steel were examined. Viscous flow behavior of powdered samples was studied with hot-stage microscopy. Effects of hydrogen atmospheres were investigated.

2:30 PM

(GOMD-SIII-034-2010) Vanadium phosphate glasses as frits for laser-sealing

R. Morena*, L. A. Lamberson, CORNING Incorporated, United States

Frit-sealing is typically accomplished using furnace heating. This process is frequently lengthy in duration, and involves heating the entire assembly to the sealing temperature, holding at this temperature to permit frit flow and bonding to occur, and then cooling at a gradual ramp to avoid excess thermal stress. Although this approach has been notably successful for many products, many new sealing applications (such as OLEDs) are degraded by exposure to even mild temperatures (~100degC). Vanadium phosphate frits are described that are capable of being sealed by a laser at speeds as fast as 100mm/sec. The resulting seals are hermetic, and have withstood high humidity for >1000 hrs. These frits have relatively low Tg (<350degC). Unlike other low Tg frits, the vanadium phosphate compositions are distinguished by low CTE (<70-80x10-7/degC). As a result, it is possible with the use of CTE-lowering fillers to expansion match alumino-silicate and boro-silicate display glasses.

2:45 PM

(GOMD-SIII-035-2010) Sealing Glasses for Applications below 200°C

L. Gambino, Rutgers University, United States; A. Jitianu, Lehman College-CUNY, United States; L. C. Klein*, Rutgers University, United States

Organic-inorganic gels have been prepared for low temperature seals and hermetic barriers in microelectronics. Using the sol-gel process, it is possible to prepare silica-based hybrid gels that are rigid at room temperature, but soften and flow repeatedly around 110°C. This softening behavior has been called melting. The ability to flow is an indication that the material is not fully cross-linked. In fact, the hybrids show glass transition behavior at temperatures below 0°C. Once these gels have been consolidated at around 160°C, they no longer show the ability to soften. Mixtures of mono-substituted siloxanes and di-substituted siloxanes have been prepared. The resulting melting gels have been characterized for their glass transition temperatures, softening temperatures and consolidation temperatures. With low-temperature sealing applications in mind, densities, porosities, vapor transport properties, hardness, dielectric constants and transparency have been measured.

3:15 PM

(GOMD-SIII-036-2010) Lithium ion diffusion in silicon-Lithium battery materials

M. Zhang*, D. A. Drabold, Ohio University, United States

Li deposition in electrolytes limits charging-discharging cycles in novel Li-Si batteries. We study this problem by performing ab initio simulation of Li+ diffusion in models representing the anode, electrolyte, and their interface. To elucidate the extrordinary diffusion of Li^+ and calibrate the method, $Si_{64}Li_m$ (m = 1, 2, 3) are modeled by density functional codes SIESTA and VASP at 4K, 200K, 400K, 1000K and 2000K. Above 400K, simulations show Li^+ to be extremely diffusive. This is in contrast to Ag^+ in chalcogenides, for which the transit time is much smaller than trapping time. The practical composition $Li_{22}Si5$ of anode is simulated by structural models $Li_{54}Si_n$ (n = 10, 12, 13). The density of states show that they are good metals, Fermi level is shifted up relative to pure lithium metal: it becomes less conductive but still an excellent anode. We consider the anode and electrolytes separately and together, to model interface effects.

3:30 PM

(GOMD-SIII-037-2010) Development of LiFePO4 glass-ceramic for cathode material of lithium ion battery

T. Nagakane*, H. Yamauchi, K. Yuki, A. Sakamoto, Nippon Electric Glass Co.,Ltd., Japan; T. Honma, T. Komatsu, Nagaoka University of Technology, Japan; M. Zou, Y. Okumura, T. Sakai, National Institute of Advanced Industrial Science and Technology, Japan

A LiFePO4 glass-ceramic for the cathode active material of lithium ion rechargeable battery was prepared through crystallizing precursor glass under reducing atmosphere. The electrode fabricated with this glass-ceramic showed discharged voltage of 3.4V (vs. Li metal) corresponding to the electrode potential of LiFePO4, and higher cell voltage at high-rate discharge than the conventional LiFePO4 ceramic produced by solid state reaction. This suggests that the internal resistance of the battery fabricated with this glass-ceramic is lower than the one with the conventional LiFePO4 ceramic. In general, it is reported that magnetic impurities involved in the LiFePO4 ceramic cause short circuit problem. It was confirmed that this glass-ceramic contains much less magnetic impurities than the ceramic through an experiment using a magnet of magnetic flux density of 300mT. This glass-ceramic is expected as a cathode material for safe lithium-ion rechargeable batteries with superior high-rate performance.

3:45 PM

(GOMD-SIII-038-2010) Proton Conduction of Sol-Gel Derived Monolithic Electrolytes for use in Mid-Temperature Proton Exchange Fuel Cells

A. Feldman*, J. Kieffer, University of Michigan, United States

Ionically conductive sol-gel derived glasses are desirable in the design of mid-temperature, low humidity fuel cells due to their chemical sensitivity and environmental robustness. In order to better understand the conduction pathways through this class of electrolytes we synthesize phosphosilicate systems via ambient sol-gel methods and characterize them using a combination of inelastic light scattering techniques coupled with impedance spectroscopy. The structural evolution of the electrolyte is monitored via Brillouin and Raman scattering. The latter is used to track the development of structural moieties and the former to

study the connectivity between these building blocks. Conductivity, measured by impedance spectroscopy, is correlated with the multi-aspect structural characterization based on inelastic light scattering. We present data for a range of phosphosilicate glass compositions processed to varying degrees of densification.

4:00 PM

(GOMD-SIII-039-2010) Dielectric Breakdown of Alkali-Free Boroaluminosilicate Glass Thin Films

J. Serra*, M. Lanagan, C. Pantano, Penn State University, United States

High quality, commercial alkali-free boroaluminosilicate wafer glasses have emerged as potential candidates for use in high energy density capacitors. In recent work, near intrinsic breakdown strength was reported for thin (10- 30μm) alkali-free glass; the dielectric breakdown strength is found to increase with decreasing thickness of the glass. To extend this study of thickness dependence, and to confirm the intrinsic value, thin films have been fabricated using radio frequency magnetron sputter deposition to allow measurements at thicknesses less than 5μm thick. The film composition and dielectric properties have been obtained and compared to the bulk glass properties using x-ray photoelectron spectroscopy, Fourier Transform Infrared spectroscopy, microscopy and dielectric measurements.

4:15 PM

(GOMD-SIII-040-2010) Transition- and Post-Transition Metal doped Glasses and Glass Ceramics for Energy Efficient Lighting (Invited)

L. Wondraczek*, M. Peng, Universitat Erlangen-Nurnberg, Germany

Using glasses and glass ceramics, respectively, as phosphor materials in energy efficient light sources may offer various advantages with respect to processing and recycling as well as color versatiliy. In this context, transition and post-transition metal ion doped materials will be discussed in this talk. Particular focus is given to Mn2+ and Bi2+-doped materials which presently receive, on the one side, significantly less consideration than rare-earth dopants whereas, on the other side, they have a long history as synthetic or natural phosphors (Mn2+) and exhibit unique optoelectronic properties (both), respectively.

4:45 PM

(GOMD-SIII-041-2010) Removal of Chromium(VI) Ion from a Solution by Barium Borosilicate Glass

I. Baek*, C. Kim, Inha University, Korea, Republic of

The Cr(VI) compounds in wastewater are highly toxic chemicals that cause serious problems. Current methods for Cr(VI) ion removal from wastewater are mostly too expensive and have operational difficulties. In this study, therefore, Cr(VI) ion was removed by using barium borosilicate glasses. When glass is reacted with a solution containing Cr(VI) ions, Ba^{2+} ions leached out of the glass surface combine with Cr(VI) ions in a solution to precipitate $BaCrO_4$ crystals on the glass surface. The Cr(VI) ions can thereby be removed from the solution. Various glasses with different amounts of BaO and B_2O_3 in the SiO_2-B_2O_3-BaO-Na_2O glass system have been prepared. After the reaction, the concentration of the Cr(VI), Si, B, Ba and Na ions remained in the reacted solution were measured by ICP-OES. The reacted glass surface were analyzed by using a XRD, SEM, and EDS. The removal efficiency increases with BaO and B_2O_3 content in the glass. The pH of the solution for optimum removal of Cr(VI) ions was 3.0~5.0.

Symposium IV: Glass Corrosion

Short-term Corrosion Issues I

Room: Carder
Session Chair: Nathan Mellott, Alfred University

1:00 PM

(GOMD-SIV-001-2010) Glass Corrosion 101 (Invited)

C. Pantano*, Pennsylvania State University, United States

This tutorial will focus on the phenomenological aspects of glass corrosion and leaching in silicate based systems, including the most important dependences on pH and glass composition. An emphasis will be placed on how corrosion alters the surface structure and properties of the glass, and likewise, how the surface influences the corrosion kinetics at short and long times. Selected examples of corrosion behavior in simple, complex and commercial glasses will be used to exemplify the basic phenomena and the consequences of glass corrosion in manufacturing and service.

2:00 PM

(GOMD-SIV-002-2010) Practical Aspects of Corrosion in Glass Fiber (Invited)

J. F. Bauer*, J Bauer Consulting, United States

Commercial applications of glass fibers are often limited by their susceptibility to aqueous corrosion reactions. Direct attack on fiber surfaces typically leads to embrittlement and loss of fiber tensile strength. Corrosion can also contribute to chemistry changes at interfaces with polymeric coatings resulting in poor initial cure or subsequent de-coupling. However corrosion isn't always bad! Today manufacturers may deliberately build in a certain amount of "corrodibility" into their glasses for purposes such as enhanced biodecomposition in the lung , hydrolytic bonding in wet laid fiber papers, or for actually improving adhesion through the creation of more reactive surface sites. The key lies in understanding the chemical and physical nature of fiber surfaces which can be quite different from that of the bulk glass. Balancing these issues with the traditional constraints of cost and manufacturability can be a challenge for glass scientists and engineers – examples to be given.

2:30 PM

(GOMD-SIV-003-2010) Effects of leaching at glass/polymer interfaces

J. Banerjee*, Pennsylvania State University, United States; J. Hamilton, Johns Manville, United States; C. Pantano, Pennsylvania State University, United States

Application of a water-based polymer onto an alkali-rich multi-component silicate glass has been found to influence the interfacial adhesion relative to its behavior on silica. We developed a method to study the interfacial phenomena by using thin films of polymer to create a model interface with the glass where surface sensitive characterization tools could be applied. The effect of processing conditions and exposure to environmental duress on interfacial chemistry and stability with respect to sodium content of the glass was investigated. X-ray Photoelectron Spectroscopy was used to provide complementary chemical composition information for samples that were characterized by Infrared Reflectance spectroscopy. IR analysis showed that sodium leached from the glass into the interfacial region, saturated the carboxylic acid functional groups in the polymer by forming carboxylates. The formation of sodium carboxylates reduced the concentration of carboxylic functional groups necessary for curing.

Short-term Corrosion Issues II

Room: Carder
Session Chair: Nathan Mellott, Alfred University

3:15 PM

(GOMD-SIV-004-2010) On the Mechanisms of Corrosion Induced Roughening of Silicate Glass Surfaces

N. P. Mellott*, K. Kalac, Alfred University, United States; C. G. Pantano, The Pennsylvania State University, United States

Throughout their processing and service lifetime, glasses are exposed to a wide variety of corrosive environments, many of which are aqueous based. Therefore, glass surface properties as a function of aqueous corrosion are of both importance and significant interest. In this study, atomically smooth fiber and melt surfaces are reacted under a wide range of aqueous conditions. Such surfaces allow direct investigation of the molecular/microscopic effects of corrosion on surface roughness without the influence of surface preparation artifacts. In particular, atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS), and solution analysis by inductively coupled plasma mass spectrometry (ICP-MS) were used to investigate what molecular scale processes are responsible for the roughening of glass surfaces observed with aqueous corrosion.

3:30 PM

(GOMD-SIV-005-2010) Acid-induced alteration of Alkali Borosilicate frit

P. Marques*, R. M. Morena, Corning Sas, France

The alteration behavior of an alkali borosilicate glass in both sintered frit and bulk forms was studied following static leach tests in hot nitric acid solution using bending strength testing of polished specimens before and after acid exposure as a measure of degradation. SEM was used to examine changes in failure origin and in surface morphology associated with the acid exposure for both sets of specimens. The results indicate that the degradation resistance of the bulk glass is superior to that of the sintered frit, and that the alteration mechanism of both materials is dissimilar. The breakage origins of the sintered frit were associated with etched surface craters formed during firing of the frit with alumina-rich contaminants.

3:45 PM

(GOMD-SIV-006-2010) Aqueous corrosion of the GeSe4 chalcogenide glass:surface properties and corrosion mechanism

Y. Niu, J. Guin*, T. Rouxel, CNRS-Université de Rennes 1, France; A. Abdelouas, Ecole des mines de Nantes, France; J. Troles, Université de Rennes 1, France; F. Smektala, Université de Bourgogne, France

The aqueous corrosion behavior of the GeSe4 glass was studied over time under various conditions (temperature, pH). The evolution of the surface topography by atomic force microscopy and properties such as the surface hardness and reduced modulus as well as the optical transmission (1-16 μm)were followed as a function of corrosion time. It was found that the durability of GeSe4 is drastically affected by an increase of both temperature and pH. Furthermore during the corrosion mechanism pure Selenium nanoparticles were formed which nature - amorphous or crystallized (hexagonal phase) - depends on temperature. A reaction mechanism is proposed and the activation energy of the reaction of corrosion in deionized water is determined from the measurement, over time and for different temperatures, of the optical loss of a fiber made of the same glass composition and placed in deionized water.

4:00 PM

(GOMD-SIV-007-2010) Analytical modeling of the aqueous dissolution behavior of phosphate glasses

M. L. Schmitt*, L. Ma, R. Brow, Missouri S&T, United States

An analytical corrosion model was developed to predict dissolution rates for phosphate glasses in aqueous environments by considering reactions between water and individual bonds that constitute the glass structure. Thermodynamic principals, such as free energy of hydration, as well as compositional and structural properties, including field strength effects and bond basicities, were considered in the derivation of the model. Experimental dissolution results of alkali-alkaline earth phosphate glasses were used in model fitting. Modeling predictions for iron and zinc phosphate glasses are compared to empirical dissolution rates for validation of the model and show promising results.

Symposium V: Glass Structure and Properties

Glass Structure and Properties II: Simulations and Chalcogenides

Room: Keuka
Session Chair: Randall Youngman, Corning Incorporated

1:15 PM

(GOMD-SV-010-2010) Understanding the structures and properties of silicate and aluminosilicate glasses from classical and ab initio molecular dynamics simulations (Invited)

J. Du*, University of North Texas, United States

With ever increasing computing power and maturing simulation algorithms, computer simulations have become an important part of research in understanding the structure and properties of glasses complement to the experimental efforts. In this paper, I will present recent progresses of applying classical and ab initio molecular dynamics simulations of silicate and aluminosilicate glasses. The focus will be given to the interpretation, using these computer simulations, of the experimental structural data such as X-ray and neutron diffractions to understand the short and medium range structures of these glasses. Calculations of ion diffusion properties, mechanical properties, and electronic properties based the structure models from simulations and understanding the structure - property relationships of these glasses will also be presented.

1:45 PM

(GOMD-SV-011-2010) Mechanical Behavior of Water-Containing Glass by MD simulation

S. Ito*, T. Taniguchi, Asahi Glass Co., Ltd, Japan

Structure and mechanical property of water-containing (Li, Na, K)2O-Al2O3-SiO2 glasses were investigated by molecular dynamics simulation. The glasses with various content of water, such as OH and H2O, were prepared by substituting H for alkali ion and/or adding H2O molecules. The packing density of the glasses became smaller and larger, respectively, with increasing OH content and H2O content. The number of network rings decreased slightly with increasing both OH and H2O contents. Bulk and Young's modulus decreased remarkably with increasing OH content, whereas bulk modulus increased and Young's modulus decreased slightly with increasing H2O content. Under stress, the water-containing glasses deformed easily compared to the water-free glasses. The role of OH and H2O for flow and densification under stress will be discussed in terms of glass composition and structure.

2:00 PM

(GOMD-SV-012-2010) Structural Association of Ga and P in Selenide Glass

B. Aitken*, S. Currie, R. Youngman, C. Ponader, Corning Inc., United States

Ga improves the durability of P-containing sulfide glasses, where its incorporation leads to the formation of associated GaS4/2 and PS4/2 tetrahedra. In this study of GeGaP selenide glass, we examine the effect of Ga on the extent of glass formation as well as physical property and structural trends using viscometry, dilatometry, Raman and NMR spectroscopy. The thermal expansion coefficient and Tg of 66.7GeSe2:xGa2Se3:(33.3-xP2Se5) glasses decrease and increase, respectively, with rising Ga content, indicating an increase in network connectivity, while molar volume attains a maximum near x=16.7, suggesting a structural transition as Ga replaces P. With increasing Ga content, Raman spectra show a decrease in the intensity of the P=Se stretch-

ing mode, while 31P MAS NMR spectra reveal the concomitant emergence of a resonance assigned to PSe4/2 groups. The results indicate the gradual conversion of Se=PSe3/2 units into PS4/2 species with increasing Ga concentration, similar to the case of the analogous sulfide glasses.

2:15 PM

(GOMD-SV-013-2010) Influence of iso-structural substitutions on physical properties in Ge(As,Sb)(S,Se) glasses

G. Guery*, D. Musgraves, K. Richardson, L. Petit, clemson university, United States; E. Fargin, University of Bordeaux, France

Chalcogenide glasses present exceptional infrared transparency, large non-linear refractive indexes and low phonon energies, making them good candidates for infrared optical applications. We report results of a systematic study examining the relationship of the physical properties to the structure of glasses in the Ge(As,Sb)(S,Se) system , in order to elucidate the effect of the substitution of Sb for As on the nonlinear behaviour as well as on the thermal, mechanical and optical characteristics of the glass. Verification of the composition by Energy Dispersive X-Ray Spectroscopy is coupled with thermomechanical characterization via Differential Scanning Calorimetery, Fourier Transform Infrared and UV-Visible spectroscopies, and by the Vickers hardness. The structural properties are investigated using Raman Spectroscopy. Lastly, this paper reports the viscosity-temperature behaviour of glasses with x = 30 and 60 using a beam bending and a parallel plate viscometer.

2:30 PM

(GOMD-SV-014-2010) High-resolution 77Se NMR investigation of the structure of GexSe100-x glasses

E. L. Gjersing, S. Sen*, University of California Davis, United States; B. Aitken, Corning Inc., United States

77Se MAS NMR spectroscopy has been conducted at 11.7 T to investigate the short-and intermediate- range structure and chemical order in binary GexSe100-x glasses with x=5-40. Four distinct Se environments are observed for the first time, corresponding to Se-Se-Se, Ge-Se-Se, Ge-Se-Ge in corner-shared GeSe4 tetrahedra, and Ge-Se-Ge in edge-shared GeSe4 tetrahedra. Analysis of the compositional variation of the relative concentrations of these Se sites indicates a structure that is partially clustered with regions rich in GeSe4 tetrahedra separated by those consisting predominantly of Se chains especially for compositions with x≥17. In addition, the percentage of edge-sharing Se sites was calculated from the fits and is seen to increase from 8% at Ge13Se87 up to 23% at Ge33Se67 glass, consistent with Raman spectroscopic and neutron diffraction results.

2:45 PM

(GOMD-SV-015-2010) Impact of Chalcogen Deficiency in GeAsPS and GeGaPS Glasses

R. Youngman*, B. Aitken, S. Currie, Corning Incorporated, United States

Chalcogenide glasses are unique in that the metal:chalcogen ratio can vary significantly from stoichiometry, resulting in materials with substantial homopolar bonding. Chalcogen-deficient glasses therefore typically display metal-metal bonding. However, in P-containing sulfide glasses, e.g. GeAsPS with Ge:As:P = 5:1:1, P speciation is sufficiently flexible to absorb large S deficiency without metal-metal bond formation by converting S=PS3/2 tetrahedra to trigonal PS3/2 groups. At lower S levels, P-P bonding is required, leading to a red shift of the absorption edge, which is relatively unaffected by the initial reductions in S. Using NMR, we compare this behavior with that of Ga-containing glasses with Ge:Ga:P = 5:1:1, where Ga stabilizes P in symmetric PS4/2 tetrahedra in the stoichiometric glass. With decreasing S, there is a marked increase in the concentration of trigonal PS3/2 units, but PS4/2 groups remain an important structural unit, even after formation of P-P bonding in the most S-deficient compositions.

Glass Structure and Properties III: Phosphates

Room: Keuka

Session Chair: Randall Youngman, Corning Incorporated

3:15 PM

(GOMD-SV-016-2010) Properties and Structures of Tin Phosphate Glasses modified with Ga2O3 and Sb2O3

J. Lim*, R. K. Brow, Missouri S&T, United States; H. Yang, National United University, Taiwan

The properties and structure of xSnO*(1-x)P2O5(0.5≤x≤0.7) glasses and 0.67SnO*0.33P2O5 glass modified with up to 16 mole % Ga2O3 and Sb2O3 compositions are reported. The glasses were prepared in vitreous carbon crucible by melting under argon between 900 and 1000°C. All glasses were characterized by differential thermal analysis(DTA) and dissolution rates in deionized water were determined. The refractive index was measured at three different wavelengths using a prism coupling technique and transmission spectra were collected from ultraviolet to the near infrared. The effects of Ga2O3 and Sb2O3 oxide additions on these properties of glass were studied. Glasses with refractive index (nd) over 1.8 and glass transition temperatures under 350°C could be prepared from these systems. Raman spectroscopy indicates that progressively shorter phosphate chains are present in the structures of the binary Sn-phosphate glasses with increasing SnO-contents, and with increasing Ga- and Sb- oxide contents.

3:30 PM

(GOMD-SV-017-2010) Structure-Property Relationships in Cerium Aluminophosphate and Silicophosphate Glasses

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

The high solubility of cerium in binary phosphate glasses and their good chemical durability suggest that this cation may act as a network intermediate rather than a modifier. To investigate the structure of cerium in phosphate glasses, cerium coordination shells will be determined by Ce L3-edge EXAFS, and the network-forming cations studied by 29Si, 27Al, and 31P NMR, in two series of glasses: Al(PO3)3 - Ce(PO3)3 and Ce(PO3)3 - SiP2O7. Six-coordinated silicon cations are known to occur in binary silicophosphate glasses and ternary silicophosphate glasses containing alkali or alkaline earth cations. Thus, it is noteworthy that in both of these series, 6-coordinated cerium, found in binary cerium phosphate glasses, may directly substitute for silicon and aluminum, and possibly explain the poor durability of the high silica-content glasses. Additionally, basic properties, as well as chemical and thermal stability, of these glasses will be investigated.

3:45 PM

(GOMD-SV-018-2010) Raman Spectra and the Structure of Iron-Phosphate Compounds and Glasses

L. Zhang*, J. Lim, R. K. Brow, M. E. Schlesinger, Missouri S&T, United States

Ferrous and ferric phosphate compounds were studied using Raman spectroscopy. Peak assignments were based on compound structures. The P-O stretching mode for orthophosphate compounds ($FePO_4$ and $Fe_7(PO_4)_6$) produces one very strong peak located at 1000-1050cm^{-1}, whereas several P-O stretching modes are present for pyrophosphate compounds ($Fe_2P_2O_7$, $Fe_3(P_2O_7)_2$ and $Fe_4(P_2O_7)_2$) in the range from 1000 to 1200cm^{-1}, with the strongest peak located ~1050-1150cm^{-1}. Metaphosphate compounds exhibit one intense peak near 1200cm^{-1}. These results are used to interpret the Raman spectra collected for iron phosphate glasses. For ferric orthophosphate glass, there is no evidence for the existence of P-O-P linkages. For the pyro- and metaphosphate series, Fe(II) enhances the relative intensity of P-O-P mode located in the range of 700-900cm^{-1}. The similarity and difference between the structure of iron phosphate glasses and compounds and the effects of composition on structure will be discussed.

4:00 PM

(GOMD-SV-019-2010) Structural and Dispersive Aspects of the Photoelasticity of Glass

V. Martin*, S. Thomas, V. Dickinson, B. Chen, U. Werner-Zwanziger, R. Dunlap, J. Zwanziger, Dalhousie University, Canada

The photoelasticity (stress-optic response) of glass is investigated through structure-property correlations and dispersive measurements. Structure is determined with a combination of solid-state NMR and Moessbauer spectroscopy in alkali and tin phosphates and silicates. Strengths and limitations of the empirical model for the relationship between structure and photoelasticity recently proposed by our laboratory are presented. The dispersion of the induced birefringence is also presented, and differences between the phosphate and silicate systems are analyzed in terms of the structure around nonbridging oxygen.

4:15 PM

(GOMD-SV-020-2010) WITHDRAWN

4:30 PM

(GOMD-SV-021-2010) Structure of Sodium Borophosphate Glasses

R. Christensen*, G. Olson, Iowa State University, United States; A. Matic, Chalmers University of Technology, Sweden; V. Petkov, Central Michigan University, United States; S. W. Martin, Iowa State University, United States

Ion-conducting glasses hold the potential for widespread use in batteries, fuel cells, sensors, and thermionic devices. It has been found 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, a study of multiple ternary systems properties and structures has been undertaken. Glass properties and qualitative structural studies of IR and Raman spectroscopy have been reported elsewhere. Quantitative structural studies on mixed glass former $y(Na_2O)$-$(1-y)[xB_2O_3$- $(1-x)P_2O_5]$ [y = 0.35, 0.50, x =0, 0.1, 0.2…1] glasses will be reported. Short-range structures were investigated using Neutron Diffraction and Nuclear Magnetic Resonance. Medium range structures were investigated using X-ray Diffraction. These results show changing structure based on changing concentration of the glass formers, confirming the findings of previous studies.

Wednesday, May 19, 2010

Symposium II: Glass Science

Topology and Rigidity II

Room: Cayuga

Session Chair: Matthieu Micoulaut, Universite Pierre-et-Marie Curie

8:00 AM

(GOMD-SII-038-2010) Spatial correlations in amorphous networks and their electronic consequences: an emerging theory of the Urbach tail (Invited)

D. Drabold*, Ohio University, United States; F. Inam, International Center for Theoretical Physics, Italy; Y. Li, Ohio University, United States

In this talk, we discuss the existence of subtle spatial correlations in good quality continuous random network models of a-Si, a-Si:H, a-silica and other systems. In a-Si, we have shown that spatially correlated long (short) bonds are associated with the electronic conduction (valence) tails [Y. Pan, F. Inam. M. Zhang and D. Drabold, Phys. Rev. Lett. 100 206403 (2008), ibid. J. Non. Cryst. Sol. 354 3480 (2008)]. We explore the static and finite-temperature aspects of these correlations, both topological and electronic, and further analyze the connection between these structures and the Urbach edges.

8:30 AM

(GOMD-SII-039-2010) The non-trivial structure of disordered network-forming materials unraveled by first-principles molecular dynamics (Invited)

C. Massobrio*, IPCMS, France

Realistic modelling of behaviors inherent in network-forming disordered materials (existence of structural order beyond the first shell of neighbors, appearance of an intermediate phase separating mean-field accessible topological patterns) requires a precise description of chemical bonding properties. This allow to capture subtle features of the topological organizations in systems otherwise escaping a quantitative characterization. In this talk we shall provide specific examples of network-forming disordered materials for which the predictive power of first-principles molecular dynamics has allowed to highlight atomic-scale structural organization. Key methodological issues (role of the exchange-correlation functional, system size effects, adequacy of the statistical sampling) will also be addressed.

9:00 AM

(GOMD-SII-040-2010) Evolution of the potential-energy surface of amorphous silicon

H. Kallel, N. Mousseau*, F. Schiettekatte, Universite de Montréal, Canada

The link between the energy surface of bulk systems and their dynamical properties is generally difficult to establish. Using the activation-relaxation technique (ART nouveau), we follow the change in the barrier distribution of a model of amorphous silicon as a function of the degree of relaxation. We find that while the barrier-height distribution, calculated from the initial minimum, is a universal function that depends only on the level of distribution, the reverse-barrier height distribution, calculated from the final state, is independent of the relaxation, following a different universal function. Moreover, the resulting gained or released energy distribution is a simple convolution of these two distributions indicating that the activation and relaxation part of a mechanism are independent. This characterized energy landscape can be used to explain nanocalorimetry measurements of amorphous silicon models.

9:15 AM

(GOMD-SII-041-2010) Characterizing the sodium environnement in amorphous silicates

M. Bauchy*, M. Micoulaut, Université Pierre et Marie Curie, France

Recently, it has been found that sodium silicates were displaying the same phenomenology as in network chalcogenide glasses, i.e. a stressed rigid phase for glasses having a silica rich content, an intermediate phase between 18 and 22% sodium oxide, and a flexible phase for higher sodium content. In order to apply bond constraint algorithms to this system, a preliminary question deals with the definition of the sodium environment. We focus on the latter using Molecular Dynamics Simulations of a NS2 glass. Results show that the sodium neighbours (bridging and non-bridging oxygens) are not equivalent. Moreover, partial angular distributions show that the angular excursion of the sodium is much larger than the one found for atoms having intact bonding constraints. Pressure effects are also presented.

9:30 AM

(GOMD-SII-042-2010) Molecular structure of ideal chalcohalide glasses

P. Boolchand, S. Bhosle*, Univ of Cincinnati, United States

Alloying Iodine in bulk GetSe100-t glasses leads to a collapse (almost to a critical triple point) of the ideal glass forming composition range, the so called Intermediate Phase (IP) 1,2. We have now synthesized ternary GexSe90-xI10 bulk alloy glasses at a fixed (10 mole %) Iodine concentration across a range of Ge concentrations encompassing the mean-field rigidity transition composition, xmf = 23%. Raman scattering displays rich lineshapes1,2 revealing modes of Corner-Sharing and Edge Sharing tetrahedra of the base network along with those of the Iodine modified mixed tetrahedral units GeSe4-mIm with m = 1-4 . Quenched glasses are Tg-cycled, and evolution of glass structure as a function of

Ge content in the 21.5% < x < 24% range and thermal cycling studied in Raman scattering and calorimetric measurements. Results of these experiments dwelling on the nature of network structure prevailing in the IP will be reviewed. 1 Phys. Rev. Lett. 87, 185503 (2001). 2 J. Phys.: Condens. Matter 19, 226201(2007).

9:45 AM

(GOMD-SII-043-2010) Hidden structure in amorphous and glassy materials Y Li, S. Chakraborty and D A Drabold

Y. Li*, S. Chakraborty, D. Drabold, Ohio University, United States

Recently[1] we have shown that amorphous silicon and glassy silica exhibit extended spatial correlations of specific topological units (long and short bonds in a-Si, and certain O-O and Si-Si correlations in silica). Furthermore, in both cases we associate these correlations with the Urbach edges seen in optical or electronic experiments. In this talk, we present new results on a chalcogenide glass, a-As2Se3, and further examine the case of a-Si to consider the dynamics of these structures in amorphous silicon. Results will be presented for various temperatures, and we will compare these results with the temperature dependence of the bandtails in a-Si:H. [1] Y. Pan, F. Inam, M. Zhang and D. A. Drabold, Atomistic origin of Urbach tails in amorphous silicon, Phys. Rev. Lett. 100 206403 (2008); F. Inam, J. P. Lewis and D. A. Drabold, Hidden structure in amorphous solids, Phys. Stat. Sol. a (in press).

10:00 AM

(GOMD-SII-044-2010) Intermediate phase in ternary GexSbxSe100-2x bulk alloy glasses

P. Boolchand, K. Gunasekera*, P. Chen, Univ of Cincinnati, United States

Ternary GexSbxSe100-2x alloy glasses are synthesized by melt quenching over a wide composition range, 0 < x < 25%, and examined in modulated DSC, Raman scattering and molar volume experiments. The enthalpy of relaxation at Tg shows the opening of a reversibility window or Intermediate Phase (IP) in the 13% < x < 18% range, or 2.40 < r < 2.54 mean coordination number range, where r = 2 + 3x. FT- Raman studies reveal frequency of the CS mode of GeSe4 tetrahedra to steadily blue shift with increasing x, and we are investigating variation of optical elasticity from these data. In ternary GexAsxSe100-2x glasses the IP resides in the 2.28 < r < 2.54 range1. The narrower IP in the present glasses suggests that Sb takes on only a 3-fold coordinated pyramidal local structure. 1 Jour. Non-Cryst. Solids 355, 1773 (2009).

Glass Transition and Relaxation I

Room: Cayuga
Session Chair: Prabhat Gupta, The Ohio State University

10:30 AM

(GOMD-SII-045-2010) Structural Relaxation in the Glassy State: Further Evidence for the Path Dependence of the Relaxation Time (Invited)

F. Begum, S. Simon*, Texas Tech University, United States

An important assumption made in the TNM and KAHR models of structural recovery is that the nonlinearity of the response can be accounted for by allowing the relaxation time to depend on the instantaneous structure of the glass. Using mercury immersion dilatometry, we examine this assumption by performing down-jumps from various temperatures to a given aging temperature, thereby changing the nonlinearity of the response. We find that the time required to reach equilibrium for down jumps is a strong function of the jump size. The results are not consistent with the TNM/KAHR models of structural recovery and seem to indicate that the relaxation time depends on path and not on the instantaneous structure of the glass. This conclusion is corroborated by the results of prior measurements made to elucidate the tau-effective paradox, as well as results of unique temperature perturbation experiments made in our laboratory.

11:00 AM

(GOMD-SII-046-2010) Microscopic Aspects of Stretched Exponential Relaxation (SER) (Invited)

J. C. Phillips*, Rutgers, United States

I review experiment and theory of SER (discovered in 1854!), as represented by a growing body of time- and temperature-dependent data. Many electrical and optical phenomena exhibit SER with probe relaxation $I(t) \sim \exp[-(t/\tau)\beta]$, with $0 < \beta < 1$. Here τ is a material-sensitive parameter, useful for discussing chemical trends. The "shape" parameter β is dimensionless and plays the role of a non-equilibrium scaling exponent; its value, especially in glasses, is both practically useful for quality control and theoretically significant. The mathematical complexity of SER is such that rigorous derivations of this peculiar function were not achieved until the 1970's. Universal values of β reflect competition between short- and long-range forces. Examples discussed include inorganic network glasses (the "simplest" case), polymers, electronic glasses, and patterns of 600 million world-wide 20th century citations across all natural sciences.

11:30 AM

(GOMD-SII-047-2010) Logarithmic Relaxation of Stress Correlator in Supercooled Liquids

J. Eapen*, North Carolina State University, United States

Slowly relaxing materials are classified as strong or fragile with the latter displaying a pronounced non-linear variation in viscosity with temperature. While viscosities are easily measured in an experiment, the attendant relaxations of stresses are not readily accessible. This paper describes a Molecular Dynamics (MD) investigation of the relaxation of the stress correlator in a binary supercooled system. The stress correlator in the model fragile system portrays three characteristic variations as a function of temperature with three identifiable cross-over temperatures – T0, Tx and Tc. The stress correlator transitions from a power law behavior at high temperatures to an incipient logarithmic behavior at a cross-over temperature – T0. Upon decreasing the temperature, the logarithmic relaxation grows in time and finally breaks down at a second cross-over temperature – Tx. In the temperature range between T0 and Tx, the slow logarithmic relaxation emanates from a homogeneous crowding mechanism.

11:45 AM

(GOMD-SII-048-2010) Modeling the enthalpy relaxation of glasses far from equilibrium

X. Guo*, Aalborg University, Denmark; J. Mauro, Corning Incorporated, United States; Y. Yue, Aalborg University, Denmark

Existing phenomenological models such as the Tool-Narayanaswamy-Moynihan (TNM) approaches are not able to describe the enthalpy relaxation of the glasses far from equilibrium. To enable accurate modeling over a wider range of thermal histories, we have extended the existing models in three aspects. First, the width of glass transition region is a function of the cooling rate. Second, the relaxation time distribution consists of at least two regimes, corresponding to alpha and beta relaxation processes. Third, a reasonable configurational entropy function is determined by evaluating the performance of various viscosity equations, i.e., Adam-Gibbs, Vogel-Fulcher-Tammann, Avramov-Milchev, and the newly developed Mauro-Yue-Ellison-Gupta-Allan expression. The model performance is evaluated during both annealing and dynamic heating and cooling processes. We show that the enthalpy relaxation of several oxide glass-formers far from equilibrium can be described accurately using our extended modeling approach.

Symposium III: Glass Technology

Melting & Process Modeling

Room: Seneca
Session Chairs: Olus Boratav, Corning Incorporated; Li Yang, Corning Incorporated

8:15 AM

(GOMD-SIII-042-2010) The batch-to-melt conversion - mineralogical, caloric and kinetic aspects (Invited)
R. Conradt*, RWTH Aachen University, Germany

The paper focuses on optimizing both the energy and time demand of the batch-to-melt conversion. It is shown that the choice of individual raw materials yielding a given glass composition has a major impact on the intrinsic, and hence, on the overall heat demand. The time demand is a quantity totally independent of the intrinsic heat demand, but it has a strong influence on the efficiency of heat exploitation and thus also has a major impact on the overall heat demand Viewed from a macroscopic point of view, the time demand is influenced by the temperature level in the tank, the intensity of convection, and reactor space utilization. Microscopically, it is a function of atomic mobility, the intensity of grain-to-grain contact, and the kind of primary phases formed. Specific case studies are given comprising calculations, lab scale experiments, and industrial campaigns.

8:45 AM

(GOMD-SIII-043-2010) Full conversion of glass furnace to oxygen-fuel combustion
X. He*, M. J. Watson, M. E. Habel, Air Products and Chemicals, Inc., United States; J. Rossi, Fiberglass Industries, Inc., United States

Oxy-fuel combustion has become an attractive technology for glass melting in recent years. As a major industrial oxygen supplier, Air Products is dedicated to bringing industry preferred combustion technology to customers in the glass industry. The HRi™ high radiation burner is a result of this effort. The HRi™ burners provide highly radiative luminous flames utilizing a patented staging technology. The result is highly efficient directional heating that delivers the major fraction of the energy to the melt. Air Products has supplied this combustion technology and oxygen to many full and partial conversion oxy-fuel glass furnaces worldwide. These conversions achieved an average fuel saving of 30%~50% compared with air-fuel operations. In this paper, a case study in Fiberglass Industries will be presented. The case study compares the furnace efficiency before and after it was converted from air-fuel to oxy-fuel combustion. We will also show how we used the CFD simulation to optimize the furnace design and operation.

9:00 AM

(GOMD-SIII-044-2010) Bubble Concentration Model
W. W. Johnson*, Corning Incorporated, United States

Present-day glass-melting furnace models typically assume glass is a homogeneous fluid, with density being only a function of temperature. Thermally induced density gradients drive molten-glass convection. However, in the actual process, gas release and segregation during melting, volatilization, and refractory dissolution work against the ideal view of the melting furnace. Bubbles and chemical inhomogeneities affect density and can overwhelm the thermal effect. An improved model will be described that adds the effect of bubble concentration to the buoyancy source term. The utility of the model will be illustrated by examples.

9:15 AM

(GOMD-SIII-045-2010) Draw Resonance in Viscous Sheets
O. Boratav*, Z. Zheng, Corning Incorporated, United States; A. Amosov, Corning Incorporated, Russian Federation

The instability known as the "draw resonance" in literature is studied for a viscous sheet considering the visco-gravity balances (Stokes number) and the heating/cooling effects (Stanton number). The analysis considers thin-film approximation for continuity, momentum and energy equations and determines the critical draw ratio for a range of Stokes numbers and Stanton numbers. The critical draw ratio is very sensitive to the variation of Stokes and Stanton numbers. It is shown that the decrease in Stokes number and/or the increase in Stanton number results in a decrease in the critical draw ratio.

9:30 AM

(GOMD-SIII-046-2010) The Liquidus Temperature; its Critical Role in Glass Manufacturing (Invited)
F. T. Wallenberger*, A. Smrček, Consultant, United States

The liquidus temperature plays such a critical role in the fiberglass manufacturing process that it had to be included since 1997, alongside viscosity, in designing new energy-friendly fiberglass compositions by the trend line design model. The effect of fiber, flat and container glass compositions will be analyzed relative to the forming and liquidus temperature at the furnace exit, and on glass compositions during bending, forming and pressing. New energy friendly fiberglass compositions are already being used commercially. Further research must establish if the viscosity (energy) of commercial glass compositions can also by reduced by reformulation without causing devit or crystallization at the liquidus temperature.

Optical Materials I

Room: Seneca
Session Chairs: Hong Li, Schott North America, Inc.; Amanda Young, Sandia National Laboratories

10:15 AM

(GOMD-SIII-047-2010) Optical Materials for Harsh Ionizing-Radiation Environments (Invited)
K. Simmons-Potter*, University of Arizona, United States

The proliferation of optical materials and components in advanced and self-diagnostic space systems has necessitated the development of targeted materials and devices that can withstand harsh ambient ionizing radiation environments. Prior research has demonstrated that optical materials that are subjected to large total doses, and/or high dose rates, of ionizing radiation exhibit substantial optical photodarkening. This induced loss can be sufficient to preclude optical device operation following irradiation. Toward this end the optical response of a subset of critical materials to large fluxes of ionizing radiation has been investigated. Specifically, both passive and active optical fibers, active laser and Q-switch materials and optical filters have been tested and, in many cases, materials band structure and defects have been engineered to produce radiation-hardened components. This talk will review progress in radiation-hardening strategies and materials design for key devices.

10:45 AM

(GOMD-SIII-048-2010) Use of Gadolinium Oxide for Neutron Detection in Glasses
K. Goetschius*, J. Shelby, Alfred University, United States; A. Huston, S. Rychnovsky, B. Wright, Naval Research Laboratory, United States

Radiation sensitive glasses were fabricated with gadolinium oxide, yttrium oxide and samarium oxide as the capture species and either Tb, Ce or Eu as the fluorescent ion. Various combinations were made using an aluminosilicate, an aluminoborate or an aluminogermanate matrix. All samples were tested in both a gamma radiation and a thermal neutron radiation field. In the both fields, Tb doped samples exhibited the strongest sensitivity, particularly when paired with gadolinium oxide. These results are consistent with the large Z number and thermal neutron capture cross section of Gd. Furthermore, the neutron sensitivity was found to be relatively constant as the Gd/Tb concentration was varied. These glasses were characterized using UV/Vis, IR and fluorescence spectroscopy. Radiation sensitivity measurements were done in conjunction with Naval Research Laboratories in Washington, DC using a photomultiplier tube in photon counting mode to measure fluorescent output during radiation exposure.

11:00 AM

(GOMD-SIII-049-2010) Yb-doped oxide glasses under ionizing irradiation: a relaxation processes study

N. Ollier*, V. Puhkhaya, LSI, France; J. Doualan, R. Moncorgé, CIMAP, France

Yb-doped oxide glasses are of significant interest because of their use in high-power fiber laser. Under, ionizing irradiation, the valence state of the doping element can be modified by a reduction process. Moreover, at high irradiation doses (>1 GGy), the coordination number or site symmetry around the doping ion can also be changed. Our approach is thus using ionizing irradiation (electrons and gamma rays) to: 1) Induce new properties in Yb-doped oxide glasses such as optical properties 2) Bring new results on the glass aging under irradiation (i.e photodarkening). We will present here results about the evolution of the Yb3+ environment under irradiation and the formation of point defect by EPR spectroscopy. Luminescence properties evolution of Yb3+ (The IR emission spectrum and 2F5/2 excited state lifetime) will be also discussed. We will particularly emphasize new results obtained on the relaxation processes.

11:15 AM

(GOMD-SIII-052-2010) Crystalline Semiconductor Core Optical Fibers

S. Morris*, J. Ballato, T. Hawkins, P. Foy, C. McMillen, R. Stolen, Clemson University, United States; R. Rice, Northrop Grumman Space Technology, United States

Rapid advances in semiconductor-based photonics have generated interest in the eventual integration of electronics and optics. The extension from a planar waveguide to an optical fiber platform would be a significant progression to 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. In the case of the Si fibers, X-ray diffraction and Raman scattering analyses indicated that the core was highly crystalline. More than 250 meters of Ge fiber were fabricated, possessing a 15 micrometer core within a 150 micrometer diameter glass cladding. X-ray diffraction and Raman spectroscopy confirmed the core to be phase-pure, highly crystalline, and with a nominal amount of oxygen diffused into the core from the cladding. Such highly crystalline semiconductor core optical fibers have significant potential for Raman fiber devices, mid- and long-wave infrared sensing and power delivery, and terahertz guided wave structures.

11:30 AM

(GOMD-SIII-051-2010) Sub-Micron Grained Highly Transparent Y_2O_3 Ceramics: Synthesis, Processing, and Properties

K. Serivalsatit*, B. Kokuoz, B. Yazgan Kokouz, M. Kennedy, J. Ballato, Clemson University, United States

Y_2O_3 transparent ceramics are being developed as alternative to single crystals for high-power solid-state laser systems. In this work, we present the synthesis of Y_2O_3 nanopowders by solution precipitation using ammonium hydroxide and yttrium nitrate as precursors. Characterizations of as-prepared and calcined nanopowders were performed using Fourier transform infrared spectroscopy (FTIR), X-ray diffractometry (XRD), and transmission electron microscope (TEM). The subsequent processing of these nanopowders into sub-micron transparent ceramics was accomplished by modifying the two-step sintering approach. These transparent ceramics exhibited equivalent transparency to that of the single crystal beyond 1200 nm wavelength. The microhardness and fracture toughness of the modified two-step sintered ceramic exceeded those of conventionally sintered ceramic by 25% and 70%, respectively.

11:45 AM

(GOMD-SIII-050-2010) Effect of Bromine on NaF Crystallization in Photo-Thermo-Refractive Glass

G. P. Souza, V. Fokin, C. Baptista, E. D. Zanotto, Federal University of San Carlos, Brazil; J. Lumeau*, L. Glebova, L. B. Glebov, University of Central Florida, United States

Photo-thermo-refractive (PTR) glass is a photo-sensitive multicomponent silicate optical glass which contains a small amount (<1 mol%) of bromine. PTR glass undergoes crystallization of NaF nanocrystals after UV-exposure followed by thermal treatment, resulting in permanent refractive index change. In this study we show that bromine decreases the solubility of NaF in PTR glass, i.e. increases the super-saturation of NaF. This fact was demonstrated by a decrease of the maximum volume fraction of crystallized NaF with decreasing bromine content in the parent glass. The evolution of the glass transition temperature, Tg, with increasing isothermal treatment time revealed a minimum resulted from interplay between two concurring processes, liquid-liquid phase separation that led to decrease in Tg and NaF crystallization that acted in the opposite direction. In glasses with lower bromine content fewer crystals appeared, having a larger size, and surface-initiated crystallization was dominant.

Symposium IV: Glass Corrosion

Ancient and Analogue Glasses

Room: Carder

Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

8:15 AM

(GOMD-SIV-008-2010) The Morphology of Weathering on Ancient Glasses (Invited)

R. H. Brill*, Corning Museum of Glass, United States

This paper will review the surprisingly wide variety of weathering effects found on historical glass artifacts that have been exposed to different environmental conditions for long periods of time. The extent of weathering, as well as the nature of the effects observed, will be described in terms of certain intrinsic properties of the artifacts and environmental factors. Examples of weathering on objects selected from some 3500 years of glass history will be illustrated.

9:00 AM

(GOMD-SIV-009-2010) Some thoughts on the use of ancient glasses in performance assessment of nuclear waste glass disposal (Invited)

D. Strachan*, Pacific Northwest National Laboratory, United States; R. Brill, Corning Museum of Glass, United States

Glasses have been used for treasured articles for at least the last 3000 y. The ancient people who produced these glasses and glass artifacts unwittingly started 'experiments' that can we can use. There are two parts to the assessment to which ancient glasses could provide valuable information – the glass dissolution mechanism and the transport of. Ancient glasses, while having simple compositions relative to nuclear waste glasses, do dissolve with the same. These glasses have been found in a variety of different environments. The characterization of the alteration products and dissolution depths can yield important information on the dissolution mechanism. In this paper, we discuss the types of glasses that might be included in such an effort, the compositions of those glasses, the areas where these glasses might be found, and what analyses might be used on the glasses that are found and on those that are currently in museum collections.

9:30 AM

(GOMD-SIV-010-2010) The use of Roman glass to predict the long-term behavior of HLW (Invited)

S. Gin, CEA, France; A. Verney-Carron, CNRS, France; P. Frugier*, CEA, France

The predictability of models describing long-term nuclear glass behavior in a geological repository can be tested by means of natural or archaeological analogs. This study covers fractured archaeological glass blocks from a shipwreck discovered near the French island of Embiez. The laboratory investigation led to the development and subsequent validation on archaeological objects of a geochemical model capable of accurately simulating the coupling between chemistry and transport to account for the alteration state of the cracks according to their geometric characteristics. The analogous behavior of Roman and nuclear glass and the similarities in their crack networks allow us to consider applying the model to nuclear glasses under geological repository conditions.

This investigation of old samples clearly shows that the internal crack network does not play a major role in the overall long-term alteration of glass blocks. We discuss here implications of such conclusion on the long-term behavior of nuclear glass.

10:00 AM

(GOMD-SIV-011-2010) The surface and beyond: new insights in old glass

H. Roemich*, New York University, United States

Glass objects have been produced for more than 5,000 years and form now an important part of our cultural heritage, with prominent objects such as glass beads from Mesopotamia, perfume bottles from Egypt, drinking glasses from the Roman period and stained glass windows in European Gothic cathedrals. Depending on their composition and the exposure environment, historic glasses develop degradation phenomena, ranging from thin hydrated surface layers up to complete cracking all through the sample. Historic glasses from archaeological context and samples taken from naturally weathered stained glass windows were examined to compare the weathering phenomena and degree of degradation. Laboratory experiments were performed to simulate degradation phenomena on model glasses with compositions similar to historic glasses.

Modeling

Room: Carder
Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

10:30 AM

(GOMD-SIV-012-2010) Interaction of Water with Multi-Component Silicate Glass Surfaces (Invited)

A. Cormack*, Alfred University, United States; A. Tilocca, University College London, United Kingdom

The adsorption of water onto glass surfaces plays a critical role in many properties of glasses. Probing the adsorption mechanisms requires an understanding of the atomic scale surface structure of the glass; although this is still difficult to extract from experiments, atomistic simulations have progressed to the point where accurate models may be produced. In this presentation, we discuss some quantum mechanical simulations of the interaction of water molecules with a multi-component silicate glass used in biomedical applications. We have performed calculations involving single water molecules, dimers and trimers, as well as a complete film of water covering the glass surface. Both physisorption and chemisorption mechanisms are observed. We describe surface structural features which promote chemisorption, and compare these to structural features of silica surfaces. We find the chemistry of the glass to play an important role, and will discuss the implications of this result, with respect to other glasses.

11:00 AM

(GOMD-SIV-013-2010) Delayed failure of oxide glasses (Invited)

M. Tomozawa*, RPI, United States

Glasses exhibit static fatigue, or delayed failure, with the strength decreasing with the time of static loading in the presence of moist atmosphere. This is due to slow crack growth in the presence of moist atmosphere under sub-critical stress. The phenomenon is attributed to stress corrosion of glass, namely the tensile stress-accelerated reaction between glass and water but the exact nature of the reaction is not clear. Various different possible stress corrosion reactions will be considered including glass dissolution into water, glass-water reaction, and water diffusion into glass. From the stress dependence of the reactions, water diffusion into glass is considered the likely mechanism. When water enters into glasses, it causes the reduction of elastic modulus and the strength of the glass. Even though oxide glasses have been considered to be perfectly brittle, possibility of the strength reduction by the yield strength reduction will be explored.

11:30 AM

(GOMD-SIV-014-2010) DFT MD Simulations of Proton Attack on a Silica Surface (Invited)

J. D. Kubicki*, The Pennsylvania State University, United States

Hydrolysis of Si-O-Si linkages catalyzed by proton attack is thought to be the rate-controlling step for dissolution of silicates. Previous work has modeled this process with the cluster approximation and limited solvation. In this work, results of DFT-MD simulations using the program VASP are presented that include a periodic silica surface and a bulk water phase. The energetics of proton adsorption at the Si-O-Si site and subsequenty hydrolysis reaction are predicted and discussed in comparison with experimental data on silicate dissolution. The role of H-bonding from the water to the silica surface and among atoms on the silica surface itself is critical in stabilizing the protonated Si-O-Si group. In addition, charge-balancing by the chloride ion has a significant effect on calculated reaction energetics.

Symposium V: Glass Structure and Properties

Photoinduced Structural Changes in Glass

Room: Keuka
Session Chair: Pierre Lucas, University of Arizona

8:00 AM

(GOMD-SV-022-2010) Determination of structural defects in chalcogenide glasses by high-resolution XPS (Invited)

H. Jain*, A. Kovalskiy, R. Golovchak, Lehigh University, United States

In view of the limited usefulness of X-ray diffraction, high resolution X-ray photoelectron spectroscopy (XPS) is shown to be one of the most insightful tools for determining the defects in amorphous solids. Using the examples of chalcogenide glasses we demonstrate that the analysis of the core level spectra provides the number of chemical environments for a specific element, its oxidation states and the chemical identity of its neighboring atoms. The valence band spectra offer the features of bonding states, confirmation of bond hybridization or phase separation in investigated disordered materials. The XPS data can be effectively used to characterize evolution of defect structure under in situ laser irradiation, the role of lone-pair electrons in these processes, etc. The ratio of the homo- and heteropolar chemical bonds in bulk and thin films is established quantitatively.

8:30 AM

(GOMD-SV-023-2010) In situ Observation of the Photoinduced Atomistic Changes in Chalcogenide Glasses

D. Zhao*, H. Jain, Lehigh University, United States

Contrasting photoinduced changes are observed in arsenic vs. germanium sulfide glassy films. We have sought the atomistic origin of this difference by determining their local atomic structure by in-situ EXAFS where synchrotron X-rays probe the structure while the samples are subjected to laser irradiation. It is found that germanium sulfide glasses are very stable upon laser illumination while the arsenic sulfide glasses present remarkable changes. There is no observable reversible structural change in all the investigated glasses after removal of the laser, nor is there any further change upon altering the laser polarization. Overall, a clear evidence of differences in photoinduced atomistic changes has been obtained for arsenic and germanium sulfides. However, the absence of transient changes in atomic structure does not correlate with the transient reversible changes in optical properties, indicating predominantly electronic processes as the source of the latter.

8:45 AM

(GOMD-SV-024-2010) Photosensitivity in As-S-Se mixed chalcogen glasses: the relative role of selenium versus sulfur

P. Lucas*, F. Lin, Z. Yang, University of Arizona, United States

The lone pair states of chalcogen atoms are known to lie at the top of the valence band and to contribute a great deal to the photosensitivity of these glasses under sub-bandgap illumination. The mechanism of many photostructural effects has been studied in mixed chalcogenide glasses in order to identify the relative contribution of selenium versus sulfur. Power dependent and wavelength dependent measurements indicate that the selenium-rich glasses are more photosensitive than the sulfur counterparts. An in-situ Raman study of a mixed 50%Se-50%S glass confirm that selenium is the major actor in the photostructural process. The origin of this phenomenon is associated with the higher energy of selenide lone pairs states.

9:00 AM

(GOMD-SV-025-2010) Dynamic equilibrium under light irradiation shown through photoinduced fluidity

Y. Gueguen*, J. Sangleboeuf, V. Keryvin, T. Rouxel, Université de Rennes 1, France; C. Boussard-Plédel, B. Bureau, J. Troles, UMR CNRS 6226, France; P. Lucas, University of Arizona, United States

15 years ago, H.Fritzsche postulates [Philos. Mag. B 1993 68 561-572], in his model of photoinduced structural changes in chalcogenides glasses, that a dynamic equilibrium exists resulting from the competition between the photoinduced increase of the local configuration energy and the thermal relaxation of this energy. 4 years ago, P.Lucas et al. [Phys. Rev. B 2005 71 104207] show through calorimetric studies, that this equilibrium exists, and that the structural relaxation is eased by photoinduced structural changes. Here we show first that this competition even exists at very low light intensity in Ge-Se glasses. We have developed dedicated experimental setups to measure all the strain components of viscous flow under light irradiation (elasticity, delayed elasticity, inelasticity), and we show through the evolution of all these components, as for example through the stability of the viscosity over months, the equilibrium of mechanical properties under irradiation.

9:15 AM

(GOMD-SV-026-2010) Photofluidity and Optical Microfrabrication of Tapers in Low-Loss Chalcogenide Fibers

P. Lucas*, E. Lepine, Z. Yang, University of Arizona, United States; Y. Gueguen, J. Sangleboeuf, B. Bureau, X. Zhang, University of Rennes I, France

Chalcogenide glasses undergo a photoinduced decrease in viscosity upon irradiation with sub-bandgap light. We study photofluidity in Ge-Se glass fibers and demonstrate its use for producing tapers in low-loss chalcogenide fibers with fine control on the diameter and geometry. The tapers produced this way act as a sensing zone along a chalcogenide glass fiber used for evanescent wave spectroscopy. The photoinduced viscosity is studied as a function of irradiation wavelength. Tappered produce this way permit to increase the sensing sensitivity by almost two orders of magnitude.

9:30 AM

(GOMD-SV-027-2010) Dynamics of femtosecond laser modification in glass

J. J. Witcher*, L. Fletcher, N. Troy, D. Krol, UC Davis, United States

The use of femtosecond lasers to modify the bulk of transparent materials has proven to be an important method for the fabrication of all-optical integrated circuits. In order to advance this technology it is necessary to better understand the modification process. Using a pump-probe setup with the fs-laser we have studied the dynamics of femtosecond laser modification in fused silica glass. The transmission of a broadband probe was measured as a function of pump-probe delay time. By comparing the transmission results with theoretical modeling of plasma properties both the electron density created by the absorption of the fs-laser pump pulse and the timescales of the modification process were determined. We will discuss the results in relation to the morphology and structural changes in the glass after fs laser-induced modification.

9:45 AM

(GOMD-SV-028-2010) Mechanisms of Laser Induced Modification of Lead and Barium Vanadate Glasses

M. Affatigato*, R. Dongol, L. Tweeton, C. Faris, S. Feller, Coe College, United States

We report on our investigations on the mechanisms for structural and morphological change in lead and barium vanadate glasses modified by 785 nm laser irradiation. The fundamental process is thermal in nature, leading to phase decomposition, phase changes, and mass transport in the center of the irradiated region, as well as the formation of lead- or barium-rich debris zones. Crystallization is also a consequence of the exposure to the laser light. We further report on pre-irradiation experiments in which low-power exposure above a determined energy threshold results in structural changes that bridge the gap between the amorphous state and the ultimate crystalline arrangement. Finally, we discuss the application of the laser irradiation in the making of vanadate microspheres. This work was supported by the National Science Foundation under grant Nos. DMR-RUI-0904615, DMR-MRI-0722682, DMR-MRI-0420539, and DMR-MRI-0320861. Coe College is also thanked for its financial support.

10:00 AM

(GOMD-SV-029-2010) Photoinduced Molecular Assembly in Dip-Coated Films via In-Situ Illuminations

Z. Schneider*, K. Simmons-Potter, B. G. Potter, University of Arizona, United States; T. Boyle, Sandia National Laboratories, United States

Dip-coating techniques are employed to create thin films from photosensitive titanium alkoxide precursor solutions via in-situ illuminations at and above the meniscus to control molecular assembly at the on-set of material formation. Photoexcitation at different points in the dip-coating process have been used to manipulate the micro- and nanostructure of the photodeposited films due to changes in the mobility of the reactants from the evaporation and gravitational draining of the solvent. SEM micrographs have been acquired to monitor the micro- and nanostructure of these films as a function of exposure height above the meniscus. The vibrational and electronic structure has also been examined to identify the changes in the ligands at different stages in the illuminated dip-coating process. This work was supported by the US Department of Energy, Office of Basic Energy Sciences, the University of Arizona, State of Arizona, TRIF Optics Initiative program and by Sandia National Laboratories.

10:30 AM

(GOMD-SV-030-2010) Polarized infrared studies of silica glass exposed to polarized excimer laser irradiation (Invited)

C. M. Smith*, N. F. Borrelli, J. E. Tingley, Corning Incorporated, United States

The use of polarized infrared spectroscopy to elucidate the permanent, anisotropic response of silica glass to polarized excimer laser irradiation will be discussed. From the interpretation of the results we propose a model where the anisotropic laser-induced volume expansion is associated with light-induced formation of hydrogen-bonded OH species along with concomitant bleaching of non-hydrogen bonded OH species. This model is supported by the measured anisotropy in the infrared spectra that is well-correlated with anisotropic changes in silica bulk properties.

11:00 AM

(GOMD-SV-031-2010) Study of ionization of cerium in multicomponent silicate glasses

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

Photo-Thermo-Refractive (PTR) glass is a photosensitive multicomponent silicate glass which provides refractive index change after UV-exposure (photoionization of cerium ions) and thermal development. The

origin of photosensitivity of this glass is usually explained by thermal precipitation of sodium fluoride crystals inside the glass matrix. This feature of PTR glass is successfully used for phase hologram recording. However, mechanisms of photoionization of cerium are still unclear. To study this effect, glass matrix doped with cerium was fabricated and its absorption spectra were studied after excitation using different wavelengths. Method for analyzing spectra of cerium is first introduced. Then, structure of induced absorption spectra is shown to depend on the excitation wavelength demonstrating the existence of several types of Ce3+. Such structure is also studied by deconvolution of spectra to Gaussian components. Specific absorption spectra of photoionized Ce3+ and of electron centers are thus analyzed.

11:15 AM

(GOMD-SV-032-2010) Femtosecond Laser Waveguide Writing in Erbium Doped Phosphate Glass

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

Permanent structural changes induced by femtosecond laser pulses inside active glasses can be used to fabricate waveguide lasers. Phosphate glasses are excellent glass systems for achieving high rare-earth oxide concentrations, and are ideal for fabricating compact waveguide lasers that operate in the C-band. Previous research with zinc phosphate glasses has demonstrated that the bulk glass structure is important in determining the resulting morphological changes as well as the waveguide quality. Waveguides have been fabricated inside erbium doped and undoped zinc polyphosphate glasses using tightly focused fs laser pulses from a regeneratively amplified Ti:sapphire, 1 kHz, 180 fs laser system with pulse energies ranging from 0.2 μJ – 4 μJ. Near field guiding profiles and white light images as well as insertion losses were measured after waveguides were written. Laser-induced structural changes in the glass were characterized using confocal fluorescence and Raman microscopy.

11:30 AM

(GOMD-SV-033-2010) Analysis of Radiation-Induced Darkening in Ce-doped Phosphate Glasses

R. Woodman*, J. Belcher, C. Ferreira, L. Gonzalez, Infoscitex Corporation, United States; C. Pantano, J. Rygel, The Pennsylvania State University, United States; J. Du, L. Kokou, University of North Texas, United States

To evaluate radiation-induced darkening of Ce-doped phosphate glasses, optical transmittance spectra were measured before and after radiation exposure. Phosphate hosts were doped with varying amounts of cerium and co-dopants. Samples were exposed to combined proton-electron-ultraviolet, electron, or gamma radiation. Phosphate glasses exhibited shorter-wavelength ultraviolet absorption edges than silicates. However, after radiation exposure, the absorption edge shifts more in the phosphate glasses than the silicates, so that the post-exposure edge is at longer wavelengths in the phosphates than the silicates. The nature of the radiation-induced shift in absorption edge varies with the type of radiation (photonic vs. corpuscular) in the phosphates, but not the silicates. By combining the optical spectroscopy with MD simulations of the Ce environment and spectroscopic analysis of the oxidation state of Ce, the large shift in phosphates can be attributed to structural features of the Ce environment.

Symposium II: Glass Science

Glass Transition and Relaxation II

Room: Cayuga
Session Chair: Prabhat Gupta, The Ohio State University

1:15 PM

(GOMD-SII-049-2010) Structural Aspects of Relaxation in Oxide Glasses (Invited)

J. F. Stebbins*, Stanford University, United States

"Unrelaxed" states in glasses can be obtained in many ways, including raising the fictive temperature (Tf) by rapid cooling, inducing anisotropy by shear, changing populations of defects by radiation, and inelastic densification at high pressure. These all have consequences in glass technology; all must also be recorded by alteration of the structure. This may include changes that relax at a wide range of rates and have wide ranges of effects on bulk properties. Experiments that quantitatively characterize the structural differences between "unrelaxed" and "relaxed" states are thus the key starting points and are becoming more common; detailed studies that map specific structural relaxation kinetics to those of bulk properties are just beginning. Given the importance of boro- and aluminosilicate glasses, it is fortunate that both B and Al cation coordinations, as measured by high-field NMR, can be especially sensitive to changes in the relaxation state, particularly as induced by high P and high Tf.

1:45 PM

(GOMD-SII-050-2010) Understanding liquids and glass transition on the basis of elastic waves (Invited)

K. Trachenko*, University of Cambridge, United Kingdom

No expression for liquid heat capacity exists in textbooks. The reason for this was summarized by Landau as "liquids have no small parameter". I formulate and solve the problem in the language of phonons. The resulting equation relates liquid heat capacity to its viscosity with no fitting parameters. I subsequently address the problem of glass transition and propose that the key is the range of propagation of high-frequency waves in a liquid, d. d measures the range over which local atomic jumps interact with each other via the elastic waves they induce. The non-trivial point is that d increases with liquid relaxation time τ, contrary to the usual decrease of d with τ for commonly discussed hydrodynamic waves. Small at high temperature, d increases on lowering the temperature, setting the cooperativity of molecular relaxation. I show how this increase gives the Vogel-Fulcher-Tammann law and discuss the absence of divergence at the VFT temperature, the origin of dynamic crossovers and liquid fragility.

2:15 PM

(GOMD-SII-051-2010) Viscoelastic dynamics of network-forming sodium ultraphosphate liquids: a dynamic light scattering study

D. Sidebottom*, R. Fabian, Creighton University, United States

The viscoelastic relaxation of glass forming (Na2O)x(P2O5)1-x liquids was measured by photon correlation spectroscopy at temperatures near the glass transition for compositions extending from pure phosphorus pentoxide to the metaphosphate (x = 0.5). Over this compositional range, alkali addition produces a continuous depolymerization of the covalently-bonded structure from one of a 3-dimensional network to that of polymer chains. Substantial increases in the fragility accompany the depolymerization and are shown to be identical to those seen in certain ion-free chalcogenide glass formers suggesting a common topological origin. The relaxation is non-exponential and the stretching exponent shows a complex variation with regards to both composition and temperature that is believed to arise from a decoupling of ionic motions from those of the network occurring as the glass transition is approached.

2:30 PM

(GOMD-SII-052-2010) The Glass Transition at the Nanoscale

Y. P. Koh, S. Simon*, Texas Tech University, United States

The effects of nanoconfinement on Tg of polymeric and low molecular weight glass forming materials have been extensively investigated in the literature. On the other hand, the Tg depression of materials synthesized under nanoconfinement has not been well studied, nor has the influence of conversion and crosslinking been characterized. To this end, we examine the trimerization reaction of monofunctional and difunctional cyanate esters in nanopores to form a low molecular cyanurate and a crosslinked polycyanurate, respectively. For the monofunctional reactant, there is no possibility for the intracyclization side reactions that can occur in the difunctional system. Using differential scanning calorimetry (DSC), we find a Tg depresssion for both of the reactants and their products. The magnitude of the depression increases with in-

creasing conversion and with increasing crosslink density and seems to be related to the size and stiffness of the molecule being confined relative to the confinement size.

2:45 PM

(GOMD-SII-053-2010) Universality of Boson Peaks in Lithium Borate Glasses

S. Kojima*, Y. Matsuda, M. Kawashima, S. Aramomi, University of Tsukuba, Japan; M. Kodama, Sojo University, Japan

The composition dependence of boson peaks has been studied by Raman scattering in lithium borate glass xLi2O-(1-x)B2O3. The peak positions markedly increase with the increase of Li2O composition, and clearly correlate with the shear modulus below x=0.28. The composition variation of boson peak intensity is stronger than Debye level. The boson peak spectra of all compositions are well scaled by the master curve. It indicates that the function of the distribution of V-DoS remains the same with the increase of Li2O composition. The universality of Raman results are discussed in comparison with those of neutron inelastic scattering and low-temperature heat capacity measurements.

Glass Transition and Relaxation III

Room: Cayuga
Session Chair: Roger Loucks, Alfred University

3:15 PM

(GOMD-SII-054-2010) Landscape View of Sub-Tg Relaxation (Invited)

P. Gupta*, J. Mauro, The Ohio State University, United States

Glass objects are frequently exposed to temperatures below the glass transition temperature (Tg) for a variety of reasons either during the finishing stages of their manufacture or during use. In such sub-Tg treatments, physical dimensions and properties change with time as a consequence of structural relaxation. The present understanding of sub-Tg relaxation remains poor. On one hand, there exists a wide spread belief that changes occuring in glasses at low temperatures are insignificant. On the other hand, there is ample evidence of measurable changes taking place over long times. In this paper, we develop a generic phenomenology of sub-Tg relaxation using the energy landscape formalism. Our analysis shows that the landscape view provides a sound basis for formulating a comprehensive, generic, and detailed theory for rationalizing such diverse phenomena as aging, cold flow (iso-structural viscosity), creep, and delayed elasticity.

3:45 PM

(GOMD-SII-055-2010) Cadmium manganese telluride: optical & magnetic properties

J. McCloy*, T. Droubay, B. Riley, J. Ryan, Pacific Northwest National Laboratory, United States

Optical and magnetic properties of single crystals of Cd1-xMnxTe (x=0.05, 0.25, 0.33, 0.50) were investigated for their potential as non-traditional radiation detectors. Transmission measurements in the visible confirmed the band-gap expected by the composition. Far-infrared reflectance and backwards-wave oscillator transmission measurements investigated the zero-field optical properties near the phonon resonances. Electron spin resonance, magnetic susceptibility (field-cooled/zero-field cooled), vibrating sample magnetometry, and magnetoresistance measurements show the different behavior from this material at different magnetic dopant levels. The spin glass behavior of CMT is discussed in light of these results.

4:00 PM

(GOMD-SII-056-2010) Nonmonotonic Evolution of Density Fluctuations During Glass Relaxation

J. C. Mauro*, Corning Incorporated, United States; S. Soyer Uzun, University of California—Davis, United States; W. Bras, Netherlands Organization for Scientific Research (NWO), France; S. Sen, University of California—Davis, United States

A fundamental understanding of glass relaxation behavior is vital to the glass and polymer science communities. While prior work has focused on relaxation of first-order thermodynamic properties such as enthalpy and density, we present theoretical and experimental results showing that fluctuations in enthalpy and density relax non-monotonically. These results provide direct evidence for dynamical heterogeneities and their close association with density fluctuations. Our results imply that density fluctuations, and hence light scattering, can be minimized through design of thermal history.

4:15 PM

(GOMD-SII-057-2010) Fictive Temperature and the Glassy State

R. J. Loucks*, Alfred University, United States; J. C. Mauro, Corning Incorporated, United States; P. K. Gupta, The Ohio State University, United States

It is common to describe the state of a glass in terms of a fictive temperature or distribution of fictive temperatures. However, a number of definitions of fictive temperature are being practiced in the field. At least three definitions are possible: (a) microscopic, (b) macroscopic, and (c) kinetic. Of these, the microscopic definition offers the possibility of writing a simplified statistical mechanical model of the nonequilibrium glassy state in terms of a linear combination of equilibrium liquid states. However, we show that the microscopic physics of a glass cannot, in general, be described in this manner, and the fictive temperature description of the glassy state is only rigorous under special circumstances.

4:30 PM

(GOMD-SII-058-2010) The Thermodynamic Significance of Order Parameters

R. J. Araujo*, J. C. Mauro, Corning Incorporated, United States

The thermodynamic state of a glass is often described in terms of a number of order parameters, each of which evolves toward its equilibrium value during glass relaxation. The problem comes in identifying these order parameters and determining their physical significance. The authors argue that the order parameters in a glass can be defined in terms of a set of configurational temperatures, each corresponding to a particular mode of energy storage. The evolution of glass properties can then be calculated using a coupled set of rate equations describing the relaxation of the configurational temperatures toward their equilibrium values, viz., the reservoir temperature. The authors illustrate the concept of configurational temperatures by considering the free energy of mixing in alkali borate and silicate glasses.

4:45 PM

(GOMD-SII-059-2010) Heat Capacity, Enthalpy Fluctuations, and Configurational Entropy in Broken Ergodic Systems

B. D. Esham*, Alfred University, United States; J. C. Mauro, Corning Incorporated, United States; S. Sen, University of California—Davis, United States; R. J. Loucks, G. J. McGowan, Alfred University, United States

The traditional method of calculating configurational entropy from heat capacity curves assumes equilibrium thermodynamics and reversible processes ($\Delta G = 0$). However, the glass transition is not a reversible process and glass, by definition, is nonequilibrium. We present an alternative method for computing the configurational entropy of glass from heat capacity data that accounts for the nonequilibrium nature of glass. Our method, based on the underlying enthalpy fluctuations governing heat capacity, predicts a loss of entropy during the glass transition and zero entropy at absolute zero temperature.

5:00 PM

(GOMD-SII-060-2010) Residual entropy : harmonization of statistical mechanics and thermodynamics

A. Takada*, Asahi Glass Company, Japan

The residual entropy of glasses is still the subject of controversy. There are two ways to define the residual entropy due to the nonergodicity on glass. One is based on the time evolution of configurations and the other is based on the sampling from the probability population. First, a simple model including the vibrational and configurational contributions of entropy is constructed. Then the residual entropies estimated from two different method; one is based on calorimetric formula and the other is based on the probability population, are compared employing the constructed model. The calculated results indicate that two estimated values of residual entropy are equivalent and non-zero. These results also support that the entropy is the state variable even in non-equilibrium. Finally, the relaxation effects are interpreted in terms of the time evolution of entropy.

Symposium III: Glass Technology

Optical Materials II

Room: Seneca

Session Chairs: Hong Li, Schott North America, Inc.; Amanda Young, Sandia National Laboratories

1:15 PM

(GOMD-SIII-053-2010) Low losses highly non linear As2S3 suspended core microstructured optical fibers (Invited)

F. Smektala*, M. El Amraoui, J. Jules, G. Gadret, J. Fatome, Université de Bourgogne, France; C. Polacchini, I. Skrypatchev, Y. Messadeq, Instituto de Quimica, Brazil; G. Renversez, Institut Fresnel, France; M. Szpulak, Institute Of Physics, Poland; J. Troles, Sciences Chimiques de Rennes, France; L. Brilland, Perfos, France

Elaboration of low-losses highly non linear chalcogenide optical fibers for the generation of efficient non linear effects in the infrared remains a challenge. In recent years, much work has been devoted to the study of microstructured fibers with different designs and various elaboration processes. Their background losses were typically of several dB/m. In this work we present our achievements in the elaboration of low-losses suspended core optical fibers elaborated from As2S3 glass. Alternatively to other processes we use a mechanical machining for preforms elaboration. The fiber drawing leads to suspended core geometry with controlled diameter core. The dispersion properties are managed and the zero dispersion wavelength is shifted until 2 μm. The background level of losses is 0.35 dB/m. By ps pumping at 1.55 μm, we observe a high non linear response with self phase modulation, Raman generation and finally a strong spectral enlargement in the infrared with an average output power of - 5 dBm.

1:45 PM

(GOMD-SIII-054-2010) Towards low loss, high-index-contrast chalcogenide glass photonics: thermal reflow and overlayer spin-coating

J. Hu*, Massachusetts Institute of Technology, United States; N. Carlie, L. Petit, Clemson University, United States; A. Agarwal, L. C. Kimerling, Massachusetts Institute of Technology, United States; K. Richardson, Clemson University, United States

High index contrast (HIC) photonic integration using chalcogenide (ChG) glasses offers unique competitive edges for sensing and nonlinear optics, such as reduced footprint and small optical mode size. The high optical loss resulting from roughness scattering, however, has been the major roadblock towards HIC ChG photonics. This work pioneers two techniques for loss reduction in chalcogenide glass waveguides and resonators using thermal reflow and overlayer spin-coating, respectively. The former approach leverages surface tension of glass to smooth roughness and eliminate scattering loss. In the latter method, an overlayer coating of chalcogenide glass is spin-coated onto as-patterned devices, and thereby creates a surface finish with significantly reduced roughness. We present a systematic study which combines kinetic theory, material analysis, and optical simulation, on both mechanisms. Experimentally, we demonstrate over 50% loss reduction using the techniques.

2:00 PM

(GOMD-SIII-055-2010) Grayscale Lithography Using Chalcogenide Glass Resists

A. Kovalskiy*, Lehigh University, United States; M. Vlcek, University of Pardubice, Czech Republic; J. Cech, H. Jain, Lehigh University, United States

Examples of applications of chalcogenide glass (ChG) thin film e-beam and photo-resists for grayscale lithography are presented. It is demonstrated that these materials can be utilized for making ultrathin (~600 nm) grayscale patterns for IR microoptics and micro(nano)-electromechanical systems (MEMS/NEMS) , which are compatible with traditional silicon chip technology. The ChG patterns can be used on the surface of the chip or transferred into the silicon. The technology is demonstrated with inexpensive and reliable fabrication of ultrathin Fresnel lenses that are transparent in the visible as well as in the IR region. The optical functionality of the Fresnel lenses is confirmed. Application of silver photodissolution in grayscale lithography for MEMS applications is also shown. A substrate to ChG/silver thickness etching ratio of ~ 10 is obtained for the transfer of patterns into silicon using reactive ion etching, more than a five-fold increase compared to traditional polymer photoresist.

2:15 PM

(GOMD-SIII-056-2010) Optimization of spin-coating parameters for optical quality chalcogenide thin films in the As-Ge(Sb)-System

N. Carlie*, L. Petit, J. D. Musgrave, K. Richardson, Clemson University, United States

Solution-based processing methods, such as spin-coating of dissolved chalcogenide-glasses, are attractive as a novel route to form thin films and coatings. In order to use this method to create optical elements it is necessary to optimize process steps to minimize sources of optical loss. To this end, we present the fabrication of thin films in the As-Ge(Sb)-S system using a three step process including: dissolution of bulk glasses, spin-coating and heat treatment of the subsequent films. The dissolution process has been optimized in order to allow the deposition of films with composition identical to that of the parent bulk, while the spin-coating and heat treatment steps have been optimized to provide films of maximum thickness and uniformity with minimum surface roughness and residual solvent content. The optical properties of these films have been examined using UV-Vis and FTIR spectroscopy, and their structure has been elucidated using micro-Raman spectroscopy.

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(GOMD-SIII-057-2010) Effects of deposition parameters on the optical properties and stability of thermally evaporated Ge-As-Se thin films

D. Bulla*, R. Wang, S. Prasad, A. V. Rode, S. J. Madden, B. Luther-Davies, Australian National University, Australia

Thin films of GexAsySe100-x-y ($5<x<33$, $10<y<30$) glasses have been thermally evaporated from bulk material and submitted to thermal treatments. The linear refractive index and optical band-gap for as-deposited and annealed films have been analyzed as function of the deposition parameters, chemical composition and mean coordination number (MCN). The film composition was found to be directly affected by deposition rate, with low rates producing films with elevated Ge and reduced As content compared with the bulk starting material. As a result films with close to the same stoichiometry as the bulk could be obtained by choosing appropriate deposition conditions. As-deposited films with $2.44 <= MCN <= 2.54$ showed refractive indices and optical band-gaps very close to those of the bulk. Upon annealing, high MCN films evolved such that their indices and band gaps approached the bulk values whereas at low MCN films resulted in no changes to the film optical properties.

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(GOMD-SIII-058-2010) Structure-Optical Property Correlations for Arsenic-Sulfide Glasses in the Visible, Infrared, and Sub-millimeter Regions

J. McCloy, B. J. Riley, S. K. Sundaram, A. Qiao, J. V. Crum, B. R. Johnson*, Pacific Northwest National Lab, United States

Structural and optical properties of AsxS100-x glasses were measured from visible to terahertz wavelengths. A series of annealed, bulk AsxS100-x glasses (x = 30 to 42) were made and their refractive indices determined at terahertz, infrared, and visible frequencies using a combination of a quasi-optical backwards wave oscillator spectrometer for terahertz measurements and a prism coupler for visible and infrared measurements. It was found that refractive index at all frequencies increases with arsenic composition up to 40 atomic % arsenic then decreases with additional arsenic. Structure in x-ray diffraction patterns support the notion of a minimum volume at 40 atomic %, while the average covalent coordination number indicates the rigidity percolation threshold is reached there. At As concentrations > 40 atomic %, the network becomes over-constrained, the molar volume increases. Correlations were drawn between the atomic structure of the glasses and their optical properties.

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(GOMD-SIII-059-2010) Chalcogenide optical fibers used for CO2 detection

F. Charpentier*, S. Maurugeon, J. Troles, V. Nazabal, L. Brilland, Universite de Rennes 1- CNRS, France; P. Camy, J. L. Doualan, CIMAP, France; C. Boussard-Pledel, X. H. Zhang, P. Lucas, B. Bureau, Universite de Rennes 1- CNRS, France

The ability to detect and analyze carbon dioxide has become increasingly important in environmental as well as planetary science. Accurate detection of CO2 in the earth's atmosphere is critical for the study of environmental processes such as global warming, while CO2 has also gained special interest in the field of extraterrestrial exploration because it is produced by living organisms and is therefore regarded as one of the markers of potential life on telluric exoplanets. Remote optical detection of CO2 involves monitoring of its two vibrational absorption bands at 4.3μm and 16μm and therefore requires advanced infrared technologies. In that framework, chalcogenide glasses are matchless materials. Nevertheless, different chalcogenide glass optical devices have to be developed depending on the targeted vibrational absorption band. First, among the measures to reduce CO2 emissions, capture and geological storage holds out promise for the future in the fight against climate change.

3:30 PM

(GOMD-SIII-060-2010) Chalcogenide waveguides integrated microfluidic sensor device

M. L. Brandily-Anne*, Universite de Rennes, France; F. Charpentier, Universite de Rennes 1, France; H. Lhermitte, Universite de Rennes, France; J. Charrier, FOTON, France; B. Bureau, V. Nazabal, Universite de Rennes 1, France

Chalcogenide glasses are of great interest for microphotonics applications due to their wide range of optical properties, large capacity for doping, high non linear capacity and their wide transparency window stretching from the visible to the far-infrared. These properties make them ideal candidates for sensing, as most of chemical and biological species have their fingerprints in the mid and far-infrared range. The development of high quality waveguides, made of chalcogenide glasses, will be presented in this presentation. Sulphide or Selenide thin films have been deposited onto oxided silicon wafers by RF-sputtering Channel waveguides have been defined using reactive ion etching technique under a CF4 plasma. Those waveguides yield an attenuation of 0.5 dB.cm-1 for Se-glasses and 0.7 dB.cm-1 for S-glasses (measured at 1550 nm). A microfluidic sensor device has been developed where waveguides are encapsulated with a resin SU8 and sealed via a polydimethylsiloxane (PDMS)

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(GOMD-SIII-061-2010) Utilizing Rare Earth Doped Nanoparticles to Tailor Emission Spectrum of Optical Fiber

T. L. James, C. Kucera, B. Kokuoz, E. Garber, D. Edmonson, Clemson university, United States; D. Griese, M. Miller, E. Chasteen, M. Goodson, Furman University, United States; A. James, Clemson university, United States; W. Baker, Furman University, United States; J. Ballato*, Clemson university, United States

Modified chemical vapor deposition derived silica preforms were solution doped with nanoparticles comprised of a variety of host materials (LaF3, CaF2, SrF2, BaF2) and rare earth dopants. The glass was examined to determine the effects of spatially localizing dissimilar dopants to control energy transfer and the impact of vibrational energy of host materials in resultant optical fiber. Preforms prepared with Eu3+/Tb3+ co-doped LaF3 nanoparticles exhibited energy transfer from the Tb3+ to the Eu3+ ions, whereas the preform containing individually doped particles yielded only discretely Tb3+ or Eu3+ emissions. The extension of this work to broadband amplifiers and lasers will also be discussed.

4:00 PM

(GOMD-SIII-062-2010) Structural and Compositional Modification of Glass Surfaces by Thermal Poling

N. J. Smith*, C. G. Pantano, Pennsylvania State University, United States

Thermal poling is a thermo-electric treatment method used primarily to modify glasses for second-order nonlinearity (SON), wherein a micron-scale modified layer is induced on the anode side of the glass, usually with some evidence of cation depletion and (often subtle) structural alterations. In pursuit of new methods of glass surface modification, we have been evaluating thermal poling under conditions outside the range typically used to induce SON (eg. poling temperature/atmosphere/electrode), but wherein more substantial structural and compositional modifications of the surface may be achieved by electrolysis of constituent cations and anions within the glass network in the near-surface region. Such modifications are realized in several multicomponent silicates (including alkali-free glasses), and the strong dependence of surface composition, structure, and nonlinear optical properties on such conditions—as shown by XPS, vibrational spectroscopy, and Maker Fringe techniques—will be reported.

4:15 PM

(GOMD-SIII-063-2010) Fabrication and Applications of Thin, Free-Standing Borophosphosilicate Glass (BPSG) Films

C. L. Trivelpiece*, J. S. Brenizer, C. G. Pantano, The Pennsylvania State University, United States

Thin, free-standing BPSG films (< 1.5 μm thick) were fabricated (Penn State NSF-NNIN Nanofab) for use as neutron converters in an ultra-high spatial resolution neutron imaging system. To date, several large area (10 mm^2 – 25 mm^2), free-standing thin films have been produced with localized surface roughness RMS values of 10 – 20 nm. Stress has been observed near the edges of these films via birefringence methods, and a proposed annealing schedule is being implemented to determine if this stress can be relaxed. This work focuses on the processing techniques used to fabricate the films, the analyses used to evaluate the processed films, and issues associated with film deformation due to residual stress. Other applications of these thin, free-standing BPSG films – aside from neutron imaging – will also be discussed.

4:30 PM

(GOMD-SIII-064-2010) Nanophase semiconductor-transparent conductive oxide composite thin films for photovoltaic applications

G. H. Shih*, C. G. Allen, B. G. Potter, University of Arizona, United States

We investigate the morphological evolution and concomitant modification of optical and electronic behavior in quantum-scale germanium (Ge) structures embedded within an indium-tin-oxide (ITO) matrix. Samples are prepared using a multisource, sequential RF magnetron sputter technique. Deposition condition controls coupled with post-deposition heat-treatment are shown to impact phenomena of direct importance to the use of these films as active elements in photovoltaic

devices. The incorporation of the nanocrystalline semiconductor is associated with enhanced thermally generated (dark) carrier density and increased photoconduction, compared to a single phase ITO. Moreover, variation in the Ge phase assembly is correlated with a quantum-size induced blue-shift in the optical absorption. These results demonstrate the significance of multi-length scale structural control on the optical and optoelectronic properties of these semiconductor-based nanocomposite thin films.

4:45 PM

(GOMD-SIII-065-2010) Development of an original process for the realization of multi-materials optical fibres

S. Leparmentier, J. Auguste*, G. Humbert, F. Gérôme, C. Restoin, J. Blondy, XLIM, France; B. Desruelle, DGA, France

In this communication, the realization of original optical fibres using a process based on powdered glass materials is demonstrated. The concept of these 'multi-materials' fibres is to link the strong points of the two main glass families used for usual optical fibres: pure silica for the fibre cladding (microstructured or not) and an other optical glass (silica or non-silica glass) for the core. To realize such fibres, we have developed an original process based on powdered glasses. Materials are mainly manufactured as powder allowing a larger choice for the fibres core. With this process, we can insert one or many glasses into micrometric structures by simply filling thin capillary tubes with powder and stacking them to realize original designs which are impossible to achieve by standard processes. Low loss step-index and microstructured 'multi-materials' optical fibres with lanthano-alumino-silicate and borosilicate glasses are first proofs of this new original route.

5:00 PM

(GOMD-SIII-066-2010) Photo luminescence properties of copper ion doped alkali borosilicate glasses in metastable immiscibility region

A. Yasumori*, F. Tada, D. Takemoto, N. Matsui, T. Kishi, Tokyo University of Science, Japan

The various approaches for preparation of warm color light emitted glasses or glass ceramics excited by near ultraviolet (NUV) light emitted diodes (LEDs) are investigated in order to achieve high power warm white LEDs, which requires high thermal and UV light durability. In this study, alkali-borosilicate glasses (R_2O-B_2O_3-SiO_2, R=Li, Na, K) in metastable immiscibility region containing Cu^+-Cu^+ clusters as yellow color light emission center were prepared by a conventional melting method. The photo luminescent (PL) and light absorption properties of the obtained Cu ion doped glasses were mainly examined. The blue light emission due to isolated Cu^+ ions and the yellow light one due to Cu^+-Cu^+ clusters by UV light irradiation were observed and the emission spectra changed with the glass composition, Cu_2O and SnO contents. The existence of phase separation structure in the glass matrix was very effective in forming of Cu^+-Cu^+ clusters in R_2O-B_2O_3 rich phase.

Symposium IV: Glass Corrosion

Long-term Corrosion Testing

Room: Carder

Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

1:15 PM

(GOMD-SIV-015-2010) Modeling Alteration of Borosilicate High-Level Waste Glass Networks in a Radiation Environment (Invited)

L. Dewan, L. Hobbs*, Massachusetts Institute of Technology, United States; R. Cherifi, Université Pierre et Marie Curie, France; J. Delaye, CEA Valrhô-Marcoule, France

Glass network alterations in a simplified Na aluminoborosilicate model nuclear-waste-glass were investigated in a simulated waste environment using molecular dynamics (MD) codes and efficient topological assessment algorithms. Collision cascades were initiated ballistically (1~70 keV initial kinetic energy, dissipated elastically) and carried out using DL_POLY2 MD codes incorporating both two-body Buckingham and three-body Born-Mayer-Huggins potentials verified in the GULP atomistic simulation package. Network topologies of the initial and resulting altered glass structures were determined by enumerating the primitive-ring-based local cluster atom complement at each atom site. The topological description is seen to provide a revealing assessment of network structural changes in the simulated radiation environment that can be potentially related to observable macroscopic changes, such as swelling, viscosity change and radiation-induced devitrification.

1:45 PM

(GOMD-SIV-016-2010) Initial dissolution rate of P0798 simulated HLW glass as a function of pH and temperature measured by using micro-reactor flow-through test (Invited)

Y. Inagaki*, H. Makigaki, Kyushu University, Japan; S. Mitsui, JAEA, Japan; K. Idemitsu, T. Arima, Kyushu University, Japan; K. Noshita, Hitachi, Ltd, Japan

A new type of flow-through test method using micro-reactor was developed and applied to measurement of dissolution kinetics for a Japanese simulated HLW glass, P0798. In this method, a coupon shaped glass is placed on a Teflon plate with a micro-channel (20mm x 2mm x 0.16mm), and a solution is injected into the inlet of the channel at a constant flow rate. The outlet solution, which reacted with glass through the channel, is retrieved to be analyzed for determination of the dissolution rate. By using this method we measured the initial dissolution rate as a function of pH and temperature. The results showed that the initial dissolution rate has "V-shaped" pH dependence at any temperature from 25 to 90°C similar to that for R7T7 glass evaluated by CEA, France. However, a certain difference was observed between them in the temperature dependence at high pHs. Based on the results and comparison, we discussed the dissolution kinetics.

2:15 PM

(GOMD-SIV-017-2010) Isotopic Enrichment Studies to Determine Elemental Diffusion Profiles Through an Established Alteration Layer

J. V. Ryan*, A. Mitroshkov, D. M. Strachan, Pacific Northwest National Laboratory, United States

Research into new spent nuclear fuel cycles by the Department of Energy Fuel Cycle R&D program may result in a repository inventory where HLW glass would play a deterministic role in models of radionuclide release. One of the key remaining questions is the mechanism and extent by which alteration layers present a barrier to corrosion. In order to investigate the diffusion of ions and their rate of dissolution/reprecipitation from glasses in a mature state of corrosion, isotopically enriched glasses and those with natural elemental abundances were both synthesized and allowed to corrode in equivalent conditions. Following the development of a mature alteration layer, the solutions will be swapped and the diffusion of individual isotopes through the corrosion products monitored. This talk presents the initial experiments to ensure the proper characterization of the main test later this year.

2:30 PM

(GOMD-SIV-018-2010) Long-Term Durability Testing of Glasses for the Stabilization of Closed Nuclear Fuel Cycle Waste Streams

A. L. Billings*, J. C. Marra, C. C. Crawford, Savannah River National Laboratory, United States

The Fuel Cycle Research and Development program is sponsored by the US DOE to develop and demonstrate a process for the recycling of spent nuclear fuel in order to achieve a closed nuclear fuel cycle. Borosilicate glass was selected as the baseline technology for immobilization of the Cs/Sr/Ba/Rb, lanthanide and transition metal fission product waste steams. Long term corrosion behavior is not well established for these type of waste glasses. These studies were aimed to develop and test glasses which could successfully immobilize the waste streams and have acceptable chemical durability. Long-term durability was simulated using the Product Consistency Testing (PCT) at a high surface area of glass to volume of water ratio and elevated temperatures. Chemical composition analyses and other characterization techniques were used on the leached glasses to examine the altered surfaces of the glasses after 6 months of treatment.

2:45 PM

(GOMD-SIV-019-2010) Evaluating the long-term weathering of minerals and engineered materials across a range of spatial and temporal-scales

E. M. Pierce*, Pacific Northwest National Lab, United States

Use of mineral and glass dissolution rates measured in the laboratory experiments to predict the weathering of primary minerals and volcanic glass in field studies and to advance our understanding of element cycles in the environment has been of interest to the geochemical community for decades. The construction of valid rate models to describe the dissolution of rock forming minerals, the evolution of soils, and the corrosion resistance of engineered materials in numerous applications lies at the heart of predictive science of geochemistry. Improvements to these rate models require an understanding of the key processes that control mineral- and glass-water reaction across multiple scales (e.g., spatial and temporal). This presentation will discuss the current approach being used to predict the long-term weathering of glass as well as highlight the current science gaps that need to be filled to improve these continuum-scale simulations of key processes.

3:00 PM

(GOMD-SIV-020-2010) Molecular Modeling of Aluminosilicate Glass Dissolution for High-Level Nuclear Waste Repository Science

L. J. Criscenti*, Sandia National Laboratories, United States; J. D. Kubicki, S. L. Brantley, Pennsylvania State University, United States

Safe, long-term storage of high-level nuclear waste in glass is dependent upon the rate at which the glass dissolves or "weathers". Currently, there are seven different models for long-term glass dissolution used in performance assessment. The main reason for this disagreement is a poor understanding of the controlling mechanisms in glass dissolution. Quantum mechanics calculations can provide activation energies for elementary reaction steps that can be compared with experimental data. Using cluster calculations, we showed that (1) a change in Al coordination from four-fold to six-fold at the glass–water interface is energetically possible as a dissolution step and (2) Q3Si-O bond breaking requires more energy than the experimentally-derived activation barrier (Criscenti et al. 2005, 2006), therefore, this reaction is not a rate-limiting step. A matrix of calculated energies for breaking glass bonds will provide key mechanistic information to understand glass dissolution.

Symposium V: Glass Structure and Properties

Glass Structure and Properties IV: More Fun with the Vitreous State

Room: Keuka

Session Chair: Morten Smedskjaer, Aalborg University

1:15 PM

(GOMD-SV-034-2010) Elasticity, Compression Behavior, and Vibrational Properties of Silicate Glasses under High Pressures: A Review (Invited)

M. H. Manghnani*, University of Hawaii, United States

An understanding of the physical and structural properties of glasses under both the static and dynamic pressures is important for optimizing their armor use. The purpose of this paper is to correlate the structure-property relations of selected glasses under static and dynamic pressures. Using high precision ultrasonic interferometry and Brillouin scattering techniques, the elastic properties and equation of state (pressure-density relations) of selected silicate glasses of various compositions (soda-lime silicate, borosilicate, and system SiO2-TiO2) have been determined under static high pressures up to 20 GPa. To understand the pressure dependencies of the non-linear and anomalous compression behavior, the structural bonding (e.g., Si-O-Si, Si-O-B and Si-O-Ti), based on vibrational properties of these glasses, were probed under *in situ* hydrostatic pressure environments in a diamond anvil cell by Raman spectroscopy. These results are compared with the available shock wave data.

1:30 PM

(GOMD-SV-035-2010) A chemical probe for measuring glass densification under sharp contact?

J. Guin*, Y. Niu, T. Rouxel, CNRS-Université de Rennes 1, France; A. Abdelouas, Ecole des mines de Nantes, France

Densification under a sharp contact is a well known and well studied permanent deformation mechanism in glass. Such a densification phenomenon involves structural changes in the glassy network (number of SiO4 units per ring, Si-O-Si angle, Si coordination) that may, or not, enhance chemical reactions such as the aqueous dissolution rate of the silica network. Such an enhanced reaction may be used to probe and get an insight regarding the shape and size of the densified volume. Such an enhanced reaction coupled with 3 dimensional AFM measurements were used to study the densified zone under crack free Vickers, Berkovich and Knoop indentations made on a silica glass and a soda lime silicate glass. The volume and the shape of the densified zone are compared to results collected by other techniques such as 3 dimensional Raman cartography of indentations and full recovery of the densified volume by thermal treatment at 0.9*Tg. Both techniques were used on the same glass compositions.

1:45 PM

(GOMD-SV-036-2010) High frequency sound and boson peak in glasses

B. Rufflé*, University Montpellier II, France

A rather intriguing feature in the physics of glasses is the anomalous behavior of the low-frequency part of the vibration spectrum and the corresponding thermal properties. The boson peak (BP) is an excess in the vibrational density of states (VDOS), observed in many glasses at frequencies of the order of one THz. It appears as a hump in the reduced VDOS $g(\omega)/\omega^2$, above the acoustic Debye level. This excess produces the well-known specific heat anomaly of glasses at temperatures $T \approx h\omega_{BP} / 5\, k_B \sim 10$ K. It is generally agreed that the BP is a vibrational signature of the disordered structure of glasses beyond the nm scale. Its correct understanding is thus of considerable importance. Because of the development of new experimental techniques allowing one to perform Brillouin scattering measurements in the THz range, as well as pertinent md simulations, the question concerning the nature of the modes in the BP region has gained much additional interest recently. In this talk I will present recent progress on these questions.

2:00 PM

(GOMD-SV-037-2010) Optical basicity revisited: theory and application to optical properties and crystallization (Invited)

J. McCloy*, Pacific Northwest National Laboratory, United States

The concept of optical basicity has proven very fruitful to glass science since its introduction into the chemistry community in 1971. In this presentation, the theoretical background of optical basicity is reviewed, emphasizing the relative merits of 3scales which have been proposed in the literature based on optical properties or chemical bonding. Results for various cations are considered and compared among the various scales and to ionic field strength, allowing estimation of basicity parameters not currently assigned in the literature. Some applications of optical basicity are then considered, including prediction of refractive index through consideration of oxygen polarizability and relative state of redox of multivalent cations. Finally, the potential application of optical basicity towards the understanding crystallization in oxide nuclear waste glasses is offered.

2:15 PM

(GOMD-SV-038-2010) Correlation of Network Structure with Devitrification Mechanism in Lithium and Sodium Diborate Glasses

B. Chen, U. Werner-Zwanziger, J. Zwanziger*, Dalhousie University, Canada; M. Nascimento, L. Ghussn, E. Zanotto, Federal University of Sao Carlos, Brazil

The intermediate-range structure of the network former in lithium and sodium diborate was studied using nuclear magnetic resonance spectroscopy. Specifically, B-11/B-10 rotational-echo double resonance experiments were employed to determine the distribution of dipole couplings between these isotopes and in this way determine whether the intermediate range order of the borate network was the same in the glasses as in the crystal forms of these compounds. It was found that in the lithium diborate case the networks are in fact similar between glass and crystal, while in sodium diborate they differ substantially. Because lithium diborate shows homogeneous nucleation and growth on the laboratory time scale while sodium diborate does not, it was concluded that structural similarity between glass and crystal of the glass former correlates strongly with nucleation mechanism.

2:30 PM

(GOMD-SV-039-2010) Structural Studies of Alkali Tungstate and Molybdate Glasses by X-ray Absorption Spectroscopy

C. W. Ponader*, K. Adib, B. G. Aitken, Corning Incorporated, United States

Bulk alkali tungstate or molybdate glasses, with Li, Na and K, are of interest because of the absence of traditional glassforming components. Mixed-alkali tungstate and molybdate glasses containing 52.5 to 62.5% (W,Mo)O3 have been characterized with X-ray absorption spectroscopy of tungsten and molybdenum. Tungsten occupies both tetrahedral and octahedral sites in tungstate glasses. The site distribution varies with the tungsten content: the tetrahedral site fraction increases as shown by a 14% rise in the intensity of the pre-edge peak as the alkali content increases from 38.5 to 45%. Molybdenum also appears to occur in these two types of sites; but the distribution does not seem to be sensitive to molybdenum concentration. Molybotungstate glasses can be made by partially replacing MoO3 with WO3, resulting in a slight extension of the glass-forming region to higher RO3. The tungsten and molybdenum speciation in these glasses is found to be independent of the Mo/W ratio.

2:45 PM

(GOMD-SV-040-2010) Vanadium-51 and Boron-11 NMR Study of Ionically Conducting Alkali Borovanadate Glasses

V. K. Michaelis*, University of Manitoba, Canada; J. North, A. Ramm, S. Feller, Coe College, United States; S. Kroeker, University of Manitoba, Canada

In the search for better battery materials, glasses have become attractive alternatives to the heavy, toxic and expensive CoO_2 cathode materials used now. V_2O_5 can be vitrified with B_2O_3, forming a homogeneous borovanadate matrix to host mobile cations. The V_2O_5/B_2O_3 ratio can be adjusted to tune the properties, resulting in lower metal content and reduced processing temperatures. A series of such materials has been investigated by high-resolution NMR spectroscopy to illuminate the network structure and ionic mobility. ^{11}B and ^{51}V MAS NMR at both 14.1 & 21.1T reveal valuable information about the local environments of the network-forming cations. Fast MAS is necessary to resolve multiple ^{51}V sites, which can be interpreted with the aid of ab initio chemical shift calculations. 2D ^{7}Li and ^{133}Cs exchange spectroscopy is used to characterize the timescales of ionic motion in these materials, demonstrating a few promising candidates for further development as cathode materials.

3:15 PM

(GOMD-SV-041-2010) Intermediate-range Order in Nanostructured Silica

G. Chen*, C. Wan, B. Prasai, D. A. Drabold, Ohio University, United States

The sol-gel processing provides an effective approach to fabricate nanostructured glasses. An obvious feature associated with these glasses is their large specific surface area, which could have impact on the atomic structure. To understand the intermediate-range order (IRO) in nanostructured silica, we conducted small/wide angle x-ray scattering on a variety of sol-gel derived silica glasses, including nano-colloidal and periodic mesoporous silica. By analyzing the first sharp diffraction peak of these glasses, we found that their IRO not only differs from that of the melt-quenched silica, but also depends on specific nanoscale structure. IRO of the sol-gel derived silica was studied as a function of annealing temperature and doping concentration, and the results are compared with those obtained form molecular dynamic simulations. The combined experimental and theoretical studies shed light on the defective nature of the IRO in sol-gel-derived nanostructured silica.

3:30 PM

(GOMD-SV-042-2010) Interactions of Small Molecules with Oxide Surfaces: Models for Polymer Binding on Glass Fibers

K. T. Mueller*, L. Ortiz-Rivera, D. L. Suchy, J. Stapleton, C. G. Pantano, Penn State University, United States

Improvements in the performance of many fiberglass-based materials depends on an understanding of the specific binding of soft materials (such as polymers) to reaction sites on a multicomponent oxide surface. Properties of small organic molecules on oxide surfaces are being investigated in this study to understand the different binding sites present at the glass/polymer interface, as well as to probe the resulting chemical structures found for adsorbent complexes. We follow interfacial reactions with a combination of solid-state nuclear magnetic resonance (NMR), infrared spectroscopy (IR), and temperature programmed desorption inverse gas chromatography (TPD-IGC) methods. Spectroscopic data are mapped onto TPD-IGC results that reveal multiple desorption events. These results support our hypothesis that both physical and chemical absorption processes are occurring at these interfaces, and we correlate these processes to oxide composition and adsorbate chemical functionality.

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*** Denotes Presenter**

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