conference program

2015

GLASS & OPTICAL MATERIALS DIVISION and DEUTSCHE GLASTECHNISCHE GESELLSCHAFT

ACerS GOMD–DGG Joint Meeting

May 17 – 21

Hilton Miami Downtown
Miami, Florida, USA

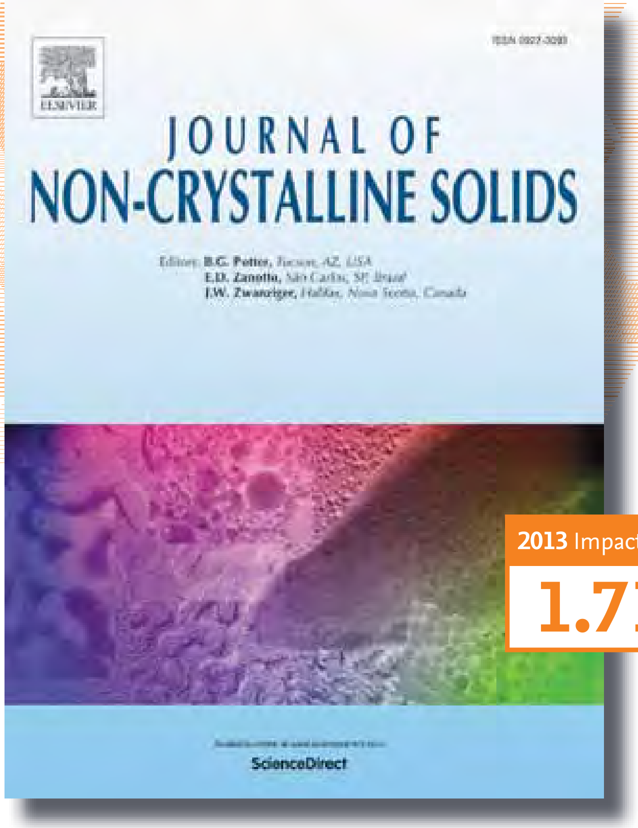
ceramics.org/gomd-dgg

The American Ceramic Society
www.ceramics.org

ELSEVIER

JOURNAL OF NON-CRYSTALLINE SOLIDS

PROUD SPONSOR OFTHE GOMD 2015 POSTER SESSION



JOURNAL OF NON-CRYSTALLINE SOLIDS

Editors: **B.G. Potter**, *Tucson, AZ, USA*
E.D. Zanotto, *São Carlos, SP, Brazil*
J.W. Zwanziger, *Halifax, Nova Scotia, Canada*

ScienceDirect

2013 Impact Factor*

1.716

MEET THE EDITORS:

B. G. Potter, *University of Arizona, Arizona Materials Laboratory, Tucson, AZ, USA*

E. D. Zanotto, *Universidade Federal de São Carlos, Vitreous Materials Lab, São Carlos, SP, Brazil*

J.W. Zwanziger, *Dept. of Chemistry, Dalhousie University, Halifax, Canada*

TIME & DATE:

Date: Monday, May 18

Time: 6.30 – 8.30 pm

Announcing the 2015 W.H. Zachariasen Award

The Young Scientist Award for Outstanding Research on Non-Crystalline Solids

The winner will be announced during the conference banquet on Tuesday, May 19.

FOR MORE INFORMATION

www.elsevier.com/locate/jnoncrysol

Welcome

On behalf of The American Ceramic Society and the Deutsche Glastechnische Gesellschaft, welcome to the 2nd Joint ACerS GOMD–DGG Meeting. Building on the success of the 2014 joint meeting, GOMD–DGG 2015 will continue to strengthen ties between the European and US glass communities.

We have a record number of presentations and posters that explore the fundamental nature of the glassy state, glass applications in healthcare, energy and environment, glass manufacturing challenges, nuclear waste immobilization, optical and optoelectronic materials, and more. With over 400 submissions, GOMD–DGG 2015 will provide a unique opportunity for glass scientists and technologists to interact.

GOMD–DGG 2015 includes five symposia with more than 20 sessions led by technical leaders from industry, government laboratories, and academia covering the latest advances in glass science and technology. The poster session will highlight late-breaking research and feature the annual student poster contest.

Several special activities are planned in addition to the technical program:

- Renew acquaintances and get to know new faces within the GOMD community during the Welcome Reception on Sunday from 6:00 p.m. – 8:00 p.m.
- Special Award Lectures: The Stookey Lecture of Discovery Award (Monday morning), the George W. Morey Award (Tuesday morning), the Norbert J. Kreidl Award for Young Scholars (Tuesday at noon), the Darshana and Arun Varshneya Frontiers of Glass Science lecture (Wednesday morning) and the Darshana and Arun Varshneya Frontiers of Glass Technology lecture (Thursday morning).
- Continue your learning experience by attending the Poster Session and Student Poster Competition on Monday from 6:30 p.m. – 8:30 p.m.
- GOMD attendees are invited to be our guests and continue networking with their colleagues during the conference dinner on Tuesday from 7:00 p.m. – 10:00 p.m.

Special thanks to our sponsors, including PPG Industries Inc. for sponsoring the George W. Morey Award, Schott North America, Inc. for sponsoring the Norbert J. Kreidl Award, Corning Incorporated and Coe College for sponsoring the Stookey Lecture of Discovery, and Saint-Gobain for sponsoring the "Panel Discussion for Students - Advice From the Experts on Publishing Your Scientific Research." We also thank the Journal of Non-Crystalline Solids, Dias Infrared Systems, Mo-Sci Corporation, AdValue Technology, the International Journal of Applied Glass Science, Irradiance Glass, American Elements and Ohio University for their generous support. Corning Incorporated also sponsors the Student Poster Competition.

The Hilton Downtown Miami is steps away from the Metromover, Miami's free electric rail system that will connect you to all the major destinations, including the Perez Museum of Art and the Bayside Marketplace. Check out the Miami Duck Tours to see and learn about Miami from land or by sea.

The American Ceramic Society and the Deutsche Glastechnische Gesellschaft thank you for participating in this year's meeting.

Gang Chen
Ohio University, USA

Steve W. Martin
Iowa State University, USA

Reinhard Conradt
RWTH Aachen University, Germany

save the date

October 4 – 8, 2015

MS&T15

MATERIALS SCIENCE & TECHNOLOGY

Greater Columbus Convention Center | Columbus, Ohio USA

Technical Meeting and Exposition

The technical program covers:

- Biomaterials
- Ceramic and Glass Materials
- Electronic and Magnetic Materials
- Energy Issues
- Fundamentals and Characterization
- Iron and Steel
- Materials – Environment Interactions
- Materials Performance
- Nanomaterials
- Processing and Product Manufacturing

matscitech.org

Organized by:

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AIST Association for Iron & Steel Technology

ASM International

TMS The Minerals, Metals & Materials Society

Sponsored by:

NACE International The Corrosion Society

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Final Program

GOMD Officers

Division Chair
Steven A. Feller
Coe College

Vice Chair
Edgar Zanotto
Federal University of São Carlos

Chair-Elect
Randy Youngman
Corning Incorporated

Secretary
Pierre Lucas
University of Arizona

2015

ACERS GOMD–DGG JOINT MEETING

award speakers

Stookey Lecture of Discovery

Monday, May 18, 2015 | 8 – 9 a.m.

N. B. Singh, University of Maryland, Baltimore County, USA

Title: *Development of multifunctional chalcogenide and chalcopyrite crystals and glasses*

Sponsored by **Corning Incorporated** and **Coe College**

George W. Morey Lecture

Tuesday, May 19, 2015 | 8 – 9 a.m.

Jianrong Qiu, South China University of Technology, China

Title: *Control of the metastable state of glasses*

Sponsored by **PPG Industries, Inc.**

Norbert J. Kreidl Lecture

Tuesday, May 19, 2015 | Noon – 1 p.m.

Michael J. Guerette, Rensselaer Polytechnic Institute, USA

Title: *Structure of nonlinear elasticity of silica glass fiber under high strains*

Sponsored by **Schott North America, Inc.**

Varshneya Frontiers of Glass Science Lecture

Wednesday, May 20, 2015 | 8 – 9 a.m.

Sabyasachi Sen, University of California, Davis, USA

Title: *Structural aspects of relaxational dynamics in glasses and supercooled liquids*

Varshneya Frontiers of Glass Technology Lecture

Thursday, May 21, 2015 | 8 – 9 a.m.

Steven B. Jung, Mo-Sci Corporation, USA

Title: *The present and future of glass in medicine*

Schedule At A Glance

Saturday, May 16, 2015

Nucleation, growth and crystallization in glasses—Fundamentals and applications short course*	1:00 p.m. – 5:00 p.m.

Sunday, May 17, 2015

Nucleation, growth and crystallization in glasses—Fundamentals and applications short course*	8:00 a.m. – 12:00 p.m.
AACS' What's new in ancient glass research workshop**	9:00 a.m. – 5:20 p.m.
GOMD-DGG Registration	4:00 p.m. – 7:00 p.m.
Welcome reception	6:00 p.m. – 8:00 p.m.

Monday, May 18, 2015

GOMD-DGG Registration	7:00 a.m. – 5:30 p.m.
Stookey Lecture of Discovery	8:00 a.m. – 9:00 a.m.
Concurrent Sessions	9:20 a.m. – 5:40 p.m.
Lunch provided	12:00 p.m. – 1:20 p.m.
GOMD General Business Meeting	5:45 p.m. – 6:30 p.m.
Poster Session (Sponsored by Journal of Non-Crystalline Solids) & Student Poster Competition	6:30 p.m. – 8:30 p.m.

Tuesday, May 19, 2015

GOMD-DGG Registration	7:30 a.m. – 5:30 p.m.
George W. Morey Award Lecture	8:00 a.m. – 9:00 a.m.
Concurrent Sessions	9:20 a.m. – 6:00 p.m.
The Norbert J. Kreidl Award for Young Scholars Lecture	12:00 p.m. – 1:00 p.m.
Lunch on own	12:00 p.m. – 1:30 p.m.
Conference Banquet	7:00 p.m. – 10:00 p.m.

Wednesday, May 20, 2015

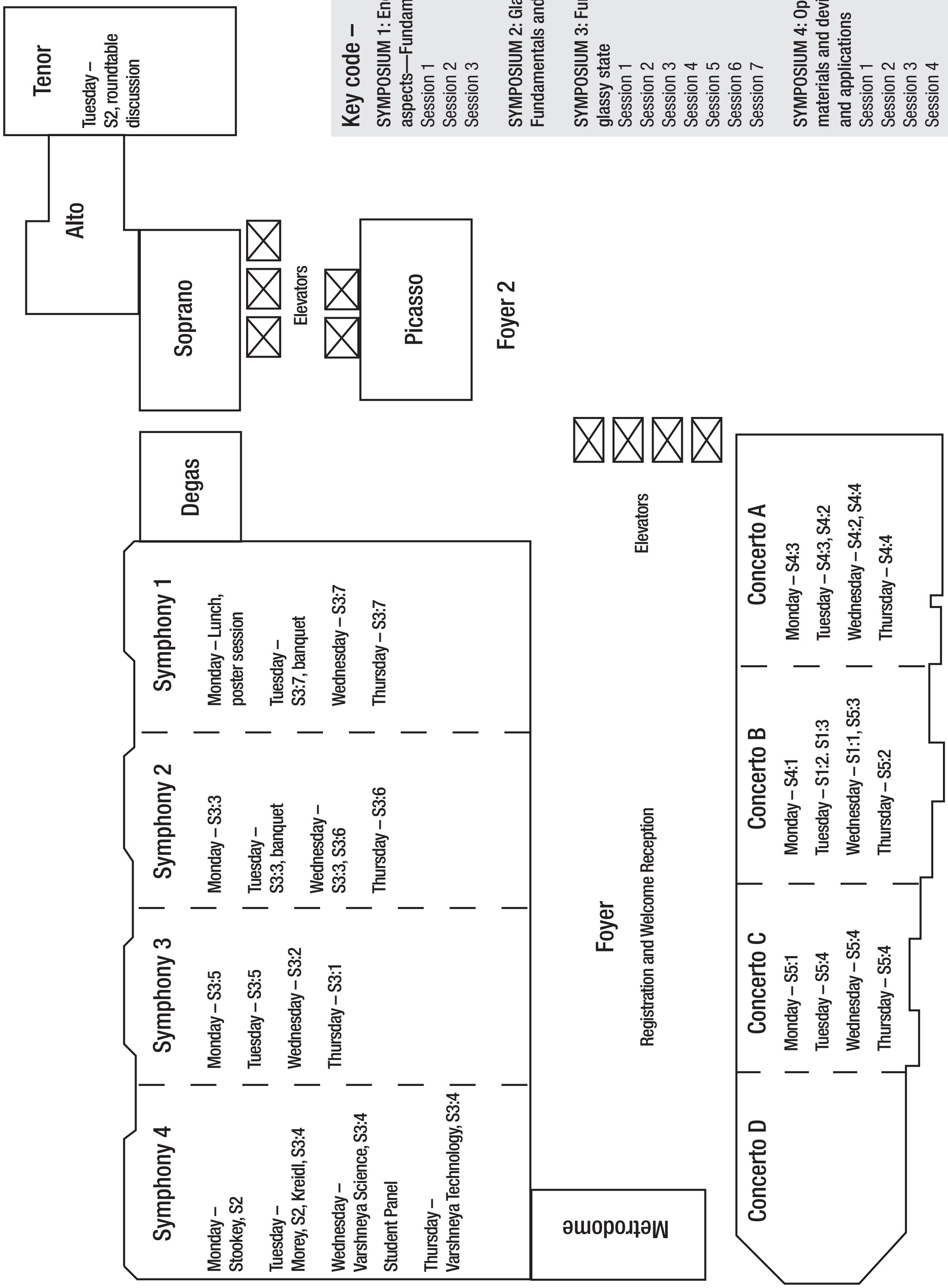
GOMD-DGG Registration	7:30 a.m. – 5:00 p.m.
Darshana and Arun Varshneya Frontiers of Glass Science Lecture	8:00 a.m. – 9:00 a.m.
Concurrent Sessions	9:20 a.m. – 5:40 p.m.
Panel Discussion for Students: Advice From the Experts on Publishing Scientific Research (Sponsored by Saint-Gobain and ACerS GGRN)	12:00 p.m. – 1:20 p.m.
Lunch on own	12:00 p.m. – 1:30 p.m.

Thursday, May 21, 2015

GOMD-DGG Registration	7:30 a.m. – 12:00 p.m.
Darshana and Arun Varshneya Frontiers of Glass Technology Lecture	8:00 a.m. – 9:00 a.m.
Concurrent Sessions	9:20 a.m. – 12:00 p.m.

* separate registration required
** separate registration required, this workshop is at the Hyatt Regency Miami

Floor Plan



Key code –

SYMPOSIUM 1: Energy and environmental aspects—Fundamentals and application
Session 1
Session 2
Session 3

SYMPOSIUM 2: Glasses in healthcare—Fundamentals and application

SYMPOSIUM 3: Fundamentals of the glassy state
Session 1
Session 2
Session 3
Session 4
Session 5
Session 6
Session 7

SYMPOSIUM 4: Optical and electronic materials and devices—Fundamentals and applications
Session 1
Session 2
Session 3
Session 4

SYMPOSIUM 5: Glass technology and cross-cutting topics
Session 1
Session 2
Session 3
Session 4

Local transportation –

Getting around town - Miami boasts a fully integrated mass transit system in order to get just about anywhere within the region. You can pick up the free Miami Metromover and the Miami Trolley from early morning to midnight. Ask the hotel staff for directions.

Panel Discussion for Students | Advice From the Experts on Publishing Your Scientific Research

Brought to you by SAINT-GOBAIN and ACerS' Global Graduate Researcher Network (GGRN)

ALL STUDENT ATTENDEES ARE INVITED TO ATTEND A PANEL DISCUSSION
WEDNESDAY, MAY 20, 12 – 1:20 p.m, during the GOMD - DGG 2015 meeting

Experts in the journal editing field will provide students with advice on scientific publishing. The panel discussion will be moderated by Mark Mecklenborg, Director of Membership, Meetings, and Technical Publications, The American Ceramic Society, and there will be three panelists:

1. **Matteo Cavalleri** is the managing editor for The American Ceramic Society's Journal portfolio, and is editor-in-chief, *International Journal of Quantum Chemistry*, at John Wiley & Sons, in Hoboken, New Jersey.
2. **L. David Pye** is Dean and Professor of Glass Science, Emeritus, Alfred University, and Editor of the *International Journal of Applied Glass Science*. He is Past President and Distinguished Life Member of The American Ceramic Society, Past President of the International Commission on Glass, and an aspiring stained glass artist.
3. **Josef W. Zwanziger** holds the Tier 1 Canada Research Chair in NMR Studies of Materials at Dalhousie University, in Halifax, Canada. His lab studies glass structure and optical properties with a range of techniques. He is one of the Editors of the *Journal of Non-Crystalline Solids.*

Lunch will be provided on a first come, first served basis. RSVP for the event is required. If you are interested in attending the panel discussion, please contact a representative at the registration desk to inquire if there is still space available.

GOMD Student Poster Contest Information

Sponsored by CORNING

MONDAY, MAY 18 | 6:30–8:30 p.m. | SYMPHONY BALLROOM

The GOMD Student Poster Contest, sponsored by Corning Incorporated, will again be held as part of the GOMD-DGG joint meeting in Miami. The contest will take place on Monday evening as part of the regular poster session that runs from 6:30 - 8:30 p.m. in Symphony Ballroom I. This year's contest is organized by **Yiquan Wu** of Alfred University.

Students need to set up their posters anytime from 3:20 – 5:00 p.m. Pins will be provided. Each contest participant should check the meeting program to find the paper number for their poster then look for the corresponding number on the poster boards. Students are expected to remain with their poster during the poster session so the judges can ask questions as needed. All posters must be removed from the boards at 8:30 p.m. that evening. Posters that are left on the boards will not be mailed back to students.

Winners of the poster contest will be announced at the conference dinner on Tuesday evening from 7:00 – 10:00 p.m. so please plan to attend.

Remember that the poster set-up time is 3:20 – 5:00 pm on Monday. Good luck to all students, and thanks to Corning for their generous sponsorship!

Save the date

APRIL 25–26, 2016 | CLEVELAND, OHIO

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- Panel discussions, moderated "fireside" chats, and talks
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CeramicTechToday FROM THE AMERICAN CERAMIC SOCIETY

2016 GLASS AND OPTICAL MATERIALS DIVISION

The Madison Concourse Hotel and Governor’s Club
Madison, Wisconsin

save the date

May 22 –26, 2016

Tentative Symposia

– Energy Applications of Glass—Fundamentals and Applications

– Health, Medical, Biological Aspects—Fundamentals and Applications

– Fundamentals of the Glassy State

– Optical and Electronic Materials and Devices—Fundamentals and Applications

– Glass Technology and Cross-cutting Topics

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Oral Presenters

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A				
Affatigato, M.	21-May	10:20AM	Symphony Ballroom I	34
Ahmad, N.	19-May	2:00PM	Concerto C	27
Ahmad, S.	19-May	2:20PM	Concerto B	24
Ahmed, I.	18-May	9:50AM	Symphony Ballroom IV	15
Alderman, O.	19-May	11:10AM	Symphony Ballroom II	22
Ali, S.	20-May	3:00PM	Symphony Ballroom II	30
Allix, M.	21-May	11:00AM	Concerto A	35
Almeida, R.M.	19-May	4:50PM	Concerto B	24
Alrasheedi, N.	20-May	2:40PM	Symphony Ballroom II	30
Amma, S.	20-May	10:00AM	Symphony Ballroom II	28
Angeli, F.	20-May	10:40AM	Concerto C	29
B				
Backhouse, D.J.	19-May	2:20PM	Concerto C	27
Balachandran, B.	19-May	2:40PM	Concerto B	24
Balasubramanian, P.	19-May	11:00AM	Symphony Ballroom IV	22
Baroni, A.	19-May	4:20PM	Symphony Ballroom IV	25
Bartolomey, S.	21-May	10:50AM	Symphony Ballroom III	33
Bassiri-Gharb, N.	20-May	2:50PM	Concerto B	32
Bauchy, M.	20-May	4:40PM	Symphony Ballroom IV	30
Beall, G.H.	20-May	9:20AM	Symphony Ballroom III	28
Benmore, C.J.	19-May	11:30AM	Symphony Ballroom II	22
Benmore, C.J.	20-May	9:50AM	Symphony Ballroom I	28
Bergmann, G.	18-May	4:00PM	Concerto C	19
Bergmann, G.	18-May	5:00PM	Concerto C	19
Bischoff, C.	18-May	3:00PM	Symphony Ballroom II	17
Bista, S.	20-May	2:40PM	Symphony Ballroom I	31
Biswas, P.	18-May	9:50AM	Concerto B	16
Bouzid, A.	18-May	4:00PM	Concerto B	18
Bouzid, A.	20-May	4:10PM	Symphony Ballroom I	31
Bradt, R.C.	19-May	9:20AM	Symphony Ballroom III	23
Brandt, J.	19-May	2:30PM	Symphony Ballroom IV	24
Brauer, D.S.	19-May	1:20PM	Symphony Ballroom IV	24
Bréhault, A.	18-May	10:50AM	Concerto A	16
Brow, R.	19-May	10:30AM	Symphony Ballroom IV	22
Buff, A.K.	20-May	3:40PM	Symphony Ballroom III	29
Busch, R.	20-May	1:20PM	Symphony Ballroom II	30
Bychkov, E.	19-May	1:50PM	Concerto B	24
C				
Cabral, A.A.	20-May	4:40PM	Symphony Ballroom III	29
Caillaud, C.	19-May	4:20PM	Concerto A	26
Cardinal, T.	18-May	9:50AM	Concerto A	16
Caurant, D.	19-May	10:30AM	Symphony Ballroom II	22
Chahal, R.	21-May	10:10AM	Symphony Ballroom II	34
Champagnon, B.	19-May	1:50PM	Symphony Ballroom III	25
Champagnon, B.	20-May	1:50PM	Symphony Ballroom I	31
Chapman, C.L.	18-May	4:40PM	Symphony Ballroom IV	17
Charpentier, T.	20-May	9:20AM	Symphony Ballroom IV	33
Chaysuwan, D.	19-May	2:50PM	Symphony Ballroom IV	25
Chen, G.	19-May	1:50PM	Symphony Ballroom II	25
Chen, W.W.	21-May	10:40AM	Concerto B	35
Chen, X.	20-May	4:20PM	Concerto A	31
Chinaglia, C.R.	18-May	4:20PM	Symphony Ballroom IV	17
Chinnam, R.	20-May	9:40AM	Concerto C	29
Choi, D.	19-May	2:00PM	Concerto A	26
Christie, J.K.	18-May	10:40AM	Symphony Ballroom IV	15
Christmann, A.I.	18-May	10:20AM	Concerto C	16
Cicconi, M.	20-May	11:20AM	Symphony Ballroom II	28
Corkhill, C.L.	19-May	1:40PM	Concerto C	26
Cormier, L.	20-May	10:50AM	Symphony Ballroom I	28
Cormier, L.	20-May	3:00PM	Symphony Ballroom III	29
Courtheoux, L.	20-May	2:10PM	Concerto B	32
Crawford, C.	19-May	10:50AM	Concerto C	23
Curtis, B.	19-May	11:30AM	Concerto B	22
D				
Danto, S.	19-May	4:40PM	Concerto A	26
Dasmahapatra, A.	20-May	11:00AM	Symphony Ballroom IV	33
Davis, M.J.	20-May	10:50AM	Symphony Ballroom III	28
Davis, M.J.	21-May	9:50AM	Concerto B	35
Day, D.	19-May	9:20AM	Symphony Ballroom IV	22
de Camargo, A.	18-May	4:00PM	Concerto A	19
de Ligny, D.	20-May	10:20AM	Symphony Ballroom I	28
Deinhardt, A.	18-May	10:20AM	Symphony Ballroom II	15
Deinhardt, A.	20-May	10:00AM	Concerto B	27
Dejneka, M.	18-May	11:20AM	Symphony Ballroom III	16
Dejneka, M.	21-May	10:40AM	Concerto A	34
deng, L.	19-May	3:40PM	Symphony Ballroom IV	25
Desmoulin, J.	19-May	10:10AM	Concerto A	23
Deubener, J.	19-May	4:30PM	Concerto B	24
Deubener, J.	20-May	2:20PM	Symphony Ballroom III	29
Diegeler, A.	20-May	4:20PM	Symphony Ballroom III	29
Dixon, D.	20-May	4:50PM	Concerto C	32
Dongol, R.	18-May	11:10AM	Concerto A	16
Dousti, M.	18-May	10:30AM	Concerto A	16
Drabold, D.	18-May	11:00AM	Concerto B	16
Dronskowski, R.V.	18-May	1:20PM	Concerto B	18
Du, J.	19-May	11:10AM	Concerto C	24
Du, Q.	19-May	1:20PM	Concerto A	26
Dubiel, M.	19-May	11:30AM	Concerto A	23
Duclere, J.	21-May	9:40AM	Concerto A	34
Dunn, B.	20-May	1:20PM	Concerto B	32
Duran, A.	20-May	4:50PM	Concerto B	32
Durschang, B.R.	20-May	11:20AM	Concerto B	27
Dussauze, M.	18-May	2:40PM	Concerto A	19
E				
Ebert, W.	19-May	5:20PM	Concerto C	27
Eckert, H.	18-May	4:50PM	Symphony Ballroom II	18
Eden, M.	18-May	1:20PM	Symphony Ballroom II	17
Elhadj, S.	19-May	10:50AM	Concerto A	23
Esteban, L.	19-May	1:50PM	Symphony Ballroom IV	24
Evans, A.	21-May	10:00AM	Concerto A	34
F				
Fargin, E.	18-May	10:10AM	Concerto A	16
Fayon, F.	18-May	9:50AM	Symphony Ballroom II	15
Feller, S.	18-May	3:40PM	Symphony Ballroom II	17
Ferrand, K.	19-May	2:40PM	Concerto C	27
Ford, D.C.	19-May	11:30AM	Concerto C	24
Foret, M.	21-May	10:40AM	Symphony Ballroom I	34
Fu, Q.	18-May	1:50PM	Symphony Ballroom IV	17
Fuhrmann, S.	20-May	9:20AM	Symphony Ballroom II	28
G				
Gan, H.	21-May	9:40AM	Concerto C	35
George, J.	19-May	11:20AM	Symphony Ballroom IV	22
Gin, S.	19-May	9:50AM	Concerto C	23
Glaesemann, G.S.	18-May	9:20AM	Symphony Ballroom III	15
Gleason, B.	21-May	10:50AM	Symphony Ballroom II	34
Goel, A.	21-May	11:00AM	Concerto C	35
Golovchak, R.	21-May	11:30AM	Symphony Ballroom III	33
Gomez, S.	18-May	10:40AM	Symphony Ballroom III	15
Gong, Y.	19-May	4:40PM	Concerto C	27
Gouillart, E.	20-May	5:00PM	Symphony Ballroom III	29
Gross, T.M.	18-May	11:00AM	Symphony Ballroom III	16
Guerette, M.J.	19-May	12:00PM	Symphony Ballroom IV	24
Guillen, D.P.	20-May	5:10PM	Concerto C	33
Gulbiten, O.	20-May	4:20PM	Symphony Ballroom II	30
Guo, X.	18-May	5:10PM	Symphony Ballroom II	18
Gupta, P.	19-May	3:20PM	Symphony Ballroom III	26
H				
Haaks, M.	19-May	10:20AM	Concerto B	22
Han, S.	21-May	11:20AM	Symphony Ballroom IV	34
Hannon, A.C.	19-May	10:10AM	Symphony Ballroom II	22
Harrison, M.	19-May	1:20PM	Concerto C	26
Hayashi, A.	19-May	1:20PM	Concerto B	24
He, H.	18-May	4:30PM	Symphony Ballroom III	18
Hench, L.L.	18-May	9:20AM	Symphony Ballroom IV	15
Heske, C.	19-May	3:40PM	Concerto B	24
Horbach, J.	20-May	2:40PM	Symphony Ballroom IV	30

Presenting Author List

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Huang, L.	19-May	2:30PM	Symphony Ballroom III	25
Huang, L.	21-May	11:40AM	Symphony Ballroom I	34
Huang, W.	19-May	4:10PM	Concerto B	24
Hubert, M.	18-May	11:00AM	Concerto C	16
Hubert, M.	18-May	4:20PM	Concerto C	19
Hunault, M.	19-May	3:40PM	Symphony Ballroom II	25
Hupa, L.	18-May	10:10AM	Symphony Ballroom IV	15

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Name	Date	Time	Room	Page Number
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Ito, S.	19-May	1:20PM	Symphony Ballroom III	25

J

Name	Date	Time	Room	Page Number
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Jain, V.	20-May	3:40PM	Concerto C	32
Jantzen, C.M.	19-May	10:10AM	Concerto C	23
Jin, T.	20-May	3:00PM	Concerto C	32
Johnson, B.S.	19-May	10:50AM	Symphony Ballroom II	22
Jones, J.	18-May	1:20PM	Symphony Ballroom IV	17
Jung, S.	18-May	3:40PM	Symphony Ballroom IV	17
Jung, S.	21-May	8:00AM	Symphony Ballroom IV	33

K

Name	Date	Time	Room	Page Number
Karlsson, S.	18-May	1:50PM	Symphony Ballroom III	18
Kaseman, D.C.	20-May	4:00PM	Symphony Ballroom II	30
Kasper, A.M.	18-May	11:40AM	Concerto C	17
Keles, O.	18-May	11:20AM	Symphony Ballroom IV	15
Kerisit, S.	19-May	3:40PM	Concerto C	27
Kieffer, J.	20-May	1:20PM	Symphony Ballroom III	29
Kim, C.	21-May	11:40AM	Concerto C	35
Kim, D.	20-May	2:40PM	Concerto C	32
Kim, D.	20-May	5:00PM	Symphony Ballroom IV	30
Kim, S.	20-May	5:40PM	Symphony Ballroom IV	30
Kim, S.H.	19-May	9:50AM	Symphony Ballroom III	23
Kim, W.	19-May	5:00PM	Concerto A	26
Kim, W.	20-May	2:10PM	Concerto A	31
Klein, L.C.	20-May	2:30PM	Concerto B	32
König, J.	20-May	10:50AM	Concerto B	27
Koudelka, L.	18-May	1:50PM	Symphony Ballroom II	17
Kovalskiy, A.	19-May	10:30AM	Concerto A	23
Kramer, D.	19-May	2:30PM	Symphony Ballroom II	25
Krenkel, S.	19-May	3:10PM	Symphony Ballroom IV	25
Kroeker, S.	18-May	2:30PM	Symphony Ballroom II	17
Kroll, P.	20-May	10:20AM	Symphony Ballroom IV	33
Krüger, S.	20-May	2:40PM	Symphony Ballroom III	29

L

Name	Date	Time	Room	Page Number
LaComb, M.	18-May	4:10PM	Symphony Ballroom II	17
Lamberson, L.	18-May	2:30PM	Symphony Ballroom III	18
Lampin, E.	20-May	1:20PM	Symphony Ballroom IV	30
Laux, S.	18-May	4:40PM	Concerto C	19
Lee, S.	19-May	1:20PM	Symphony Ballroom II	25
Lee, S.	19-May	9:50AM	Concerto B	22
Lepicard, A.	18-May	3:00PM	Concerto A	19
Lepry, W.C.	19-May	10:10AM	Symphony Ballroom IV	22
Lezzi, P.J.	18-May	3:30PM	Symphony Ballroom III	18
Li, K.	18-May	3:40PM	Concerto A	19
Li, L.	19-May	1:40PM	Concerto A	26
Li, N.	21-May	11:00AM	Symphony Ballroom IV	33
Li, Y.	20-May	1:50PM	Concerto A	31
Limbach, R.	18-May	10:20AM	Symphony Ballroom III	15
Liu, Q.	18-May	9:20AM	Concerto A	16
Liu, Y.	20-May	3:40PM	Concerto A	31
Lonnroth, N.	20-May	2:20PM	Symphony Ballroom I	31
Lubitz, G.	18-May	9:20AM	Concerto C	16
Lucas, P.	18-May	1:50PM	Concerto B	18
Lucas, P.	20-May	11:40AM	Symphony Ballroom II	28
Lucas, P.	20-May	3:40PM	Symphony Ballroom II	30
Luo, J.	18-May	4:50PM	Symphony Ballroom III	18

M

Name	Date	Time	Room	Page Number
Ma, L.	20-May	11:20AM	Concerto C	29
Mao, A.	20-May	5:20PM	Symphony Ballroom II	31
Marple, M.A.	19-May	11:10AM	Concerto B	22
Masselin, P.	19-May	9:20AM	Concerto A	23
Massobrio, C.	20-May	5:00PM	Symphony Ballroom II	30
Masuno, A.	21-May	11:00AM	Symphony Ballroom I	34
Matlack, K.S.	21-May	10:20AM	Concerto C	35
Matthias, A.	19-May	5:30PM	Concerto B	24
Mauro, J.C.	21-May	10:20AM	Symphony Ballroom IV	33
McCloy, J.	20-May	2:50PM	Concerto A	31
McCloy, J.	21-May	11:20AM	Concerto C	35
McLaren, C.	19-May	4:10PM	Symphony Ballroom I	26
Merdrignac-Conanec, O.	20-May	1:20PM	Concerto A	31
Micoulaut, M.	18-May	3:00PM	Concerto B	18
Micoulaut, M.	20-May	1:50PM	Symphony Ballroom III	29
Micoulaut, M.	20-May	3:40PM	Symphony Ballroom IV	30
Micoulaut, M.	20-May	4:40PM	Symphony Ballroom I	31
Miguez Pacheco, V.	18-May	2:30PM	Symphony Ballroom IV	17
Mitra, I.	20-May	9:50AM	Symphony Ballroom III	28
Mitsui, S.	19-May	10:30AM	Concerto C	23
Mizoguchi, T.	19-May	2:50PM	Symphony Ballroom II	25
Mohd-Noor, F.	19-May	9:50AM	Symphony Ballroom II	22
Møller, U.	20-May	9:20AM	Concerto A	28
Möncke, D.	20-May	10:40AM	Symphony Ballroom II	28
Montagne, L.	20-May	9:20AM	Concerto B	27
Morin, E.	18-May	4:30PM	Symphony Ballroom II	17

N

Name	Date	Time	Room	Page Number
Nakane, S.	20-May	10:20AM	Symphony Ballroom III	28
Neeway, J.J.	20-May	9:20AM	Concerto C	29
Neuville, D.R.	19-May	4:00PM	Symphony Ballroom II	25
Neuville, D.R.	21-May	9:50AM	Symphony Ballroom III	33
Neyret, M.	20-May	1:40PM	Concerto C	32
Niessen, V.	18-May	10:40AM	Concerto C	16
Nommeots-Nomm, A.	18-May	2:10PM	Symphony Ballroom IV	17
Novak, S.	19-May	2:20PM	Concerto A	26

O

Name	Date	Time	Room	Page Number
Oelgoetz, J.R.	20-May	5:20PM	Symphony Ballroom IV	30
Opila, E.J.	21-May	9:50AM	Symphony Ballroom I	34
Ori, G.	21-May	9:20AM	Symphony Ballroom IV	33
Orzol, D.	18-May	2:00PM	Concerto C	19

P

Name	Date	Time	Room	Page Number
Pacaud, F.	19-May	4:00PM	Symphony Ballroom IV	25
Pandey, A.	18-May	10:20AM	Concerto B	16
Pegg, I.L.	20-May	4:10PM	Concerto C	32
Pföss, B.	18-May	11:00AM	Symphony Ballroom IV	15
Pletser, D.	20-May	5:30PM	Concerto C	33
Podraza, N.	18-May	9:20AM	Concerto B	16
Poletto Rodrigues, B.	20-May	4:20PM	Symphony Ballroom IV	30
Pönitzsch, A.	18-May	2:10PM	Symphony Ballroom III	18
Potter, A.	20-May	11:00AM	Symphony Ballroom II	28
Pradel, A.	19-May	9:20AM	Concerto B	22
Prasai, K.	18-May	10:40AM	Concerto B	16
Prewitz, M.	20-May	11:40AM	Concerto B	27
Priven, A.	20-May	4:00PM	Symphony Ballroom IV	30
Prokhorenko, O.	18-May	2:40PM	Concerto C	19
Prokhorenko, O.	18-May	3:00PM	Concerto C	19
Prokhorenko, O.	21-May	11:40AM	Symphony Ballroom IV	34
Pukhkaya, V.	18-May	2:50PM	Symphony Ballroom III	18

Q

Name	Date	Time	Room	Page Number
Qiu, J.	19-May	8:00AM	Symphony Ballroom IV	21

R

Name	Date	Time	Room	Page Number
Raedlein, E.	18-May	2:20PM	Concerto C	19
Rahaman, M.N.	18-May	2:50PM	Symphony Ballroom IV	17
Rahaman, M.N.	19-May	9:50AM	Symphony Ballroom IV	22

Oral Presenters

Name	Date	Time	Room	Page Number
Rampf, M.	19-May	2:10PM	Symphony Ballroom IV	24
Rani, N.	19-May	5:40PM	Concerto C	27
Raty, J.	18-May	2:40PM	Concerto B	18
Reinsch, S.	19-May	11:30AM	Symphony Ballroom III	23
Reiser, J.	20-May	10:20AM	Concerto C	29
Rice, J.	19-May	5:00PM	Concerto C	27
Rimsza, J.M.	20-May	10:00AM	Symphony Ballroom IV	33
Rodrigues, A.M.	20-May	4:00PM	Symphony Ballroom III	29
Rodriguez, C.P.	20-May	2:20PM	Concerto C	32
Rodriguez, V.	18-May	1:20PM	Concerto A	18
Ronchetto, E.	18-May	3:50PM	Symphony Ballroom III	18
Rosales Sosa, G.A.	18-May	11:40AM	Symphony Ballroom III	16
Rössler, C.	19-May	10:50AM	Symphony Ballroom III	23
Roth, J.	19-May	4:30PM	Symphony Ballroom I	26
Ruffle, B.	20-May	3:00PM	Symphony Ballroom I	31
Ruffle, B.	21-May	10:20AM	Symphony Ballroom III	33
Ryan, J.V.	19-May	9:20AM	Concerto C	23
		S		
Saitoh, A.	20-May	10:20AM	Concerto A	29
Salmon, P.	19-May	9:20AM	Symphony Ballroom II	22
Salmon, P.	20-May	9:20AM	Symphony Ballroom I	28
Savytskyy, D.	19-May	9:50AM	Concerto A	23
Schaut, R.A.	19-May	4:50PM	Symphony Ballroom I	26
Schuller, S.	21-May	10:00AM	Concerto C	35
Seaman, J.H.	19-May	10:30AM	Symphony Ballroom III	23
Sen, S.	18-May	11:10AM	Symphony Ballroom II	15
Sen, S.	20-May	4:40PM	Symphony Ballroom II	30
Sen, S.	20-May	8:00AM	Symphony Ballroom IV	27
Serbena, F.C.	20-May	11:30AM	Symphony Ballroom III	28
Seuthe, T.	19-May	11:50AM	Concerto A	23
Sglavo, V.M.	19-May	5:00PM	Symphony Ballroom III	26
Sheth, N.	19-May	2:10PM	Symphony Ballroom II	25
Shoulders, T.	20-May	4:00PM	Concerto A	31
Sidebottom, D.	21-May	11:10AM	Symphony Ballroom III	33
Singh, N.B.	18-May	8:10AM	Symphony Ballroom IV	15
Sisken, L.	21-May	9:20AM	Concerto A	34
Skinner, L.	20-May	11:20AM	Symphony Ballroom IV	33
Smedskjaer, M.M.	21-May	9:20AM	Symphony Ballroom I	34
Smektala, F.	20-May	10:00AM	Concerto A	29
Smith, C.	20-May	11:50AM	Symphony Ballroom III	28
Smith, C.	21-May	9:50AM	Symphony Ballroom II	34
Smith, N.J.	19-May	4:20PM	Symphony Ballroom II	25
Somorowsky, F.N.	19-May	3:00PM	Concerto B	24
Sorin, F.	20-May	10:40AM	Concerto A	29
Stebbins, J.F.	18-May	9:20AM	Symphony Ballroom II	15
Su, X.	20-May	1:50PM	Concerto B	32
Sundararajan, M.	20-May	4:10PM	Concerto B	32
Suratwala, T.	18-May	2:20PM	Concerto A	19
Suratwala, T.	19-May	10:10AM	Symphony Ballroom III	23
Suratwala, T.	19-May	3:40PM	Symphony Ballroom I	26
Svenson, M.N.	21-May	11:20AM	Symphony Ballroom I	34
Swab, J.	21-May	10:20AM	Concerto B	35
		T		
Takebe, H.	20-May	9:40AM	Concerto B	27
Talimian, A.	19-May	4:40PM	Symphony Ballroom III	26
Tandia, A.	21-May	10:00AM	Symphony Ballroom IV	33
Tanguy, A.	20-May	3:40PM	Symphony Ballroom I	31
Tao, G.	19-May	3:40PM	Concerto A	26
Thapar, P.	19-May	5:10PM	Concerto B	24
Thiele, S.	18-May	11:20AM	Concerto C	16

Name	Date	Time	Room	Page Number
Trivelpiece, C.L.	18-May	4:20PM	Concerto A	19
Trivelpiece, C.L.	19-May	3:00PM	Concerto C	27
Trivelpiece, C.L.	19-May	4:00PM	Concerto C	27
Troles, J.	21-May	10:30AM	Symphony Ballroom II	34
		V		
van Wüllen, L.	18-May	10:40AM	Symphony Ballroom II	15
Vargheese, K.D.	20-May	2:00PM	Symphony Ballroom IV	30
Varshneya, A.	19-May	3:40PM	Symphony Ballroom III	26
Varshneya, A.	19-May	4:00PM	Symphony Ballroom III	26
Varshneya, A.	19-May	4:20PM	Symphony Ballroom III	26
Veber, A.	19-May	11:10AM	Concerto A	23
Vienna, J.	21-May	9:20AM	Concerto C	35
Vu, A.	18-May	3:40PM	Concerto C	19
		W		
Wall, N.A.	20-May	10:00AM	Concerto C	29
Wang, W.	20-May	4:30PM	Concerto B	32
Wang, W.	20-May	9:40AM	Symphony Ballroom II	28
Watson, D.	19-May	10:50AM	Concerto B	22
Weaver, J.L.	21-May	10:40AM	Concerto C	35
Weber, R.	18-May	1:50PM	Concerto A	19
Wei, S.	20-May	1:50PM	Symphony Ballroom II	30
Weigand, R.	18-May	1:20PM	Concerto C	19
Weigand, R.	18-May	1:40PM	Concerto C	19
Wereszczak, A.	21-May	11:00AM	Concerto B	35
Wereszczak, A.	21-May	9:20AM	Concerto B	35
Wiederhorn, S.	19-May	11:10AM	Symphony Ballroom III	23
Woelffel, W.	18-May	9:40AM	Concerto C	16
Woelffel, W.	20-May	10:20AM	Symphony Ballroom II	28
Wondraczek, L.	20-May	1:20PM	Symphony Ballroom I	31
Wondraczek, L.	20-May	10:20AM	Concerto B	27
Wondraczek, L.	21-May	9:20AM	Symphony Ballroom II	34
Wu, J.	18-May	2:10PM	Symphony Ballroom II	17
Wu, W.	20-May	2:20PM	Symphony Ballroom IV	30
		X		
Xu, K.	20-May	2:00PM	Concerto C	32
		Y		
Yang, Y.	20-May	2:30PM	Concerto A	31
Yano, T.	20-May	1:20PM	Concerto C	32
Yano, T.	20-May	11:00AM	Concerto C	29
Yildirim, C.	20-May	5:10PM	Symphony Ballroom I	31
Yoshida, S.	18-May	9:50AM	Symphony Ballroom III	15
Youngman, R.	18-May	11:40AM	Symphony Ballroom II	15
Youngman, R.	20-May	11:10AM	Symphony Ballroom III	28
Yu, Y.	20-May	10:40AM	Symphony Ballroom IV	33
Yue, Y.	20-May	11:20AM	Symphony Ballroom I	28
Yue, Y.	20-May	2:10PM	Symphony Ballroom II	30
Yue, Y.	21-May	9:20AM	Symphony Ballroom III	33
		Z		
Zamurs, A.Z.	18-May	10:00AM	Concerto C	16
Zanotto, E.D.	20-May	5:20PM	Symphony Ballroom III	29
Zeidler, A.	19-May	4:40PM	Symphony Ballroom IV	25
Zhang, J.	18-May	4:20PM	Concerto B	18
Zhang, L.	20-May	3:40PM	Concerto B	32
Zhang, X.	18-May	2:10PM	Concerto B	18
Zu, Q.	18-May	4:10PM	Symphony Ballroom III	18
Zwanziger, J.	18-May	1:20PM	Symphony Ballroom III	18
Zwanziger, J.	19-May	2:10PM	Symphony Ballroom III	25

Poster Presenters

Name	Date	Time	Room	Page Number
Amir, F.	18-May	6:00PM	Symphony Ballroom I	20
Bacha, M.G.	18-May	6:00PM	Symphony Ballroom I	21
Balasubramanian, P.	18-May	6:00PM	Symphony Ballroom I	20
Bischoff, C.	18-May	6:00PM	Symphony Ballroom I	21
Bréhault, A.	18-May	6:00PM	Symphony Ballroom I	20
Bychkov, E.	18-May	6:00PM	Symphony Ballroom I	20
Caurant, D.	18-May	6:00PM	Symphony Ballroom I	21
Cheng, K.	18-May	6:00PM	Symphony Ballroom I	20
Cho, J.	18-May	6:00PM	Symphony Ballroom I	21
Cook, J.	18-May	6:00PM	Symphony Ballroom I	20
Danto, S.	18-May	6:00PM	Symphony Ballroom I	20
de Ligny, D.	18-May	6:00PM	Symphony Ballroom I	21
Dechandt, I.C.	18-May	6:00PM	Symphony Ballroom I	20
Diegeler, A.	18-May	6:00PM	Symphony Ballroom I	21
Dongol, R.	18-May	6:00PM	Symphony Ballroom I	21
Fernandes, R.G.	18-May	6:00PM	Symphony Ballroom I	20
Ferreira, E.B.	18-May	6:00PM	Symphony Ballroom I	21
Fox, K.M.	18-May	6:00PM	Symphony Ballroom I	21
Freudenberger, P.T.	18-May	6:00PM	Symphony Ballroom I	20
Fuhrmann, S.	18-May	6:00PM	Symphony Ballroom I	21
Gong, Y.	18-May	6:00PM	Symphony Ballroom I	20
Hakari, T.	18-May	6:00PM	Symphony Ballroom I	20
Heffner, W.R.	18-May	6:00PM	Symphony Ballroom I	20
Hellmann, K.	18-May	6:00PM	Symphony Ballroom I	20
Hutchison, C.	18-May	6:00PM	Symphony Ballroom I	20
Ihalawela, C.A.	18-May	6:00PM	Symphony Ballroom I	20
Ito, Y.	18-May	6:00PM	Symphony Ballroom I	20
Kaseman, D.C.	18-May	6:00PM	Symphony Ballroom I	21
Kölker, K.	18-May	6:00PM	Symphony Ballroom I	19
Kroll, P.	18-May	6:00PM	Symphony Ballroom I	21
Lepicard, A.	18-May	6:00PM	Symphony Ballroom I	20
Manzani, D.	18-May	6:00PM	Symphony Ballroom I	19, 21
Marcial, J.	18-May	6:00PM	Symphony Ballroom I	20
Matsuyama, T.	18-May	6:00PM	Symphony Ballroom I	20
Pandey, A.	18-May	6:00PM	Symphony Ballroom I	21
Philipps, K.	18-May	6:00PM	Symphony Ballroom I	20
Prasai, K.	18-May	6:00PM	Symphony Ballroom I	20
Riley, B.	18-May	6:00PM	Symphony Ballroom I	21
Roth, N.	18-May	6:00PM	Symphony Ballroom I	20
Saturday, L.	18-May	6:00PM	Symphony Ballroom I	21
Schuller, S.	18-May	6:00PM	Symphony Ballroom I	21
Seuthe, T.	18-May	6:00PM	Symphony Ballroom I	21
Sidebottom, D.	18-May	6:00PM	Symphony Ballroom I	20
Souza, M.T.	18-May	6:00PM	Symphony Ballroom I	20
Stamminger, M.	18-May	6:00PM	Symphony Ballroom I	21
Svenson, M.N.	18-May	6:00PM	Symphony Ballroom I	20
Thai, A.	18-May	6:00PM	Symphony Ballroom I	21
Thirion, L.	18-May	6:00PM	Symphony Ballroom I	21
Wang, B.	18-May	6:00PM	Symphony Ballroom I	21
wang, J.	18-May	6:00PM	Symphony Ballroom I	21
Wang, R.	18-May	6:00PM	Symphony Ballroom I	20
Weaver, J.L.	18-May	6:00PM	Symphony Ballroom I	20
Whale, A.	18-May	6:00PM	Symphony Ballroom I	20
Wondraczek, L.	18-May	6:00PM	Symphony Ballroom I	21
Yu, Y.	18-May	6:00PM	Symphony Ballroom I	21
Zamyatin, O.	18-May	6:00PM	Symphony Ballroom I	21
Zu, Q.	18-May	6:00PM	Symphony Ballroom I	21

Monday, May 18, 2015

Stookey Lecture of Discovery Award

Room: Symphony Ballroom IV

8:00 AM

Introduction

8:10 AM

(GOMD-AL-001-2015) Development of multifunctional chalcogenide and chalcopyrite crystals and glasses (Invited)

N. B. Singh*[1]; 1. University of Maryland, Baltimore County

8:50 AM

Presentation of Award

9:00 AM

Break

Symposium 2: Glasses in Healthcare - Fundamentals and Applications

Design of Glasses for Biomedical Applications

Room: Symphony Ballroom IV

Session Chairs: Leena Hupa, Åbo Akademi University

9:20 AM

(GOMD-S2-001-2015) Bio-Ceramics: Unmet Challenges (Invited)

L. L. Hench*[1]; 1. University of Florida, USA

9:50 AM

(GOMD-S2-002-2015) Resorbable Glass Microspheres for Applications in Regenerative Medicine

I. Ahmed*[1]; Z. K. Hossain[1]; V. Sottile[1]; D. Grant[1]; B. Scammell[1]; 1. University of Nottingham, United Kingdom

10:10 AM

(GOMD-S2-003-2015) Tailoring bioactive glasses for various products (Invited)

L. Hupa*[1]; 1. Åbo Akademi University, Finland

10:40 AM

(GOMD-S2-004-2015) Structure of Mg-based bulk metallic glass

J. K. Christie*[1]; 1. University College London, United Kingdom

11:00 AM

(GOMD-S2-005-2015) Structuring surfaces of bioactive glasses at the micro scale by mould casting

B. Pföss*[1]; M. Höner[2]; M. Wirth[1]; T. Vossel[1]; H. Fischer[2]; A. Bührig-Polaczek[1]; R. Conradt[1]; 1. RWTH Aachen University, Germany; 2. University Hospital RWTH Aachen, Germany

11:20 AM

(GOMD-S2-006-2015) Modeling fracture behavior of porous glass

O. Keles*[1]; R. Garcia[2]; K. J. Bowman[1]; 1. Illinois Institute of Technology, USA; 2. Purdue University, USA

Symposium 3: Fundamentals of the Glassy State

Session 3: Structural Characterization of Glasses I

Room: Symphony Ballroom II

Session Chair: Hellmut Eckert, University of Sao Paulo

9:20 AM

(GOMD-S3-001-2015) Structure and dynamics in oxide glasses and glass-forming liquids: NMR progress and prognoses (Invited)

J. F. Stebbins*[1]; 1. Stanford University, USA

9:50 AM

(GOMD-S3-002-2015) Disorder in Strontium Aluminosilicate Glasses and Transparent Polycristalline Ceramics (Invited)

F. Fayon*[1]; K. Al Saghir[1]; S. Chenu[2]; E. Véron[1]; C. Genevoix[1]; G. Matzen[1]; D. Massiot[1]; M. Allix[1]; 1. CNRS, France; 2. limoges university, France

10:20 AM

(GOMD-S3-003-2015) Spectroscopic study on the influence of hydroxide ions on the UV-transparency of soda-lime silicate glass

A. Deinhardt*[1]; M. Kilo[1]; G. Sextl[2]; H. Eckert[3]; 1. Fraunhofer Institute for Silicate Research ISC, Germany; 2. University of Würzburg, Germany; 3. University of Münster, Germany

10:40 AM

(GOMD-S3-004-2015) The structure of glasses and its evolution above T_g – crystallisation, phase separation and species exchange: lessons from *in situ* MAS-NMR (Invited)

L. van Wüllen*[1]; S. Venkatachalam[1]; J. Holzinger[1]; M. Engelmayer[1]; 1. Augsburg University, Germany

11:10 AM

(GOMD-S3-005-2015) Probing glass/liquid structure and dynamics with novel NMR spectroscopic techniques (Invited)

S. Sen*[1]; D. C. Kaseman[1]; T. Edwards[1]; I. Hung[2]; Z. Gan[2]; 1. University of California, Davis, USA; 2. National High Field Magnetic Laboratory, USA

11:40 AM

(GOMD-S3-006-2015) Impact of Sodium Addition on the Structure and Properties of AlP Silicate Glasses

R. Youngman*[1]; B. Aitken[1]; 1. Corning Incorporated, USA

Session 5: Mechanical Properties of Glasses I

Room: Symphony Ballroom III

Session Chair: Lothar Wondraczek, University of Jena

9:20 AM

(GOMD-S3-007-2015) A History of Optical Fiber Strength and Reliability for the Benefit of Emerging Flexible Glass Applications (Invited)

G. S. Glaesemann*[1]; 1. Corning Incorporated, USA

9:50 AM

(GOMD-S3-008-2015) In-Situ Evaluation of Elastic and Inelastic Deformations of Glasses under Some Indenters (Invited)

S. Yoshida*[1]; S. Sasaki[1]; K. Wada[1]; M. Kato[1]; A. Yamada[1]; J. Matsuoka[1]; N. Soga[1]; 1. The University of Shiga Prefecture, Japan

10:20 AM

(GOMD-S3-009-2015) Plasticity, crack initiation and defect resistance in alkali-borosilicate glasses: From normal to anomalous behavior

R. Limbach*[1]; A. Winterstein-Beckmann[1]; A. Dellith[2]; D. Möncke[1]; L. Wondraczek[1]; 1. Friedrich Schiller University of Jena, Germany; 2. Leibnitz Institute of Photonic Technologies IPhT, Germany

10:40 AM

(GOMD-S3-010-2015) Structural study of alkali boroaluminosilicate glass: response to damage

S. Gomez*[1]; I. Dutta[1]; G. G. Moore[1]; M. P. Carson[1]; 1. Corning Incorporated, USA

11:00 AM

(GOMD-S3-011-2015) Structure and Mechanics of NBO-Free Calcium Boroaluminosilicate Glasses with B_2O_3 substituted for SiO_2

T. M. Gross*[1]; 1. Corning Inc., USA

11:20 AM

(GOMD-S3-012-2015) Damage Resistant Glasses with High Strength

M. Dejneka*[1]; T. Gross[1]; 1. Corning Incorporated, USA

11:40 AM

(GOMD-S3-013-2015) Crack Resistant Al_2O_3–SiO_2 Glasses Fabricated by Containerless Processing

G. A. Rosales Sosa*[1]; A. Masuno[1]; H. Inoue[1]; Y. Higo[2]; S. Kojima[3]; K. Tae Hyun[3]; K. Matsumoto[3]; 1. Institute of Industrial Science, The University of Tokyo, Japan; 2. The Japan Synchrotron Radiation Research Institute, Japan; 3. University of Tsukuba, Japan

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 1: Amorphous Semiconductors: Electronic Properties, Transport and Modeling

Room: Concerto B

Session Chair: Xiang-Hua Zhang, University of Rennes / CNRS

9:20 AM

(GOMD-S4-001-2015) Impact of Optical and Electrical Properties on Performance of Hydrogenated Silicon Based Photovoltaic and Microbolometer Devices (Invited)

N. Podraza*[1]; 1. University of Toledo, USA

9:50 AM

(GOMD-S4-002-2015) Hydrogen microstructure in amorphous silicon: A joint analysis from experimental data and *ab initio* interactions (Invited)

P. Biswas*[1]; 1. The University of Southern Mississippi, USA

10:20 AM

(GOMD-S4-003-2015) RMC-Force: toward a new strategy for materials modeling

A. Pandey*[1]; P. Biswas[2]; D. Drabold[1]; 1. Ohio Univeristy, USA; 2. University of Southern Mississippi, USA

10:40 AM

(GOMD-S4-004-2015) Band gap engineering: a computational approach

K. Prasai*[1]; P. Biswas[2]; D. Drabold[1]; 1. Ohio University, USA; 2. University of Southern Mississippi, USA

11:00 AM

(GOMD-S4-005-2015) Physics of a-Si:H night-vision devices (Invited)

D. Drabold*[1]; A. Pandey[1]; 1. Ohio University, USA

Session 3: Novel Optical Glass Materials

Room: Concerto A

Session Chair: Shibin Jiang, AdValue Photonics Inc

9:20 AM

(GOMD-S4-006-2015) Nanoparticles in matrixes to induce enhancement of optical nonlinearity (Invited)

Q. Liu*[1]; M. Song[1]; 1. Wuhan University, China

9:50 AM

(GOMD-S4-007-2015) Structure and optical properties of gallium oxide containing phosphate glasses

T. Cardinal*[1]; P. Hee[1]; M. Vangheluwe[2]; J. Desmoulin[1]; Y. Ledemi[3]; S. Danto[1]; Y. Petit[1]; S. Kroeker[4]; L. Canioni[2]; Y. Messaddeq[3]; R. Vallee[3]; 1. ICMCB, France; 2. LOMA, France; 3. COPL, Canada; 4. University of Manitoba, Canada

10:10 AM

(GOMD-S4-008-2015) A new system of gallate glasses: Ga_2O_3-GeO_2-Na_2O-BaO
Candidates for optical applications in the near infrared

E. Fargin*[1]; P. Hee[1]; Y. Ledemi[2]; M. Dussauze[3]; T. Skopak[1]; T. Cardinal[1]; S. Kroeker[4]; Y. Messaddeq[2]; 1. Institut de Chimie de la Matière Condensée de Bordeaux, France; 2. Centre d'Optique, Photonique et Laser, Canada; 3. Institut des Sciences Moléculaires, France; 4. University of manitoba, Canada

10:30 AM

(GOMD-S4-009-2015) Optical and spectroscopic properties of tungsten phosphate glasses containing silver nanoparticles

M. Dousti*[1]; A. de Camargo[1]; 1. Universidade de São Paulo, Brazil, Brazil

10:50 AM

(GOMD-S4-010-2015) Moldable multispectral glasses transparent from the visible up to the thermal infrared region

A. Bréhault*[1]; L. Calvez[1]; X. Zhang[1]; 1. Université de Rennes 1, France

11:10 AM

(GOMD-S4-011-2015) Molecular Dynamics Simulation of Glasses for Photomultiplier Tubes in Neutrino Detection

R. Dongol*[1]; T. Adama[2]; S. Sundaram[1]; 1. Alfred University, USA; 2. Corning Incorporated, USA

Symposium 5: Glass Technology and Cross-cutting Topics

Session 1: Challenges in Glass Manufacturing I

Room: Concerto C

Session Chair: Hong Li, PPG Industries, Inc.

9:20 AM

(GOMD-S5-001-2015) Container glass: Where have we been and where are we going?

G. Lubitz*[1]; 1. Vetropack Holding AG, Switzerland

9:40 AM

(GOMD-S5-002-2015) Physical and chemical mechanisms happening in soda-lime batch melting followed by *in situ* imaging

W. Woelffel*[1]; M. Chopinet[1]; M. J. Toplis[2]; E. Véron[4]; E. Boller[3]; E. Gouillart[1]; 1. Saint-Gobain Recherche/CNRS, France; 2. Observatoire Midi-Pyrénées, France; 3. European Synchrotron Radiation Facility, France; 4. Conditions Extrêmes et Matériaux : Haute Température et Irradiation, France

10:00 AM

(GOMD-S5-003-2015) The Use of Hot Stage Microscopy to Observe and Analyze Glass Formation Behavior

A. Z. Zamurs*[1]; 1. Rio Tinto Minerals, USA

10:20 AM

(GOMD-S5-004-2015) Influence of alumina and boron raw materials on the melt formation in sodium aluminoborosilicate batches

A. I. Christmann*[1]; O. Hochrein[2]; J. Deubener[1]; 1. Clausthal University of Technology, Germany; 2. SCHOTT AG, Germany

10:40 AM

(GOMD-S5-005-2015) Characterization of Accelerated Batch Melting by Using an Up-Scaling Method

V. Niessen*[1]; R. Conradt[1]; 1. RWTH Aachen University, Germany

11:00 AM

(GOMD-S5-006-2015) Factors influencing quality of reduced glasses and their experimental evaluation

M. Hubert*[1]; M. Rongen[1]; P. Marson[1]; A. Suarez Barcena[1]; M. van Kersbergen[1]; A. Faber[1]; S. Lessmann[1]; 1. CelSian Glass & Solar, Netherlands

11:20 AM

(GOMD-S5-007-2015) Mechanisms related to cleaning of boron containing flue gases

S. Thiele*[1]; R. Conradt[1]; 1. RWTH Aachen University, Germany

11:40 AM

(GOMD-S5-008-2015) Iron equilibrium in the float glass process
A. M. Kasper*[1]; 1. Saint Gobain, Germany

Symposium 2: Glasses in Healthcare - Fundamentals and Applications

Bioactive Glass Scaffolds and Implants for Bone Repair I

Room: Symphony Ballroom IV
Session Chair: Delbert Day, Missouri University of Science and Technology

1:20 PM

(GOMD-S2-007-2015) Bioactive glass scaffolds : sol-gel v melt-derived (Invited)
J. Jones*[1]; 1. Imperial College London, United Kingdom

1:50 PM

(GOMD-S2-008-2015) Bioactive glass for regeneration of large bone defects
Q. Fu*[1]; A. Tomsia[2]; 1. Corning Incorporated, USA; 2. Lawrence Berkeley National Laboratory, USA

2:10 PM

(GOMD-S2-009-2015) Porous bioactive glass foam scaffolds: Comparison of 3 compositions by 2 Processing Methods
A. Nommeots-Nomm*[1]; P. Lee[2]; E. Saiz[1]; J. Jones[1]; 1. Imperial College London, United Kingdom; 2. University of Manchester, United Kingdom

2:30 PM

(GOMD-S2-010-2015) Development and characterization of COPPER and NIOBIUM releasing silicate bioactive glasses
V. Miguez Pacheco*[1]; D. de Ligny[1]; D. S. Brauer[2]; K. Rottenbacher[2]; A. R. Boccaccini[1]; 1. University of Erlangen Nuremberg, Germany; 2. Friedrich Schiller University Jena, Germany

2:50 PM

(GOMD-S2-011-2015) Potential of Bioactive Glass Scaffolds as Implants for Structural Bone Repair
M. N. Rahaman*[1]; S. Bal[2]; L. F. Bonewald[3]; 1. Missouri S&T, USA; 2. University of Missuri-Columbia, USA; 3. University of Missouri-Kansas City, USA

3:10 PM

Break

Bioactive Glass Scaffolds and Implants for Bone Repair II

Room: Symphony Ballroom IV
Session Chair: Julian Jones, Imperial College London

3:40 PM

(GOMD-S2-012-2015) Review of a Commercial Bioactive Glass Scaffold Used in Human Spine Applications
S. Jung*[1]; 1. Mo-Sci Corporation, USA

4:00 PM

(GOMD-S2-013-2015) Cell-bioactive glass scaffold interactions: The role of substrate nano-structure
T. J. Kowal[1]; T. Chokshi[1]; R. Holovchak[1]; M. M. Falk[1]; H. Jain*[1]; 1. Lehigh University, USA

4:20 PM

(GOMD-S2-014-2015) Bactericide Action of a Titanium Surface Biofunctionalized with a Novel Bioactive Glass
C. R. Chinaglia*[1]; L. Campanini[1]; L. H. Pitaluga[1]; N. S. Silva[1]; C. W. Souza[1]; O. Peitl[1]; E. D. Zanotto[1]; 1. Federal University of São Carlos, Brazil

4:40 PM

(GOMD-S2-015-2015) Antimicrobial behavior of ion-exchanged silver in glass – the physics and chemistry
C. L. Chapman*[1]; C. Kosik Williams[1]; N. Borrelli[1]; Y. Wei[1]; O. Petzold[1]; 1. Corning Incorporated, USA

Symposium 3: Fundamentals of the Glassy State

Session 3: Structural Characterization of Glasses II

Room: Symphony Ballroom II
Session Chair: Randall Youngman, Corning Incorporated

1:20 PM

(GOMD-S3-014-2015) Rationalizing Composition-Structure Trends of Rare-Earth Aluminosilicate Glasses by Solid-State NMR and Molecular Dynamics Simulations (Invited)
A. Jaworski[1]; B. Stevensson[1]; B. Pahari[1]; S. Iftekhar[1]; M. Eden*[1]; 1. Stockholm University, Sweden

1:50 PM

(GOMD-S3-015-2015) Structure-property relationships in barium borophosphate glasses modified with niobium oxide
L. Koudelka*[1]; P. Kalenda[1]; P. Mosner[1]; L. Montagne[2]; B. Revel[2]; 1. University of Pardubice, Czech Republic; 2. University of Lille, France

2:10 PM

(GOMD-S3-016-2015) Effects of temperature and composition on boron-containing glass network structure
J. Wu*[1]; J. F. Stebbins[2]; 1. Corning Inc., USA; 2. Stanford University, USA

2:30 PM

(GOMD-S3-017-2015) High-Temperature NMR Spectroscopy of Phase Separation in Model Nuclear Waste Glasses (Invited)
S. Kroeker*[1]; J. Wren[1]; B. J. Greer[1]; 1. University of Manitoba, Canada

3:00 PM

(GOMD-S3-018-2015) Comparison of Sodium Phosphate and Thiophosphate Glass Structure
C. Bischoff*[1]; R. Brow[1]; S. Martin[2]; 1. Missouri University of Science and Technology, USA; 2. Iowa State University, USA

3:20 PM

Break

Session 3: Structural Characterization of Glasses III

Room: Symphony Ballroom II
Session Chair: Leo van Wüllen, Augsburg University

3:40 PM

(GOMD-S3-019-2015) Intermediate Range Order of Borate Glasses Found From ^{10}B NMR (Invited)
S. Feller*[1]; K. Goranson[1]; M. Faaborg[1]; E. Troendle[1]; N. Barnes[1]; M. Chace[1]; R. Rice[2]; M. Affatigato[1]; D. Holland[3]; M. Smith[4]; 1. Coe College, USA; 2. Simpson College, USA; 3. University of Warwick, United Kingdom; 4. University of Lancaster, United Kingdom

4:10 PM

(GOMD-S3-020-2015) Oxygen Speciation in Strontium Borate Glasses and Crystals: High Resolution ^{11}B and ^{17}O MAS NMR Analysis
M. LaComb*[1]; J. Stebbins[1]; 1. Stanford University, USA

4:30 PM

(GOMD-S3-021-2015) Changes of Al coordination with temperature in aluminoborosilicate glasses: effects of B concentration
E. Morin*[1]; J. F. Stebbins[1]; 1. Stanford University, USA

4:50 PM

(GOMD-S3-022-2015) Structure/Property Correlations in Fluorophosphate and Fluoroborate Glasses Studied by Solid State NMR

H. Eckert*[1]; M. de Oliveira[1]; A. de Camargo[1]; 1. University of Sao Paulo, Brazil

5:10 PM

(GOMD-S3-023-2015) Structure and Properties of Quaternary Network Former Glasses $20B_2O_3$-$8Al_2O_3$-xP_2O_5-$(72-x)SiO_2$

X. Guo*[1]; R. Youngman[1]; C. L. Hogue[1]; J. C. Mauro[1]; J. Wang[1]; 1. Corning Incorporated, USA

Session 5: Mechanical Properties of Glasses II

Room: Symphony Ballroom III

Session Chair: Scott Glaesemann, Corning Incorporated

1:20 PM

(GOMD-S3-024-2015) Adding topology to the Makishima-Mackenzie Modelsil (Invited)

M. Plucinski[1]; J. Zwanziger*[1]; 1. Dalhousie University, Canada

1:50 PM

(GOMD-S3-025-2015) Mechanical Properties of TiO_2 doped Soda-Lime-Silicate Glasses

S. Karlsson*[1]; R. Limbach[2]; K. Lundstedt[1]; L. Wondraczek[2]; 1. Glafo - the Glass Research Institute, Sweden; 2. Friedrich Schiller University of Jena, Germany

2:10 PM

(GOMD-S3-026-2015) Micromechanical properties in aluminophosphate glasse

A. Pönitzsch*[1]; J. Deubener[1]; 1. Institute for Non-Metallic Materials, Germany

2:30 PM

(GOMD-S3-027-2015) Influence of Atomic Structure on Mechanical Properties in Calcium-Aluminosilicate Glasses

L. Lamberson*[1]; R. Youngman[1]; S. Baker[2]; 1. Corning Incoporated, USA; 2. Cornell University, USA

2:50 PM

(GOMD-S3-028-2015) Plastic deformation of Na-aluminosilicate glasses under micro and nano-indentation

V. Pukhkaya*[1]; J. Teisseire[1]; M. Heili[2]; C. Martinet[2]; V. Martinez[2]; B. Champagnon[2]; G. Kermouche[3]; E. Barthel[4]; 1. Saint Gobain Recherche, France; 2. UMR5306 CNRS, France; 3. Ecole des Mines de Saint-Etienne, CNRS, France; 4. ESPCI, France

3:10 PM

Break

3:30 PM

(GOMD-S3-029-2015) Mechanical degradation and surface crystallization of silica glass fibers

P. J. Lezzi*[1]; E. E. Evke[1]; E. M. Aaldenberg[1]; M. Tomozawa[1]; 1. RPI, USA

3:50 PM

(GOMD-S3-030-2015) Aging and Fatigue of Soda-Lime-Silicate Glass Fiber

E. Ronchetto*[1]; R. K. Brow[1]; 1. Missouri University of Science and Technology, USA

4:10 PM

(GOMD-S3-031-2015) Mechanical properties of HS high strength glass fibers

Q. Zu*[1]; J. Liu[1]; Y. Zhang[1]; J. Zhou[1]; J. Li[1]; 1. Sinoma Science & Technology Co.,Ltd., China

4:30 PM

(GOMD-S3-032-2015) Effects of Counter-surface and Humidity on the Mechanochemical Wear of Soda Lime Glass

H. He*[1]; L. Qian[1]; C. Pantano[2]; S. Kim[2]; 1. Southwest Jiaotong University, China; 2. Pennsylvania State University, USA

4:50 PM

(GOMD-S3-033-2015) Effects of thermal poling on structural and mechanical properties of soda-lime glass surface

J. Luo*[1]; H. He[3]; C. G. Pantano[2]; S. H. Kim[1]; 1. Pennsylvannia State University, USA; 2. Department of Material Science, USA; 3. Southwest Jiaotong, China

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 1: Phase Change and Other Chalcogenide Materials

Room: Concerto B

Session Chairs: Parthapratim Biswas; David Drabold, Ohio University

1:20 PM

(GOMD-S4-012-2015) A chemical (bonding) perspective on phase-change and related materials (Invited)

R. V. Dronskowski*[1]; 1. RWTH Aachen University, Germany

1:50 PM

(GOMD-S4-013-2015) Doping of As-Te glassy semiconductors with transition metal elements

P. Lucas*[1]; B. Potter[1]; G. Coleman[1]; B. Bureau[2]; C. Boussard[2]; J. Adam[2]; 1. University of Arizona, USA; 2. University of Rennes, France

2:10 PM

(GOMD-S4-014-2015) Semiconducting chalcogenide glass ceramics with internal heterojunctions (Invited)

X. Zhang*[1]; Y. Xu[1]; Q. Shen[2]; B. Fan[1]; X. Qiao[2]; X. Fan[2]; L. Calvez[1]; H. Ma[1]; M. Cathelinaud[1]; 1. University of Rennes / CNRS, France; 2. Zhejiang University, China

2:40 PM

(GOMD-S4-015-2015) Aging mechanisms in amorphous GeTe

J. Raty*[1]; W. Zhang[2]; J. Luckas[2]; R. Mazzarello[2]; C. Bichara[3]; M. Wuttig[2]; 1. University of Liege, Belgium; 2. RWTH Aachen University, Germany; 3. CNRS and Aix-Marseille University, France

3:00 PM

(GOMD-S4-016-2015) Quantitative measure of tetrahedral-sp^3 geometries in amorphous Ge-Te and Ge-Si-Te phase change alloys

M. Micoulaut*[1]; P. Boolchand[2]; S. Ravindren[2]; K. Gunasekera[2]; 1. Universite Pierre-et-Marie Curie, France; 2. University of Cincinnati, USA

3:20 PM

Break

3:40 PM

(GOMD-S4-017-2015) Size Dependent Phase Transition Behavior of Amorphous Phase-change Sb_2Te_3 Nanowires

C. A. Ihalawela*[1]; M. Sundararajan[1]; X. Lin[2]; M. Kordesch[1]; G. Chen[1]; 1. Ohio University, USA; 2. Argonne National Lab, USA

4:00 PM

(GOMD-S4-018-2015) First principles study of the amorphous Ga4Sb6Te3 phase change alloy

A. Bouzid*[1]; S. Gabardi[2]; M. Boero[1]; C. Massobrio[1]; M. Bernasconi[2]; 1. Institut de physique et chimie des matériaux de Strasbourg, France; 2. Dipartimento di Scienza dei Materiali, Italy

4:20 PM

(GOMD-S4-019-2015) Near and mid-infrared emission from composite of PbSe quantum dots and chalcogenide glasses

J. Zhang*[1]; C. Liu[1]; X. Zhao[1]; J. Heo[2]; 1. Wuhan University of Technology, China; 2. Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), Republic of Korea

Session 3: Optical Material Processing and Characterization

Room: Concerto A

Session Chair: Shibin Jiang, AdValue Photonics Inc

1:20 PM

(GOMD-S4-020-2015) What can we learn in glass materials combining conventional infrared and Raman with unconventional hyper-Raman and hyper-Rayleigh techniques? (Invited)

V. Rodriguez*[1]; M. Dussauze[1]; S. Sirotkin[1]; G. Guéry[1]; T. Cardinal[1]; K. Richardson[2]; 1. University of Bordeaux, France; 2. University of Central Florida, USA

1:50 PM

(GOMD-S4-021-2015) Aerodynamic Levitator at the NOMAD Instrument for *in-situ* Investigation of Structure in Liquids and Glasses Formed in Extreme Conditions (Invited)

R. Weber*[1]; J. Neuefeind[2]; 1. Materials Development, Inc., USA; 2. Spallation Neutron Source, Oak Ridge National Laboratory, USA

2:20 PM

(GOMD-S4-022-2015) Towards understanding and controlling surface microroughness during glass polishing

T. Suratwala*[1]; R. Steele[1]; M. Feit[1]; R. Dylla-Spears[1]; R. Desjardin[1]; L. Wong[1]; N. Shen[1]; P. Miller[1]; 1. Lawrence Livermore Nat'l Lab, USA

2:40 PM

(GOMD-S4-023-2015) Thermally poled glasses: Towards a control of their structure and second order optical properties at the micrometer scale

M. Dussauze*[1]; A. Lepicard[1]; F. Adamietz[1]; K. Richardson[2]; T. Cardinal[1]; E. Fargin[1]; V. Rodriguez[1]; 1. University of Bordeaux, France; 2. University of Central Florida, USA

3:00 PM

(GOMD-S4-024-2015) Control of surface reactivity in borosilicate glasses using thermal poling

A. Lepicard*[1]; T. Cardinal[1]; V. Rodriguez[1]; K. Richardson[2]; M. Dussauze[1]; 1. University of Bordeaux, France; 2. University of Central Florida, USA

3:20 PM

Break

Session 3: Luminescent and Doped Glasses

Room: Concerto A

Session Chair: Juejun Hu, MIT

3:40 PM

(GOMD-S4-025-2015) Laser Properties of Tm^{3+}-doped Tellurite-Phosphate Glass Composite Fiber

K. Li*[1]; L. Hu[1]; P. Kuan[1]; X. Fan[1]; L. Zhang[1]; 1. Shanghai Institute of Optics and Fine Mechanics, China

4:00 PM

(GOMD-S4-026-2015) Efficient red emission of Eu^{3+}-doped new tungsten phosphate glasses

M. Dousti[2]; G. Y. Poirier[1]; A. de Camargo*[2]; 1. Institute of Science and Technology, Federal University of Alfenas, Brazil; 2. Physics Institute of São Carlos, University of São Paulo, Brazil

4:20 PM

(GOMD-S4-027-2015) Scintillating Glass/Polymer Composite Neutron Detectors

C. L. Trivelpiece*[1]; I. Jovanovic[1]; M. Mayer[1]; J. Nattress[1]; 1. Pennsylvania State University, USA

Symposium 5: Glass Technology and Cross-cutting Topics

Session 1: Challenges in Glass Manufacturing II

Room: Concerto C

Session Chairs: Irene Peterson, Corning Incorporated; Hong Li, PPG Industries, Inc.

1:20 PM

(GOMD-S5-009-2015) Optimized radiative heat transfer and service life of the crown in glass furnaces

R. Weigand*[1]; H. Hessenkemper[1]; A. Rössel[1]; D. Tritschel[1]; 1. TU Bergakademie Freiberg, Germany

1:40 PM

(GOMD-S5-010-2015) Lowering of refractory corrosion in enamel production

R. Weigand*[1]; H. Hessenkemper[1]; A. Rössel[1]; D. Tritschel[1]; 1. TU Bergakademie Freiberg, Germany

2:00 PM

(GOMD-S5-011-2015) Tribological investigations of the glass-metal contact in glass-container production

D. Orzol*[1]; C. Roos[2]; L. Wondraczek[1]; 1. Otto Schott Instute, FSU Jena, Germany; 2. IPGR, Switzerland

2:20 PM

(GOMD-S5-012-2015) Droplet formation in altered silicate glass surface

E. Raedlein*[1]; 1. Technische Universität Ilmenau, Germany

2:40 PM

(GOMD-S5-013-2015) Model of Continuous Fiber Drawing. II. Extended Parametric Study

O. Prokhorenko*[1]; 1. L.G.P. International, USA

3:00 PM

(GOMD-S5-014-2015) Model of Continuous Fiber Drawing. III. Criteria of Fiber Breakage

O. Prokhorenko*[1]; 1. L.G.P. International, USA

3:20 PM

Break

3:40 PM

(GOMD-S5-015-2015) An Integrative Approach for the Numerical Modeling-assisted Design of Non-isothermal Glass Molding Process for Complex Glass Optics

A. Vu*[1]; H. Kreilkamp[1]; G. Liu[1]; O. Dambon[1]; F. Klocke[1]; 1. Fraunhofer Institute for Production Technology, Germany

4:00 PM

(GOMD-S5-016-2015) Measurements and calculations for the production of lightweight hollow ware

G. Bergmann*[1]; N. Löber[1]; J. Simon[1]; H. Müller-Simon[1]; 1. Hüttentechnische Vereinigung der deutschen Glasindustrie e.V., Germany

4:20 PM

(GOMD-S5-017-2015) Energy efficiency improvements for glass furnaces

O. Verheijen[1]; A. Habraken[1]; L. Thielen[1]; J. van der Dennen[1]; M. van Kersbergen[1]; M. Hubert*[1]; 1. CelSian Glass & Solar, Netherlands

4:40 PM

(GOMD-S5-018-2015) Operating Experience with OPTIMELT™ Heat Recovery Technology on a Commercial Glass Furnace

S. Laux*[1]; A. Gonzalez Rodriguez[2]; H. Kobayashi[1]; A. Francis[1]; R. Bell[1]; E. Evenson[1]; 1. Praxair Inc, USA; 2. Grupo Pavisa, Mexico

5:00 PM

(GOMD-S5-019-2015) Scientific work and industrial research as an effective tool for being in step with glass industry

G. Bergmann*[1]; 1. Hüttentechnische Vereinigung der deutschen Glasindustrie e.V., Germany

Posters

Student Poster Competition

Room: Symphony Ballroom I

6:00 PM

(GOMD-SP-P001-2015) Specialty optical fibers for temperature sensing based on spontaneous Raman scattering

D. Manzani*[1]; H. Ebendorff-Heidepriem[2]; S. J. Ribeiro[1]; T. M. Monro[2]; 1. Institute of Chemistry, Brazil; 2. Institute for Photonics and Advanced Sensing, Australia

(GOMD-SP-P002-2015) Development Strategies for Fibre Glasses

K. Kölker*[1]; R. Conradt[1]; 1. RWTH Aachen University, Germany

(GOMD-SP-P003-2015) Na-based sulfide glasses for solid electrolyte

A. Bréhault*[1]; S. Cozic[1]; R. Boidin[2]; L. Calvez[1]; P. Masselin[3]; O. Bošák[4]; V. Labas[4]; E. Bychkov[3]; X. Zhang[1]; D. Le Coq[1]; 1. University of Rennes 1, France; 2. University of Pardubice, Czech Republic; 3. University of Littoral Côte d'Opale, France; 4. Slovak University of Technology, Slovakia

(GOMD-SP-P004-2015) Pressure-Induced Changes in Inter-Diffusivity, Compressive Stress, and Hardness in Chemically Strengthened Glass

M. N. Svenson*[1]; L. Thirion[2]; R. Youngman[2]; J. Mauro[2]; S. Rzoska[3]; M. Bockowski[3]; M. Smedskjær[1]; 1. Aalborg University, Denmark; 2. Corning Incorporated, USA; 3. Polish Academy of Sciences, Poland

(GOMD-SP-P005-2015) Phase Theoretical Development of Fiber Glasses

K. Hellmann*[1]; R. Conradt[1]; 1. RWTH Aachen Institute of Mineral Engineering, Germany

(GOMD-SP-P006-2015) Red Mud Recycling for Reinforcement Glass Fibers

S. V. Krogel[1]; K. Hellmann*[1]; S. Bunk[1]; F. M. Kaussen[1]; R. Conradt[1]; B. Friedrich[1]; 1. RWTH Aachen University, Germany

(GOMD-SP-P007-2015) Investigation of short range order and elastic properties of multicomponent oxide glasses

K. Philipps*[1]; R. P. Stoffel[1]; R. Conradt[1]; R. Dronskowski[1]; 1. RWTH Aachen University, Germany

(GOMD-SP-P008-2015) New Bioactive Glass Fibers for Soft Tissue Regeneration

M. T. Souza*[1]; O. Peitl[1]; M. Puzzi[2]; E. Dutra Zanotto[1]; 1. Universidade Federal de São Carlos, Brazil; 2. State University of Campinas, Brazil

(GOMD-SP-P009-2015) Atomic-Level Structure of Rare-Earth Doped (0.2 - 2 at%) Sodium Phosphate Glasses

F. Amir*[1]; C. Yoo[1]; E. S. Gunapala[1]; G. Marasinghe[1]; P. Akhter[4]; L. Skinner[2]; C. Benmore[2]; C. U. Segre[3]; K. Zhang[1]; T. Shibata[3]; R. K. Brow[5]; 1. University of North Dakota, USA; 2. Argonne National Laboratory, USA; 3. Illinois Institute of Technology, USA; 4. State University New york, USA; 5. Missouri University of Science and Technology, USA

(GOMD-SP-P010-2015) Tellurite glasses for the near-IR: from material design to fiber fabrication

S. Danto*[1]; T. Billotte[1]; N. Lo[1]; F. Désévédavy[2]; C. Strutynski[2]; S. Chenu[3]; M. Dussauze[1]; V. Rodriguez[1]; G. Délaizir[3]; J. Duclere[3]; P. Thomas[3]; F. Smektala[2]; K. Richardson[4]; E. Fargin[1]; T. Cardinal[1]; 1. University of Bordeaux, France; 2. University of Burgundy, France; 3. University of Limoges, France; 4. College of Optics & Photonics-UCF, USA

(GOMD-SP-P011-2015) The Structure and Properties of Glasses in the ZnO-B_2O_3-P_2O_5 System

P. T. Freudenberger*[1]; 1. Missouri University of Science and Technology, USA

(GOMD-SP-P012-2015) Rubidium Ion Conducting Glasses for Solid State Alkali Atom Sources

A. Whale*[1]; S. W. Martin[1]; J. Bernstein[2]; 1. Iowa State University, USA; 2. Charles Stark Draper Laboratory, USA

(GOMD-SP-P013-2015) Dynamic Light Scattering in Aluminophosphate Glass-forming Melts

A. Keller[1]; D. Sidebottom*[1]; 1. Creighton University, USA

(GOMD-SP-P014-2015) The shape of diopside glass particles probed by crystallization kinetics and DSC

R. G. Fernandes*[1]; E. B. Ferreira[1]; 1. University of São Paulo, Brazil

(GOMD-SP-P015-2015) A Sampling Method for Semi-Quantitative and Quantitative Electron Microprobe Analysis of Glass Surfaces

J. L. Weaver*[1]; J. Reiser[1]; O. Neill[1]; J. McCloy[1]; N. Wall[1]; 1. Washington State University, USA

(GOMD-SP-P016-2015) Structure of S-rich Binary As-S Spin-Coated Thin Films

J. Cook*[3]; P. Xiong-Skiba[3]; M. Vlcek[1]; H. Jain[2]; A. Kovalskiy[3]; 1. University of Pardubice, Czech Republic; 2. Lehigh University, USA; 3. Austin Peay State University, USA

(GOMD-SP-P017-2015) Evolution of Sodium Borosilicate Glasses in Humid Environments

Y. Gong*[1]; C. Yatongchai[1]; A. W. Wren[1]; C. Durucan[2]; N. P. Mellott[1]; 1. Alfred University, USA; 2. Middle East Technical University, Turkey

(GOMD-SP-P018-2015) The effect of heat treatment schedule on the composition and microstructure of aluminosilicate crystals in High-Alumina High-Level Nuclear Waste glasses

J. Marcial*[1]; J. S. McCloy[1]; O. K. Neill[1]; 1. Washington State University, USA

(GOMD-SP-P019-2015) Characterization of Na_2S-P_2S_5 glassy electrolyte thin films preparesd by pulsed laser deposition

Y. Ito*[1]; A. Hayashi[1]; M. Tatsumisago[1]; 1. Osaka Prefecture University, Japan

(GOMD-SP-P020-2015) Second Harmonic Generation stability in Chalcogenide glasses

A. Lepicard*[2]; V. Rodriguez[1]; K. Richardson[2]; M. Dussauze[1]; 1. University of Bordeaux, France; 2. University of Central Florida, USA

(GOMD-SP-P021-2015) Heterogeneous Nucleation on Palladium doped $Li_2O.2SiO_2$ glass by Differential Thermal Analysis

N. Roth*[1]; K. S. Ranasinghe[1]; 1. Southern Polytechnic State University, USA

(GOMD-SP-P022-2015) Growth Mechanism of Amorphous Sb_2Te_3 Thin Films and Nanowires Prepared by Electrochemical Deposition

C. A. Ihalawela*[1]; M. Sundararajan[1]; X. Lin[2]; M. Kordesch[1]; G. Chen[1]; 1. Ohio University, USA; 2. Argonne National Lab, USA

(GOMD-SP-P023-2015) Simulations of silver-doped germanium-selenide glasses and their response to radiation

K. Prasai*[1]; D. Drabold[1]; 1. Ohio University, USA

(GOMD-SP-P024-2015) Corrosion Study of a Glass Composite Material for Intermediate Level waste Disposal

C. Hutchison*[1]; 1. Imperial College London, United Kingdom

(GOMD-SP-P025-2015) Characterization of silicate bioactive glasses with combined polyvalent ions

F. Stölzel[2]; A. Lenhart[2]; R. detsch[1]; A. hoppe[1]; P. Balasubramanian*[1]; A. R. Boccaccini[1]; 1. University of Erlangen-Nuremberg, Germany; 2. Technische Hochschule Nürnberg Georg-Simon Ohm, Germany

Poster Session

Room: Symphony Ballroom I

6:00 PM

(GOMD-S1-P001-2015) Preparation of Composite Positive Electrodes with Li_3PS_4 Glass as Active Material for All-Solid-State Lithium Secondary Batteries

T. Hakari*[1]; M. Nagao[1]; A. Hayashi[1]; M. Tatsumisago[1]; 1. Osaka Prefecture University, Japan

(GOMD-S1-P002-2015) Comparison of electrochemical performance between amorphous and crystalline TiS_3 positive electrodes in all-solid-state lithium batteries with sulfide solid electrolytes

T. Matsuyama*[1]; M. Deguchi[1]; A. Hayashi[1]; M. Tatsumisago[1]; T. Ozaki[2]; Y. Ishii[1]; Y. Togawa[1]; S. Mori[1]; 1. Osaka Prefecture University, Japan; 2. Technology Research Institute of Osaka Prefecture, Japan

(GOMD-S1-P003-2015) Ion transport and atomic structure of rubidium chloride doped sulphide glasses

M. Bokova[1]; F. Hindle[1]; A. Cuisset[1]; E. Bychkov*[1]; I. Alekseeev[2]; A. M. Whale[3]; S. W. Martin[3]; 1. University of Littoral, France; 2. St Petersburg University, Russian Federation; 3. Iowa State University, USA

(GOMD-S2-P004-2015) Sol-gel preparation of calcium sulphate/bioglass composite and its in vitro evaluation

K. Cheng*[1]; Q. Lv[1]; X. He[1]; W. Weng[1]; 1. Zhejiang University, China

(GOMD-S2-P005-2015) Bioactivity of $2Na_2O.1CaO.3SiO_2$-P_2O_5 glasses

I. C. Dechandt*[1]; G. D. Dogado[1]; F. C. Serbena[1]; 1. State University of Ponta Grossa, Brazil

(GOMD-S3-P006-2015) Role of glass homogeneity in Ge-As-Se system

R. Wang*[1]; Z. Yang[1]; B. Luther-Davies[1]; 1. Australian National University, Australia

(GOMD-S3-P007-2015) Exploring relaxation and the glass transition with sugar glasses and home-built apparatus

W. R. Heffner*[1]; K. E. Calay[1]; 1. Lehigh University, USA

(GOMD-S4-P008-2015) Teaching Nano-particle Fluorescence in Glass with Candy

W. R. Heffner*[1]; D. Wright III[2]; 1. Lehigh University, USA; 2. Oakwood University, USA

(GOMD-S3-P009-2015) Crystallization versus temperature in an iron-rich lead aluminosilicate composition: a contribution to the understanding of French Renaissance glazes preparation
N. Capobianco[1]; G. Wallez[1]; A. Bouquillon[2]; D. Caurant*[1]; C. Doublet[2]; P. Lehuédé[2]; 1. CNRS, France; 2. C2RMF, France

(GOMD-S3-P010-2015) Evaluation of critical cooling rate of silicate melts by the guided random parameterization method
E. B. Ferreira*[1]; E. D. Zanotto[2]; 1. Engineering School of São Carlos/USP, Brazil; 2. UFSCar, Brazil

(GOMD-S3-P011-2015) Thermooptical devices for the investigation of the properties of glass at high temperatures
M. Kilo[1]; A. Diegeler*[1]; F. Raether[2]; B. Durschang[1]; M. Krauss[1]; 1. Fraunhofer ISC, Germany; 2. Fraunhofer HTL, Germany

(GOMD-S3-P012-2015) Thermal analysis of novel multifunctional glasses and glass-ceramics for IR photonics
L. Saturday*[1]; C. Johnson[1]; Y. Shpotyuk[2]; R. Golovchak[1]; 1. Austin Peay State University, USA; 2. University of Rennes, France

(GOMD-S3-P013-2015) The effect of Li2O, Na2O, and ZnO on phase separation of TeO2 glass towards porous tellurite microsphere in vapor adsorption application
J. wang*[1]; 1. NSYSU University, Taiwan

(GOMD-S3-P015-2015) NMR Structural Investigation of Zinc Borophosphate Glasses
C. Bischoff*[1]; P. T. Freudenberger[1]; R. Brow[1]; 1. Missouri University of Science and Technology, USA

(GOMD-S3-P016-2015) Relaxation processes of densified silica glass: structural approach
A. Cornet[1]; C. Martinet[1]; B. Champagnon[1]; V. Martinez[1]; D. de Ligny*[2]; 1. Institut Lumière Matière, France; 2. Universität Erlangen-Nuremberg, Germany

(GOMD-S3-P017-2015) Study of Bi and Ga incorporation in glassy selenides and tellurides
A. Thai*[1]; R. Golovchak[1]; Y. Shpotyuk[2]; W. R. Heffner[3]; H. Jain[3]; 1. Austin Peay State University, USA; 2. Université de Rennes 1, France; 3. Lehigh University, USA

(GOMD-S3-P018-2015) Structure-Property Relationships in Chalcogenide Glasses: Novel Insights from 2D High-Resolution ^{77}Se NMR Spectroscopy
D. C. Kaseman*[1]; I. Hung[2]; Z. Gan[2]; B. Aitken[3]; S. Sen[1]; 1. University of California Davis, USA; 2. National High Magnetic Field Laboratory, USA; 3. Corning Inc, USA

(GOMD-S3-P019-2015) Glass Transition and Reversibility in Silicate Glasses
Y. Yu*[1]; B. Wang[1]; Y. Lee[1]; M. Micoulaut[2]; M. Bauchy[1]; 1. UCLA, USA; 2. Université Pierre et Marie Curie, France

(GOMD-S3-P020-2015) Rigidity Theory Applied to Amorphization of Nano-Materials
B. Wang*[1]; Y. Yu[1]; M. Bauchy[1]; 1. University of California, Los Angeles, USA

(GOMD-S3-P021-2015) Structural Rigidity During Radiation-Induced Amorphization
B. Wang*[1]; Y. Yu[1]; M. Bauchy[1]; 1. University of California, Los Angeles, USA

(GOMD-S3-P022-2015) Combining Ab-Initio GIPAW Calculations and Experimental ^{29}Si NMR Spectra to Analyze the Structure of Amorphous Silicon Oxycarbides
J. P. Nimmo[1]; P. Kroll*[1]; 1. UT Arlington, USA

(GOMD-S3-P023-2015) Mechanical properties and thermal history dependence of melt quenched glass in comparison to amorphized zeolite material
T. Palenta[1]; S. Fuhrmann*[1]; M. Mackovic[2]; E. Spiecker[2]; L. Wondraczek[1]; 1. University Jena Otto-Schott Institute for Materials Research, Germany; 2. Friedrich-Alexander University Erlangen; Center for Nanoanalysis and Electron Microscopy, Germany

(GOMD-S3-P024-2015) Strength of SiO_2-$A1_2O_3$-MgO glass fibers at high temperature
Q. Zu*[1]; Y. Zhang[1]; S. Huang[1]; W. Song[1]; 1. Sinoma Science & Technology Co.,Ltd., China

(GOMD-S4-P027-2015) Electrical Activity of Boron and Phosphorous in Hydrogenated Amorphous Silicon
A. Pandey*[1]; B. Cai[2]; D. Drabold[1]; 1. Ohio Univeristy, USA; 2. Washington University School of Medicine, USA

(GOMD-S4-P028-2015) Optical thermometry based on visible upconversion luminescence of Er^{3+} and Er^{3+}/Yb^{3+} co-doped tellurite glasses and optical fibers
D. Manzani*[1]; K. Nigoghossian[1]; V. A. Rivera[2]; S. J. Ribeiro[1]; 1. Institute of Chemistry, Brazil; 2. Instituto de Física de São Carlos, Brazil

(GOMD-S4-P029-2015) Ultraviolet transmission spectrum of synthetic fused silica containing molecular oxygen
M. Stamminger*[1]; 1. Heraeus, Germany

(GOMD-S4-P030-2015) Precipitation of divalent Pd and metallic Pd nanostructures in glass for UV plasmonics
D. Bust[1]; S. Fuhrmann[1]; K. Wondraczek[4]; D. Möncke[1]; H. Ebendorff-Heidepriem[3]; E. Spiecker[2]; L. Wondraczek*[1]; 1. University of Jena, Germany; 2. University of Erlangen-Nuremberg, Germany; 3. University of Adelaide, Australia; 4. Leibniz Institute of Photonic Technologies, Germany

(GOMD-S4-P031-2015) Effect of oxide buffer layer and microstructure on the optical properties of VO_2 film deposited on soda lime silicate window glass
J. Cho*[1]; H. Koo[1]; C. Park[1]; 1. Seoul National University, Republic of Korea

(GOMD-S4-P032-2015) Relaxation phenomena in fs-laser modified glass studied by μ-Raman-spectroscopy
T. Seuthe*[1]; A. Mermillod-Blondin[2]; M. Grehn[3]; J. Bonse[4]; M. Eberstein[1]; 1. Fraunhofer IKTS, Germany; 2. Max-Born-Institute for Nonlinear Optics and Short Pulse Spectroscopy, Germany; 3. Technische Universität Berlin, Germany; 4. BAM - Federal Institute for Materials Research and Testing, Germany

(GOMD-S4-P033-2015) Compressive Stress Profiles of Chemically Strengthened Glass After Exposure to High Voltage Electric Fields
L. Thirion*[1]; E. Streltsova[1]; M. He[1]; J. Mauro[1]; 1. Corning Incorporated, USA

(GOMD-S4-P034-2015) Impurity absorption of *d*-elements in tellurite-molybdate glasses
O. Zamyatin*[1]; A. Sibirkin[1]; M. Churbanov[1]; E. Torokhova[1]; 1. Lobachevsky State University of Nizhni Novgorod, Russian Federation

(GOMD-S4-P035-2015) Infrared-Transparent Glass Ceramics: an Exploratory Study
B. Riley*[2]; J. McCloy[1]; D. A. Pierce[2]; 1. Washington State University, USA; 2. Pacific Northwest National Laboratory, USA

(GOMD-S5-P036-2015) Sintering of glasses with concurrent crystallization assisted by DC electric field
M. G. Bacha*[1]; E. B. Ferreira[1]; 1. University of São Paulo, Brazil

(GOMD-S5-P037-2015) Insight into chemical reactivity during nuclear glass synthesis
E. Boué[1]; S. Schuller*[1]; A. Mesbah[2]; T. Charpentier[1]; S. Poissonnet[1]; M. Toplis[3]; 1. CEA, France; 2. ICSM, France; 3. CNRS, France

(GOMD-S5-P038-2015) Advanced Nuclear Waste Glass Development for the DOE Hanford Site
K. M. Fox*[1]; D. K. Peeler[1]; A. A. Kruger[2]; 1. Savannah River National Laboratory, USA; 2. U.S. Department of Energy Office of River Protection, USA

(GOMD-S5-P039-2015) Comparison of corrosion of rare earth oxides containing borophosphate and borosilicate glasses
M. Wang[1]; W. Deng[2]; R. Dongol*[2]; B. Clark[2]; P. Tumurugoti[2]; N. Mellott[2]; S. Sundaram[2]; 1. Inner Mongolia University of Science and Technology, China; 2. New York State College of Ceramics, Alfred University, USA

Tuesday, May 19, 2015

George W. Morey Award Lecture

Room: Symphony Ballroom IV

8:00 AM

(GOMD-AL-001-2015) Control of the metastable state of glasses (Invited)
J. Qiu*[1]; 1. South China University of Technology, China

8:50 AM

Presentation of Award

9:00 AM

Break

Symposium 1: Energy and Environmental Aspects - Fundamentals and Applications

Session 2: Glassy Solid Electrolytes I

Room: Concerto B

Session Chair: Steve Martin, Iowa State University

9:20 AM

(GOMD-S1-001-2015) Ion conducting borophosphate glasses and development of all solid state batteries (Invited)

A. Pradel*[1]; M. Ribes[1]; A. Piarristeguy[1]; G. Silly[1]; 1. Université Montpellier 2, France

9:50 AM

(GOMD-S1-002-2015) Silicon-based Lihium Superionic Conductor for Solid-State Lithium Metal Battery (Invited)

S. Lee*[1]; 1. University of Colorado Boulder, USA

10:20 AM

(GOMD-S1-003-2015) ^{7}Li NMR studies of lithium ion dynamics in ceramics (Invited)

M. Haaks*[1]; R. Riedel[1]; S. Martin[2]; M. Vogel[1]; 1. TU Darmstadt, Germany; 2. Iowa State University of Science & Technology, USA

10:50 AM

(GOMD-S1-004-2015) The Mixed Glass Former Effect in Glassy Solid State Electrolytes: Structural Properties, Physical Properties and Ionic Conductivities of the $0.5Na_2S + 0.5[xSiS_2 + (1-x) PS_{5/2}]$ glass system

D. Watson*[1]; B. Curtis[1]; S. Martin[1]; 1. Iowa State University, USA

11:10 AM

(GOMD-S1-005-2015) Glass formation and fast Ag ion conduction in the system Ag_2Se-Ga_2Se_3-$GeSe_2$

M. A. Marple*[1]; S. Kim[1]; B. Aitken[2]; S. Sen[1]; 1. University of California Davis, USA; 2. Corning Incorporated, USA

11:30 AM

(GOMD-S1-006-2015) Physical and Structural Properties of Glassy Solid State Electrolytes of the $0.2Na_2O + 0.8[xB_2O_3 + (1-x) GeO_2]$ Series

B. Curtis*[1]; S. Keizer[2]; J. Wang[2]; M. Dettman[2]; D. Hynek[2]; S. Feller[2]; S. Martin[1]; 1. Iowa State University, USA; 2. Coe College, USA

Symposium 2: Glasses in Healthcare - Fundamentals and Applications

Borate-based Bioactive Glass

Room: Symphony Ballroom IV

Session Chairs: Steven Jung, Mo-Sci Corporation; Qiang Fu, Corning Incorporated

9:20 AM

(GOMD-S2-016-2015) Angiogenic Response of Bioactive Borate Glass Beads and Microfibers in "Hairless" Mice (Invited)

R. Watters[1]; R. Brown[1]; D. Day*[1]; 1. Missouri University of Science and Technology, USA

9:50 AM

(GOMD-S2-017-2015) In Vitro and In Vivo Evaluation of Borate Bioactive Glass Microfibers for Soft Tissue Repair

M. N. Rahaman*[1]; W. Huang[2]; C. Zhang[3]; 1. Missouri S&T, USA; 2. Tongji University, China; 3. Shanghai Jiaotong University, China

10:10 AM

(GOMD-S2-018-2015) Gel-Derived Borate Glasses for Bone Tissue Engineering

W. C. Lepry*[1]; M. James-Bhasin[1]; S. Nazhat[1]; 1. McGill University, Canada

10:30 AM

(GOMD-S2-019-2015) Dissolution Kinetics and Conversion to Hydroxyapatite of Bioactive Borate Glasses (Invited)

R. Brow*[1]; J. George[1]; K. Goetschius[1]; 1. Missouri S&T, USA

11:00 AM

(GOMD-S2-020-2015) Development, Characterization and In Vitro Bioactivity Study of Boron-containing Silicate, Borosilicate and Borate Bioactive Glass Scaffolds

P. Balasubramanian*[1]; B. Jokić[2]; A. Malchere[3]; L. Gremillard[3]; J. Jones[4]; J. Chevalier[3]; A. Boccaccini[1]; 1. University of Erlangen-Nuremberg, Germany; 2. University of Belgrade, Serbia; 3. INSA Lyon, France; 4. Imperial College London, United Kingdom

11:20 AM

(GOMD-S2-021-2015) *In-vitro* dissolution of a bioactive borate glass under dynamic conditions

J. George*[1]; R. K. Brow[1]; 1. Missouri University of Science and Technology, USA

Symposium 3: Fundamentals of the Glassy State

Session 3: Structural Characterization of Glasses IV

Room: Symphony Ballroom II

Session Chair: Gang Chen, Ohio University

9:20 AM

(GOMD-S3-034-2015) Identifying and characterising the different structural length scales in glassy materials (Invited)

P. Salmon*[1]; A. Zeidler[1]; 1. University of Bath, United Kingdom

9:50 AM

(GOMD-S3-035-2015) Isotope Substitution Neutron Diffraction Study of the Lithium and Tellurium Environments in Binary Li_2O-TeO_2 Glasses

F. Mohd-Noor*[1]; D. Holland[1]; A. Hannon[2]; E. R. Barney[3]; 1. University of Warwick, United Kingdom; 2. Rutherford Appleton Laboratory, United Kingdom; 3. University of Nottingham, United Kingdom

10:10 AM

(GOMD-S3-036-2015) The Structure of Arsenic Sulphide Glasses: Evidence for Tetrahedral Units?

A. C. Hannon*[1]; A. Cuisset[2]; E. Bychkov[2]; 1. ISIS Facility, United Kingdom; 2. Université du Littoral, France

10:30 AM

(GOMD-S3-037-2015) Structural investigations on glasses belonging to the SiO_2-B_2O_3-La_2O_3 system

D. Caurant*[1]; H. Trégouët[1]; O. Majérus[1]; T. Lerouge[1]; L. Cormier[2]; T. Charpentier[3]; H. Vezin[4]; 1. CNRS, France; 2. UPMC, France; 3. CEA, France; 4. Université de Lille1, France

10:50 AM

(GOMD-S3-038-2015) Study of Fluorophlogopite Crystallization using *in-situ* X-ray Diffraction and Pair Distribution Function

B. S. Johnson*[1]; C. Chung[1]; J. L. Jones[1]; 1. North Carolina State University, USA

11:10 AM

(GOMD-S3-039-2015) Local structure of molten borates: testing the temperature dependent predictions of thermodynamic models

O. Alderman*[1]; C. Benmore[2]; L. Skinner[2]; M. Liška[3]; J. Macháček[4]; A. Tamalonis[1]; A. Lin[5]; R. Weber[1]; 1. Materials Development Inc., USA; 2. Advanced Photon Source, Argonne National Laboratory, USA; 3. Vitrum Laugaricio – Joint Glass Center of IIC SAS, TnUAD, and FChPT STU, Slovakia; 4. Institute of Chemical Technology, Czech Republic; 5. Northwestern University, USA

11:30 AM

(GOMD-S3-040-2015) Advances in high energy x-ray scattering from glasses (Invited)

C. J. Benmore*[1]; L. Skinner[2]; O. Alderman[3]; R. Weber[3]; 1. Argonne National Laboratory, USA; 2. Stony Brook University, USA; 3. Materials Development Inc., USA

Session 5: Mechanical Properties of Glasses III

Room: Symphony Ballroom III

Session Chair: Satoshi Yoshida, The University of Shiga Prefecture

9:20 AM

(GOMD-S3-041-2015) The Crack Tip in SLS and FS Glass from a Fracture Mechanics Perspective (Invited)

R. C. Bradt*[1]; 1. University of Alabama, USA

9:50 AM

(GOMD-S3-042-2015) Glass-water interactions – lessons from surface-sensitive spectroscopy, indentation, and scratch tests

N. Surdyka[1]; H. He[1]; J. Luo[1]; L. Bradley[1]; N. Sheth[1]; C. Pantano[1]; S. H. Kim*[1]; 1. Pennsylvania State University, USA

10:10 AM

(GOMD-S3-043-2015) Chemical-mechanical characteristics & the formation of the Bielby layer on polished glass surfaces

T. Suratwala*[1]; N. Shen[1]; R. Steele[1]; M. Feit[1]; L. Wong[1]; R. Dylla-Spears[1]; R. Desjardin[1]; P. Miller[1]; 1. Lawrence Livermore Nat'l Lab, USA

10:30 AM

(GOMD-S3-044-2015) Modeling Crack Growth Behavior of Glass Strengthened by a Sub-Critical Tensile Stress

J. H. Seaman*[1]; T. A. Blanchet[1]; P. J. Lezzi[1]; M. Tomozawa[1]; 1. Rensselaer Polytechnic Institute, USA

10:50 AM

(GOMD-S3-045-2015) Sub-critical crack growth in hydrous borate and silicate glasses

C. Rössler*[1]; U. Bauer[2]; A. Pönitzsch[1]; J. Deubener[1]; H. Behrens[2]; S. Reinsch[3]; R. Müller[3]; 1. TU Clausthal, Germany; 2. Leibnitz University of Hannover, Germany; 3. Federal Institute for Materials Research and Testing, Germany

11:10 AM

(GOMD-S3-046-2015) Volume Expansion caused by Water Penetration into Silica Glass

S. Wiederhorn*[2]; F. Yi[2]; D. Lavan[2]; T. Fett[1]; L. Richter[2]; 1. Karlsruhe Institute of Technology, Germany; 2. NIST, USA

11:30 AM

(GOMD-S3-047-2015) Mechanical spectroscopy studies on hydrous borate and silicate glasses

S. Reinsch*[1]; U. Bauer[2]; C. Rössler[3]; R. Müller[1]; H. Behrens[2]; J. Deubener[3]; 1. BAM Federal Institute for Materials Research and Testing, Germany; 2. Leibniz University of Hannover, Germany; 3. Clausthal University of Technology, Germany

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 3: Laser Processing and Photostructuring

Room: Concerto A

Session Chair: Juejun Hu, MIT

9:20 AM

(GOMD-S4-028-2015) Point by point direct laser writing of waveguide in chalcogenide glass (Invited)

P. Masselin*[1]; D. Le Coq[2]; E. Bychkov[1]; 1. Université du Littoral Côte d'Opale, France; 2. Université de Rennes 1, France

9:50 AM

(GOMD-S4-029-2015) Rotatory laser-induced single crystal growth of Sb_2S_3 on the surface of Sb-S-I glass

D. Savytskyy*[1]; N. Tamura[2]; V. Dierolf[1]; H. Jain[1]; 1. Lehigh University, USA; 2. Lawrence Berkeley National Laboratory, USA

10:10 AM

(GOMD-S4-030-2015) Direct Laser Writing surface microstructuring of silver-doped phosphate glasses for new functionalities

J. Desmoulin*[1]; T. Cardinal[1]; S. Danto[1]; M. Vangheluwe[2]; Y. Petit[1]; M. Dussauze[1]; M. Lahaye[1]; L. Canioni[1]; V. Rodriguez[1]; R. Vallée[2]; 1. University of Bordeaux, France; 2. University of Laval, Canada

10:30 AM

(GOMD-S4-031-2015) Features of Photostructural Response in Spin-Coated Chalcogenide Glass Thin Films

A. Kovalskiy*[1]; J. Cook[1]; R. Golovchak[1]; S. Slang[3]; K. Palka[3]; L. Loghina[3]; M. Vlcek[3]; H. Jain[2]; 1. Austin Peay State University, USA; 2. Lehigh University, USA; 3. University of Pardubice, Czech Republic

10:50 AM

(GOMD-S4-032-2015) Optical damage performance of widegap semiconductor transparent electrodes

S. Elhadj*[1]; J. Bude[1]; J. Adams[1]; M. Menor[1]; J. Yoo[1]; T. Olson[1]; J. Lee[1]; A. Samanta[1]; C. Stolz[1]; 1. Lawrence Livermore National Laboratory, USA

11:10 AM

(GOMD-S4-033-2015) Glass surface texturing by demixing under CO_2-laser irradiation

A. Veber*[1]; M. R. Cicconi[1]; N. Travitzky[1]; D. de Ligny[1]; 1. Universität Erlangen-Nürnberg, Germany

11:30 AM

(GOMD-S4-034-2015) Implantation of gold into pure and silver containing glass by means of ArF-excimer laser irradiation

M. Dubiel*[1]; M. Heinz[1]; J. Meinertz[2]; J. Ihlemann[2]; 1. Martin Luther University Halle-Wittenberg, Germany; 2. Laser-Laboratorium Göttingen e.V., Germany

11:50 AM

(GOMD-S4-035-2015) Structural changes and relaxation phenomena responsible for the permanent refractive index change of glasses after fs-laser modification

T. Seuthe*[1]; A. Mermillod-Blondin[2]; M. Grehn[3]; J. Bonse[4]; M. Eberstein[1]; 1. Fraunhofer IKTS, Germany; 2. Max-Born-Institute for Nonlinear Optics and Short Pulse Spectroscopy, Germany; 3. Technische Universität Berlin, Germany; 4. BAM - Federal Institute for Materials Research and Testing, Germany

Symposium 5: Glass Technology and Cross-cutting Topics

Session 4: Waste Glass Corrosion I

Room: Concerto C

Session Chair: James Marra, SRNL

9:20 AM

(GOMD-S5-020-2015) Hydration-induced morphological evolution at glass-liquid interfaces: a new model of long-term glass corrosion (Invited)

J. V. Ryan*[1]; 1. Pacific Northwest National Laboratory, USA

9:50 AM

(GOMD-S5-021-2015) How nanoporous alteration layers can make borosilicate glasses very durable?

S. Gin*[1]; P. Jollivet[1]; 1. CEA, France

10:10 AM

(GOMD-S5-022-2015) Stage III Dissolution of High Level Waste (HLW) and Low Activity Waste (LAW) Glasses Triggered by Leachate Interactions

C. M. Jantzen*[1]; C. Crawford[1]; 1. Savannah River National Laboratory, USA

10:30 AM

(GOMD-S5-023-2015) Preparation of an Information Basis for Development of Practical Performance Assessment Models on Waste Glass Corrosion in Geological Disposal

S. Mitsui*[1]; T. Ohe[2]; Y. Inagaki[3]; T. Ohkubo[4]; S. Kurosawa[5]; T. Goto[5]; M. Inagaki[5]; K. Ishiguro[5]; H. Takase[6]; H. Takahashi[6]; 1. Japan Atomic Energy Agency, Japan; 2. Tokai University, Japan; 3. Kyushu University, Japan; 4. Chiba University, Japan; 5. Nuclear Waste Management Organization of Japan, Japan; 6. Quintessa Japan, Japan

10:50 AM

(GOMD-S5-024-2015) Formulation and durability testing of glass ceramics for immobilization of waste products from used fuel reprocessing

C. Crawford*[1]; J. Crum[2]; J. Marra[1]; 1. SRNL, USA; 2. PNNL, USA

11:10 AM

(GOMD-S5-025-2015) Structure and diffusion properties of boroaluminosilicate nuclear waste glasses
J. Du*[1]; L. deng[1]; M. Ren[1]; 1. University of North Texas, USA

11:30 AM

(GOMD-S5-026-2015) First-Principles Based Modeling Of Borosilicate Glass Hydrolysis
D. C. Ford*[1]; H. He[2]; P. Zapol[1]; 1. Argonne National Laboratory, USA; 2. Valparaiso University, USA

Norbert J. Kreidl Award Lecture

Room: Symphony Ballroom IV

12:00 PM

(GOMD-AL-002-2015) Structure and Nonlinear Elasticity of Silica Glass Fiber under High Strains
M. J. Guerette*[1]; 1. Rensselaer Polytechnic Institute, USA

12:50 PM

Presentation of Award

Symposium 1: Energy and Environmental Aspects - Fundamentals and Applications

Session 2: Glassy Solid Electrolytes II

Room: Concerto B
Session Chair: Annie Pradel, Université Montpellier 2

1:20 PM

(GOMD-S1-007-2015) Glass-Based Na_3PS_4 Solid Electrolytes for All-Solid-State Sodium Batteries (Invited)
A. Hayashi*[1]; M. Tatsumisago[1]; 1. Osaka Prefecture University, Japan

1:50 PM

(GOMD-S1-008-2015) Heavy vs. Light Cation Chalcogenide Glasses: Ion transport and Structural Features (Invited)
E. Bychkov*[1]; 1. University of Littoral, France

2:20 PM

(GOMD-S1-009-2015) Rare-earth aluminosilicate glasses as solders for joining of silicon carbide components via laser supported process
S. Ahmad*[1]; M. Herrmann[2]; W. Lippmann[2]; M. M. Ahmed[1]; M. Steinbrück[1]; H. J. Seifert[1]; 1. Karlsruhe Institute of Technology, Germany; 2. Technical University of Dresden, Germany

2:40 PM

(GOMD-S1-010-2015) Development of Flexible Glass Capacitors for Power Inverters in Electric Drive Vehicles
B. Balachandran*[1]; B. Ma[1]; M. Pyrz[2]; M. Lanagan[2]; S. Garner[3]; P. Cimo[3]; 1. Argonne National Laboratory, USA; 2. Pennsylvania State University, USA; 3. Corning, Inc, USA

3:00 PM

(GOMD-S1-011-2015) Porous Vycor®-Glass: Alternative leaching techniques for new applications
F. N. Somorowsky*[1]; B. R. Durschang[1]; M. Kilo[1]; G. Sextl[1]; 1. Fraunhofer Institute for Silicate Research ISC, Germany

3:20 PM

Break

Session 3: Thin Film Technologies

Room: Concerto B
Session Chair: B.G. Potter, University of Arizona

3:40 PM

(GOMD-S1-012-2015) Helping to optimize Solar Energy-Conversion Devices with Soft X-Ray and Electron Spectroscopies (Invited)
C. Heske*[1]; 1. University of Nevada, Las Vegas (UNLV) and Karlsruhe Institute of Technology (KIT), USA

4:10 PM

(GOMD-S1-013-2015) CdTe-ZnO Nanocomposite Thin-Film Spectral Sensitizers in Hybrid Photovoltaic
W. Huang*[1]; S. De Valle[1]; K. Simmon-Potter[1]; B. Potter[1]; 1. University of Arizona, USA

4:30 PM

(GOMD-S1-014-2015) High temperature effects on AR-coated silica glass for solar tower receivers
G. Helsch[1]; R. Uhlig[2]; H. Bornhöft[1]; J. Deubener*[1]; 1. Clausthal University of Technology, Germany; 2. Institute of Solar Research, DLR, Germany

4:50 PM

(GOMD-S1-015-2015) Sol-gel Derived Materials for Yb Disk Lasers
T. Ribeiro[1]; L. F. Santos[1]; M. Goncalves[1]; R. M. Almeida*[1]; 1. Instituto Superior Técnico / UL, Portugal

5:10 PM

(GOMD-S1-016-2015) Exceptional Kinetic Stability of Vapor Deposited As_2S_3 Films
P. Thapar*[1]; D. Savytskii[1]; W. R. Heffner[1]; H. Jain[1]; 1. Lehigh University, USA

5:30 PM

(GOMD-S1-017-2015) Density dependence of refractive index of nanoparticle-derived titania films on glass
A. Matthias*[1]; N. Raicevic[2]; R. D. Tchana[1]; J. Deubener[1]; D. Kip[2]; 1. Clausthal University of Technology, Germany; 2. Helmut Schmidt University, Germany

Symposium 2: Glasses in Healthcare - Fundamentals and Applications

Bioactive Glass in Dental and Medical Applications

Room: Symphony Ballroom IV
Session Chair: Delia Brauer, Friedrich-Schiller-Universität

1:20 PM

(GOMD-S2-022-2015) Influence of Mg and Zn substitution on bioactive glass dissolution at neutral and acidic pH (Invited)
D. S. Brauer*[1]; M. Blochberger[1]; 1. Friedrich-Schiller-Universität, Germany

1:50 PM

(GOMD-S2-023-2015) Glass-fibers with antimicrobial properties for bone defects restoration
L. Esteban*[1]; B. Cabal[2]; R. Torrecillas[2]; C. Prado[2]; R. López[2]; F. Quintero[3]; J. Pou[3]; J. Panide[3]; J. Moya[1]; 1. Consejo Superior de Investigaciones Científicas, Spain; 2. Nanomaterials and Nanotechnology Research Center, Spain; 3. Universidad de Vigo, Spain

2:10 PM

(GOMD-S2-024-2015) Twofold internal crystallization of lithium disilicate and fluorapatite in the SiO_2-Li_2O-Al_2O_3-CaO/SrO-K_2O-P_2O_5-F system for dental restorations
M. Rampf*[1]; C. Ritzberger[1]; M. Schweiger[1]; W. Höland[1]; 1. Ivoclar Vivadent AG, Liechtenstein

2:30 PM

(GOMD-S2-025-2015) Influence of bioactive glasses on self-restoring potential of dentin adhesive systems
J. Brandt*[1]; R. Göbel[2]; A. Rzanny[2]; D. S. Brauer[1]; 1. Friedrich-Schiller-University, Germany; 2. University Hospital Jena, Germany

2:50 PM

(GOMD-S2-026-2015) Development of mica-based glass-ceramics for dental applications

D. Chaysuwan*[1]; T. Srichumpong[1]; K. Suputtamongkol[2]; 1. Kasetsart University, Thailand; 2. Mahidol University, Thailand

3:10 PM

(GOMD-S2-027-2015) Manufacturing of highly porous, anisotropic glass monoliths with a honeycomb-like structure

S. Krenkel*[1]; H. Uhlig[2]; D. Enke[2]; E. Rädlein[1]; 1. Ilmenau University of Technology, Germany; 2. University of Leipzig, Germany

Glasses in Healthcare: Current Applications and Future Potential

Room: Tenor

Session Chairs: Mohamed Rahaman, Missouri S&T

3:40 PM

Roundtable Discussion

Symposium 3: Fundamentals of the Glassy State

Session 3: Structural Characterization of Glasses V

Room: Symphony Ballroom II

Session Chair: Philip Salmon, University of Bath

1:20 PM

(GOMD-S3-048-2015) Oxide glasses under extreme compression and 2 dimensional confinement (Invited)

S. Lee*[1]; 1. Seoul National University, Republic of Korea

1:50 PM

(GOMD-S3-049-2015) Structure and Mechanical Properties of Nanoporous Glasses Characterized by X-ray Scattering

M. Sundararajan[1]; C. A. Ihalawela[1]; G. Chen*[1]; 1. Ohio University, USA

2:10 PM

(GOMD-S3-050-2015) Usable Strength of Glass—Surface Chemistry Perspective

N. Sheth*[1]; N. Surdyka[1]; J. Luo[1]; J. Barnerjee[1]; C. Pantano[1]; S. Kim[1]; 1. Pennsylvania State University, USA

2:30 PM

(GOMD-S3-051-2015) Surface Studies of Calcium Aluminosilicate Glasses

D. Kramer*[1]; C. Pantano[1]; C. Trivelpiece[1]; 1. Pennsylvania State University, USA

2:50 PM

(GOMD-S3-052-2015) Atomic scale investigation of dopant in glass using aberration corrected STEM-EELS

T. Mizoguchi*[1]; A. Masuno[1]; H. Inoue[1]; 1. University of Tokyo, Japan

3:10 PM

Break

Session 3: Structural Characterization of Glasses VI

Room: Symphony Ballroom II

Session Chair: Steve Martin, Iowa State University

3:40 PM

(GOMD-S3-053-2015) Combining optical and x-ray absorption spectroscopies: application to medieval stained glasse

M. Hunault*[1]; F. Bauchau[2]; C. Loisel[2]; M. Hérold[3]; G. Calas[1]; 1. University Pierre and Marie Curie, France; 2. Laboratoiry of Research on Historical Monuments, France; 3. Centre André Chastel, France

4:00 PM

(GOMD-S3-054-2015) Structure and properties of strontium aluminosilicate glasses and melts

D. R. Neuville*[1]; A. Novikov[2]; P. Florian[2]; L. Hennet[2]; 1. CNRS-IPGP, France; 2. CNRS-CEMHTI, France

4:20 PM

(GOMD-S3-055-2015) Structure in Surface Depletion Layers formed on Sodium Aluminosilicate Glasses by Thermal Poling

N. J. Smith*[1]; I. Dutta[1]; C. W. Ponader[1]; 1. Corning Incorporated, USA

Session 4: Modeling and Simulations of Glasses I

Room: Symphony Ballroom IV

Session Chairs: Jincheng Du, University of North Texas; Walter Kob, Universite Montpellier 2

3:40 PM

(GOMD-S3-056-2015) Molecular dynamics simulations of borate and borosilicate glasse

L. deng*[1]; J. Du[1]; 1. University of North Texas, USA

4:00 PM

(GOMD-S3-057-2015) Physicochemical properties of nuclear glasses (SiO_2-B_2O_3-Na_2O-La_2O_3) by Molecular Dynamics simulations

F. Pacaud*[1]; M. Salanne[1]; J. Delaye[2]; 1. Phenix Laboratory, France; 2. CEA Marcoule, France

4:20 PM

(GOMD-S3-058-2015) Transport anomalies, structure and ring structure in densified liquid B_2O_3

A. Baroni*[1]; G. Ferlat[1]; M. Salanne[1]; M. Micoulaut[1]; 1. Paris Sorbonne Universités, France

4:40 PM

(GOMD-S3-059-2015) The role of oxygen packing in the structural transformations of oxide glasses (Invited)

A. Zeidler*[1]; P. S. Salmon[1]; 1. University of Bath, United Kingdom

Session 5: Mechanical Properties of Glasses IV

Room: Symphony Ballroom III

Session Chairs: Richard Bradt, University of Alabama; Morten Smedskjaer, Aalborg University; Stefan Karlsson, Glafo - the Glass Research Institute

1:20 PM

(GOMD-S3-060-2015) Mechanical Property and Nanostructure of Anisotropic Glass (Invited)

S. Ito*[1]; S. Inaba[1]; H. Hosono[2]; J. Endo[1]; 1. Asahi Glass Co., Ltd., Japan; 2. Tokyo Institute of Technology, Japan

1:50 PM

(GOMD-S3-061-2015) Silica deformation under a uniaxial stress: a non-isotropic material behavior

B. Champagnon*[1]; S. Degioanni[1]; C. Martinet[1]; 1. Université Lyon1, France

2:10 PM

(GOMD-S3-062-2015) Unit polarizability as a predictor of stress-optic response

J. Galbraith[1]; J. Zwanziger*[1]; 1. Dalhousie University, Canada

2:30 PM

(GOMD-S3-063-2015) Mechanical Properties of Densified Silica Glass (Invited)

L. Huang*[1]; 1. RPI, USA

3:00 PM

Break

3:20 PM

(GOMD-S3-064-2015) Thermodynamics of the Dilation Anomaly in Ion Exchange Strengthening

P. Gupta*[1]; P. Kreski[1]; A. Varshneya[1]; 1. Saxon Glass Technologies, Inc, USA

3:40 PM

(GOMD-S3-065-2015) Mechanical models for viscoelastic relaxation during ion exchange in glass

A. Varshneya*[1]; P. K. Kreski[1]; G. A. Olson[1]; P. K. Gupta[1]; 1. Saxon Glass Technologies, Inc., USA

4:00 PM

(GOMD-S3-066-2015) Warp reduction during chemical strengthening of float-produced thin flat soda lime silicate glasses: I, Thermal treatment

A. Varshneya*[1]; P. Kreski[1]; G. Olson[1]; 1. Saxon Glass Technologies, Inc., USA

4:20 PM

(GOMD-S3-067-2015) Warp reduction during chemical strengthening of float-produced thin flat soda lime silicate glasses: II, Differential methods

P. Kreski[1]; T. Goldberg[1]; A. Varshneya*[1]; 1. Saxon Glass Technologies, Inc., USA

4:40 PM

(GOMD-S3-068-2015) Electric field assisted ion exchange of soda lime silicate and borosilicate glass tubes

A. Talimian*[1]; V. M. Sglavo[1]; 1. Universitá degli Studio di Trento, Italy

5:00 PM

(GOMD-S3-069-2015) Effect of KNO_3 molten bath Na enrichment on the mechanical performances of ion-exchanged soda-lime-silicate float glass

V. M. Sglavo*[1]; H. Hassani[1]; 1. University of Trento, Italy

Session 7: Response of Glass to Extreme Conditions

Room: Symphony Ballroom I

Session Chair: Mario Affatigato, Coe College

3:40 PM

(GOMD-S3-070-2015) Surface interactions on glass optics during fabrication, post-processing & laser operation (Invited)

T. Suratwala*[1]; 1. Lawrence Livermore Nat'l Lab, USA

4:10 PM

(GOMD-S3-071-2015) Extreme-condition response of glass under moderate electric field, temperature and stress

C. McLaren*[1]; W. Heffner[1]; H. Jain[1]; 1. Lehigh University, USA

4:30 PM

(GOMD-S3-072-2015) High Temperature Infrared Glasses for Optical Fiber Sensing

J. Roth*[1]; S. Martin[1]; J. Ballato[2]; 1. Iowa State University, USA; 2. Clemson University, USA

4:50 PM

(GOMD-S3-073-2015) Chemical durability of 'forbidden' glasses

R. A. Schaut*[1]; S. A. Tietje[1]; 1. Corning Incorporated, USA

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 3: Optical Thin Film and Planar Devices

Room: Concerto A

Session Chair: Juejun Hu, MIT

1:20 PM

(GOMD-S4-037-2015) Nanophotonic chalcogenide glass device fabrication using electron beam lithography

Q. Du*[1]; H. Lin[2]; C. Smith[3]; K. Richardson[3]; J. Hu[1]; 1. MIT, USA; 2. University of Delaware, USA; 3. University of Central Florida, USA

1:40 PM

(GOMD-S4-038-2015) Flexible chalcogenide glass waveguide-integrated photodetectors

L. Li*[1]; H. Lin[1]; Q. Du[2]; C. Smith[3]; K. Richardson[3]; J. Hu[1]; 1. University of Delaware, USA; 2. Massachusetts Institute of Technology, USA; 3. University of Central Florida, USA

2:00 PM

(GOMD-S4-039-2015) Hydrogenated amorphous silicon for nonlinear optic applications

D. Choi*[1]; X. Gai[1]; B. Luther-Davies[1]; 1. Australian National University, Australia

2:20 PM

(GOMD-S4-040-2015) Deposition of luminescent quantum dot doped chalcogenide glass films from solution

S. Novak*[1]; W. Liyanage[2]; C. Li[3]; H. Hodei[3]; C. Smith[3]; N. McClenaghan[4]; M. Khajavikhan[3]; M. Nath[2]; W. Deng[3]; K. Richardson[3]; 1. Clemson University, USA; 2. Missouri S&T, USA; 3. University of Central Florida, USA; 4. Universite Bordeaux, France

2:40 PM

Break

Session 2: Optical Fibers I

Room: Concerto A

Session Chair: Frederic Smektala, Universite de Bourgogne

3:40 PM

(GOMD-S4-041-2015) Advances in infrared fibers (Invited)

G. Tao*[1]; A. F. Abouraddy[1]; 1. University of Central Florida, USA

4:20 PM

(GOMD-S4-042-2015) All-solid chalcogenide microstructured optical fibers exhibiting photonic bandgap propagation

C. Caillaud*[1]; G. Renversez[3]; L. Brilland[2]; D. Mechin[2]; J. Adam[1]; J. Troles[1]; 1. Institut des Sciences Chimiques de Rennes - University of Rennes 1, France; 2. PERFOS - R&D Platform of Photonics Bretagne, France; 3. Aix-Marseille Université - CNRS - Centrale Marseille - Institut Fresnel UMR 7249, France

4:40 PM

(GOMD-S4-043-2015) Photo-inscriptible silver-containing phosphate glass fibers

S. Danto*[1]; J. Desmoulin[1]; F. Désévédavy[2]; F. Smektala[2]; Y. Petit[1]; L. Canioni[1]; M. Dussauze[1]; V. Rodriguez[1]; E. Fargin[1]; T. Cardinal[1]; 1. University of Bordeaux, France; 2. University of Burgundy, France

5:00 PM

(GOMD-S4-044-2015) Cladded single crystal fibers for high power single frequency fiber lasers

W. Kim*[1]; B. Shaw[1]; C. Askins[1]; J. Peele[2]; D. Gibson[1]; S. Bowman[1]; S. Bayya[1]; J. Sanghera[1]; 1. Naval Research Laboratory, USA; 2. Sotera Defense Solutions, USA

Symposium 5: Glass Technology and Cross-cutting Topics

Session 4: Waste Glass Corrosion II

Room: Concerto C

Session Chair: Stephane Gin, CEA

1:20 PM

(GOMD-S5-027-2015) The effect of high sodium waste streams on the product quality of UK vitrified high level waste

M. Harrison*[1]; C. Steele[2]; 1. National Nuclear Lab (UK), United Kingdom; 2. Sellafield Ltd, United Kingdom

1:40 PM

(GOMD-S5-028-2015) Dissolution of UK high level nuclear waste glass under conditions relevant to geological disposal

C. L. Corkhill*[1]; N. Cassingham[1]; C. Mann[1]; D. J. Backhouse[1]; R. Hand[1]; N. Hyatt[1]; 1. The University of Sheffield, United Kingdom

2:00 PM

(GOMD-S5-029-2015) Characterisation of Corroded Simulant UK Magnox HLW Glass using ToF-SIMS

N. Ahmad*[1]; S. Fearn[1]; J. R. Jones[1]; W. E. Lee[1]; 1. Imperial College London, United Kingdom

2:20 PM

(GOMD-S5-030-2015) Effect of Ca and Mg Addition on the Aqueous Durability of Glasses in High-pH Environments

R. Hand[1]; D. J. Backhouse*[1]; C. L. Corkhill[1]; N. Hyatt[1]; 1. University of Sheffield, United Kingdom

2:40 PM

(GOMD-S5-031-2015) Glass alteration in alkaline conditions: comparison between SON68 and ISG

K. Ferrand*[1]; S. Liu[1]; K. Lemmens[1]; 1. sck-cen, Belgium

3:00 PM

(GOMD-S5-032-2015) Simulating Stage II → Stage III Dissolution with Saturated Glass Solutions

C. L. Trivelpiece*[1]; C. Pantano[1]; Y. Zhang[1]; 1. Pennsylvania State University, USA

3:20 PM

Break

Session 4: Waste Glass Corrosion III

Room: Concerto C

Session Chair: Mike Harrison, National Nuclear Lab (UK)

3:40 PM

(GOMD-S5-033-2015) Low-Temperature Alkali Diffusion in Boroaluminosilicate Nuclear Waste Glasses

S. Kerisit*[1]; J. J. Neeway[1]; Z. Zhu[1]; J. V. Ryan[1]; 1. Pacific Northwest National Laboratory, USA

4:00 PM

(GOMD-S5-034-2015) The Effects of Lithium Ion Counter-Diffusion on Glass Dissolution

C. L. Trivelpiece*[1]; C. Pantano[1]; 1. Pennsylvania State University, USA

4:20 PM

(GOMD-S5-035-2015) Dissolution Rate of Borosilicate Glass SON68: A Method of Quantification Based upon Interferometry

J. P. Icenhower*[1]; 1. Sandia National Laboratory, USA

4:40 PM

(GOMD-S5-036-2015) Evaluation of Glass Melt Surfaces with Aqueous Corrosion: An Atomic Force Microscopy Approach

Y. Gong*[1]; N. P. Mellott[1]; 1. Alfred University, USA

5:00 PM

(GOMD-S5-037-2015) Study of Composition Effects on Stage III Dissolution Using Glass Fiber

J. Rice*[1]; C. Trivelpiece[1]; C. Pantano[1]; 1. The Pennsylvania State University, USA

5:20 PM

(GOMD-S5-038-2015) An Interlaboratory Study on the Precision of ASTM C1285 Tests

W. Ebert*[1]; 1. Argonne National Lab, USA

5:40 PM

(GOMD-S5-039-2015) Sr ion implantation in the obsidian glass for its performance assessment as a waste form under hydrothermal-like conditions in geological repository

N. Rani*[1]; P. Kumar[2]; R. Sharma[2]; S. Chopra[2]; G. Roonwal[2]; J. Shrivastava[1]; 1. UNIVERSITY OF DELHI, India; 2. IUAC, India

Wednesday, May 20, 2015

Varshneya Frontiers of Glass Science Lecture

Room: Symphony Ballroom IV

8:00 AM

(GOMD-AL-003-2015) Structural aspects of relaxational dynamics in glasses and supercooled liquids (Invited)

S. Sen*[1]; 1. University of California, Davis, USA

8:50 AM

Presentation of Award

9:00 AM

Break

Symposium 1: Energy and Environmental Aspects - Fundamentals and Applications

Session 1: Flat Glasses, Capillaries, Foams and Enamels

Room: Concerto B

Session Chair: Joachim Deubener, Clausthal Univeristy of Technology

9:20 AM

(GOMD-S1-018-2015) Evidence for self-healing effect in a multi-layer glass / vanadium boride coating

L. Montagne*[1]; T. Carlier[1]; F. Méar[1]; R. Podor[2]; S. Saitzek[1]; R. Desfeux[1]; J. Blach[1]; 1. University of Lille, France; 2. ICSM, France

9:40 AM

(GOMD-S1-019-2015) Compositional Dependence of Alkali Resistance in $CaO–Al_2O_3–SiO_2$ Glasses

H. Takebe*[1]; S. Takahashi[1]; 1. Ehime University, Japan

10:00 AM

(GOMD-S1-020-2015) Influence of network modifiers on the glass system $ZnO-Al_2O_3-B_2O_3-SiO_2$

A. Deinhardt*[1]; M. Kilo[1]; S. Senger[1]; G. Sextl[1]; 1. Fraunhofer Institute for Silicate Research ISC, Germany

10:20 AM

(GOMD-S1-021-2015) Large-area fluidic windows (Invited)

L. Wondraczek*[1]; 1. University of Jena, Germany

10:50 AM

(GOMD-S1-022-2015) Improving the thermal insulation properties of the foam glasses (Invited)

J. König*[1]; R. R. Petersen[1]; Y. Yue[1]; 1. Aalborg University, Denmark

11:20 AM

(GOMD-S1-023-2015) New Glass-Seal-Type for Solid Oxide Fuel Cells

B. R. Durschang*[1]; M. Kilo[1]; M. Müller[2]; S. Hornauer[2]; 1. Fraunhofer ISC, Germany; 2. ElringKlinger AG, Germany

11:40 AM

(GOMD-S1-024-2015) Glass capillaries for hydrogen storage (Invited)

M. Prewitz*[1]; P. Ried[1]; M. Gaber[1]; R. Müller[1]; K. Holtappels[1]; C. Marotzke[1]; 1. Federal Institute for Materials Research and Testing, Germany

Symposium 3: Fundamentals of the Glassy State

Session 2: Glass-ceramics

Room: Symphony Ballroom III

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

9:20 AM

(GOMD-S3-074-2015) Don Stookey (1915-2014): Pioneering Researcher and Adventurer (Invited)

G. H. Beall*[1]; 1. Corning Incorporated, USA

9:50 AM

(GOMD-S3-075-2015) Current topics in glass-ceramics R&D - an industrial perspective (Invited)

I. Mitra*[1]; 1. SCHOTT AG, Germany

10:20 AM

(GOMD-S3-076-2015) Recent research in low thermal expansion glass-ceramics for new application (Invited)

S. Nakane*[1]; 1. Nippon Electric Glass, Japan

10:50 AM

(GOMD-S3-077-2015) Characterization of Pd-doped CMAS-TiO_2 Glass-Ceramics

M. J. Davis*[1]; P. Vullo[1]; M. Reich[2]; R. Golovchak[3]; C. Saiyasombat[4]; H. Jain[4]; 1. SCHOTT North America, Inc., USA; 2. SCHOTT AG, Germany; 3. Austin Peay State University, USA; 4. Lehigh University, USA

11:10 AM

(GOMD-S3-078-2015) Element Partitioning and Residual Glass in Beta-Spodumene Glass-Ceramics

R. Youngman*[1]; C. Smith[1]; Q. Fu[1]; M. Comte[1]; 1. Corning Incorporated, USA

11:30 AM

(GOMD-S3-079-2015) Crystallization Toughening in Lithium Disilicate Glass-Ceramic

F. C. Serbena*[1]; I. Mathias[1]; C. E. Foerster[1]; E. D. Zanotto[2]; 1. State University of Ponta Grossa, Brazil; 2. Federal University of São Carlos, Brazil

11:50 AM

(GOMD-S3-080-2015) Nepheline glass-ceramics

C. Smith*[1]; G. H. Beall[1]; S. A. Tietje[1]; A. Ellison[1]; 1. Corning Incorporated, USA

Session 3: Structural Characterization of Glasses VII

Room: Symphony Ballroom II

Session Chair: John McCloy, Washington State University

9:20 AM

(GOMD-S3-081-2015) Pure network former SiO_2-P_2O_5 glass Topological aspects of $[PO_4]^{4-}$ incorporation and nanoscale homogeneity of the glassy network

S. Fuhrmann*[1]; C. Domscheit[1]; S. Unger[2]; K. Schuster[2]; L. Wondraczek[1]; 1. University Jena Otto-Schott Institute for Materials Research, Germany; 2. Leibnitz Institute of Photonic Technology, Germany

9:40 AM

(GOMD-S3-082-2015) Elastic Properties of Mixed-Network Former Glasses

W. Wang*[1]; R. Christensen[2]; J. Byer[2]; G. Olson[2]; S. Martin[2]; J. Kieffer[1]; 1. University of Michigan, USA; 2. Iowa State University of Science & Technology, USA

10:00 AM

(GOMD-S3-083-2015) Composition Effects on Ionic Transport in Alkali - Alkaline-Earth - Aluminosilicate Glass

S. Amma*[1]; M. T. Lanagan[2]; S. H. Kim[2]; C. G. Pantano[2]; 1. Asahi Glass co. ltd, Japan; 2. The Pennsylvania State University, USA

10:20 AM

(GOMD-S3-084-2015) Statistical deconvolution of soda-lime glasses Raman spectra

W. Woelffel*[1]; C. Claireaux[1]; E. Burov[1]; É. Barthel[2]; M. Toplis[2]; E. Gouillart[1]; 1. Saint-Gobain Recherche/CNRS, France; 2. CNRS, France

10:40 AM

(GOMD-S3-085-2015) Transition and Post-Transition Metal-Borate Glasses: Structure-Property Correlation, Cluster Formation and Borate Ligand Speciation

D. Möncke*[1]; D. Palles[2]; E. I. Kamitsos[2]; L. Wondraczek[1]; 1. Friedrich-Schiller University Jena, Germany; 2. National Hellenic Research Foundation, Greece

11:00 AM

(GOMD-S3-086-2015) Investigation of the Glass Transition Widths in Alkali and Alkaline-Earth Germanate and Borate Glass Systems at Low Modifier Loading

A. Potter*[1]; J. Bainbridge[1]; D. Starkenburg[1]; B. Perez[1]; D. Hynek[1]; C. Wilkinson[1]; D. Shadle[1]; M. Franke[1]; M. Affatigato[1]; S. Feller[1]; 1. Coe College, USA

11:20 AM

(GOMD-S3-087-2015) Transition elements in glasses at dilute levels

M. Cicconi*[1]; D. de Ligny[1]; 1. University of Erlangen-Nürnberg, Germany

11:40 AM

(GOMD-S3-088-2015) Structure of molten $ZnCl_2$ salts: a combined theoretical and experimental study.

P. Lucas*[1]; A. Al Sayoud[1]; A. Edwards[1]; K. Muralidharan[1]; V. Manga[1]; P. deymier[1]; 1. University of Arizona, USA

Session 7: Glass under Extreme Conditions I

Room: Symphony Ballroom I

Session Chair: Benoit Ruffle, Montpellier University

9:20 AM

(GOMD-S3-089-2015) Network glass-forming materials at high pressures and temperatures (Invited)

P. Salmon*[1]; A. Zeidler[1]; 1. University of Bath, United Kingdom

9:50 AM

(GOMD-S3-090-2015) High energy x-ray measurements at extreme conditions (Invited)

C. J. Benmore*[1]; L. Skinner[2]; O. Alderman[3]; R. Weber[3]; R. Mayanovic[4]; A. Anderson[5]; L. Lazareva[2]; J. Parise[2]; 1. Argonne National Laboratory, USA; 2. Stony Brook University, USA; 3. Materials Development Inc., USA; 4. Missouri State University, USA; 5. St. F.X. University, Canada

10:20 AM

(GOMD-S3-091-2015) Using Prince Rupert's drops to induce extreme tensile stress in glasses, a Raman spectroscopy study (Invited)

D. de Ligny*[1]; A. Posch[2]; F. Kalkowski[1]; J. Ernst[3]; A. Nowak[3]; D. R. Neuville[4]; A. Lenhart[2]; 1. University Erlangen-Nürnberg, Germany; 2. Georg-Simon-Ohm-Hochschule Nürnberg, Germany; 3. Fraunhofer Institute for Integrated Circuits IIS, Germany; 4. Institut de Physique du Globe CNRS, France

10:50 AM

(GOMD-S3-092-2015) Experimental investigations at high temperature of the glass / melt structures (Invited)

L. Cormier*[1]; G. Lelong[1]; L. Hennet[2]; 1. CNRS - UPMC, France; 2. CNRS, France

11:20 AM

(GOMD-S3-093-2015) Impact of extreme forming conditions on glass properties (Invited)

Y. Yue*[1]; 1. Aalborg University, Denmark

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 2: Optical Fibers II

Room: Concerto A

Session Chair: Johann Troles, University de Rennes I

9:20 AM

(GOMD-S4-045-2015) Entering the mid-infrared with supercontinuum generated in chalcogenide fibers (Invited)

U. Møller*[1]; C. Petersen[1]; I. Kubat[1]; O. Bang[1]; 1. Technical University of Denmark, Denmark

10:00 AM

(GOMD-S4-046-2015) Atmospheric Aging of As_2S_3 Microstructured Fibers: Optical, Structural, Surface Issues and their Impact on Mid-Infrared Supercontinuum Generation

O. Mouawad[1]; F. Desevedavy[1]; J. Jules[1]; G. Gadret[1]; F. Amrani[1]; B. Kibler[1]; J. Fatome[1]; O. Heintz[1]; E. Lesniewska[1]; F. Smektala*[1]; 1. Universite de Bourgogne, France

10:20 AM

(GOMD-S4-047-2015) Optical fiber fabrication of zero photoelastic $ZnO–SnO–P_2O_5–B_2O_3$ glasses

A. Saitoh*[1]; Y. Oba[1]; G. Tricot[2]; H. Takebe[1]; 1. Ehime University, Japan; 2. Université de Lille 1, France

10:40 AM

(GOMD-S4-036-2015) Innovative fabricaiton approaches of multi-material nanostructured glass-based photonic systems (Invited)

F. Sorin*[1]; 1. Ecole Polytechnique Federale de Lausanne, Switzerland

Symposium 5: Glass Technology and Cross-cutting Topics

Session 4: Waste Glass Corrosion IV

Room: Concerto C

Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

9:20 AM

(GOMD-S5-040-2015) Dissolution Behavior of High-Sodium and High-Sulfate Glasses Designed for Immobilization of Hanford Low-Activity Waste

J. J. Neeway*[1]; J. V. Ryan[1]; R. M. Asmussen[1]; N. P. Qafoku[1]; 1. Pacific Northwest National Laboratory, USA

9:40 AM

(GOMD-S5-041-2015) Corrosion in Surface and Bulk Cracks of an ILW Glass Composite Material

R. Chinnam*[1]; B. Lee[1]; 1. Imperial College London, United Kingdom

10:00 AM

(GOMD-S5-042-2015) Effect of hematite, solution compositions, and surface/volume ratio on the alteration of SON68 and ISG glasses

N. A. Wall*[1]; T. Lemesle[1]; J. Neeway[2]; J. V. Ryan[2]; Q. Nikolla[2]; J. McCloy[1]; 1. Washington State University, USA; 2. Pacific Northwest National Laboratory, USA

10:20 AM

(GOMD-S5-043-2015) Glass Corrosion in the Presence of Iron-Bearing Materials and Potential Corrosion Suppressors

J. Reiser*[1]; L. Neill[1]; J. Weaver[1]; B. Parruzot[1]; C. Musa[1]; J. Neeway[2]; J. Ryan[2]; N. Qafoku[2]; S. Gin[3]; N. Wall[1]; 1. Washington State University, Chemistry Department, USA; 2. Pacific Northwest National Lab, Energy and Environment Directorate, USA; 3. CEA Marcoule DTCD SECM LCLT, F-30207, France

10:40 AM

(GOMD-S5-044-2015) Structure and chemical durability of molybdenum-bearing sodium borosilicate glass

E. Nicoleau[1]; F. Angeli*[1]; P. jollivet[1]; S. Schuller[1]; A. Le Gac[1]; M. Fournier[1]; T. Charpentier[2]; 1. CEA Marcoule, France; 2. CEA Saclay, France

11:00 AM

(GOMD-S5-045-2015) Surface Alternation of Cr_2O_3-CoO-Al_2O_3-doped Iron-Phosphate Glasses Containing Fission Products During Immersion in Water and Heating in Vacuum

T. Yano*[1]; H. Tateno[1]; T. Kishi[1]; K. Matsuyama[2]; T. Okita[2]; S. Miyamoto[2]; H. Kofuji[3]; M. Myochin[3]; 1. Tokyo Institute of Technology, Japan; 2. Toshiba Corporation, Japan; 3. Japan Atomic Energy Agency, Japan

11:20 AM

(GOMD-S5-046-2015) Dissolution behavior of $Na_2O–FeO–Fe_2O_3–P_2O_5$ glasses

L. Ma*[1]; R. K. Brow[1]; M. E. Schlesinger[1]; 1. Missouri University of Science and Technology, USA

Symposium 3: Fundamentals of the Glassy State

Session 2: Nucleation, Growth and Overall Crystallization

Room: Symphony Ballroom III

Session Chair: Edgar Zanotto, Federal University of São Carlos

1:20 PM

(GOMD-S3-094-2015) Formation and Coexistence of Crystalline Motifs in Supercooled Liquids and Glasses (Invited)

J. Kieffer*[1]; 1. University Of Michigan, USA

1:50 PM

(GOMD-S3-095-2015) Problems in simulations of crystal nucleation in glass-forming liquids: a review (Invited)

M. Micoulaut*[1]; 1. Universite Pierre-et-Marie Curie, France

2:20 PM

(GOMD-S3-096-2015) Tammann curves of crystallization: from textbook to current research in multi-component glass-ceramics

S. Krüger[1]; M. Dressler[1]; J. Deubener*[1]; 1. Clausthal University of Technology, Germany

2:40 PM

(GOMD-S3-097-2015) Heterogeneous surface nucleation of lithium disilicate: An isothermal DSC study

S. Krüger*[1]; J. Deubener[1]; 1. Clausthal University of Technology, Germany

3:00 PM

(GOMD-S3-098-2015) Nucleating agents: is there any specific site for nucleation?

L. Cormier*[3]; O. Dargaud[1]; G. Calas[3]; C. Jousseaume[2]; S. Papin[2]; 1. Cité de la céramique – Sèvres et Limoges, France; 2. Saint-Gobain Recherche, France; 3. UPMC - CNRS, France

3:20 PM

Break

3:40 PM

(GOMD-S3-099-2015) The Effects of Phase Morphology on Nucleation and Growth Behavior in $GeSe_2$-As_2Se_3-PbSe Glasses

A. K. Buff*[1]; C. Smith[1]; A. Swisher[2]; A. Pogrebnyakov[2]; M. Kang[2]; T. Mayer[2]; K. Richardson[1]; 1. University of Central Florida, USA; 2. The Pennsylvania State University, USA

4:00 PM

(GOMD-S3-100-2015) Crystallization kinetics of a non-stoichiometric glass monitored by electrical conductivity measurements

T. S. Bello[1]; A. M. Rodrigues*[1]; E. D. Zanotto[1]; V. M. Fokin[2]; 1. Federal University of São Carlos, Brazil; 2. S.I. Vavilov State Optical Institute, Russian Federation

4:20 PM

(GOMD-S3-101-2015) Investigations towards an automated detection of the crystallization of high-performance glasses using thermooptical methods

M. Kilo[1]; A. Diegeler*[1]; I. Göbel[1]; G. Maas-Diegeler[1]; F. Raether[2]; M. Straub[1]; 1. Fraunhofer ISC, Germany; 2. Fraunhofer HTL, Germany

4:40 PM

(GOMD-S3-102-2015) Non-Isothermal Crystallization and Glass Stability on Heating in some Silicate Systems

G. M. Melo[1]; A. A. Cabral*[1]; 1. FEDERAL INSTITUTE OF MARANHÃO, Brazil

5:00 PM

(GOMD-S3-103-2015) Hydrodynamic coarsening observed by in-situ tomography in barium borosilicate melts

E. Gouillart*[1]; D. Bouttes[2]; O. Lambert[1]; W. Woelffel[1]; D. Vandembroucq[2]; E. Boller[3]; 1. Joint Unit CNRS/Saint-Gobain, France; 2. PMMH, France; 3. ESRF, France

5:20 PM

(GOMD-S3-104-2015) The breakdown of the Stokes-Einstein-Eyring equation versus fragility of oxide glasses

D. R. Cassar[1]; M. L. Nascimento[1]; V. M. Fokin[1]; N. Natalia Vedishcheva[2]; E. D. Zanotto*[1]; 1. Federal University of São Carlos, Brazil; 2. Institute of Silicate Chemistry, Russian Federation

Session 4: Modeling and Simulations of Glasses III

Room: Symphony Ballroom IV

Session Chairs: Walter Kob, Universite Montpellier 2; Carlo Massobrio, Institut de Physique de Chimie des Matériaux

1:20 PM

(GOMD-S3-105-2015) A new method to model heat transfers at the atomic scale: the approach-to-equilibrium molecular dynamics (Invited)

E. Lampin*[1]; P. Palla[1]; F. Cleri[1]; 1. IEMN, France

2:00 PM

(GOMD-S3-106-2015) Molecular Dynamics Simulations of Ion-Exchanged Glass

K. D. Vargheese*[1]; A. Tandia[1]; J. Mauro[1]; 1. Corning Inc, USA

2:20 PM

(GOMD-S3-107-2015) Simulation of Ion Implantation into Fractal Aerogel Structures

W. Wu*[1]; J. Kieffer[1]; 1. University of Michigan, USA

2:40 PM

(GOMD-S3-108-2015) Anomalous transport and shear bands in glass-forming systems under shear (Invited)

J. Horbach*[1]; P. Chaudhuri[2]; G. P. Shrivastav[1]; 1. Heinrich Heine University of Duesseldorf, Germany; 2. Institute of Mathematical Sciences, India

3:20 PM

Break

Session 4: Modeling and Simulations of Glasses IV

Room: Symphony Ballroom IV

Session Chairs: Jincheng Du, University of North Texas; Walter Kob, Universite Montpellier 2

3:40 PM

(GOMD-S3-109-2015) Structural properties of As-Se glasses and melts: insight from ab initio simulations

M. Bauchy[2]; A. Kachmar[3]; M. Micoulaut*[1]; 1. Universite Pierre-et-Marie Curie, France; 2. University of California, USA; 3. Qatar Fundation, Qatar

4:00 PM

(GOMD-S3-110-2015) Challenges in glass property prediction

A. Priven*[1]; 1. Corning Korea, Republic of Korea

4:20 PM

(GOMD-S3-111-2015) Bond constraint modelling of the mixed-alkali-effect on the Tg of ternary metaphosphates

B. Poletto Rodrigues*[1]; L. Wondraczek[1]; 1. Otto Schott Institute of Materials Research, Germany

4:40 PM

(GOMD-S3-112-2015) Topological Origin of the Fracture Toughness of Silicate Glasses

M. Bauchy*[1]; Y. Yu[1]; B. Wang[1]; J. Mauro[2]; 1. University of California, Los Angeles, USA; 2. Corning Inc., USA

5:00 PM

(GOMD-S3-113-2015) Thermodynamic Optimization and Experimental Study of the K_2O-Na_2O-CaO-MgO-Al_2O_3-SiO_2 System

D. Kim*[1]; M. Van Ende[1]; I. Jung[1]; 1. McGill University, Canada

5:20 PM

(GOMD-S3-114-2015) Benchmarking the Cation-Interlinking Network Cluster Approach (CINCA) with larger calculations

J. R. Oelgoetz*[1]; L. Judy[1]; R. Golovchak[1]; A. Kovalskiy[1]; 1. Austin Peay State University, USA

5:40 PM

(GOMD-S3-115-2015) Prediction of Long Term Mechanical Reliability of Curved Display Panels considering Glass Fatigue

S. Kim*[1]; H. Lee[1]; 1. Samsung Display Co. Ltd., Republic of Korea

Session 6: Non-Oxide and Metallic Glasses I

Room: Symphony Ballroom II

Session Chair: Pierre Lucas, University of Arizona

1:20 PM

(GOMD-S3-116-2015) Liquid-liquid transition in metallic melts (Invited)

R. Busch*[1]; 1. Saarland University, Germany

1:50 PM

(GOMD-S3-117-2015) Connection Between Structure and Fragility of Metallic Glass-forming Liquids

S. Wei*[1]; O. Gross[1]; M. Stolpe[1]; Z. Evenson[1]; I. Gallino[1]; W. Hembree[1]; J. Bednarcik[2]; J. Kruzic[3]; R. Busch[1]; 1. Saarland University, Germany; 2. Deutsches Elektronen-Synchrotron DESY, Germany; 3. Oregon State University, USA

2:10 PM

(GOMD-S3-118-2015) Microscopic origin of the fragile-to-strong transition in glass-forming liquids (Invited)

Y. Yue*[1]; L. Hu[2]; 1. Aalborg University, Denmark; 2. Shandong University, China

2:40 PM

(GOMD-S3-119-2015) On the Modelling of the Transient Flow Behaviour of Metallic Glasses: Analogy with Portevin–Le Chatelier effect

N. Alrasheedi*[1]; K. Hajlaoui[1]; 1. IMAM University, Saudi Arabia

3:00 PM

(GOMD-S3-120-2015) Effects of nitrogen on glass properties

S. Ali*[1]; 1. Linnæus University,, Sweden

3:20 PM

Break

Session 6: Non-Oxide and Metallic Glasses II

Room: Symphony Ballroom II

Session Chair: Lothar Wondraczek, University of Jena

3:40 PM

(GOMD-S3-121-2015) Compositional homogeneity during synthesis of chalcogneide glasses

P. Lucas*[1]; B. Bureau[3]; S. Sen[2]; G. Coleman[1]; 1. University of Arizona, USA; 2. UC Davis, USA; 3. University of Rennes, France

4:00 PM

(GOMD-S3-122-2015) Direct Observation of Sequential Lifting of Rotational Constraints in a Molecular Glass-Forming Liquid

D. C. Kaseman*[1]; B. G. Aitken[2]; S. Sen[1]; 1. University of California Davis, USA; 2. Corning Inc, USA

4:20 PM

(GOMD-S3-123-2015) Heat Capacity Spectroscopy Analysis of Structural Heterogeneity in As-Se and Ge-Se Glasses

O. Gulbiten*[1]; P. Lucas[2]; B. Aitken[1]; 1. Corning Incorporated, USA; 2. University of Arizona, USA

4:40 PM

(GOMD-S3-124-2015) Structural anisotropy in supercooled Ge_5Se_{95} liquid under uniaxial loading

S. Sen*[1]; D. C. Kaseman[1]; 1. University of California, Davis, USA

5:00 PM

(GOMD-S3-125-2015) First-principles modelling of chalcogenide glasses: how to achieve a quantitative structural characterization

C. Massobrio*[1]; A. Bouzid[1]; M. Boero[1]; G. Ori[1]; E. Lampin[2]; 1. Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), 23 rue du Loess, F-67034, France; 2. Institut d'Electronique, de Microélectronique et de Nanotechnologies, Avenue Poincaré, BP 60069, F - 59652, France

5:20 PM

(GOMD-S3-126-2015) Structure of chalcogenide glasses in the system BaSe-Ga_2Se_3-$GeSe_2$: Role of Stoichiometry

A. Mao*[1]; B. Aitken[2]; S. Sen[1]; 1. University of California at Davis, USA; 2. Corning Incorporated, USA

Session 7: Glass under Extreme Conditions II

Room: Symphony Ballroom I

Session Chair: Morten Smedskjaer, Aalborg University

1:20 PM

(GOMD-S3-127-2015) Pressure effects in borosilicate glasses (Invited)

L. Wondraczek*[1]; 1. University of Jena, Germany

1:50 PM

(GOMD-S3-128-2015) A-thermal and a-tensile silicate glasses obtained from high pressure experiments (Invited)

B. Champagnon*[1]; S. Degioanni[1]; C. Sonneville[1]; M. Heili[1]; C. Martinet[1]; V. Martinez[1]; D. Vouagner[1]; J. Le Brusq[1]; M. Rabia[2]; D. de Ligny[3]; 1. Université Lyon1, France; 2. Laboratoire de Physique des Rayonnements, Algeria; 3. Universitat Erlangen-Nurnberg, Germany

2:20 PM

(GOMD-S3-129-2015) Pressure induced changes to titanium phosphate glass

N. Lonnroth*[1]; R. Youngman[1]; M. N. Svenson[2]; B. Aitken[1]; M. M. Smedskjaer[2]; 1. Corning Incorporated, USA; 2. Aalborg University, Denmark

2:40 PM

(GOMD-S3-130-2015) Aluminum and boron coordination changes and densification of high pressure aluminosilicate and aluminoborosilicate glasses

S. Bista*[1]; J. F. Stebbins[1]; W. B. Hankins[2]; T. W. Sisson[2]; 1. Stanford University, USA; 2. USGS, USA

3:00 PM

(GOMD-S3-131-2015) Elasticity of vitreous silica under fluid pressure

B. Coasne[3]; C. Weigel[1]; A. Polian[2]; M. Kint[1]; J. Rouquette[4]; J. Haines[4]; M. Foret[1]; R. Vacher[1]; B. Ruffle*[1]; 1. Montpellier University, France; 2. Université P. et M. Curie, France; 3. Massachusetts Institute of Technology, USA; 4. Université Montpellier 2, France

3:20 PM

Break

Session 7: Modeling of Glass under Extreme Conditions

Room: Symphony Ballroom I

Session Chair: Liping Huang, Rensselaer Polytechnic Institute

3:40 PM

(GOMD-S3-132-2015) Constitutive Laws and Raman Spectroscopy of Silica Glasses submitted to High Mechanical Stresses (Invited)

A. Tanguy*[1]; E. Barthel[2]; N. Shcheblanov[1]; B. Mantisi[3]; G. Kermouche[4]; 1. Institut Lumière Matière, France; 2. ESPCI, France; 3. université Paris 6, France; 4. Ecole des Mines de St Etienne, France

4:10 PM

(GOMD-S3-133-2015) Amorphous $GeSe_2$ and $GeSe_4$ under high pressure: A first principles study (Invited)

A. Bouzid*[1]; S. Le Roux[1]; C. Tugène[1]; M. Boero[1]; C. Massobrio[1]; 1. Institut de physique et chimie des matériaux de Strasbourg, France

4:40 PM

(GOMD-S3-134-2015) Relaxation and thermodynamic reversibility in glasses and liquids under pressure (Invited)

M. Micoulaut*[1]; M. Bauchy[2]; 1. Universite Pierre-et-Marie Curie, France; 2. University of California, USA

5:10 PM

(GOMD-S3-135-2015) Structural properties of densified Ge_xSe_{1-x} glasses (Invited)

C. Yildirim*[1]; M. Micoulaut[1]; J. Raty[2]; 1. Universite Pierre-et-Marie Curie, France; 2. Université de Liège, Belgium

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 4: Optical Ceramics I

Room: Concerto A

Session Chair: Yiquan Wu, Alfred University

1:20 PM

(GOMD-S4-048-2015) Hot-Pressed ZnS Infrared Ceramics: Correlating Precursor Synthesis Method To Sinterability and Transparency (Invited)

O. Merdrignac-Conanec*[1]; N. Hakmeh[1]; X. Zhang[1]; J. Adam[1]; 1. University of Rennes 1, France

1:50 PM

(GOMD-S4-049-2015) Cr^{2+} doped ZnS polycrystalline transparent ceramics

Y. Li*[1]; Y. Wu[1]; 1. Alfred University, USA

2:10 PM

(GOMD-S4-050-2015) Optical ceramics for high power solid state lasers

W. Kim*[1]; C. Baker[1]; G. Villalobos[1]; J. Frantz[1]; B. Shaw[1]; M. Hunt[2]; S. Bayya[1]; B. Sadowski[3]; I. Aggarwal[3]; J. S. Sanghera[1]; 1. Naval Research Laboratory, USA; 2. Unversity Research Foundation, USA; 3. Sotera Defense Solutions, USA

2:30 PM

(GOMD-S4-051-2015) Processing and characterization of Eu: $Ba_2Zr_2Si_3O_{12}$ optical ceramics

Y. Yang*[1]; Y. Wu[1]; 1. Alfred University, USA

2:50 PM

(GOMD-S4-052-2015) Scintillation and luminescence in transparent colorless single and polycrystalline bulk ceramic ZnS

J. McCloy*[1]; M. Bliss[2]; B. W. Miller[2]; Z. Wang[2]; S. Stave[2]; 1. Washington State University, USA; 2. Pacific Northwest National Laboratory, USA

3:10 PM

Break

Session 4: Optical Ceramics II

Room: Concerto A

Session Chair: Yiquan Wu, Alfred University

3:40 PM

(GOMD-S4-053-2015) Spectroscopic and electrical properties of $CuAlO_2$ optical ceramics

Y. Liu*[1]; Y. Wu[1]; 1. Alfred University, USA

4:00 PM

(GOMD-S4-054-2015) Compaction of Barium Chloride Transparent Ceramics at Low Temperature and High Pressure

T. Shoulders*[1]; M. Gascon[2]; G. Bizarri[2]; E. Bourret[2]; R. Gaume[1]; 1. University of Central Florida, USA; 2. Lawrence Berkeley National Laboratory, USA

4:20 PM

(GOMD-S4-055-2015) Combustion synthesis of lead oxide nanopowders for the preparation of PMN-PT transparent ceramics

X. Chen*[1]; S. Chen[2]; P. Clequin[2]; W. T. Shoulders[1]; R. Gaume[2]; 1. University of Central Florida, USA; 2. CREOL, USA

Symposium 5: Glass Technology and Cross-cutting Topics

Session 3: Liquid Synthesis and Sol-gel-derived Materials

Room: Concerto B

Session Chairs: Rui Almeida, Instituto Superior Técnico; Alicia Duran, CSIC

1:20 PM

(GOMD-S5-047-2015) Sol-Gel Materials For Energy Applications (Invited)

B. Dunn*[1]; 1. UCLA, USA

1:50 PM

(GOMD-S5-048-2015) $BaTiO_3$/Low Melting Glass Core-Shell Nanocomposite for High Energy Storage Capacitor Applications

X. Su*[1]; B. Riggs[2]; M. Tomozawa[1]; J. K. Nelson[1]; D. Chrisey[2]; 1. Rensselaer Polytechnic Institute, USA; 2. Tulane University, USA

2:10 PM

(GOMD-S5-049-2015) Soft chemistry route to nanostructured GeS_2 hybrid materials

L. Courtheoux*[1]; R. Mathiaud[1]; G. Silly[1]; H. Albadri[2]; J. Levillain[2]; A. Gaumont[2]; M. Ribes[1]; A. Pradel[1]; 1. University of Montpellier, France; 2. ENSICAEN, France

2:30 PM

(GOMD-S5-050-2015) Effect of Tetraethoxy- and Tetramethoxysilane (TEOS/TMOS) on Melting Gel Behavior

L. C. Klein*[1]; K. Al-Marzoki[1]; A. Jitianu[2]; 1. Rutgers University, USA; 2. Lehman College-CUNY, USA

2:50 PM

(GOMD-S5-051-2015) Chemical Solution-Processed Ferroelectric Thin Films and Nanostructure (Invited)

N. Bassiri-Gharb*[1]; 1. Georgia Institute of Technology, USA

3:20 PM

Break

3:40 PM

(GOMD-S5-052-2015) Novel nanostructured phosphate glasses derived by sol-gel route: from optical to environmental applications (Invited)

L. Zhang*[1]; J. He[1]; Y. Wang[1]; J. Ren[1]; 1. Shanghai Institute of Optics and Fine Mechanics, CAS, China

4:10 PM

(GOMD-S5-053-2015) Stress Manipulation of Mesoporous Titanium Phosphate Glass

M. Sundararajan*[1]; G. Chen[1]; 1. Ohio University, USA

4:30 PM

(GOMD-S5-054-2015) Sol-Gel Derived Solid State Lithium Ion Conducting Organic-Inorganic Hybrid Electrolytes

W. Wang*[1]; J. Kieffer[1]; 1. University of Michigan, USA

4:50 PM

(GOMD-S5-055-2015) Influence of surface pretreatment of magnesium alloy on the deposition of glass-like cerium coatings obtained by sol-gel

A. Duran*[1]; 1. CSIC, Spain

Session 4: Waste Glass Melting Processes - Experimental Studies and Modeling

Room: Concerto C

Session Chair: Vijay Jain, Savannah River Remediation LLC

1:20 PM

(GOMD-S5-056-2015) Laboratory-scale cold cap analysis for liquid-fed ceramic melter using high-temperature X-ray CT

T. Yano*[1]; K. Watanabe[1]; K. Mori[1]; T. Amagasa[1]; R. Nakata[1]; J. Ogata[1]; T. Kishi[1]; K. Takeshita[1]; Y. Miura[2]; N. Kanehira[2]; 1. Tokyo Institute of Technology, Japan; 2. Japan Nuclear Fuel Limited, Japan

1:40 PM

(GOMD-S5-057-2015) Non-Newtonian behavior of nuclear glass melts containing Platinum Group Metal particles

M. Neyret*[2]; J. Puig[2]; B. Penelon[2]; P. Marchal[1]; O. Pinet[2]; 1. CNRS, France; 2. CEA, France

2:00 PM

(GOMD-S5-058-2015) Specific Surface Area Change of a High-Alumina HLW Melter Feed during Vitrification

K. Xu*[1]; P. Hrma[1]; M. Schweiger[1]; 1. Pacific Northwest National Laboratory, USA

2:20 PM

(GOMD-S5-059-2015) Thermal diffusivity of melter feed for a high-alumina high-level waste glass

C. P. Rodriguez*[1]; J. Chun[1]; M. J. Schweiger[1]; P. Hrma[1]; 1. Pacific Northwest National Lab, USA

2:40 PM

(GOMD-S5-060-2015) Effects of Melter Processing Parameters on Technetium Retention in Glass during Waste Vitrification

D. Kim*[1]; A. A. Kruger[2]; 1. PNNL, USA; 2. Office of River Protection, USA

3:00 PM

(GOMD-S5-061-2015) Rhenium/Technetium Partitioning and Nitrate Decomposition during Melting of Simplified Low Activity Waste Glass Feeds

T. Jin*[1]; D. Kim[1]; M. J. Schweiger[1]; A. Kruger[2]; 1. Pacific Northwest National Laboratory, USA; 2. U.S. Dept of Energy, USA

3:20 PM

Break

Session 4: Vitrification Operations and Melter Studies

Room: Concerto C

Session Chair: John Vienna, PNNL

3:40 PM

(GOMD-S5-062-2015) Status of High-Level Radioactive Waste Vitrification in the United States (Invited)

V. Jain*[1]; 1. Savannah River Remediation LLC, USA

4:10 PM

(GOMD-S5-063-2015) Technetium Behavior During Hanford LAW Vitrification

I. L. Pegg*[1]; K. S. Matlack[1]; H. Abramowitz[1]; M. Brandys[1]; 1. The Catholic University of America, USA

4:30 PM

(GOMD-S5-064-2015) Volume, density, and void fraction changes as glass batch converts to molten glass

P. Hrma*[1]; 1. PNNL, USA

4:50 PM

(GOMD-S5-065-2015) Investigation of Multiple Cold-Cap Temperature Profiles with Mathematical Modeling

D. Dixon*[1]; M. Schweiger[1]; B. Riley[1]; R. Pokorny[2]; P. Hrma[1]; 1. Pacific Northwest National Laboratory, USA; 2. Institue of Chemical Technology, Czech Republic

5:10 PM

(GOMD-S5-066-2015) Integrated Heat Transfer Model of a Waste Glass Melter with Cold Cap Physics

D. P. Guillen*[1]; R. Pokorny[2]; P. Hrma[3]; 1. Idaho National Laboratory, USA; 2. Institute of Chemical Technology Prague, Czech Republic; 3. Pacific Northwest National Laboratory, USA

5:30 PM

(GOMD-S5-067-2015) Immobilisation process for contaminated zeolitic ion exchangers from Fukushima

D. Pletser*[1]; B. Lee[1]; 1. Imperial College London, United Kingdom

Symposium 3: Fundamentals of the Glassy State

Session 4: Modeling and Simulations of Glasses II

Room: Symphony Ballroom IV

Session Chairs: Carlo Massobrio, Institut de Physique de Chimie des Matériaux; Jincheng Du, University of North Texas

9:20 AM

(GOMD-S3-136-2015) New insights into oxide glass structure from a combined experimental and computational solid-state NMR approach (Invited)

T. Charpentier*[1]; F. Vasconcelos[1]; M. Salanne[2]; J. Delaye[3]; F. Pacaud[3]; F. Angeli[3]; S. Schuller[3]; 1. CEA, France; 2. UPMC Paris VI, France; 3. CEA, DEN, France

10:00 AM

(GOMD-S3-137-2015) Development and analysis of amorphous calcium pyrophosphate structure models

J. M. Rimsza*[1]; J. Du[1]; C. Bonhomme[2]; C. Gervais[2]; C. Coelho Diogo[3]; C. Sassoye[2]; 1. The University of North Texas, USA; 2. UniversiteParis 06, France; 3. Universite Paris 06, France

10:20 AM

(GOMD-S3-138-2015) First-Principles Nuclear Magnetic Resonance of 29Si for Structural Analysis of Metal-Silicate Glasses

A. Dasmahapatra[1]; J. P. Nimmo[1]; P. Kroll*[1]; 1. UT Arlington, USA

10:40 AM

(GOMD-S3-139-2015) Surface Reactivity of Silicate Glasses: New Insights from Reactive Potentials

Y. Yu*[1]; B. Wang[1]; Y. Lee[1]; M. Bauchy[1]; 1. UCLA, USA

11:00 AM

(GOMD-S3-140-2015) Clustering in Metal Silicate Glasses

A. Dasmahapatra*[1]; P. Kroll[1]; 1. UT Arlington, USA

11:20 AM

(GOMD-S3-141-2015) Structural transitions in oxides at extreme temperatures: From Silica to molten Uranium dioxide (nuclear fuel) (Invited)

L. Skinner*[1]; C. Benmore[2]; R. J. Weber[3]; O. L. Alderman[3]; 1. stony brook university, USA; 2. Argonne Nat. Lab., USA; 3. Materials Development Inc., USA

Thursday, May 21, 2015

Varshneya Frontiers of Glass Technology Lecture

Room: Symphony Ballroom IV

8:00 AM

(GOMD-AL-004-2015) The present and future of glass in medicine (Invited)

S. Jung*[1]; 1. Mo-Sci Corporation, USA

8:50 AM

Presentation of Award

9:00 AM

Break

Symposium 3: Fundamentals of the Glassy State

Session 1: Glass Heterogeneities and Structural Relaxation

Room: Symphony Ballroom III

Session Chair: Dominique de Ligny, University Erlangen-Nürnberg

9:20 AM

(GOMD-S3-142-2015) Structural heterogeneity in glass: Insight from relaxation studies (Invited)

Y. Yue*[1]; 1. Aalborg University, Denmark

9:50 AM

(GOMD-S3-143-2015) Viscosity of silicate melts: a key to understand the structure of melts: (Invited)

D. R. Neuville*[1]; 1. CNRS-IPGP, France

10:20 AM

(GOMD-S3-144-2015) Atomic scale network relaxation observed in a silicate glass by XPCS (Invited)

B. Ruffle*[1]; 1. Montpellier University, France

10:50 AM

(GOMD-S3-145-2015) Two Complementary Approaches for the Quantification of Inhomogeneities in Glasses

S. Bartolomey*[1]; R. Conradt[1]; 1. RWTH Aachen University, Germany

11:10 AM

(GOMD-S3-146-2015) Some Theoretical Approaches to Understanding a Universal Pattern in the Fragility of Network-forming Glasses

D. Sidebottom*[1]; T. Tran[1]; S. Schnell[1]; 1. Creighton University, USA

11:30 AM

(GOMD-S3-147-2015) Structural relaxation in network glasses: do we need a new paradigm?

R. Golovchak*[1]; 1. Austin Peay State University, USA

Session 4: Modeling and Simulations of Glasses V

Room: Symphony Ballroom IV

Session Chairs: Carlo Massobrio, Institut de Physique de Chimie des Matériaux; Walter Kob, Universite Montpellier 2

9:20 AM

(GOMD-S3-148-2015) Atomic Scale Modeling of Amorphous Chalcogenide Surfaces (Invited)

G. Ori*[3]; B. Coasne[2]; M. Boero[1]; C. Massobrio[1]; 1. CNRS, France; 2. Massachusetts Institute of Technology, USA; 3. IPCMS-CNRS, France

10:00 AM

(GOMD-S3-149-2015) Glass surface properties enhancement with thermal poling: a molecular dynamics study

A. Tandia*[1]; K. Vargheese[1]; 1. Corning Incorporated, USA

10:20 AM

(GOMD-S3-150-2015) Distinguishability of Particles in Glass-Forming Systems

J. C. Mauro*[1]; M. M. Smedskjaer[2]; 1. Corning Incorporated, USA; 2. Aalborg University, Denmark

10:40 AM

(GOMD-S3-151-2015) Structural simulations of oxy-fluoride glasses

H. Inoue*[1]; A. Masuno[1]; 1. The Univeristy of Tokyo, Japan

11:00 AM

(GOMD-S3-152-2015) Large Scale Simulation of Structure and Properties of Slicate and Metallic Glass (Invited)

N. Li*[1]; X. Zhao[1]; 1. Wuhan University of Technology, China

11:20 AM

(GOMD-S3-153-2015) Source of instability in amorphous semiconducting oxides (Invited)

S. Han*[1]; 1. Seoul National University, Republic of Korea

11:40 AM

(GOMD-S3-154-2015) State of the Surface of a Thin Sheet of Glass, and its Strength

O. Prokhorenko*[1]; 1. L.G.P. International, USA

Session 6: Non-Oxide and Metallic Glasses III

Room: Symphony Ballroom II

Session Chair: Ozgur Gulbiten, Corning Incorporated

9:20 AM

(GOMD-S3-155-2015) Structure and Properties of Sulfophosphate Glasses (Invited)

L. Wondraczek*[1]; 1. University of Jena, Germany

9:50 AM

(GOMD-S3-156-2015) Investigation of Structure and Properties in the $GeSe_2$-As_2Se_3-PbSe System with Varying PbSe

C. Smith*[1]; K. Chamma[1]; D. McClane[1]; L. Sisken[1]; A. K. Buff[1]; A. Swisher[2]; A. Pogrebnyakov[2]; T. Mayer[2]; K. Richardson[1]; 1. University of Central Florida, USA; 2. Pennsylvania State University, USA

10:10 AM

(GOMD-S3-157-2015) Rare earth doped chalcogenide glasses for environmental sensing

R. Chahal*[1]; F. Starecki[1]; C. Boussard-Pledel[1]; J. Doualan[7]; L. Quetel[2]; K. Michel[3]; S. Marre[8]; S. Morais[8]; Y. Garrabos[8]; C. Prestipino[1]; A. Trapananti[4]; A. Moreac[5]; G. Tricot[6]; A. Braud[7]; P. Camy[7]; B. Bureau[1]; V. Nazabal[1]; 1. Institut des Sciences Chimiques de Rennes UMR CNRS 6226, France; 2. IDIL Fibres Optiques, France; 3. Bureau des Recherches Geologiques et Minieres (BRGM), France; 4. ESRF, France; 5. Institut de Physique de Rennes UMR CNRS 6251, France; 6. ENSC Lille Unite de Catalyse et Chimie du Solide UMR 8181, France; 7. Centre de Recherche sur les Ions, les Materiaux et la Photonique (CIMAP) UMR 6252 CEA-CNRS-ENSICaen, France; 8. Institut de Chimie de la Matiere Condensee de Bordeaux CNRS (ICMCB) UPR 9048, France

10:30 AM

(GOMD-S3-158-2015) Viscosity of $As_{40}Se_{60}$ glass during the fiber drawing process

J. Troles*[1]; G. yang[1]; B. Bureau[1]; C. Boussard[1]; P. Houizot[1]; C. Sangleboeuf[1]; T. Rouxel[1]; 1. University of Rennes 1, France

10:50 AM

(GOMD-S3-159-2015) Optical Property Extrema and Correlation in GeAsSe ternary glass forming system

B. Gleason*[1]; L. Sisken[2]; C. Smith[2]; R. Whitsitt[2]; A. Qiao[3]; N. Anheier[3]; K. Richardson[2]; 1. Clemson University, USA; 2. University of Central Florida, USA; 3. Pacific Northwest National Laboratory, USA

Session 7: Glass under Extreme Conditions III

Room: Symphony Ballroom I

Session Chair: Anne Tanguy, Université Lyon 1

9:20 AM

(GOMD-S3-160-2015) Unique Effects of Pressure and Thermal History: Implications for Glass Mechanics and Chemical Strengthening (Invited)

M. M. Smedskjaer*[1]; M. Bauchy[2]; M. N. Svenson[1]; J. C. Mauro[3]; L. M. Thirion[3]; S. J. Rzoska[4]; M. Bockowski[4]; 1. Aalborg University, Denmark; 2. University of California, Los Angeles, USA; 3. Corning Incorporated, USA; 4. Polish Academy of Sciences, Poland

9:50 AM

(GOMD-S3-161-2015) Transport in thermally grown borosilicate glasses (Invited)

E. J. Opila*[2]; K. Shugart[1]; B. McFarland[2]; M. Wilson[2]; 1. Air Force Research Lab, USA; 2. University of Virginia, USA

10:20 AM

(GOMD-S3-162-2015) Density of Silicate Glass Melts and Glasses Using Aerolevitation

M. Affatigato*[1]; P. Pinchuk[1]; A. Kline[2]; M. Welninski[1]; G. Wehr[1]; S. Feller[1]; 1. Coe College, USA; 2. Iowa State University, USA

10:40 AM

(GOMD-S3-163-2015) Raman spectroscopy of *v*-SiO_2 under rare gas compression

C. Weigel[1]; B. Hehlen[1]; M. Foret*[1]; M. Kint[1]; R. Vacher[1]; B. Ruffle[1]; 1. University of Montpellier, France

11:00 AM

(GOMD-S3-164-2015) Optical properties of permanently densified silica glass

A. Masuno*[1]; N. Nishiyama[2]; F. Sato[3]; T. Taniguchi[4]; H. Inoue[1]; 1. The University of Tokyo, Japan; 2. Deutsches Elektronen-Synchrotron, Germany; 3. Nippon Electric Glass Co., Ltd., Japan; 4. National Institute for Materials Science, Japan

11:20 AM

(GOMD-S3-165-2015) Structural Relaxation of Isostatically Compressed Sodium-Borate Glass

M. N. Svenson*[3]; M. M. Smedskjær[3]; Y. Yue[3]; R. Youngman[1]; S. Rzoska[2]; M. Bockowski[2]; L. R. Jensen[3]; 1. Corning Incorporated, USA; 2. Polish Academy of Sciences, Poland; 3. Aalborg University, Denmark

11:40 AM

(GOMD-S3-166-2015) Structure and Properties of Silica Glass Densified by Pressure-quenching

M. Guerette[1]; L. Huang*[1]; 1. RPI, USA

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 4: Glass Ceramics

Room: Concerto A

Session Chair: Yiquan Wu, Alfred University

9:20 AM

(GOMD-S4-056-2015) Effects of Thermal Processing Parameters on Material Properties for Chalcogenide Glass Ceramics in the Ge-As-Pb-Se System

L. Sisken*[1]; C. Smith[1]; P. Wachtel[2]; K. Chama[1]; A. K. Buff[1]; K. Richardson[1]; 1. University of Central Florida, USA; 2. Irradiance Glass, USA

9:40 AM

(GOMD-S4-057-2015) Glass-ceramics based on the bulk formation of “anti-glass” spherulites in the TeO_2-Nb_2O_5-Bi_2O_3 system

M. Shimoda[2]; A. Bertrand[1]; J. Carreaud[1]; G. Delaizir[1]; J. Duclere*[1]; M. Colas[1]; J. Cornette[1]; T. Hayakawa[2]; O. Masson[1]; C. Genevois[3]; E. Véron[3]; M. Allix[3]; P. Thomas[1]; 1. Laboratoire SPCTS, France; 2. Nagoya Institute of Technology, Japan; 3. Conditions Extrêmes et Matériaux : Haute Température et Irradiation (CEMHTI), France

10:00 AM

(GOMD-S4-058-2015) The effect of trivalent iron on the properties of fluorochlorozirconate glass ceramic

A. Evans*[1]; J. Hah[1]; R. Leonard[1]; C. Johnson[1]; J. A. Johnson[1]; 1. University of Tennessee Space Institute, USA

10:20 AM

(GOMD-S4-059-2015) Scratch resistance of glass-ceramics in the MgO-Al_2O_3-SiO_2 (MAS) system

B. Hota*[1]; O. Hochrein[2]; I. Burger[2]; I. Mitra[2]; M. Bockmeyer[2]; J. Deubener[1]; 1. Clausthal University of Technology, Germany; 2. SCHOTT AG, Germany

10:40 AM

(GOMD-S4-060-2015) Fusion Formable Glass-Ceramics with High Strength

M. Dejneka*[1]; I. Dutta[1]; C. Smith[1]; 1. Corning Incorporated, USA

11:00 AM

(GOMD-S4-061-2015) Tailoring Nanoscale Phase Separation in New Gallogermanate and Gallosilicate Oxide Glasses: Application to Highly Transparent Glass-ceramics (Invited)

M. Allix*[1]; S. Chenu[1]; E. Véron[1]; C. Genevois[1]; G. Matzen[1]; 1. Laboratoire CEMHTI - CNRS, France

Symposium 5: Glass Technology and Cross-cutting Topics

Session 2: Transparent Protective Systems

Room: Concerto B

Session Chairs: Andrew Wereszczak, Oak Ridge National Laboratory; Parimal Patel, Army Research Laboratory

9:20 AM

(GOMD-S5-068-2015) Responses of Silicate Glasses to High Pressure

A. Wereszczak*[1]; T. Morrissey[2]; M. Ferber[1]; K. Bortle[2]; E. Rodgers[2]; G. Tsoi[3]; Y. Vohra[3]; 1. Oak Ridge National Laboratory, USA; 2. ORISE, USA; 3. University of Alabama @ Birmingham, USA

9:50 AM

(GOMD-S5-069-2015) Laser-shock spall testing of glass and glass-ceramics

M. J. Davis*[1]; C. Weinhold[1]; P. Vullo[1]; 1. SCHOTT North America, Inc., USA

10:20 AM

(GOMD-S5-070-2015) Equibiaxial Flexure Strength of Glass: Influence of Glass Plate Size and Equibiaxial Ring Ratio

J. Swab*[1]; P. Patel[1]; S. Kilczewski[1]; 1. U.S. Army Research Laboratory, USA

10:40 AM

(GOMD-S5-071-2015) Investigation of failure mechanisms in glass under dynamic loading using high speed x-ray contrast imaging

N. Parab[1]; W. W. Chen*[1]; 1. Purdue University, USA

11:00 AM

(GOMD-S5-072-2015) Internal Pores in Thick Silicate Glasses Revealed by High-Strain-Energy Fracture

A. Wereszczak*[1]; S. Waters[1]; L. D. Pye[2]; 1. Oak Ridge National Laboratory, USA; 2. Alfred University, USA

Session 4: Waste Glass Chemistry

Room: Concerto C

Session Chair: Kevin Fox, Savannah River National Laboratory

9:20 AM

(GOMD-S5-073-2015) Sulfur Solubility in Hanford Waste Glass Melts

J. Vienna*[1]; D. Kim[1]; A. Kruger[2]; 1. PNNL, USA; 2. DOE-ORP, USA

9:40 AM

(GOMD-S5-074-2015) Effects of Chloride on Sulfate Solubility in LAW Glass Melts

H. Gan*[1]; Z. Feng[1]; I. L. Pegg[1]; 1. the Catholic University of America, USA

10:00 AM

(GOMD-S5-075-2015) Current state of knowledge of yellow phase in HLW glasses

S. Schuller*[1]; E. Boué[1]; E. Régnier[1]; 1. CEA, France

10:20 AM

(GOMD-S5-076-2015) Retention of Iodine in Hanford Waste Glasses

K. S. Matlack*[1]; I. L. Pegg[1]; 1. The Catholic University of America, USA

10:40 AM

(GOMD-S5-077-2015) Alkali Technetium Oxides as Model Compounds for ^{99}Tc Incorporation in Glass

J. L. Weaver*[1]; J. McCloy[1]; N. Wall[1]; C. Soderquist[2]; 1. Washington State University, USA; 2. Pacific Northwest National Labratory, USA

11:00 AM

(GOMD-S5-078-2015) Crystallization kinetics of Na_2O-Al_2O_3-Fe_2O_3-SiO_2 glasses

Y. Shahrayar[1]; E. Han[1]; A. Maron[1]; J. Marcial[2]; J. Weaver[2]; J. McCloy[2]; A. Goel*[1]; 1. Rutgers - The State University of New Jersey, USA; 2. Washington State University, USA

11:20 AM

(GOMD-S5-079-2015) Nepheline crystallization in boron-rich alumino-silicate glasses as investigated by multi-nuclear NMR, Raman, & Mössbauer spectroscopies

J. McCloy*[1]; N. Washton[3]; P. Gassman[2]; J. Marcial[1]; J. Weaver[1]; R. Kukkadapu[3]; 1. Washington State University, USA; 2. Pacific Northwest National Laboratory, USA; 3. Environmental Molecular Sciences Laboratory, USA

11:40 AM

(GOMD-S5-080-2015) Iron Phosphate Waste Forms for Simulated Fission Products Waste Streams

C. Kim*[1]; L. Ma[2]; R. K. Brow[2]; 1. MO-SCI Corporation, USA; 2. Missouri University of Science and Technology, USA

*Denotes Presenter

Monday, May 18, 2015

Stookey Lecture of Discovery Award

Room: Symphony Ballroom IV

8:00 AM

(GOMD-AL-001-2015) Development of multifunctional chalcogenide and chalcopyrite crystals and glasses (Invited)

N. B. Singh*[1]; 1. University of Maryland, Baltimore County

In this presentation we will summarize merits and demerits of by providing examples of AO, NLO and filter devices and their performance for variety of applications. Over past several years, we have grown, fabricated and studied extensively crystals of gallium selenide (GaSe), thallium arsenic selenide (Tl_3AsSe_3), thallium arsenic sulfide (Tl_3AsS_4), thallium phosphorous selenide (Tl_3PSe_4), silver thallium sulfide ($AgTlS_2$), silver gallium sulfide ($AgGaS_2$), silver gallium selenide ($AgGaSe_2$), and silver gallium germanium selenide ($AgGaGe_3Se_8$ and $AgGaGe_5Se_{12}$). Among this class of materials GaSe has strong tendency of cleaving due to Vander Waal forces along –C direction. The ternary and quaternary materials have a large flexibility to design transparency, damage threshold and effective performance. Tl_3AsSe_3 and quaternary compounds $AgGaGe_3Se_8$ and $AgGaGe_5Se_{12}$ do not require annealing, show very large transparency range and have extremely low absorption coefficient. In addition to the bulk crystal growth we have made significant progress in developing the engineered structures of quasi phase matched (QPM) for frequency conversion. We chose ZnSe because of its large transparency, low absorption and other favorable properties. In this paper we will describe growth and performance of these bulk and QPM materials for laser development and acousto-optical hyperspectral imaging.

Symposium 2: Glasses in Healthcare - Fundamentals and Applications

Design of Glasses for Biomedical Applications

Room: Symphony Ballroom IV

Session Chairs: Aldo Boccaccini, University of Erlangen-Nuremberg; Leena Hupa, Åbo Akademi University

9:20 AM

(GOMD-S2-001-2015) Bio-Ceramics: Unmet Challenges (Invited)

L. L. Hench*[1]; 1. University of Florida, USA

Affordable healthcare for an aging society will not be achieved by legislation and taxation. Ever increasing desires cannot be met by ever decreasing resources. The only viable solution to the rising costs of healthcare is to achieve revolutions in healthcare technology, distribution, expectations and priorities. Previous revolutions in healthcare, prevention of death and replacement of tissues, need to be augmented with two new, innovative revolutions: tissue regeneration and prevention of tissue deterioration. This lecture addresses the past, present and future revolutions in healthcare and outlines the potential for bioceramics in various forms to be able to provide the scientific and industrial foundation for these revolutionary technological changes to maintain a high quality of life without increasing cost of care. The emphasis is on the following topics: 1) bioactive glasses and ceramics for regeneration of tissues followed by 2) numerous unmet challenges; e.g., control of angiogenesis, soft tissue applications of bioactive ceramics and repair of chronic wounds, and 3) use of innovative bio-photonics technology for rapid, inexpensive, predictive human cell based screening of bioceramics-cell and tissue interactions.

9:50 AM

(GOMD-S2-002-2015) Resorbable Glass Microspheres for Applications in Regenerative Medicine

I. Ahmed*[1]; Z. K. Hossain[1]; V. Sottile[1]; D. Grant[1]; B. Scammell[1]; 1. University of Nottingham, United Kingdom

There has been a major shift in emphasis from tissue repair to tissue regeneration as a solution to the ever-growing need for long-term orthopaedic care. The aim of this work study was to investigate the feasibility of manufacturing resorbable phosphate-glass microspheres as cell carriers for applications in bone regenerative medicine. Phosphate-based glasses were investigated due to their easily controlled degradation profiles. The glass composition investigated was based on the system 40 P_2O_5, 16 CaO, 24 MgO and 20 Na_2O (in mol%) produced using the following precursors, NaH_2PO_4, $CaHPO_4$ and $MgHPO_4.3H_2O$ (Sigma Aldrich, U.K.), which were mixed together and melted at 1150 0C for 1.5 h. The glass was poured onto a steel plate and left to cool to room temperature, then ground and sieved into varying particle size ranges for manufacture of glass microspheres via flame spheroidisation. Early trials confirmed that bulk glass microsphere production was toally feasible and yields of 95% easily produced. Follow-on studies investigated manufacture of porous microspheres and studies showed that various porosity levels were achieved. Studies utilising human mesenchymal stem cells (hMSC) showed successful attachment to and within the microspheres produced. Resorbable phosphate-based glass microspheres were manufactured (both in bulk and porous format). hMSCs were seen to successfully attach to the microspheres produced.

10:10 AM

(GOMD-S2-003-2015) Tailoring bioactive glasses for various products (Invited)

L. Hupa*[1]; 1. Åbo Akademi University, Finland

Commercial melt-derived bioactive glasses with well-specified and controlled properties are based on a few different oxides. In general, the bioactive glasses guide and stimulate growth and healing of bone tissue, and they are available in fairly simple product forms such as monoliths or granules of defined particle size distributions. In contrast to simple glass products, current research is directed to emerging areas of using the glasses in regenerative medicine, wound healing, tissue engineering, etc. In the aforementioned applications the optimal product form is usually porous and the surface area to volume ratio is high. For regenerative medicine purposes, the glass composition must be adjusted to allow for hot working into desired shape and more importantly, to provide optimized biochemical effects in the end use. Interestingly, ions released from common network-forming or network-modifying oxides play important roles in bone metabolism. Basically, the glass composition can be tailored to possess desired hot working properties, and in vivo reactivity, by merely adjusting the composition. In this presentation, the various requirements of use and manufacture considered in tailoring the bioactive glasses will be discussed. The focus is on the physical and chemical properties of the glasses, and on how these properties can be adjusted by the choice of the composition and manufacturing method.

10:40 AM

(GOMD-S2-004-2015) Structure of Mg-based bulk metallic glass

J. K. Christie*[1]; 1. University College London, United Kingdom

Mg-based alloys are potential orthopaedic implant materials, because they have similar density and elastic properties to human bone. They degrade *in vivo*, but emit hydrogen gas as they do so. Certain compositions of Mg-Zn-Ca metallic glass form a passivating surface layer, rich in zinc, which prevents the release of hydrogen, allowing for the exploitation of these glasses as implant materials. We are using molecular dynamics simulations to understand the atomic mechanism behind the formation of this layer. We have begun by exploring the atomic structure of bulk Mg-Zn-Ca glasses, intending to identify those structural parameters which correlate with the formation of this layer. Our first-principles molecular dynamics simulations show that the local structure of the glasses shows very little dependence on composition. The Mg coordination number is ~13, and that of Zn is ~11. A wide range of bonding environments are present, including the existence of Mg-centred icosahedra, identified through a characterisation of the Voronoi polyhedra. No preference for e.g. Zn-Zn bonding was observed. It seems likely, therefore, that any structural difference in these materials occur at much larger length scales which are inaccessible at this level of simulation. We will discuss progress on the development of a classical interatomic force field for these materials, which will allow for the accurate simulation of much larger models.

11:00 AM

(GOMD-S2-005-2015) Structuring surfaces of bioactive glasses at the micro scale by mould casting

B. Pföss*[1]; M. Höner[2]; M. Wirth[1]; T. Vossel[1]; H. Fischer[2]; A. Bührig-Polaczek[1]; R. Conradt[1]; 1. RWTH Aachen University, Germany; 2. University Hospital RWTH Aachen, Germany

Within an interdisciplinary project, aiming at explaining the interaction between osteoblasts and microstructured bioglass surfaces, defect-free glass surfaces with a periodical structure were prepared by different mould casting techniques. For this purpose a number of relevant process parameters were assessed for two different glass compositions. These are first the viscosity, surface tension and crystallization maximum temperature of the glass melt. Furthermore the interaction between glass melt and mould material, with the mould surface bearing the mother shape to be impressed on the glass, plays a crucial role in the process. Problems to be avoided by any means consist in mould sticking and in the occurrence of chill ripples. Pt-Au alloys showed to be the most suitable mould material. The formation of chill ripples could be avoided by suitable pre-heating of the form. During this project we have developed a new process to fabricate samples of bioactive glasses with an excellently reproducible surface structure. The topology of the surfaces was investigated by electron microscopy and 3D-laserscanning. The bioactivity and cell compatibility were proven in simulated body fluid and cell culture experiments. First experiments show an alignment of cells which makes structured bioglass a promising candidate to further improved bone replacement applications.

11:20 AM

(GOMD-S2-006-2015) Modeling fracture behavior of porous glass

O. Keles*[1]; R. Garcia[2]; K. J. Bowman[1]; 1. Illinois Institute of Technology, USA; 2. Purdue University, USA

Mechanical behavior can limit functionality and performance in glass scaffolds that are used to heal bone related fractures, defects, and lesions. In the present study, four-point bend tests on porous glass are compared to the tensile loading simulations of microstructures that has porosity levels changing from 1 to 31 vol. %, corresponding to the cortical bone porosity levels. Microstructures containing non-overlapping pores of 48, 80, 120, and 160 μm diameter were generated, which also overlaps with the Haversian and Volkmann's canal sizes of bone. We combined the finite element method and fracture mechanics to investigate the effects of crack size distribution, pore-pore stress interactions, and crack orientation on fracture behavior of porous glass. Four different crack size distributions, including an experimental, normal, and Pareto distributions, were used in the simulations. Change in fracture strength with porosity is described by a recent formula that is based on 840 unique microstructures. The effects of crack size distributions on the steepness of fracture strength decrease with porosity is investigated. The effect of porosity on Weibull modulus is explained. In addition, design strategies to improve strength and reliability of glass scaffolds are discussed.

Symposium 3: Fundamentals of the Glassy State

Session 3: Structural Characterization of Glasses I

Room: Symphony Ballroom II
Session Chair: Hellmut Eckert, University of Sao Paulo

9:20 AM

(GOMD-S3-001-2015) Structure and dynamics in oxide glasses and glass-forming liquids: NMR progress and prognoses (Invited)

J. F. Stebbins*[1]; 1. Stanford University, USA

Since early studies of boron coordination in the late 1950's by P. Bray's group, followed by high-resolution spectroscopy of Si, Al, and P speciation in the mid-1980's, NMR has blossomed into a method of choice for determining short-range environments (e.g. first and second-shell coordinations) for many critical cations (and anions!) in oxide glasses. Double- and triple-resonance NMR and other advanced methods have yielded unique information on network ordering and connectivity. In situ, high temperature NMR has in a few simple systems provided key data on the dynamics that control liquid properties such as diffusivity and viscosity, as well as constraints on changes with T in structure. The latter, required by the significant configurational heat capacities in all but the least "fragile" of glass-forming liquids, have been explored in some detail for glasses with varying fictive temperature produced by variable thermal histories, but are still not well-known, particularly at T>>Tg. Effects of pressure on structure are also beginning to be understood from NMR on quenched samples and even a few pioneering in-situ studies of compressed glasses, but remain a challenging area for the future, of deep interest for both advanced materials and geosciences. This presentation will look to the bright future of NMR studies with lessons from milestones in past and current work.

9:50 AM

(GOMD-S3-002-2015) Disorder in Strontium Aluminosilicate Glasses and Transparent Polycristalline Ceramics (Invited)

F. Fayon*[1]; K. Al Saghir[1]; S. Chenu[2]; E. Véron[1]; C. Genevoix[1]; G. Matzen[1]; D. Massiot[1]; M. Allix[1]; 1. CNRS, France; 2. limoges university, France

The structure of strontium aluminosilicate glasses and polycristalline transparent ceramics are investigated using advanced solid-state NMR methods. Through-bond and through-space correlation methods are used to characterize the local and medium range disorder in the glass structure. The structures of the glasses are then compared to that of new highly transparent polycrystalline ceramics obtained by full congruent crystallization of the parent glasses. This method is efficiently used here for the production of dense ceramics without residual porosity and with very thin grain boundaries. XDR and NMR shown that the hexagonal structures of these crystalline materials also exhibit a variable degree of local disorder related to Sr partial site occupancies and Al/Si inversion in the tetrahedral sites. DFT computations of the birefringence performed for structural models accounting for disorder reveal that the birefringence of the crystalline phase is strongly influenced by the local disorder. We show that the introduction of a controlled degree of chemical disorder in the structure can thus be used to achieve ultimate transparency reaching the theoretical limit. Using this new concept, scalable polycrystalline ceramics with non-cubic structures and micrometer scale crystal size reaching 90% transmittance in the visible range are obtained for the first time.

10:20 AM

(GOMD-S3-003-2015) Spectroscopic study on the influence of hydroxide ions on the UV-transparency of soda-lime silicate glass

A. Deinhardt*[1]; M. Kilo[1]; G. Sextl[2]; H. Eckert[3]; 1. Fraunhofer Institute for Silicate Research ISC, Germany; 2. University of Würzburg, Germany; 3. University of Münster, Germany

It is the objective of this study to develop a highly UV-transparent soda-lime derived silicate glass, which could be a cost-efficient alternative to borosilicate glass as used in the special lamp industry. Alternatively, an UV - transparent window glass would support the UV-driven generation of provitamin D_3, which positively influences the health and well-being of people. It is well known that OH - ions have a decisive influence on the network stability, so it can be assumed that it will also affect the UV transparency. In order to minimize the water content in the glass, the batches were dried and melted under inert conditions in an electrically heated furnace at 1500 °C. Afterwards the glass melt was poured onto a preheated brass plate, to rapidly cool the glass below the transformation temperature and subsequently cooled under controlled conditions. By using spectroscopic methods (UV-Vis-, IR-, Raman-, and most importantly NMR-spectroscopy) it can be shown that the OH content is a determining factor for the ultraviolet transmittance. Its influence even surpasses the influence of different network modifying ions, which were similarly prepared and analyzed. By reducing the water content it was possible to shift the UV edge of soda-lime silicate glass (50 % transmission, sample thickness: 3 mm) from 276 nm down to 260 nm.

10:40 AM

(GOMD-S3-004-2015) The structure of glasses and its evolution above T_g – crystallisation, phase separation and species exchange: lessons from *in situ* MAS-NMR (Invited)

L. van Wüllen*[1]; S. Venkatachalam[1]; J. Holzinger[1]; M. Engelmayer[1]; 1. Augsburg University, Germany

Despite considerable progress in the characterization of the structure of amorphous solids at ambient temperatures, only sparse information is available about the structure of the corresponding melts and the evolution of the structure with temperature. Changes in the atomic structure occurring during cooling of the glass melt contribute to the configurational entropy of the liquid and are thus closely linked to structural relaxation and viscous flow. Since the structure of the glass and hence its physical and chemical properties critically depend on these structural changes and the corresponding kinetics (e. g. phase separation, crystallisation), a detailed knowledge of the equilibria between different structural units and their temperature dependence constitutes a necessary ingredient to a full understanding of the glass structure at ambient conditions. In this contribution we present results obtained on a variety of glass systems including phosphate, aluminophosphate, phosphosilicate and borosilicate glasses. Structural motifs on short and intermediate length scales are identified employing a range of advanced dipolar based solid state NMR methodologies. The structural evolution with temperature is monitored employing in situ MAS NMR spectroscopy at temperatures of up to 700 °C.

11:10 AM

(GOMD-S3-005-2015) Probing glass/liquid structure and dynamics with novel NMR spectroscopic techniques (Invited)

S. Sen*[1]; D. C. Kaseman[1]; T. Edwards[1]; I. Hung[2]; Z. Gan[2]; 1. University of California, Davis, USA; 2. National High Field Magnetic Laboratory, USA

Typically spectroscopic techniques including NMR are sensitive only to the short-range order in the glass structure in terms of the nearest-neighbor coordination environments of consituent atoms. In suitable cases, the connectivity between the coordination polyhedra can also be determined. However, such a description lacks information on the distribution of local site symmetry and anisotropy. We have recently developed two-dimensional NMR techniques that correlate the isotropic and anisotropic parts of the chemical shift tensor with superior spectral resolution and consequently allow for a detailed parametrization of the nature and extent of disorder and often unequivocal identification of structural units. Furthermore, the temperature dependence of the anisotropy can reveal dynamical processes in the supercooled liquid associated with glass transition. The results of such studies on oxide and chalcogenide glasses and liquids will be presented. Additionally, we will present the first *in situ* high-pressure (up to 2 GPa) NMR results of pressure induced reversible structural changes in oxide glasses, obtained using a high-pressure NMR probe designed in our laboratory. The implications of these results in understanding various stress-induced phenomena in amorphous materials will be discussed.

11:40 AM

(GOMD-S3-006-2015) Impact of Sodium Addition on the Structure and Properties of AlP Silicate Glasses

R. Youngman*[1]; B. Aitken[1]; 1. Corning Incorporated, USA

Glasses can be formed over a wide composition region in the Al_2O_3-P_2O_5-SiO_2 system without the incorporation of modifier cations. The pronounced association between Al and P, leading to stabilization of $AlPO_4$-like tetrahedra, results in glasses with high characteristic temperatures and other silica-like properties, such as low thermal expansion. For glasses along the 70% SiO_2 join, the ratio of Al to P determines many of their properties, driven by the concentration of fully networked polyhedra. Unfortunately, one of the consequences of such behavior is that the liquidus temperature increases with the degree of polymerization. To lower liquidus temperature and thereby aid in formability, one solution is the incorporation of a modifier like Na_2O. In this work, we examine the impact of Na_2O addition on Al_2O_3-P_2O_5-SiO_2 glasses at 70 mol% SiO_2 with emphasis on which network former is more susceptible to modification by small quantities of Na. In glasses with a constant P_2O_5 content of 7.5mol%, characteristic temperatures show a weak decrease as Na replaces Al until the ratio of $Na_2O+P_2O_5$ to Al_2O_3 equals 1, at which point all characteristic temperature drop rapidly with further increase in Na_2O content. Multi-nuclear NMR data obtained for these glasses aid in understanding the change in network structure necessary to account for these property trends.

Session 5: Mechanical Properties of Glasses I

Room: Symphony Ballroom III
Session Chair: Lothar Wondraczek, University of Jena

9:20 AM

(GOMD-S3-007-2015) A History of Optical Fiber Strength and Reliability for the Benefit of Emerging Flexible Glass Applications (Invited)

G. S. Glaesemann*[1]; 1. Corning Incorporated, USA

In the late 1970's and early 1980's, optical fiber grew from research and pilot plant projects into large scale manufacturing. Due to the fragile nature of these thin strands of glass, the approach for mechanical reliability had to mature and meet the needs of a diverse portfolio of applications, while also allowing for rapid deployment of the product. The lifetime model had to be accurate and practical from an engineering point of view, and measured strength distributions had to be relevant for the intended applications. Guidance on the handling of fiber needed to be thorough yet practical. Consequently, the overall reliability strategy had to be closely linked to known glass mechanics phenomena that influence lifetime, namely, subcritical crack growth and damage mechanics. Today there are an increasing number of applications where flat glass finds itself being stressed and handled under fatigue conditions. The emerging concerns are reminiscent of the early days of optical fiber. It is contended that the experience and strategies that grew out of the optical fiber experience are relevant for these new applications of flat glass.

9:50 AM

(GOMD-S3-008-2015) In-Situ Evaluation of Elastic and Inelastic Deformations of Glasses under Some Indenters (Invited)

S. Yoshida*[1]; S. Sasaki[1]; K. Wada[1]; M. Kato[1]; A. Yamada[1]; J. Matsuoka[1]; N. Soga[1]; 1. The University of Shiga Prefecture, Japan

This study focuses on elastic and inelastic deformations of glasses during the loading and unloading indentation cycle. In order to evaluate in-situ deformation behaviors of glass during the indentation, an indenter-microscope is constructed using an inverted microscope and a self-made indenter which includes a load cell and a piezoelectric actuator to position a diamond tip. Using this set-up, the sequence of micrographs of the contact regions between the glass and the indenter is successfully obtained during the indentation cycle. From the direct observations, an experimental evidence of sinking-in during a loading half-cycle can be acquired for some glasses. It is found that both the shape of contact region and the amount of sinking-in are affected by glass composition and by indenter geometry. These deformation behaviors of glass have a close connection with the contact damage or cracking in the glass.

10:20 AM

(GOMD-S3-009-2015) Plasticity, crack initiation and defect resistance in alkali-borosilicate glasses: From normal to anomalous behavior

R. Limbach*[1]; A. Winterstein-Beckmann[1]; A. Dellith[2]; D. Möncke[1]; L. Wondraczek[1]; 1. Friedrich Schiller University of Jena, Germany; 2. Leibnitz Institute of Photonic Technologies IPhT, Germany

We report on the mechanical properties of glasses in the ternary sodium-borosilicate system, covering the wide range of compositions from pure SiO_2 to binary sodium-borates, and crossing the region of various commercially relevant specialty borosilicate glasses, such as the multi-component Duran-, and BK7-type compositions. One series of glasses with $R(Na_2O/B_2O_3) = 0.2$ contains only bridging oxygen atoms, while other glasses are characterized by an increasing number of non-bridging oxygen ions. Elastic moduli, Poisson ratio, hardness as well as the creep and crack resistance were evaluated and annealing experiments were performed to determine the contribution of densification on the indentation deformation. The mechanical properties were correlated with structural characteristics of near- and mid-range, such as the conversion of neutral $B\varnothing_3$ units into charged $[B\varnothing_4]^-$ tetrahedral groups, the formation of non-bridging oxygen ions or the connectivity between the silicate and the borate sub-network. It was found that all these aspects play an important role on the physical and mechanical properties as well as the indentation deformation and crack initiation behavior and for the generation of a full picture of this complex glass system, these phenomena have to be treated equally

10:40 AM

(GOMD-S3-010-2015) Structural study of alkali boroaluminosilicate glass: response to damage

S. Gomez*[1]; I. Dutta[1]; G. G. Moore[1]; M. P. Carson[1]; 1. Corning Incorporated, USA

The response and the structural changes that Na_2O-B_2O_3-Al_2O_3-SiO_2 glasses undergo when subjected to damage have been studied. Both, as-made and ion-exchanged glasses were evaluated. Damage in the glasses was introduced by indentation using a Vicker's diamond tip. The structural characteristics of the glasses, before and after damage, have been characterized by Raman spectroscopy and TEM/EELS. Upon indentation, both Raman and EELS show evidence of changes in the silica network, manifested by shifts associated with Si-O-Si units. The extent of the effect of indentation in the glass network increases with increasing indentation load. The work presented here will correlate structural characteristics of the studied glasses when damaged.

11:00 AM

(GOMD-S3-011-2015) Structure and Mechanics of NBO-Free Calcium Boroaluminosilicate Glasses with B_2O_3 substituted for SiO_2

T. M. Gross*[1]; 1. Corning Inc., USA

A calcium boroaluminosilicate glass series with Al_2O_3 = CaO and B_2O_3 substituted for SiO_2 was investigated. The glass structures were determined by NMR at various fictive temperatures and showed that for each instance the aluminum is primarily tetrahedrally coordinated and the boron is primarily trigonally coordinated. The Young's modulus for each glass was calculated according to the Mackenzie and Makashima model and is in close agreement with RUS measurements. For this glass series, as B_2O_3 is substituted for SiO_2, the Young's modulus decreases, the packing density increases, and the binding energy decreases. Also, as B_2O_3 is substituted for SiO_2, the Young's modulus dependence on fictive temperature increases. For thin glass applications, the high boron, low modulus glasses are advantageous over higher modulus glasses since the bend induced stress for a given bend radius is lower. The indentation damage resistance of glasses in this series was measured and the high B_2O_3, low SiO_2 glasses are also shown to have higher Vickers indentation cracking threshold than the high SiO_2, low B_2O_3 glasses. The indentation cracking behavior is discussed in terms of packing density and coordination number of network forming cations. The indentation cracking threshold is also shown to be highly dependent on indentation rate and sharpness of the indenter.

11:20 AM

(GOMD-S3-012-2015) Damage Resistant Glasses with High Strength

M. Dejneka*[1]; T. Gross[1]; 1. Corning Incorporated, USA

While chemically strengthened glasses retain their strength far better than ordinary glass, they still scratch and break. We have discovered glass compositions that increase the Vickers crack initiation threshold by a factor of five. These compositions can also be ion exchange to a compressive stress of 800 to 1000 MPa and are capable of case depths of 50 microns or greater. The resulting tough new ion exchanged glasses have a greater damage tolerance than conventional ion exchanged glasses and exhibit a Vickers crack initiation load of 30-40kgf, compared to 5 to 7 kgf for existing chemically strengthened glasses. The unique glass structure, properties, and compositional system that give rise to this remarkably high damage tolerance will be discussed.

11:40 AM

(GOMD-S3-013-2015) Crack Resistant Al_2O_3–SiO_2 Glasses Fabricated by Containerless Processing

G. A. Rosales Sosa*[1]; A. Masuno[1]; H. Inoue[1]; Y. Higo[2]; S. Kojima[3]; K. Tae Hyun[3]; K. Matsumoto[3]; 1. Institute of Industrial Science, The University of Tokyo, Japan; 2. The Japan Synchrotron Radiation Research Institute, Japan; 3. University of Tsukuba, Japan

Strong glasses are required in various technological fields. However, their brittlenes and scratchability limits their applicability. Al_2O_3–SiO_2 glasses are known as base material to make glasses with good mechanical properties including high cracking resistance, hardness and elastic moduli. Their glass forming region is usually limited to 30mol% of Al_2O_3 due to easy crystallization from the melts. In this work, transparent xAl_2O_3–$(100–x)SiO_2$ glasses with $30 \leq x \leq 60$ were fabricated by aerodynamic levitation and their mechanical properties were investigated. The density ρ of the glasses and their atomic packing density C_g increased with the Al_2O_3 content. The elastic moduli and the Vickers hardness also increased with x. Furthermore, it was found from the indentation experiments that the cracking resistance increased with x.

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 1: Amorphous Semiconductors: Electronic Properties, Transport and Modeling

Room: Concerto B
Session Chair: Xiang-Hua Zhang, University of Rennes / CNRS

9:20 AM

(GOMD-S4-001-2015) Impact of Optical and Electrical Properties on Performance of Hydrogenated Silicon Based Photovoltaic and Microbolometer Devices (Invited)

N. Podraza*[1]; 1. University of Toledo, USA

Doped and undoped amorphous and nanocrystalline hydrogenated silicon (Si:H) and its alloys are employed in thin film photovoltaics (PV) for energy generation and as the imaging layer in uncooled infrared sensing microbolometers. The infrared to ultraviolet range optical response of Si:H based materials either directly impacts device performance or is linked to material properties that do. Spectroscopic ellipsometry measurements of thin films and layers in devices have been applied from 0.19 to 38 μm (6.5 to 0.035 eV) to determine structure in the form of surface roughness and bulk film thicknesses and optical properties in the form of the complex dielectric function spectra $\varepsilon = \varepsilon_1 + i\varepsilon_2$. Variations in ε correspond to order and the presence of impurities. Real time spectroscopic ellipsometry (RTSE) has been applied in situ, during film growth by plasma enhanced chemical vapor deposition to track structural and compositional gradients reflected in ε. RTSE studies have identified thickness dependence of the evolution of crystallinity in Si:H, band gap gradients in amorphous Si:H, and the substrate dependence of growth. Spectroscopic ellipsometry studies of layers in PV devices and imaging layers for microbolometers are compared with electrical performance properties to provide guidance for device optimization.

9:50 AM

(GOMD-S4-002-2015) Hydrogen microstructure in amorphous silicon: A joint analysis from experimental data and *ab initio* interactions (Invited)

P. Biswas*[1]; 1. The University of Southern Mississippi, USA

In this talk, I will address the problem of designing complex material as an inverse problem, and show that many aspects of structural and electronic properties of amorphous materials can be understood better from an inverse or a hybrid point of view. In particular, I will discuss how the distribution of hydrogen in amorphous silicon can be obtained by inverting experimental nuclear magnetic resonance spectra in conjunction with first-principles density-functional calculations. New results concerning two important aspects of hydrogen microstructure, such as voids and molecular hydrogen, will be presented with particular emphasis on the shape and the size of voids.

10:20 AM

(GOMD-S4-003-2015) RMC-Force: toward a new strategy for materials modeling

A. Pandey*[1]; P. Biswas[2]; D. Drabold[1]; 1. Ohio Univeristy, USA; 2. University of Southern Mississippi, USA

We introduce a novel structural modeling technique (RMC-Force) which merges the Reverse Monte Carlo (RMC) method and the forces obtained from first principles or empirical potentials. It may be understood as a development of our earlier work "Experimentally Constrained molecular Relaxation" [P. Biswas et al., Phys Rev B 71 054204 (2005)]. The new scheme was used to model amorphous silicon (a-Si) and it produces a model jointly consistent with neutron diffraction data, an empirical potential and existing Wooten-Winer-Weaire models. We note that because a-Si is over-constrained in the sense of Phillips and Thorpe, it is an especially difficult test case. Details of the method and its convergence will be provided. We have extended the method to binary systems, and will also report new models of amorphous silica and other systems.

10:40 AM

(GOMD-S4-004-2015) Band gap engineering: a computational approach

K. Prasai*[1]; P. Biswas[2]; D. Drabold[1]; 1. Ohio University, USA; 2. University of Southern Mississippi, USA

The quest for novel materials with special optical, transport or electronic properties is as old as condensed matter physics itself. In this paper, we report a method designed to find atomic coordinates consistent with a desired electronic density of states. To start with, we will give a detailed report on amorphous silicon, and configurations that maximize optical gap and others that maximize metallicity. The primary challenge of the scheme is simultaneously constraining the atomic coordinates to lie in a manifold that minimizes the total energy while satisfying the desired density of states to ensure that the coordinates obtained are realistic (potentially realizable). Preliminary results suggest that new models with improved gaps are close to the traditional minimum energy models with suitable perturbations near the atoms upon which the band-edge states are localized.

11:00 AM

(GOMD-S4-005-2015) Physics of a-Si:H night-vision devices (Invited)

D. Drabold*[1]; A. Pandey[1]; 1. Ohio University, USA

For infrared (IR), "night-vision" imaging applications, doped hydrogenated amorphous silicon is of prime interest as the active material placed at the IR focal plane. The physical property that provides this utility is a high temperature coefficient of resistance. In this talk, we discuss the physical origin of this effect, and emphasize the role of the large electron-phonon coupling for states near the band edges. The electrical conductivity is estimated with the Kubo-Greenwood formula and an ab initio Hamiltonian. We also discuss the related problem of acceptor and donor doping with B and P impurities, including all relaxation effects with ab initio interactions. B is shown to enter the network with considerable strain, contributing to the broad valence tail of the material, whereas P is much more "substitutional". Mobile H is attracted to both B and P, which strongly affects the doping efficiency, and we show that H passivates the doping. Finally, we demonstrate that mobile H and a dynamic lattice induce interesting fluctuations in conductivity that might be associated with the resistivity fluctuations observed in experiments.

Session 3: Novel Optical Glass Materials

Room: Concerto A
Session Chair: Shibin Jiang, AdValue Photonics Inc

9:20 AM

(GOMD-S4-006-2015) Nanoparticles in matrixes to induce enhancement of optical nonlinearity (Invited)

Q. Liu*[1]; M. Song[1]; 1. Wuhan University, China

Any technique that permits the creation of large nonlinearity in glasses is of great interest for practical reasons or the standpoint of the underlying physics. Expensive nonlinear crystals replaced by low-cost glasses would open up the prospect of parametric frequency converters and linear electro-optic modulators that are fully integrated into optical fibers or planar glass waveguides. Second harmonic generation (SHG) was observed in glasses by electron beam irradiation, thermal/electric poling, X-ray poling, laser irradiation and thermal poling so on. The mechanisms of them were also discussed. High second-order nonlinearity was obtained through the formation of p-n junction using PECVD deposition of a-Si:H films on fused silicasubstrate without additional electrical poling to induce SHG in the isotropic amorphous materials. Recently, Ag-nanoparticles in chalcohalide matrixes by ion implantation, nonlinear nanocrystals induced by fs laser irradiation in oxide glasses, also by heat treatment in chalcogenide glasses were fabricated. The enhancement of their optical nonlinear property were observed, which indicated that ideal glasses containing nanoparticleswith optimum size and distribution parameters would show high nonlinear optical properties.

9:50 AM

(GOMD-S4-007-2015) Structure and optical properties of gallium oxide containing phosphate glasses

T. Cardinal*[1]; P. Hee[1]; M. Vangheluwe[2]; J. Desmoulin[1]; Y. Ledemi[3]; S. Danto[1]; Y. Petit[1]; S. Kroeker[4]; L. Canioni[2]; Y. Messaddeq[3]; R. Vallee[3]; 1. ICMCB, France; 2. LOMA, France; 3. COPL, Canada; 4. University of Manitoba, Canada

Following the improvement in the performances of exotic amorphous materials, the demand for adapted near-IR optical glasses grows continuously. Nowadays exotic glasses are routinely prepared and incorporated in photonic and opto-electronic devices. Aluminophosphate glasses have been widely investigated for photonic application, but little attention has been paid to gallium oxide containing phosphate glass. The structure and optical properties of gallophosphate glasses in the pseudo-binary system xGa_2O_3 – (100-x) $NaPO_3$ (x = 0 to 30 mol%), have been investigated. The effect of the progressive addition of Ga_2O_3 on the local glass structure has been evaluated using Raman, infrared and NMR spectroscopies. As a function of the Ga_2O_3 concentration, complementary informations have evidenced the modification of the distribution and the connectivity of the phosphate groups within the glass network and the progressive role of gallium oxide as glass former. Direct correlation between the structure modification and the chemical physical properties have been established. Index modification and nano-grating formations have been obtained thanks to direct femtosecond laser writing. It has been demonstrated that addition of silver ions in this glass composition led to a significant improvement of the nano-gratings formation by providing a reservoir of available free electrons.

10:10 AM

(GOMD-S4-008-2015) A new system of gallate glasses: Ga_2O_3-GeO_2-Na_2O-BaO

Candidates for optical applications in the near infrared

E. Fargin*[1]; P. Hee[1]; Y. Ledemi[2]; M. Dussauze[3]; T. Skopak[1]; T. Cardinal[1]; S. Kroeker[4]; Y. Messaddeq[2]; 1. Institut de Chimie de la Matière Condensée de Bordeaux, France; 2. Centre d'Optique, Photonique et Laser, Canada; 3. Institut des Sciences Moléculaires, France; 4. University of manitoba, Canada

The demand for glass compositions adapted for optical applications in the near infrared spectral range has increased continuously since the performances of exotic compositions are nowadays competitive. The preparation process of exotic glasses and their incorporation into photonic and opto-electronic devices are becoming increasingly efficient. Silicate, phosphate and aluminate glasses have been widely investigated but little attention has been devoted to gallates glass matrix, which is however potentially an excellent candidate. Gallates glasses in the Ga_2O_3-GeO_2-Na_2O-BaO system are offering wider transparency in the near infrared region compared to classical oxide glasses compositions. They are also interesting for nonlinear optical properties since Ga_2O_3 confers significant polarizability and hyperpolarizability. The low phonon energy of such materials also makes them of interest as host matrices for rare earth ions in lasing applications. Explorative study of these gallates glasses has been conducted through the utilization of a design of experience approach, leading to the modelling of the properties. Thermal properties, linear and nonlinear optical properties were characterized while structural investigations were conducted using NMR, infrared and Raman spectroscopies

10:30 AM

(GOMD-S4-009-2015) Optical and spectroscopic properties of tungsten phosphate glasses containing silver nanoparticles

M. Dousti*[1]; A. de Camargo[1]; 1. Universidade de São Paulo, Brazil, Brazil

Glasses based on tungsten and phosphate oxides show promising optical and physical properties. Moreover, the incorporation of metallic nanoparticles (NPs) could modify the optical properties of these high refractive index hosts due to the surface plasmon effect of the NPs. In this work, we studied the effect of Sb_2O_3 as reducing agent to increase the transparency of these glasses, with the aim of nucleating silver NPs, by varying the concentration of the silver precursor, and the duration of heat-treatments. For the glass compositions $(100\text{-}x)(NaPO_3\text{-}WO_3)\text{-}xSb_2O_3$ (mol%), by increasing the concentration of antimony oxide there was a suppression of the broad absorption band of tungsten in the visible and a shift of the UV-absorption edge towards lower energies. The surface plasmon resonance (SPR) band of silver NPs is observed for the as-quenched sample with molar ratio $M=WO_3/(WO_3+NaPO_3)=0.5$, while other compositions (e.g. M=0.2, 0.3 and 0.4) undergo such nanocrystallization upon subsequent heat-treatments at the glass transition temperature. The required heat-treatment duration depends on the concentration of NPs and the amount of tungsten oxide. It could be concluded that antimony and tungsten ions are responsible for reducing the Ag ions to Ag NPs at low and high M factor, respectively. The SPR band frequency and intensity could be controlled by M factor and heat-treatment period.

10:50 AM

(GOMD-S4-010-2015) Moldable multispectral glasses transparent from the visible up to the thermal infrared region

A. Bréhault*[1]; L. Calvez[1]; X. Zhang[1]; 1. Université de Rennes 1, France

Our study aims to develop multispectral moldable optics operating simultaneously from the visible up to the thermal infrared region for night vision application. Among chalcogenide glasses, sulfide glasses possess the largest transmission in the visible range with an infrared transmission up to 11-12µm. For this study, GeS_2-Ga_2S_3-CsCl system was selected for its good stability against crystallization and high transparency in the visible. Our results show the different properties of this system and the synthesis of two specific compositions. The optical transmissions, the refractive indices from 0.6 to 10.7µm, the dispersion and the indices as function of temperature associated with these compositions are studied. The thermal properties, molding ability and mechanical properties will be presented to complete these optical results. For these glasses, the addition of cesium chloride causes a slight degradation of optical properties due to its water sensitivity. In order to protect these glasses against the atmospheric aggression, a protective coatings of zinc sulfide has been applied by sputtering. To go further, an antireflective coating has been developed to enhance the transmission in specific ranges. These two particular compositions able us to consider the production of optics which cover a huge spectral band and propose a real optical alternative to the ZnS for optical system.

11:10 AM

(GOMD-S4-011-2015) Molecular Dynamics Simulation of Glasses for Photomultiplier Tubes in Neutrino Detection

R. Dongol*[1]; T. Adama[2]; S. Sundaram[1]; 1. Alfred University, USA; 2. Corning Incorporated, USA

Photomultiplier tubes (PMT) used in neutrino detection experiment are exposed to high-purity water at 14C and hydrostatic pressures of approximately 890 KPa. This creates a unique and detrimental environment for the glass surface as it has been shown that water is a corrosive agent for the glass and high stress can lead to brittle failure of the glass. In our study, we have applied molecular dynamics (MD) simulation to investigate the relevant properties (e.g., mechanical properties and chemical durability) for PMT glass composition range in weight%: SiO_2 = 65-70, Na_2O = 6-9, Al_2O_3 = 4-7, B_2O_3 =

15-18, BaO = 0-3, ZnO = 0-3, and CaO = 0-1. Young's, shear, bulk moduli, stress-strain analysis and nano-indentaion results will be reported as a function of glass composition. The goal of the work is to run a multi-species optimization to search for the most suitable glass composition with the best mechanical properties and chemical stability. The selected glass composition will be used for further experimental study of performance of the glass for neutrino application.

Symposium 5: Glass Technology and Cross-cutting Topics

Session 1: Challenges in Glass Manufacturing I

Room: Concerto C
Session Chair: Hong Li, PPG Industries, Inc.

9:20 AM

(GOMD-S5-001-2015) Container glass: Where have we been and where are we going?

G. Lubitz*[1]; 1. Vetropack Holding AG, Switzerland

Glass has a long history. The first glass made by mankind was in Israel/Mesopotamia in about 3,000 B.C. Over the centuries game-changing advances were made in the melting and forming processes. Productivity increased and the product range was extended. Due to automation and mass production introduced in the 18th and 19th centuries, prices continued to decrease and glass largely replaced other packaging material such as pottery. However, in the late 20th century PET and other alternative materials gained an increasing market share of soft drink, mineral water and food packaging. This led to a decreasing number of glass production lines, especially in America and Europe. Fortunately, our western "throw-away society" has recently evolved toward a healthier and more environmentally aware lifestyle. But, the last "revolutionary" step in container glass production was in 1924 with the invention of the IS forming machine. Since then only evolutionary developments have been introduced, and such gradual evolution cannot ensure the industry's long-term survival. Intensive energy use, large capital investment and weight reduction with increased strength are all issues that must be addressed. To overcome these challenges it may well become critical for the container glass industry to develop the next game-changing technology. Potential solutions will be presented.

9:40 AM

(GOMD-S5-002-2015) Physical and chemical mechanisms happening in soda-lime batch melting followed by *in situ* imaging

W. Woelffel*[1]; M. Chopinet[1]; M. J. Toplis[2]; E. Véron[4]; E. Boller[3]; E. Gouillart[1]; 1. Saint-Gobain Recherche/CNRS, France; 2. Observatoire Midi-Pyrénées, France; 3. European Synchrotron Radiation Facility, France; 4. Conditions Extrêmes et Matériaux : Haute Température et Irradiation, France

Though a fair understanding of binary batch melting has been achieved, there is still a lack of knowledge about ternary interactions in more complex batches. This study aims at understanding the physical and chemical mechanisms propagating heterogeneity throughout the melting of a glass batch, thus requiring a considerable overheating. We study glass batches composed of size-controlled grains of sand, sodium carbonate and various calcium oxide-bearing species, mostly calcium carbonate and oxide. Isothermal treatments at 900°C, 1100°C and 1300°C are used. In addition to SEM, EDX and thermodynamic modeling, ultrafast *in situ* microtomography brings key insights to understanding the coupling between granular microstructure, reactive wetting and chemistry. Our results show that limestone grains undergo transformations that strongly depend on their neighborhood: early wetting by sodium carbonate leads to mixed carbonate formation on a small scale, quickly decomposed to solid dicalcium silicates and liquid sodium silicates. Delayed wetting and incomplete calcium to mixed carbonate conversion produce lime, whose dissolution and wetting are measured to be harder than dicalcium silicate dissolution. The variety of reactional paths followed by limestone, due to the batch granular nature as well as its chemical versatility, is consequently a major source of heterogeneity persistence

10:00 AM

(GOMD-S5-003-2015) The Use of Hot Stage Microscopy to Observe and Analyze Glass Formation Behavior

A. Z. Zamurs*[1]; 1. Rio Tinto Minerals, USA

The choice of raw materials in a glass batch can influence the glass melting process, which can in turn influence processing conditions and final glass properties. Traditionally, analytical tools such as X-ray diffraction (XRD) and differential scanning calorimetry (DSC) are used to study the kinetics of the many reactions that take place during glass formation. In this work, we demonstrate the feasibility of using hot stage microscopy (HSM) to evaluate glass formation processes. We show that HSM is a complementary technique to XRD and DSC. We have used HSM to study the effect of raw materials on the transformation temperatures of glass batches with a given overall composition. The batches were also analysed using DSC, and the partially reacted batches using XRD, to determine the transformation temperatures in parallel. The conclusions from these three techniques correlate very well, which demonstrates the feasibility of using HSM to study glass batch reactions. The paper will also highlight the strengths and weaknesses of the HSM technique.

10:20 AM

(GOMD-S5-004-2015) Influence of alumina and boron raw materials on the melt formation in sodium aluminoborosilicate batches

A. I. Christmann*[1]; O. Hochrein[2]; J. Deubener[1]; 1. Clausthal University of Technology, Germany; 2. SCHOTT AG, Germany

Due to the fact, that industrial glass production is an energy-intensive process, it is a desirable goal to reduce energy consumption during the glass melting process. Therefore knowledge about the thermo-chemical reactions of specific alumina and boron raw materials in batches for aluminoborosilicate glasses during the melt down process is increasingly growing in importance. In order to determine data under these conditions a laboratory based quench method was applied. The quenched batches were analysed using Rietveld refinement of X-ray diffraction patterns with internal standard. The volume fractions of residual raw materials (a), new formed intermediate crystalline phases (b) and the evolved melt (c) were quantified. From these data the sequence of the relevant reactions and melting path were proposed. The results show that the fraction of intermediates increases using alumina raw materials in the order Al_2O_3, $Al(OH)_3$, AlOOH, while the total melting time (c = 100%) was found to be independent on the nature of the intermediate structures. Further, we show that specific boron components in the batch, such as B_2O_3, H_3BO_3 and $Na_2B_4O_7*5H_2O$ change the melting path in a characteristic way.

10:40 AM

(GOMD-S5-005-2015) Characterization of Accelerated Batch Melting by Using an Up-Scaling Method

V. Niessen*[1]; R. Conradt[1]; 1. RWTH Aachen University, Germany

Much effort has been invested to establish a highly effective arsenal of approaches to the melting behavior of industrial batches. This up-scaling method has been proved in many projects and was employed to the development of a soda-lime-batch with an accelerated batch melting performance. In this study the batch is characterized on the micro, meso and macro scale. At the micro scale, the batch is analysed by using DTA-TG and Hot-Stage Microscopy, which involve small sample sizes (< 1 g) for investigation of physical reactions of unary, binary and ternary batch systems. At the meso scale (conductometry, modified batch-free time) the local progress of batch reactions is identified. The methods yield fingerprints of the local melting process allowing a quantitatively comparison (e.g. water release, primary melt formation. With the 10 kg – test at the macro scale a batch blanket 5 cm high is exposed to radiative heating from above and to heating via batch-to-melt contact from below. In a final step, the tested batch is to be introduced to the industrial scale. This comprises an analysis of the performance of the furnace in which the batch shall be used.

11:00 AM

(GOMD-S5-006-2015) Factors influencing quality of reduced glasses and their experimental evaluation

M. Hubert*[1]; M. Rongen[1]; P. Marson[1]; A. Suarez Barcena[1]; M. van Kersbergen[1]; A. Faber[1]; S. Lessmann[1]; 1. CelSian Glass & Solar, Netherlands

The quality of the final product must be secured by an adequate industrial glass production process. All along the production process, numerous aspects have to be considered, including notably (amongst others) the choice of the glass composition and the raw materials employed, the furnace combustion atmosphere, the type of refractories used, the thermal cycle experienced by the glass melt…. In fact, under-evaluating or neglecting one or several of these aspects can highly influence the final quality of the glass and lead to undesired colour instabilities and detrimental defects, such as un-molten raw materials, blisters, seeds, or inclusions… In this presentation, the quality-determining factors in the industrial glass production will be briefly summarized, and the experimental solutions developed at CelSian for studying them will be presented. Specific attention will be focused on the influence of redox on the melting and fining of reduced glasses. Based on case studies investigated with CelSian's dedicated experimental tools, it will be shown how small changes in the redox can have a large influence on the melting process and on the final quality of the glass.

11:20 AM

(GOMD-S5-007-2015) Mechanisms related to cleaning of boron containing flue gases

S. Thiele*[1]; R. Conradt[1]; 1. RWTH Aachen University, Germany

The evaporation of volatile species from the glass batch and melt in industrial furnaces is an undesirable phenomenon. The loss of components like sodium or boron does not only have an effect on glass composition, properties and quality, but also make flue gas filters behind glass melting tanks indispensable. The operation of these filters is often based on long experience and collected empirical data, but filter corrosion or slip-through of components can still lead to enormous problems. In boron containing flue gases, the main difficulties during filter operation are the slip-through of the gaseous species $(HBO_2)_n$ and H_3BO_3 and the back-reaction of already precipitated filter dust to gaseous species. As environmental protection, and therefore the reduction of the level of emissions, has become a quest worldwide, a better understanding and reliable data for the condensates forming in the flue gas filters are necessary to assure solid a filter operation. Our study focuses on the thermodynamic and kinetic conditions in flue gases consisting of combustion gases (CO_2, H_2O, N_2, O_2) and sodium, boron and sulphur compounds. An experimental set-up is presented by which the mass transfer conditions in a flue gas channel can be simulated in such a way that the results may be transferred to the industrial scale. The data may be used to adjust filter operation in such a way that the above mentioned problems are avoided.

11:40 AM

(GOMD-S5-008-2015) Iron equilibrium in the float glass process

A. M. Kasper*[1]; 1. Saint Gobain, Germany

Iron is ubiquist in nature; float glass can contain between ca. 100 ppm and 2% Fe_2O_3 by weight. Iron is polyvalent, i.e., it can show different oxidation states in glass. In the float chamber, the glass keeps its original redox state it received during melting – except on its surfaces that are strongly reduced. In this zone the only iron species is Fe^{2+}. On the "bath side" FeO is further reduced to the metal: FeO + Sn = SnO + Fe The reaction constant is small ($K_{R(700°C\ldots 1000°C)} = 0.03$), but a reaction takes place anyway. It's not trivial to quantify this thermodynamically. The following parameters need to be quantified: > Activity of FeO in glass; > Fe metal activity in tin [presumably strongly deviating from concentration because of combinations' formation (e.g. $FeSn_2$), and low Fe solubility in tin at respective temperatures]; > Oxygen activity in tin; > Temperature dependence of the equilibriums. > Due to high glass viscosity, the equilibrium factually might freeze in still within the float bath. Respective values measured in real float baths are used to "calibrate" this calculation. The model developed is also applied onto other elements playing a rôle in the float process, and this brings some interesting insights. It makes us understand better the chemistry of the float chamber, and it helps to make the float glass production more robust.

Symposium 2: Glasses in Healthcare - Fundamentals and Applications

Bioactive Glass Scaffolds and Implants for Bone Repair I

Room: Symphony Ballroom IV

Session Chair: Delbert Day, Missouri University of Science and Technology

1:20 PM

(GOMD-S2-007-2015) Bioactive glass scaffolds : sol-gel v melt-derived (Invited)

J. Jones*[1]; 1. Imperial College London, United Kingdom

NovaBone (Bioglass particulate) has now been used in more than 1 million patients, but it is only available in a powder form. The benefit of NovaBone over bioactive ceramics is the controlled delivery of active ions, providing osteostimulation. Here, I will describe foaming methods for producing porous bioactive glass foams that have interconnected pore networks similar to porous bone. *In vivo* studies compare sol-gel and gel cast foamed melt-quenched glass scaffolds to NovaBone and Actifuse® (porous Si-HA from Apatech Ltd.). The results show that bone regeneration is dependent on the dissolution rate (glass type and composition). Bone ingrowth was quantified through histology and novel micro-CT image analysis. At 11 weeks, the percentage bone ingrowth into preconditioned 70S30C scaffolds was similar to commercial NovaBone and Actifuse. Unlike the commercial products, pre-conditioned sol-gel scaffolds degraded and were replaced with new bone. Melt-quenched glass scaffolds of certain compositions, stimulated more bone ingrowth than has been seen in porous bioceramics even though in vitro studies showed low rate of apatite formation in simulated body fluid. 3-D printing of these compositions is possible through Robocasting. In sol-gel scaffolds cation incorporation is more complicated than previously thought. New strategies for improved cation incorporation will be proposed.

1:50 PM

(GOMD-S2-008-2015) Bioactive glass for regeneration of large bone defects

Q. Fu*[1]; A. Tomsia[2]; 1. Corning Incorporated, USA; 2. Lawrence Berkeley National Laboratory, USA

Development of bioactive glass and ceramic scaffolds intended for the reconstruction of large segmental bone defects remains a challenge in materials science. The current tissue engineering approach suffers from serious drawbacks: the low mechanical strength of scaffolds, the high cost of growth factors, and a lack of optimal strategies for growth-factor delivery. Here we show that, through the use of strong and resorbable bioactive glass (13-93 and 2B6Sr) scaffolds, effective bone healing and defect bridging can be achieved in a rabbit femur segmental defect model without growth factors or bone marrow stromal cells (BMSCs). Histological and biomechanical tests confirm the excellent ability of bioactive glass to repair large bone defects similar to autologous bone graft (ABG). The preclinical evidence suggests that this novel bioactive glass approach for regeneration of segmental bone defects has significant potential for translation to large-animal model and to clinical practice.

2:10 PM

(GOMD-S2-009-2015) Porous bioactive glass foam scaffolds: Comparison of 3 compositions by 2 Processing Methods

A. Nommeots-Nomm*[1]; P. Lee[2]; E. Saiz[1]; J. Jones[1]; 1. Imperial College London, United Kingdom; 2. University of Manchester, United Kingdom

Larry Hench's original Bioglass® 45S5 composition cannot be made into porous scaffolds while maintaining an amorphous glass structure due to its susceptibility to crystallise during sintering. Melt-derived glasses have recently been developed which avoid this crystallisation, enabling bioactive glasses to be manufactured into porous constructs. The aim of this work was to compare scaffolds manufactured with three different glass compositions by two different processing routes; adapted gel casting and 3D printing. The glasses used are ICIE16 (49.46 SiO_2, 36.27 CaO, 6.6 Na_2O, 1.07 P_2O_5 and 6.6 K_2O, in mol.%), SBP-3 (4.0 NaO, 4.0 KO, 7.5 MgO, 17.80 CaO, 17.80 SrO, 4.5 PO, 44.50 SiO in mol.%), and 13-93 (6.0 NaO, 7.9 KO, 7.7 MgO, 22.1 CaO, 1.7 PO, 54.6 SiO in mol.%). These glasses were chosen due to the differences in their modified network connectivity, 2.13, 2.84 and 3.01 respectively; suggesting different levels of bioactivity. The aim was to investigate of network connectivity and pore network on bioactivity. Difference in pore morphology and tortuosity will be created through the gel-cast foaming process and by 3-D printing (Robocasting).

2:30 PM

(GOMD-S2-010-2015) Development and characterization of COPPER and NIOBIUM releasing silicate bioactive glasses

V. Miguez Pacheco*[1]; D. de Ligny[1]; D. S. Brauer[2]; K. Rottenbacher[2]; A. R. Boccaccini[1]; 1. University of Erlangen Nuremberg, Germany; 2. Friedrich Schiller University Jena, Germany

Metallic ions have been incorporated into different glass compositions to stimulate healthy bone formation by improving the biochemical properties of Bioglass® for bone tissue engineering applications. Copper has been shown to be a powerful angiogenic agent whilst Niobium has been demonstrated to enhance the mineralization and differentiation of osteogenic cells. To further investigate these effects, Cu-containing bioactive glasses (BGs) based on the 1393 formulation and melt-derived Nb-containing BGs based on the 45S5 Bioglass® formulation were prepared. 3D glass-ceramic structures were made by the foam replica method using these materials and then subjected to simulated body fluid (SBF) studies to ascertain their bioactivity. The formation of hydroxyapatite crystals on the glass surface was a strong indication of their bioactivity, observed in SEM images. Structural characterization of the glasses was carried out using FTIR and XRD techniques. The biocompatibility of the novel BGs was tested by direct culture of MG-63 osteosarcoma cells on scaffolds whilst indirect culture of fibroblasts with BG granules was performed to detect the angiogenic potential by measuring their VEGF secretion. Release of these ions into relevant fluids was measured to ascertain their effects on cell viability, proliferation and metabolism.

2:50 PM

(GOMD-S2-011-2015) Potential of Bioactive Glass Scaffolds as Implants for Structural Bone Repair

M. N. Rahaman*[1]; S. Bal[2]; L. F. Bonewald[3]; 1. Missouri S&T, USA; 2. University of Missuri-Columbia, USA; 3. University of Missouri-Kansas City, USA

The repair of structural bone defects such as segmental defects in the long bones of the limbs is a challenging clinical problem. While many commercial osteogenic filler materials are suitable for repairing contained bone defects, no satisfactory biological solution to reconstituting segmental bone loss is yet available. The results of recent studies that have been performed to evaluate the capacity of bioactive glass scaffolds to heal segmental bone defects in small animal models will be described. Current difficulties and future prospects for the use of bioactive glass scaffolds in structural bone repair will be discussed.

Bioactive Glass Scaffolds and Implants for Bone Repair II

Room: Symphony Ballroom IV
Session Chair: Julian Jones, Imperial College London

3:40 PM

(GOMD-S2-012-2015) Review of a Commercial Bioactive Glass Scaffold Used in Human Spine Applications

S. Jung*[1]; 1. Mo-Sci Corporation, USA

Design of orthopedic devices has been studied extensively in the last two decades. Much of the design work for bone regeneration revolved around making orthopedic implants that look like cancellous or cortical bone with a high relative porosity that resorbs at the same rate as bone growth. The design on the present technology utilized morsels (~2mm diameter) composed of a bioactive glass shell surrounding an inner core of bioactive glass fibers. This technology is U.S.F.D.A approved for use as bone void filler. Several human clinical cases will be presented that have utilized this bone scaffold technology in various spinal procedures.

4:00 PM

(GOMD-S2-013-2015) Cell-bioactive glass scaffold interactions: The role of substrate nano-structure

T. J. Kowal[1]; T. Chokshi[1]; R. Holovchak[1]; M. M. Falk[1]; H. Jain*[1]; 1. Lehigh University, USA

To design ideal materials for the regeneration of different tissues, we must understand the mechanisms that allow cells to not only attach to bioscaffold materials, but also to take cues from them as to what tissue should be regenerated. Here we present evidence that cells detect differences in nano-structure using two different substrates. The first, a bioactive glass with a simple composition of 30mol%CaO – 70mol%SiO_2 contains both nano- and macro-pores. The only variable between samples of this type is nano-pore size (3.7 nm vs. 17.7 nm), while total surface area is kept constant. The second, a bioactive glass with a complex composition of 24.4mol%Na_2O–26.9mol%CaO–2.6mol%P_2O_5–46.1mol%SiO_2 called 45S5 bioglass®, varies in nano-structure due to phase separation, resulting in either spinodal interconnected or droplet nucleation morphology. Cellular response to either substrate was measured by quantification of initial adhesion to the surfaces. For both substrates, cells showed a significant preference to one of the nano-structures, indicating that cells sense morphological details of substrates that are app. 1000 times smaller than cells. Research performed in our laboratories aims to uncover underlying principles that allow cells to respond to such nano-scaled substrate details, allowing to engineer superior tissue regenerative materials.

4:20 PM

(GOMD-S2-014-2015) Bactericide Action of a Titanium Surface Biofunctionalized with a Novel Bioactive Glass

C. R. Chinaglia*[1]; L. Campanini[1]; L. H. Pitaluga[1]; N. S. Silva[1]; C. W. Souza[1]; O. Peitl[1]; E. D. Zanotto[1]; 1. Federal University of São Carlos, Brazil

The objective was to produce a titanium surface with antibacterial property by biofunctionalizing it with a novel bioactive glass. The bioactive glass (BG) composition (patent BR10 20130209619) from the SiO_2-Na_2O-K_2O-MgO-CaO-P_2O_5 system, with and without silver (1wt%), were used to biofunctionalize titanium surfaces using a proprietary method (patent BR10 2014 003817 5). The antibacterial activity was evaluated by (1) the plate count method – JIS standard Z 2801:2010, and (2) by the spread plate method (evaluation of biofilm formation). We have tested the (a) *Staphylococcus aureus, (b) Staphylococcus epidermidis, (c) Escherichia coli* and (d) *Pseudomona aeruginosa.* Samples for SEM analysis, after the incubation period, were immediately fixed in 2.5% glutaraldehyde and gradually dehydrated in ascending series of alcohol. All surfaces showed a strong bactericide action for all bacteria with at least 5 CFU log reduction. Because of that the BG+Ag was not tested. The biofilm formation test exhibited a reduction of approximately 3 CFU log, for BG+Ag. The basic BG composition had a better result than the gold standard 45S5. The SEM analysis, confirm these results. It is possible to conclude that the biofunctionalized surfaces are highly bactericide and has a good potential to avoid biofilm formation. The addition of silver enhances this potential.

4:40 PM

(GOMD-S2-015-2015) Antimicrobial behavior of ion-exchanged silver in glass – the physics and chemistry

C. L. Chapman*[1]; C. Kosik Williams[1]; N. Borrelli[1]; Y. Wei[1]; O. Petzold[1]; 1. Corning Incorporated, USA

As touchscreen electronic devices such as smartphones, tablets and kiosks have become common-place in our everyday lives, there has been an increased concern associated with transfer of pathogens to and from the glass touchscreen surfaces. An engineered surface with antimicrobial functionality can address such concerns. The silver ion, Ag^{1+}, is a well-known antimicrobial agent that can be incorporated into a glass surface through ion exchange. The focus will be on the mechanism between the interaction of the microbe and silver containing glass. As well as the optimization of the factors that allow for the best antimicrobial efficacy.

Symposium 3: Fundamentals of the Glassy State

Session 3: Structural Characterization of Glasses II

Room: Symphony Ballroom II
Session Chair: Randall Youngman, Corning Incorporated

1:20 PM

(GOMD-S3-014-2015) Rationalizing Composition-Structure Trends of Rare-Earth Aluminosilicate Glasses by Solid-State NMR and Molecular Dynamics Simulations (Invited)

A. Jaworski[1]; B. Stevensson[1]; B. Pahari[1]; S. Iftekhar[1]; M. Eden*[1]; 1. Stockholm University, Sweden

Rare earth (RE) aluminosilicate glasses exhibit high chemical stability and favorable mechanical and (magneto)optical properties, primarily stemming from the presence of trivalent RE^{3+} cations in the structures. We will present our recent results on rationalizing composition/structure correlations of RE_2O_3—Al_2O_3—SiO_2 glasses (RE=La, Lu, Sc, Y), as well as the roles of the RE^{3+} ions for dictating glass properties, such as the microhardness and the fractional compactness. Unprecedented detailed structural insight was gained over both short and medium length-scales by exploiting multinuclear {^{29}Si, ^{27}Al, ^{17}O, ^{45}Sc, ^{89}Y} magic-angle-spinning (MAS) NMR combined with molecular dynamics (MD) simulations. We quantitatively monitored the speciations of the various glass building blocks and how they depend on (1) the RE^{3+} field strength (that grows along the series $La^{3+} < Y^{3+} < Lu^{3+} < Sc^{3+}$), and (2) changes in the RE/Al/Si composition of the glass. These glass networks manifest a pronounced structural disorder (significantly higher than that of analogous glasses incorporating mono/di-valent cations) that is best described by a scenario of randomly intermixed SiO_4 and AlO_p (p=4, 5, 6) polyhedra, where the AlO_5 populations grow concurrently with the RE^{3+} field strength.

1:50 PM

(GOMD-S3-015-2015) Structure-property relationships in barium borophosphate glasses modified with niobium oxide

L. Koudelka*[1]; P. Kalenda[1]; P. Mosner[1]; L. Montagne[2]; B. Revel[2]; 1. University of Pardubice, Czech Republic; 2. University of Lille, France

Phosphate glasses containing a high amount of niobium oxide exhibit non-linear optical properties which make them attractive for various optical devices. This contribution is devoted to the investigation of glasses of the series (100-x)[0.5BaO-0.1B_2O_3-0.4P_2O_5]-xNb_2O_5 with x = 0-40 mol % Nb_2O_5 and 80[0.5BaO-yB_2O_3-(0.5-y)P_2O_5]-20Nb_2O_5 with y = 0-0.25B_2O_3. Glass structure was investigated by Raman, ^{31}P and ^{11}B MAS NMR spectroscopy. Basic characteristic parameters of the prepared glasses were determined. Raman spectra revealed that at low Nb_2O_5 content a strong vibrational band of isolated NbO_6 octahedra at 904 cm^{-1} dominates the spectra. In the glasses with 30 mol% of Nb_2O_5 new bands of 646-652 and 780-810 cm^{-1} appear in the spectra. These bands were assigned to vibrations of Nb-O-Nb bonds interconnecting NbO_6 octahedra. ^{11}B MAS NMR spectra reveal a dominant role of BO_4 units in the glass structure. Crystallization of glasses with a high Nb_2O_5 content results in the formation of crystalline compound $BaNb_2P_2O_{11}$. ^{11}B MAS NMR spectra showed the relations between BO_4 and BO_3 units and the formation of B-O-Nb bonds together with B-O-B and B-O-P bonds. With an increasing Nb_2O_5 content a part of BO_4 units is converted to BO_3 units. Borate niobato-borophosphate glasses reveal very high chemical durability and also high glass transition temperatures and high values of the index of refraction.

2:10 PM

(GOMD-S3-016-2015) Effects of temperature and composition on boron-containing glass network structure

J. Wu*[1]; J. F. Stebbins[2]; 1. Corning Inc., USA; 2. Stanford University, USA

Boron-containing glasses and melts are critical in technology. Because of the ease of transition among three- and four-coordinated boron with temperature and composition, many physical properties of such glasses can be fine-tuned. Therefore, it is very important to understand how temperature and composition affect the network structure of boron-containing glasses. The effect of temperature on the structure of boron-containing liquids has been studied by ^{11}B, ^{17}O and ^{27}Al MAS NMR spectroscopy using glass samples prepared with different cooling rates and thus different fictive temperatures (T_f), as well as by high-temperature *in situ* ^{11}B MAS NMR. The abundances of BO_3 groups and of non-bridging oxygens (NBO) increase with increasing T_f, indicating that the reaction BO_4=BO_3+NBO shifts to the right at a higher temperature. The equilibrium of this boron structure reaction depends on NBO content, and thus is highly dependent on composition, e.g. on modifier type and content. The observed T dependence of N_4 (=BO_4/(BO_3+BO_4)) allows us to estimate the enthalpy of the reaction BO_4=BO_3+NBO to be 20 to 50 kJ/mol in different glass compositions. With this information, we can extrapolate the N_4 vs. T relation to a much wider temperature range and compare the structure of different glasses isothermally, which is critical for compositions that are very sensitive to temperature changes.

2:30 PM

(GOMD-S3-017-2015) High-Temperature NMR Spectroscopy of Phase Separation in Model Nuclear Waste Glasses (Invited)

S. Kroeker*[1]; J. Wren[1]; B. J. Greer[1]; 1. University of Manitoba, Canada

High-temperature nuclear magnetic resonance (NMR) spectroscopy was used to investigate the devitrification of molybdates from model nuclear waste glasses. Solid-state NMR has provided valuable information about the identity and quantities of Mo-containing precipitates in inactive nuclear waste glasses at room temperature. However, key information about the phase separation mechanism may be more directly obtained by spectroscopically monitoring the melts during heating and cooling to mimic industrial processes. Furthermore, the elevated temperatures induced by radioactive decay will influence the stability and properties of separated phases under repository conditions. The relevance of previous ex-situ NMR results is limited by the formation of hydrates and low-temperature phases not found at realistic temperatures. The high-temperature NMR experiments reveal that molybdate liquids sequester alkali cations from the glass melt and solidify into complex crystalline aggregates upon cooling. The phase profile at repository temperatures depends critically on the bulk composition but is insensitive to the cooling rate. The use of in-situ experimental probes is essential to determine cation partitioning in composite systems and to predict the long-term disposition of nuclear materials in geologic repositories.

3:00 PM

(GOMD-S3-018-2015) Comparison of Sodium Phosphate and Thiophosphate Glass Structure

C. Bischoff*[1]; R. Brow[1]; S. Martin[2]; 1. Missouri University of Science and Technology, USA; 2. Iowa State University, USA

Although the $xNa_2O + (1-x)P_2O_5$ and $xNa_2S + (1-x)P_2S_5$ glass systems are compositionally analogous, their glass-forming regions are rather dissimilar. The oxide system is capable of glass formation over a broad compositional range from roughly x = 0 to x = 0.6, while the sulfide system forms glasses from x = 0.5 to x = 0.71 and at small region at x = 0.79 using traditional melt-quench techniques. Both the oxide and sulfide glasses have been synthesized and characterized by solid state ^{31}P nuclear magnetic resonance (NMR) techniques. While the oxides have a tendency to form large networks or chains of phosphate tetrahedral linked by bridging oxygen, the sulfides form appreciable amounts of molecular anions for all x values. Structural models developed from the concentration and connectivity of the various phosphate species will be discussed.

Session 3: Structural Characterization of Glasses III

Room: Symphony Ballroom II
Session Chair: Leo van Wüllen, Augsburg University

3:40 PM

(GOMD-S3-019-2015) Intermediate Range Order of Borate Glasses Found From ^{10}B NMR (Invited)

S. Feller*[1]; K. Goranson[1]; M. Faaborg[1]; E. Troendle[1]; N. Barnes[1]; M. Chace[1]; R. Rice[2]; M. Affatigato[1]; D. Holland[3]; M. Smith[4]; 1. Coe College, USA; 2. Simpson College, USA; 3. University of Warwick, United Kingdom; 4. University of Lancaster, United Kingdom

We have made significant improvements to *SpectraFit*, a program used to simulate ^{10}B NMR powder patterns. This is an update of work done in 2012 by Khristenko et al[1]. The program takes into account the quadrupolar interaction of ^{10}B (I=3), and it allows determination of the distributions of the quadrupolar interaction parameters in amorphous and crystalline borates. The program has the ability to analyze up to two different ^{10}B environments. The two site fitting gives four quadrupole parameters for each site, as well as a relative weighing of the three and four coordinated borons. The technique is sensitive enough to find experimental variations in the boron quadrupole parameters that arise from differences in intermediate-range order. [1] Victor Khristenko, Kevin Tholen, Nathan Barnes, Evan Troendle, Mario Affatigato, Steve Feller, Diane Holland, Thomas Kemp, and Mark Smith "*SpectraFit*: A New Program to Simulate and Fit Distributed ^{10}B Powder Patterns: Application to Symmetric Trigonal Borons," *European Journal of Glass Science Part B* **53** (3) 121-127 (2012). The National Science Foundation is acknowledged for their support under NSF grants DMR 1407404, DMR 1262315, and DMR 0904615. Coe College is also thanked for their ongoing support of our glass research program.

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(GOMD-S3-020-2015) Oxygen Speciation in Strontium Borate Glasses and Crystals: High Resolution ^{11}B and ^{17}O MAS NMR Analysis

M. LaComb*[1]; J. Stebbins[1]; 1. Stanford University, USA

Oxygen triclusters, sites with three first-neighbor highly-charged tetrahedral cations, have sometimes been suggested as playing an important role in glass structure. Due to the fact that these sites are rarely found within minerals and glasses there has been little direct spectroscopic evidence proving their existence. In the previously published crystal structure of strontium tetraborate, SrB_4O_7, most commonly known for its application to photonics as a result of its high nonlinear optical coefficients, all of the borons are tetrahedrally coordinated and two of the seven oxygens are connected to three such borons, forming oxygen triclusters similar to those found in the isostructural mineral grossite, $CaAl_4O_7$. By using isotopically enriched strontium tetraborate crystals as a model compound, we were able to utilize high-resolution ^{11}B and ^{17}O MAS (magic angle spinning) and MQMAS (multiple-quantum magic angle spinning) NMR techniques to determine the isotropic chemical shift, quadrupolar coupling constant and asymmetry of the multiple types of oxygen sites present, including the oxygen tricluster site. As a result of these better constraints on site parameters, we have been able to use high-field solid-state NMR to directly investigate the presence of these non-standard oxygen species within $SrO-2B_2O_3$ glasses.

4:30 PM

(GOMD-S3-021-2015) Changes of Al coordination with temperature in aluminoborosilicate glasses: effects of B concentration

E. Morin*[1]; J. F. Stebbins[1]; 1. Stanford University, USA

Understanding the effect of temperature on speciation is a prerequisite for constructing robust structural models of oxide glasses. Yet, the extent and direction of changes in Al coordination with fictive temperature seem to vary strongly with composition. In Ca aluminosilicate glasses cooled at various rates, Al coordination increased with increased fictive temperature (T_f). Florian and coworkers *in situ* high temperature studies of La, Y aluminosilicate liquids also found that Al coordination increased with increased temperature. Conversely, in Ca, La, Y aluminoborosilicates (with B/Si= 2, 4), we found that Al coordination decreased with increased T_f. Some researchers have suggested that there is a relationship between changing Al and B coordination with temperature, leading to different behavior in B-free versus B-rich compositions. To investigate the effect of B-to-Si ratio, Y aluminosilicates (B/Si=0) and silicon-rich Ca, La, Y aluminoborosilicates (B/Si=0.2) were studied along with La aluminoborates (B/Si= ∞) *via* 18.8T ^{27}Al and 14.1T ^{11}B NMR. Whereas we observe Al coordination increasing with increasing T_f in the low B glasses with B/Si=0 and 0.2, we observe Al coordination decreasing with increasing T_f in aluminoborates, confirming trends we have previously described for B-rich aluminoborosilicates.

4:50 PM

(GOMD-S3-022-2015) Structure/Property Correlations in Fluorophosphate and Fluoroborate Glasses Studied by Solid State NMR

H. Eckert*[1]; M. de Oliveira[1]; A. de Camargo[1]; 1. University of Sao Paulo, Brazil

Non-linear changes in the physical properties of glasses containing more than one type of network former species are often exploited for optimizing the technological performance of glasses for optical applications. Issues at the structural level concern the identification of the coordination polyhedra arising from the specific interactions between the network former species involved, their connectivity distribution, and the competition of both network formers for the network modifier species. Modern solid state nuclear magnetic resonance (NMR) techniques present a new element-selective, inherently quantitative approach to this problem, as NMR is not affected by the absence of periodicity. Specifically, we have developed the site-resolved measurement and quantitative analysis of internuclear magnetic dipole-dipole interactions, which can be translated into distance information in a straightforward manner. Using this approach we have studied the mixed anion effect in a variety of fluoroborate and fluorophosphate based glass systems, providing a structural rationale for the compositional dependence of glass transition temperatures optical properties.

5:10 PM

(GOMD-S3-023-2015) Structure and Properties of Quaternary Network Former Glasses $20B_2O_3$-$8Al_2O_3$-xP_2O_5-$(72-x)SiO_2$

X. Guo*[1]; R. Youngman[1]; C. L. Hogue[1]; J. C. Mauro[1]; J. Wang[1]; 1. Corning Incorporated, USA

It is of fundamental scientific interest to better understand network former polyhedra and their interconnectivity in glasses free of modifiers. Structure data showing the role of each glass-forming cation is very limited in such systems. It is still an open question on how Al_2O_3 and B_2O_3 generally associate with P_2O_5 in network former glasses, as well as whether SiO_2 concentration leads to different behavior. In the present study, a set of glass compositions with $P_2O_5/Al_2O_3 <1$ to $P_2O_5/(B_2O_3+Al_2O_3) >1$ were examined in terms of both their physical properties and network structure. Our results are consistent with previous findings in the B_2O_3-Al_2O_3-P_2O_5-SiO_2 quaternary. When $P_2O_5/Al_2O_3 \leq 1$, all boron cations are three-fold coordinated and all phosphorus are found in Q^4 tetrahedra having close association with aluminum, as in $AlPO_4$. When $[P_2O_5]$ is more than $[Al_2O_3]$, some of the boron is converted to four-fold coordination, with all Al_2O_3 maintained in tetrahedral groups. When $[P_2O_5]$ is in excess of $[Al_2O_3+B_2O_3]$, boron is all four-fold coordinated, while the aluminum coordination number increases where all aluminum preferentially associates with phosphorus over silicon. The impact of this network structure on glass properties will also be discussed.

Session 5: Mechanical Properties of Glasses II

Room: Symphony Ballroom III
Session Chair: Scott Glaesemann, Corning Incorporated

1:20 PM

(GOMD-S3-024-2015) Adding topology to the Makishima-Mackenzie Modelsil (Invited)

M. Plucinski[1]; J. Zwanziger*[1]; 1. Dalhousie University, Canada

The Makishima-Mackenzie Model provides a simple and intuitive relationship between glass composition, structure, and elastic properties such as the Young's Modulus. While the model is reasonably accurate for silicates, it is strikingly inaccurate for borates. We believe that the model suffers from the lack of inclusion of topology in the network description. We will show computations of networks as a function of random bond deletion of different types, to show the dependence of elasticity on average coordination number and hence network topology. We also show that this factor is more important than atomic density, which the Makishima-Mackenzie model does explicitly consider. We then proposed a modified model of Makishima-Mackenzie type, which does include network topology.

1:50 PM

(GOMD-S3-025-2015) Mechanical Properties of TiO_2 doped Soda-Lime-Silicate Glasses

S. Karlsson*[1]; R. Limbach[2]; K. Lundstedt[1]; L. Wondraczek[2]; 1. Glafo - the Glass Research Institute, Sweden; 2. Friedrich Schiller University of Jena, Germany

We report on the mechanical properties of glasses in the system TiO_2-Na_2O-CaO-SiO_2. Three series of TiO_2 doped glasses were investigated, in which (i) CaO (ii) SiO_2 and (iii) CaO as well as SiO_2, respectively, was substituted by TiO_2. All glasses were prepared by melting the raw materials in Pt/Rh10 crucibles for 18 h at 1450 °C, followed by a homogenization and conditioning of the melts at 1500 °C. The glass melts were poured into a mould, and annealed for 1 h at 550-580 °C. The mechanical properties were characterized by ultrasonic echography, nano- and microindentation. Trends in the elastic properties e.g. Young's modulus and Poisson ratio, and the indentation response, e.g. hardness, strain-rate sensitivity and crack resistance, are discussed as a function of TiO_2 content.

2:10 PM

(GOMD-S3-026-2015) Micromechanical properties in aluminophosphate glasse

A. Pönitzsch*[1]; J. Deubener[1]; 1. Institute for Non-Metallic Materials, Germany

A. Pönitzsch, J. Deubener Institute of Non-Metallic Materials, Clausthal University of Technology, Germany Aluminophosphate glasses (R-Al_2O_3-P_2O_5; R = CaO, ZnO, Na_2O) consist of two network formers and exhibit a mixed former effect which is based on changes of the average aluminum coordination number with increasing alumina content. In particular it is shown that the glass transition temperature changes non-linear with an increasing alumina content. This study aims in providing knowledge to the effect of glass topology on micromechanical properties with respect to compositional ranges where a change in the aluminum coordination ($Al^{VI} \rightarrow Al^{V} \rightarrow Al^{IV}$) is expected to take place. Therefore aluminophosphate glasses of different Al_2O_3/P_2O_5 and Al_2O_3/R ratios were prepared to study elastic and inelastic properties as well as indentation induced crack initiation and propagation were studied by ultrasonic echography and Vickers indentation, respectively.

2:30 PM

(GOMD-S3-027-2015) Influence of Atomic Structure on Mechanical Properties in Calcium-Aluminosilicate Glasses

L. Lamberson*[1]; R. Youngman[1]; S. Baker[2]; 1. Corning Incoporated, USA; 2. Cornell University, USA

Silicate glasses and more specifically Aluminosilicate glasses are widely used in applications such as LCD glass, touchscreens for hand held devices and car windows. These glasses are also interesting on a fundamental level as they exhibit a non-monatomic behavior in hardness with increasing SiO_2 content in the glass. At SiO_2 contents above 85 mole% the glasses exhibit a linear increase in hardness and a linear decrease in indentation modulus. The modulus was shown to have a linear correlation to density. As the glass density increases the indentation modulus increases. Hardness on the other hand for silicate glasses up to 85 mole% was shown to be consistent with the topological constraint theory while glasses above 85mole% SiO_2 are shown to be more consistent with a plastic deformation mechanism switch from shear to densification. Understanding the plasticity in silicate glasses and linking that to unit deformation mechanisms is key to developing other lower melting temperature glasses that exhibit more desirable mechanical properties.

2:50 PM

(GOMD-S3-028-2015) Plastic deformation of Na-aluminosilicate glasses under micro and nano-indentation

V. Pukhkaya*[1]; J. Teisseire[1]; M. Heili[2]; C. Martinet[2]; V. Martinez[2]; B. Champagnon[2]; G. Kermouche[3]; E. Barthel[4]; 1. Saint Gobain Recherche, France; 2. UMR5306 CNRS, France; 3. Ecole des Mines de Saint-Etienne, CNRS, France; 4. ESPCI, France

Under μ-indentation, silica and silica-based glasses exhibit plastic response at the micrometer scale. It is still difficult to describe the plastic deformation of amorphous material at the surface. We have already quantified the densification after indentation with Raman spectroscopy, in agreement with constitutive law of silica. Here we report our efforts to extend this approach to Na-aluminosilicate glasses. A range of Na-aluminosilicate glasses with Al/Na ratio spanning the join between Na trisilicate and albite was investigated. The glass compositions were controlled by μ-probe analysis, the moduli and hardness measured by nano-indentation. We used diffused composition gradients to evaluate individual Raman partial spectra as a basis for the investigation of structure. To study the impact of plastic deformation on the glass structure, we used 2 kg Vickers indents and mapped the Raman signal. We used Si-O-Si(Al) vibrational mode evolution in Raman spectra in 300-730 cm^{-1} region to evaluate plastic strain. This study was carried out by comparison with the spectra of samples hydrostatically compressed in a DAC. With this strategy, we were able to propose an evaluation of the ratio between shear and densification. The results were used to provide an interpretation of the different distributions of plastic strains observed as a function of glass composition in terms of constitutive relations.

3:30 PM

(GOMD-S3-029-2015) Mechanical degradation and surface crystallization of silica glass fibers

P. J. Lezzi*[1]; E. E. Evke[1]; E. M. Aaldenberg[1]; M. Tomozawa[1]; 1. RPI, USA

Pristine silica glass fiber is well known to become mechanically weaker when heat-treated in air but the cause of such weakening is not presently known. The time dependence of mechanical degradation of various silica glass fibers containing varying impurity contents were studied in the range of 500°C to 1000°C. It was found that previously unobserved nano-scale surface crystallization of Cristobalite occurred readily at these low temperatures, even after short times, and the crystallization behavior of these sub-micron cristobalite single crystals was evaluated by scanning electron microscopy. It is concluded that surface crystallization may be responsible for the mechanical weakening observed in silica glass fiber surface during heat-treatment at temperatures in excess of ~800°C, while water diffusion into the glass surface is likely responsible for the strength degradation observed at lower temperatures.

3:50 PM

(GOMD-S3-030-2015) Aging and Fatigue of Soda-Lime-Silicate Glass Fiber

E. Ronchetto*[1]; R. K. Brow[1]; 1. Missouri University of Science and Technology, USA

Fibers about 100-150 microns in diameter were drawn from melts of a commercial flint soda-lime-silicate (SLS) container glass. Fibers were aged for several months in air in either wet (80%RH / 50°C) or dry (1%RH / 32°C) conditions. A third set of fibers were continuously cycled for twelve hour periods between the wet and dry conditions. Sets of fibers were removed after various times and their failure strains were determined using a two-point bend (TPB) technique, either in liquid nitrogen or in room temperature air at 40% relative. Failure strains decreased with aging time under all aging conditions, but faster under wet conditions. Fatigue parameters were determined by measuring failure strains with TPB faceplate velocities between 500 and 4000 microns/sec, and were found to be independent (15±1.5) of the aging conditions. The aged surfaces were examined with Raman spectroscopy, scanning electron microscopy, and optical microscopy and the development of Na-carbonate reaction products on the glass surface is related to the decrease in failure strains.

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(GOMD-S3-031-2015) Mechanical properties of HS high strength glass fibers

Q. Zu*[1]; J. Liu[1]; Y. Zhang[1]; J. Zhou[1]; J. Li[1]; 1. Sinoma Science & Technology Co.,Ltd., China

This article was aimed at characterizing the mechanical property of HS™ high strength glass fibers in different fiber structures and application conditions compared to different kinds of glass fiber such as S-2, R, Hiper-Tex, Advantex, E, etc. The tensile strength and modulus of single pristine filaments of different glass fiber were tested by drawing a single filament directly from a tip under the bushing. Glass yarn, roving and impregnated strand were studied by corresponding test methods for HS fibers and other glass fibers. Mechanical properties of HS fibers in the chemical medium such as acid and alkali were tested. The mechanical properties including fatigue strength of HS fibers reinforced composite materials were studied with ASTM atandards. The relationship between glass compositions and mechanical properties was analyzed in this paper. The results indicate that the mechanical properties of HS fibers are higher than R glass and R modified high module glass fibers. Fatigue life of HS fibers reinforced composite is more than ten times higher than that of E glass fiber. The tensile strength and modulus of the HS fibers are increased with the total amount of SiO_2 and Al_2O_3 increasing. The acid resistance of HS fibers can be improved by increasing SiO_2 content.

4:30 PM

(GOMD-S3-032-2015) Effects of Counter-surface and Humidity on the Mechanochemical Wear of Soda Lime Glass

H. He*[1]; L. Qian[1]; C. Pantano[2]; S. Kim[2]; 1. Southwest Jiaotong University, China; 2. Pennsylvania State University, USA

The applications of functional and engineering glasses depend on their surface mechanochemical properties. It is essential to understand the friction and wear of glass in various conditions. Generally, the friction and wear properties of materials depend on their mechanical properties; in ambient air, however, they also depend on tribochemical reactions involving water molecules impinging from the gas phase. Previous investigations confirmed that wear of glasses could be significantly affected by the humidity, but the effects of the counter-surfaces on wear of glass were not considered. Using a ball-on-flat tribometer, the effects of the counter surface on the wear of soda lime glass in humid conditions were studied by rubbing against different ball materials, namely pyrex, Si_3N_4, Al_2O_3 and steel. The experimental results show that wear of glass was very sensitive to humidity and counter surface chemistry. In dry conditions, glass was damaged mechanically, creating a rough and deep wear track. These wear behaviors are consistent with the Archard's law which predicted that a softer material would wear easily. However, in humid conditions, the ball materials that are harder than the glass were damaged. It was believed that the chemical reactivity of substrate and counter surfaces determines which side will get worn upon sliding by tribochemical reactions involving water molecules.

4:50 PM

(GOMD-S3-033-2015) Effects of thermal poling on structural and mechanical properties of soda-lime glass surface

J. Luo*[1]; H. He[3]; C. G. Pantano[2]; S. H. Kim[1]; 1. Pennsylvannia State University, USA; 2. Department of Material Science, USA; 3. Southwest Jiaotong, China

The glass surface structure and reactivity play important roles in governing mechanical properties of commercial multi-component glasses. Knowledge of the correlation between surface structure and mechanical behavior of those glasses in different environments has become crucial to develop glasses with better reliability. The effect of sodium concentration at the soda-lime silicate glass surface on its surface chemistry and mechanical properties is investigated through thermal poling that applies high electric bias on glass at high temperature. After thermal poling, the sodium concentration gradient and structural reorganization at both surfaces were confirmed with energy dispersive x-ray (EDX), specular reflection infrared (IRRS) spectroscopy, and sum-frequency-generation (SFG) vibrational spectroscopy. Nano-indentation analysis showed that anode side has lower hardness and elastic modulus compared to the pristine glass surface, while the sodium-accumulated cathode side has higher hardness and elastic modulus. In humid environments, the cathode side shows substantially less wear, which is consistent with our previous observation of unique wear resistance of pristine soda-lime silicate glass at high humidity. The structural characterization results from EDX, IRRS, and SFG analyses allowed us to establish the relation between the glass surface structure and those mechanical properties.

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 1: Phase Change and Other Chalcogenide Materials

Room: Concerto B

Session Chairs: Parthapratim Biswas; David Drabold, Ohio University

1:20 PM

(GOMD-S4-012-2015) A chemical (bonding) perspective on phase-change and related materials (Invited)

R. V. Dronskowski*[1]; 1. RWTH Aachen University, Germany

Phase-change materials (PCMs) are widely used for data storage and in other functional devices. Despite their often seemingly simple compositions, these materials exhibit intriguing microscopic complexity and a portfolio of fascinating physical properties. From a more chemical perspective, the technological success of PCMs is a simple consequence of the structural and electronic peculiarities on the atomic scale and, in particular, of their bonding nature. In fact, the chemical bonding of crystalline and amorphous PCMs and also related materials is truly worth studying, now so easily done using state-of-the-art density-functional theory and properly chosen projection techniques as implemented in the Lobster program suite. In addition, finite-temperature properties of such solid-state materials are almost routinely accessible using quasiharmonic theoretical methods from first principles. By doing so, structure-property relationships at zero Kelvin and beyond may be thoroughly analyzed for crystalline and amorphous bulk-like PCMs as well as for surfaces structures, including their oxidation products and chemically related chalcogenides.

1:50 PM

(GOMD-S4-013-2015) Doping of As-Te glassy semiconductors with transition metal elements

P. Lucas*[1]; B. Potter[1]; G. Coleman[1]; B. Bureau[2]; C. Boussard[2]; J. Adam[2]; 1. University of Arizona, USA; 2. University of Rennes, France

With the exception of a-Si, doping of amorphous solids has received limited attention due to the intrinsic difficulty in creating electrically active dopants in amorphous structures. However, the introduction of transition metals in telluride glasses can lead to electrical conductivities many orders of magnitude larger than that of conventional chalcogenide glasses. Here we show that recent measurements of electron spin resonances in metal-doped telluride glasses reveal a strong correlation between the presence of acceptor defect sites containing unpaired electrons and a strong increase in electrical conductivity. Temperature dependent measurements of optical, electrical and EPR properties are presented to elucidate the mechanism of doping in these glasses.

2:10 PM

(GOMD-S4-014-2015) Semiconducting chalcogenide glass ceramics with internal heterojunctions (Invited)

X. Zhang*[1]; Y. Xu[1]; Q. Shen[2]; B. Fan[1]; X. Qiao[2]; X. Fan[2]; L. Calvez[1]; H. Ma[1]; M. Cathelinaud[1]; 1. University of Rennes / CNRS, France; 2. Zhejiang University, China

Semiconducting materials with efficient visible light absorption, charge separation and transport are the key for improving solar energy conversion efficiency by using photovoltaic and photocatalytic effect. In this work, a new family of semiconducting materials with a unique microstructure has been obtained by controlling the crystallization of the $GeSe_2$-Sb_2Se_3-CuI chalcogenide glass. It has been found that the precursor glass is electrically isolating and that its conductivity can be increased by several orders of magnitude by generating crystals inside the glass matrix. The photoelectric properties of the glass-ceramics strongly depend on the crystallized phases and the nanostructure. The best glass-ceramic, showing the strongest photocurrent under visible illumination, is composed of interconnected conductive micro-domains, formed by low conductive rod-like n-type Sb_2Se_3 crystals, covered by relatively high conductive p-type Cu_2GeSe_3 nano-crystals. This structure results in exceptionally long lifetime of charge carriers (around 16 μs) and high photocurrent (at least 100 times higher than that of Sb_2Se_3 or Cu_2GeSe_3 separately). The conducting mechanism and potential applications of theses chalcogenide glass-ceramics will be discussed

2:40 PM

(GOMD-S4-015-2015) Aging mechanisms in amorphous GeTe

J. Raty*[1]; W. Zhang[2]; J. Luckas[2]; R. Mazzarello[2]; C. Bichara[3]; M. Wuttig[2]; 1. University of Liege, Belgium; 2. RWTH Aachen University, Germany; 3. CNRS and Aix-Marseille University, France

Aging phenomena are common to all amorphous structures, but of special importance in phase change materials (PCM) since it impedes the realization of multi-level memories. Different interpretations have been proposed, but we focus here on the structural relaxation of amorphous GeTe, chosen because it is the simplest system that is representative of the wider class of GST alloys, lying along the GeTe-Sb2Te3 composition line of the GeSbTe phase diagram. We investigate the structure of amorphous GeTe using Density Functional Theory based Molecular Dynamics, using either the standard Generalized Gradient Approximation, or more elaborate Van der Waals approximation. New insight is provided on the stability of homopolar GeGe bonds and tetrahedral Ge bonding, in relation with the resistance drift phenomenon, that is investigated experimentally using photothermal deflection spectroscopy experiments

3:00 PM

(GOMD-S4-016-2015) Quantitative measure of tetrahedral-sp^3 geometries in amorphous Ge-Te and Ge-Si-Te phase change alloys

M. Micoulaut*[1]; P. Boolchand[2]; S. Ravindren[2]; K. Gunasekera[2]; 1. Universite Pierre-et-Marie Curie, France; 2. University of Cincinnati, USA

Phase change or Ovonic memory technology has gained much interest in the past decade as a viable solution for the rapid increase in the demand for memory storage. This unique technology, first proposed by S. Ovshinsky in 1968, is based on storing information on the crystalline and amorphous phases of a material. However, while the structure of its crystalline phase is relatively well characterized as consisting of a rhombohedrally distorted rock-salt lattice, the corresponding amorphous phase remains still poorly understood.

*Denotes Presenter

Here, we show that Sn119 Mössbauer spectroscopy and angular constraint counting of simulated structures can provide a quantitative measure of the *sp*3 tetrahedral fraction of Ge or Si cation in amorphous phase-change binary tellurides Ge*x*Te1−*x* and Si*x*Te1−*x* and GexSixTe1-2x. This represents the first quantitative estimate of such local structures, and reveals the fraction to be nearly 50%, while also revealing implications for the phase-change mechanism itself. References: *1) Quantitative measure of tetrahedral-sp^3 geometries in amorphous phase change alloys* , M. Micoulaut, K. Gunasekera, S. Ravindren, P. Boolchand, Physical Review B **90**, 094207 (2014) 2) *Effect of mixed Ge/Si cross-linking on the physical properties of amorphous Ge-Si-Te networks* , K. Gunasekera, P. Boolchand, M. Micoulaut, Journal of Applied Physics **115**, 164905 (2014).

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(GOMD-S4-017-2015) Size Dependent Phase Transition Behavior of Amorphous Phase-change Sb_2Te_3 Nanowires

C. A. Ihalawela*[1]; M. Sundararajan[1]; X. Lin[2]; M. Kordesch[1]; G. Chen[1]; 1. Ohio University, USA; 2. Argonne National Lab, USA

Size, speed and efficiency are the major challenges of next generation non-volatile memory (NVM) needed to satisfy the requirements of future device applications. Reduction of effective memory cell size in conjunction with multilevel cells could be promising to achieve high data densities, but the size reduction may result in changes in material properties. If phase transition properties of the materials are also tunable with respect to the size, then more attractive solutions could be realized. The key for NV phase-change memory (PCM) is rapid switching between two stable phases with optical or electrical excitation. In this study, we report the phase transition properties of prototypical Sb_2Te_3 nanowires synthesized in anodic alumina matrices with a range of sizes from 20 to 200 nm through an electrochemical deposition method, which is the best technique to generate high aspect ratio nanostructures. Energy dispersive X-ray spectroscopy, X-ray diffraction, electron microscopy and electrical resistivity measurements were used to characterize the composition, structure, morphology, and phase transition properties. Modifications in phase transition properties respect to the different sizes of Sb_2Te_3 nanowires will be discussed in a broader perspective to obtain fundamental understanding of the size and 1D confinement effect of PCMMs.

4:00 PM

(GOMD-S4-018-2015) First principles study of the amorphous Ga4Sb6Te3 phase change alloy

A. Bouzid*[1]; S. Gabardi[2]; M. Boero[1]; C. Massobrio[1]; M. Bernasconi[2];
1. Institut de physique et chimie des matériaux de Strasbourg, France;
2. Dipartimento di Scienza dei Materiali, Italy

Phase change memory (PCM) devices based on chalcogenides have attracted much interest as a promising candidate for next generation non-volatile memory devices. In this study, we address the structural properties of the GaSbTe alloys at the peritectic composition Ga4Sb6Te3 on the GaSb–Sb2Te3 tie line. First-principles molecular dynamics simulations within the density functional theory framework were performed to generate amorphous models of the Ga4Sb6Te3 phase change alloy by quenching from the melt. Our results show that Ga-Sb and Ga-Te bonds occur predominantly with only a minor amount of Sb-Te bonds found in the network. In particular, Ga and four-fold Sb feature present a tetrahedral-like geometry, whereas three-fold Sb atoms are in a pyramidal configuration. The tetrahedral-like geometries are similar to those of the crystal phase of the two binary compounds GaTe and GaSb. A sizable fraction of Sb-Sb bonds is also present, indicating a partial nanoscale segregation of Sb. Despite the fact that the composition Ga4 Sb6 Te3 lies on the pseudobinary GaSb-Sb2Te3 tie line, the amorphous network can be seen as a mixture of the two binary compounds GaTe and GaSb with intertwined Sb.

4:20 PM

(GOMD-S4-019-2015) Near and mid-infrared emission from composite of PbSe quantum dots and chalcogenide glasses

J. Zhang*[1]; C. Liu[1]; X. Zhao[1]; J. Heo[2]; 1. Wuhan University of Technology, China; 2. Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), Republic of Korea

Transparent composite made of mono-dispersed PbSe quantum dots and As_2S_3 glasses were prepared after mixing, pressing and consolidation processes. PbSe quantum dots were synthesized by hot-injection method, and As_2S_3 glasses were fabricated by conventional melt-quenching technique. Ultra-broad near infrared emission with full width half maximum (FWHM) ~400nm was observed from the composite with different sizes of PbSe quantum dots. Transmission electron microscopy (TEM) imaged proved the quantum dots were embedded into glass matrix, and the size distributed from 3nm to 10 nm. The effects of processing parameters on the luminescence of composite were investigated, and the interactions between quantum dots and As_2S_3 glass matrix were discussed. In addition, Sn-doped PbSe quantum dots were synthesized and incorporated into As_2S_3 glass matrix for mid-infrared emission. Mid-infrared emission centered at ~3 μm was obtained. The effect of Sn addition on luminesce of colloidal quantum dots and composite were discussed. The results indicated that band gap of bulk PbSe semiconductor decreases by Sn, which resulted in long wavelength emission. Electron energy loss spectroscopy (EELS) mapping proved the incorporation of Sn into colloidal quantum dots and quantum dots in As_2S_3 glasses. The composite with new optical properties will be applied for near and mid-infrared photonic devices.

Session 3: Optical Material Processing and Characterization

Room: Concerto A
Session Chair: Shibin Jiang, AdValue Photonics Inc

1:20 PM

(GOMD-S4-020-2015) What can we learn in glass materials combining conventional infrared and Raman with unconventional hyper-Raman and hyper-Rayleigh techniques?

(Invited)

V. Rodriguez*[1]; M. Dussauze[1]; S. Sirotkin[1]; G. Guéry[1]; T. Cardinal[1]; K. Richardson[2]; 1. University of Bordeaux, France; 2. University of Central Florida, USA

Vibrational spectroscopies are suitable techniques to get structural and dynamical insights from a wide range of systems at the molecular scale. The combination of spontaneous hyper-Raman scattering (HRS), which is a nonlinear vibrational technique, to other conventional vibrational techniques as infrared (IR) and Raman scattering (RS) has enriched this field. Besides, harmonic light scattering (HLS), also called hyper-Rayleigh scattering, provides a unique additional information about the nature and structure/symmetry of the scatterers. In that frame, we have investigated a tellurite glass system (TeO_2–$TaO_{5/2}$–ZnO) which represents a good candidate for Raman gain optical fiber. The same approach has been applied on niobium borophosphate glass system ($NaPO_3$-$Na_2B_4O_7$-Nb_2O_5). Those examples demonstrate how this approach bring new insights on the relation between linear and nonlinear optical properties and the local environment but also the intermediate range structure of the glass network.

1:50 PM

(GOMD-S4-021-2015) Aerodynamic Levitator at the NOMAD Instrument for *in-situ* Investigation of Structure in Liquids and Glasses Formed in Extreme Conditions (Invited)

R. Weber*[1]; J. Neuefeind[2]; 1. Materials Development, Inc., USA; 2. Spallation Neutron Source, Oak Ridge National Laboratory, USA

Aerodynamic sample levitation with laser beam heating has recently been integrated with the NOMAD neutron scattering instrument at the Spallation Neutron Source. The new capability enables *in-situ* measurements of structure at extreme temperatures (500-3500 °C) and in conditions that completely avoid contact with container surfaces. In addition to maintaining sample purity, levitation enables deep supercooling and enhanced glass formation from a wide variety of melts and liquids. The use of neutron scattering complements other techniques and enables use of methods such as isotope substation to obtain partial structure factors. This talk will outline the current instrument capabilities and summarize recommendations of a workshop held at the Spallation Neutron Source in February 2015. The information will be presented in the context of developing interest in using the instrument from the glass materials community.

2:20 PM

(GOMD-S4-022-2015) Towards understanding and controlling surface microroughness during glass polishing

T. Suratwala*[1]; R. Steele[1]; M. Feit[1]; R. Dylla-Spears[1]; R. Desjardin[1]; L. Wong[1]; N. Shen[1]; P. Miller[1]; 1. Lawrence Livermore Nat'l Lab, USA

The influence of slurry particle size distribution (PSD) and polishing pad surface topology on the surface roughness and removal rate of polished fused silica glass workpieces is described. Fused silica glass samples were polished with various ceria and colloidal silica slurries on various polishing pads with different surface topologies. The surface microroughness of the glass was characterized by white light interferometry and by atomic force microscopy. The results show that the roughness of the polished workpiece is quantitatively correlated with both the logarithmic slope of the tail end of PSD (as measured by single particle optical sensing) and the pad topology height histogram (as measured by confocal microscopy). A polishing model, called the Ensemble Hertzian Multi-Gap (EHMG) model, based on multiple Hertzian contacts of slurry particles each removing material at the workpiece-pad interface, was used to simulate the removal rate and resulting surface microroughness. This model determines the effective interface gap using an elastic load balance for each pad asperity which then determines the load on each particle and hence its removal amount. The correlations between the model and experiment are utilized to establish guidelines for processes to economically create atomically smooth roughness surfaces (~1 Angstrom rms) while maintaining high material removal rates.

2:40 PM

(GOMD-S4-023-2015) Thermally poled glasses: Towards a control of their structure and second order optical properties at the micrometer scale

M. Dussauze*[1]; A. Lepicard[1]; F. Adamietz[1]; K. Richardson[2]; T. Cardinal[1]; E. Fargin[1]; V. Rodriguez[1]; 1. University of Bordeaux, France; 2. University of Central Florida, USA

Poled glasses are promising materials for a large variety of applications in photonics or biomaterials. However, to control their physical and chemical properties at different scales, one needs to determine and understand the different mechanisms occurring during thermal polarization treatments. To progress in this direction, we have investigated and correlated space charge implementation and structural rearrangements induced by poling treatments on a large variety of both oxide and non-oxide glasses. This large base of results has permitted significant progresses on (i) the fabrication of glassy surfaces with tailored optical and chemical properties and (ii) the control of the poling process at sub micrometric scale. In this presentation, the high potential of such process will be demonstrated through several examples in which both structure and second order optical response have been successfully micro-patterned.

3:00 PM

(GOMD-S4-024-2015) Control of surface reactivity in borosilicate glasses using thermal poling

A. Lepicard*[1]; T. Cardinal[1]; V. Rodriguez[1]; K. Richardson[2]; M. Dussauze[1]; 1. University of Bordeaux, France; 2. University of Central Florida, USA

The ability to control glass substrate surface reactivity at different scales will enable key properties needed for future “smart substrates”. Within this objective, we aim to design a surface with tailored physical and chemical properties at a sub-micron scale using a thermal poling treatment on borosilicate glasses with selected chemical compositions. The chosen glassy systems have a high level of alkali elements which diffuse in the glass during the polarization treatment. An alkali depleted layer is formed under the anode, responsible for structural changes and the formation of a frozen electric field in the glass. Structural modifications associated with the process were investigated using Raman and infrared spectroscopy. Network reorganization was linked to creation of BO_3 units replacing $[BO_4]^-$ entities after migration of alkali ions. Strength and location of the electric field has been characterized by Second Harmonic Generation (SHG) techniques: quantitative Maker fringes analysis and μSHG imaging. It has been shown that the formation of a new charged borate structure leads to a tendency of the glass to attract water at the surface. In experiments to date, the water layer stability is retained for several weeks. Micro-localized attraction of water at the surface of a glass substrate is an interesting property with direct applications for lab-on-a-chip devices and bio-reactors.

Session 3: Luminescent and Doped Glasses

Room: Concerto A
Session Chair: Juejun Hu, MIT

3:40 PM

(GOMD-S4-025-2015) Laser Properties of Tm^{3+}-doped Tellurite-Phosphate Glass Composite Fiber

K. Li*[1]; L. Hu[1]; P. Kuan[1]; X. Fan[1]; L. Zhang[1]; 1. Shanghai Institute of Optics and Fine Mechanics, China

Tellurite composite single mode fiber with a tellurite glass core and a phosphate glass cladding was fabricated successfully, the composite fiber was much stronger than pure tellurite fiber. Both carbon nanotubes (CNTs) and semiconductor saturable absorber mirror (SESAM) are inserted separately into the laser cavities as saturable absorbers to demonstrate a fiber integrated setup. In a short, 9 cm tellurite fiber, 1.86 μm pulsed lasers without self-mode-locking effect is demonstrated by in-band pumping at 1.59 μm. An average power of 84 mW is obtained in CNT pulsed laser with 860 ns duration while in SESAM pulsed laser, the average power reaches 21 mW with 516 ns pulse width.

4:00 PM

(GOMD-S4-026-2015) Efficient red emission of Eu^{3+}-doped new tungsten phosphate glasses

M. Dousti[2]; G. Y. Poirier[1]; A. de Camargo*[2]; 1. Institute of Science and Technology, Federal University of Alfenas, Brazil; 2. Physics Institute of São Carlos, University of São Paulo, Brazil

Tungsten phosphate glass compositions are interesting non-crystalline hosts for rare earth ions RE, due to their unique photophysical properties such as high refractive index, large density, good rare earth solubility and lower phonon energy than regular phosphates. Despite of that, they are still little investigated for that purpose. The low transmittance in the visible spectral region, observed in glasses with high concentrations of WO_3 can be improved by addition of oxidizing agents such as Sb_2O_3. In this work, we aimed at preparing and studying Eu^{3+}-doped tungsten phosphate glass having nominal composition (96-x)($NaPO_3$-WO_3)-4Sb_2O_3-$x$$Eu_2O_3$ where x=0, 0.1, 0.25, 0.5 and 1 mol%. The DSC profiles of bulk and powder samples revealed an endothermic glass transition at around 480°C, while their crystallization processes exhibit different performances. The optical transparency is improved after incorporation of Sb_2O_3 and Eu_2O_3 oxides. Upon excitation with 464 nm, strong red emission is observed at 610 nm ($^5D_0 \rightarrow ^7F_2$ transition) and the average emitting level's lifetime is 1.2 ms. The CIE chromaticity diagram coordinates for the 0.5 mol% doped glass under 464 nm excitation are x = 0.65 and y = 0.35 indicating a very good quality of the red color.

4:20 PM

(GOMD-S4-027-2015) Scintillating Glass/Polymer Composite Neutron Detectors

C. L. Trivelpiece*[1]; I. Jovanovic[1]; M. Mayer[1]; J. Nattress[1]; 1. Pennsylvania State University, USA

Fast neutron detectors are being fabricated and tested that employ a matrix of scintillating polyvinyl toluene (PVT) and embedded cerium-activated, scintillating glass forms to detect fast neutrons in multiple applications, especially in the active interrogation of objects for shielded special nuclear material. Three different glass geometries have been modeled using Geant4, and the results of the simulations indicate that randomly placed glass spheres with a diameter of 300-500 μm offer the optimal combination of neutron detection efficiency and gamma rejection. Work is underway to determine the best glass composition for producing the spheres while maintaining the Ce^{3+} oxidation state. In addition to modeling and optimization of glass fabrication, a prototype detector was constructed using commercially available GS20 glass rods carefully spaced within a 3D printed mold, which was backfilled with PVT and cured to form the composite detector. Initial tests with this prototype were conducted using ^{241}AmBe, ^{252}Cf, and ^{239}PuBe neutron sources along with multiple gamma sources to demonstrate the efficacy of the detector concept. The results of the initial testing show that the prototype has a sufficiently high detection efficiency and gamma rejection to be competitive with specialized homogeneous liquid and plastic scintillation fast neutron detectors, which use solely their material properties to achieve gamma rejection.

Symposium 5: Glass Technology and Cross-cutting Topics

Session 1: Challenges in Glass Manufacturing II

Room: Concerto C
Session Chairs: Irene Peterson, Corning Incorporated; Hong Li, PPG Industries, Inc.

1:20 PM

(GOMD-S5-009-2015) Optimized radiative heat transfer and service life of the crown in glass furnaces

R. Weigand*[1]; H. Hessenkemper[1]; A. Rössel[1]; D. Tritschel[1]; 1. TU Bergakademie Freiberg, Germany

The attack of the silica crown in the glass furnace is a problem which prohibits a higher temperature of the superstructure. The aim was to transfer the developed ancorro technology which increases the service life of porous refractory to that part of the furnace and to combine a higher service life with a higher radiative heat transfer. So the problem of the temperature sink after the change of the flames should be lowered. For the future a better heating of the glass and batch will be possible. The corrosion tests were realized with NaOH at 1200°C for different hours. After treating the crown material the service life rises up to 15%. To analyze the corrosion attack a 3D scanner was used for the tests. After treating the samples the modified radiative heat transfer was measured by using a pyrometer and an IR camera which is rising after the treatment of the porous refractory. The results were used for a simulation of the furnace properties. These results and the savings in the range of a few hundred thousand euros per year will be shown in the presentation.

1:40 PM

(GOMD-S5-010-2015) Lowering of refractory corrosion in enamel production

R. Weigand*[1]; H. Hessenkemper[1]; A. Rössel[1]; D. Tritschel[1]; 1. TU Bergakademie Freiberg, Germany

High temperature processes are very complex. One of the most aggressive melts are enamels which attack the refractory much more as glass melts. Due to this fact the furnace campaign of them is only a few months. The aim was to transfer the developed surface treatment technology of ancorro also to this high temperature process. By using the surface treatment technology an oxygen depression is formed in the pores of the refractory. This reducing atmosphere increases the surface tension and viscosity of the melt in the boundary layer which slows down the whole interaction between melt and refractory. Typically refractory test were realized on different types on enamel frits. After the crucible, static and dynamic finger test the service life of the refractory increases up to 50% by using the surface treatment technology. For the finger tests a 3D scanner were used to measure the corrosion effect. The next step will be the implementation into industrial scale which will rising the life time of the furnace and saves energy, CO_2 emissions and optimizes the production process.

2:00 PM

(GOMD-S5-011-2015) Tribological investigations of the glass-metal contact in glass-container production

D. Orzol*[1]; C. Roos[2]; L. Wondraczek[1]; 1. Otto Schott Instute, FSU Jena, Germany; 2. IPGR, Switzerland

Glass-metal-contact occurs at several steps during glass container production, for example during forming of the container. Different solid and liquid lubricants are used in the industry for improving the conditions in the glass-metal-contact, but many of them introduce more problems to the container glass forming process. The loading of the gob into the blank mold is a crucial step, which can be facilitated by swabbing. During the swabbing an oil and graphite based lubricant is applied in short intervals manually on the blank molds. There is still a lack of fundamental understanding in glass-metal-contact, which prohibits the avoidance of swabbing. Therefore it is of interest, to investigate the glass-metal-contact to understand the fundamentals of that process and to find new to improve glass metal surface interaction and to enable a production without swabbing. Different materials have been tested on a special test bed and fundamental understandings of the glass-metal contact in gob-loading have been derived. A realistic simulation of the gob loading regarding the gob weight, temperature state and gob speed can be used with a quantification of the friction at the same time. The fundamentals of the interactions and corresponding material parameters will be discussed, supported by trials on afore mentioned test bed.

2:20 PM

(GOMD-S5-012-2015) Droplet formation in altered silicate glass surface

E. Raedlein*[1]; 1. Technische Universität Ilmenau, Germany

One typical surface feature of silicate glasses that had been in contact to humid atmosphere or liquid water is the formation of soft droplets with diameters in the μm range that is not yet explained by the well investigated leaching and dissolution processes. Non-homogeneous water uptake is suggested to be the cause for these droplets. The conditions of droplet growth and their behavior in different environments will be described, as well as their impact on glass quality in post-processing and application. Calcium silicate hydrate formation has been the tentative interpretation for the droplets. In a recent study with different model glasses with and without CaO components, this interpretation has been ruled out. Inhomogeneous swelling of the altered surface seems to be an intrinsic property of sodium silicate glass surface, probably due to inhomogeneous distribution of sodium species

2:40 PM

(GOMD-S5-013-2015) Model of Continuous Fiber Drawing. II. Extended Parametric Study

O. Prokhorenko*[1]; 1. L.G.P. International, USA

New version of mathematical model of continuous fiber drawing process has been recently developed by L.G.P.. The model includes the following sub-models: a) one channel of the forehearth with 7 slots, b) electrically heated bushing, c) bushing plate having 4000 tips, d) cone, which forms a single filament cooled down by fins, air flow, and spray under the drawing force. The last sub-model is capable of simulation of stationary, non-stationary, and non-linear responses of the system to disturbances. The disturbances are set as periodic or random variations of several critical input parameters (hydrostatic pressure, temperature, viscosity, surface tension, winder rotation speed, etc.). Penetration of seeds or solid particles into the forming cone represents an important source of disturbances causing, in some cases, quite strong non-linear response (perturbation) of the drawing force. The present work aimed to perform parametric study of the fiber drawing process in its non-stationary state regime. Typical commercial high-modulus fiber-glass, and standard regimes of the drawing process were selected to be a starting point for the modeling case. The main task was to determine the ranges of variations of processing parameters corresponding to optimal, acceptable, and non-acceptable states of this process. Probability of fiber breakage was used as one of the major criterion of evaluation of the tested regimes.

3:00 PM

(GOMD-S5-014-2015) Model of Continuous Fiber Drawing. III. Criteria of Fiber Breakage

O. Prokhorenko*[1]; 1. L.G.P. International, USA

Breakage at continuous fiber drawing is one of the most important problems. One can find no clear criteria of resistance of a glass fiber to a sum of forces applied in the course of drawing. Mathematical model described in the present paper is capable of calculating major components of the drawing force. The first component - is a stationary drawing force. Effective value of this force is far less than pristine strength of a single fiber. Perturbations of drawing force can increase amplitude of the drawing force. They are caused by periodic disturbances of different process parameters such as the molten glass level, electric power, winder rotation, critical properties of the molten glass, intensity of cooling, and others. The most critical disturbances are those causing non-linear response. We consider two cases. Periodic disturbances, leading to growth of the drawing force to a critical level. Random disturbances initiating non-linear system response as a rapid growth of the drawing force. The main task of the modeling - is to allow the system sensitivity to various disturbances. The model is capable to determine values of drawing force at any moment of drawing in stationary, non-stationary, and non-linear regimes. The second task - is to compare spectrum of tensile strength of the fiber with the spectrum of drawing force. In case these two spectra overlap, one can calculate probability of fiber breakage.

3:40 PM

(GOMD-S5-015-2015) An Integrative Approach for the Numerical Modeling-assisted Design of Non-isothermal Glass Molding Process for Complex Glass Optics

A. Vu*[1]; H. Kreilkamp[1]; G. Liu[1]; O. Dambon[1]; F. Klocke[1]; 1. Fraunhofer Institute for Production Technology, Germany

Intensively growing demands for complex yet low-cost precision glass optics motivate industrial companies to develop an efficient and economically viable manufacture of complex shaped optics. Against state-of-the-art replication-based techniques, **Non-isothermal Glass Molding (NGM)** turns out a promising innovative technology for cost-efficient manufacturing because of raw material save, less energy consumption and high throughput from a fast process chain. However, the process dynamic and complexity of glass behavior under extreme process conditions, i.e. high temperature, fast molding with high pressure, pose major challenges for process establishment. This research introduces an innovative design concept whereby numerical modeling-assisted modules are integrated at the early stage to standardize and accelerate the entire NGM process design. Two integrative modules based on the coupled thermo-mechanical modeling are developed. Simulation results are verified by a broad range of experiments with advanced measuring techniques. This modeling provides a systematic approach for glass preform design, mold compensation, and process optimization. In conclusion, the integration of simulation modeling into the entire process chain will significantly increase the manufacturing efficiency of complex optics as well as industrial enterprises' competitiveness.

4:00 PM

(GOMD-S5-016-2015) Measurements and calculations for the production of lightweight hollow ware

G. Bergmann*[1]; N. Löber[1]; J. Simon[1]; H. Müller-Simon[1]; 1. Hüttentechnische Vereinigung der deutschen Glasindustrie e.V., Germany

The decrease of the weight of glass bottles and jars is on top of the wishlist of customers all over the world. Especially for the blow-blow-process a more uniformly distributed wall thickness distribution is the key for lightweight bottles. We analyzed temperatures of the whole system between feeder an blank with different contact and optical techniques, measured speed and geometric changes of the gobs and used free FEM software for the calculations. The paper will present a part of our experimental work and modelling of the feeder and spout at first. The influence of pull rate and the direction of rotation of the tube f.i. will be discussed. The main part will focus on the delivery system. As an result of our research we are able to characterize the inside temperature distribution of the gobs after cutting on one hand and we are able to predict the resulting temperature distribution after leaving the delivery system for gob loading on the other hand. This includes the changes of the gobs shape and speed. Some experimental data and calculations will illustrate this topic. The current research deals with an active influencing of the heat transfer coefficient in the delivery system, first experimental results will also be presented.

4:20 PM

(GOMD-S5-017-2015) Energy efficiency improvements for glass furnaces

O. Verheijen[1]; A. Habraken[1]; L. Thielen[1]; J. van der Dennen[1]; M. van Kersbergen[1]; M. Hubert*[1]; 1. CelSian Glass & Solar, Netherlands

A systematic approach is applied to analyze the energy efficiency performance of industrial glass furnaces and to quantify the energy savings potential of individual glass furnaces. Different methods and software tools are developed and applied to assess and improve glass furnace energy efficiency. These methods include energy-efficiency benchmarking, industrially validated glass furnace energy balances, simulation tools to optimize glass furnace design and operation and to improve on regenerator design, advanced process control technologies, and breakthrough energy savings technologies like thermo-chemical recuperation. This paper discusses both glass furnace energy-efficiency benchmarking and the set-up of a detailed and industrially calibrated energy balance, enabling the quantification of the energy savings potential of an individual furnace. In addition, it is demonstrated how simulation tools can support in improving the design of glass furnace regenerators in order to increase the heat recovery from hot flue gases and thereby increasing the energy efficiency of glass furnaces. Finally, an outlook is provided on new energy savings technologies in development, including the use of preheated pelletized glass batches and production of syngas from the hot flue gases by means of thermochemical recuperation. The paper is illustrated from industrial examples.

4:40 PM

(GOMD-S5-018-2015) Operating Experience with OPTIMELT™ Heat Recovery Technology on a Commercial Glass Furnace

S. Laux*[1]; A. Gonzalez Rodriguez[2]; H. Kobayashi[1]; A. Francis[1]; R. Bell[1]; E. Evenson[1]; 1. Praxair Inc, USA; 2. Grupo Pavisa, Mexico

The operation of oxy-fuel fired glass furnaces in combination with heat recovery offers significant reduction in energy consumption and emissions relative to conventional air-firing. For a large scale commercial system, Praxair's OPTIMELT™ TCR technology is expected to reduce fuel consumption more than 30% relative to an air-fired furnace and 20% relative to an oxy-fuel baseline. An oxy-fired furnace equipped with the OPTIMELT™ TCR system is operated in a similar cyclic fashion than an air-regenerative furnace although in this case fuel is heated and reformed in place of air preheat. No catalysts or separate steam generation is required and the OPTIMELT™ system regenerators are only 1/3 the size of those required for conventional air-firing making retrofit on rebuild an attractive option. Praxair and Pavisa are cooperating in the first commercial demonstration of Praxair's novel OPTIMELT™ Thermo-Chemical Regenerator (TCR) system on a 50 tpd container furnace in Mexico. The OPTIMELT system uses regenerators to preheat and reform a mixture of natural gas and recirculated flue gas in the hot regenerator checker pack. The resulting hot syngas (H_2 and CO) results in a highly luminous flame with higher combustion enthalpy than preheated natural gas alone. The first OPTIMELT™ system was installed at Pavisa in 2014 and results and operational experience will be presented and discussed.

5:00 PM

(GOMD-S5-019-2015) Scientific work and industrial research as an effective tool for being in step with glass industry

G. Bergmann*[1]; 1. Hüttentechnische Vereinigung der deutschen Glasindustrie e.V., Germany

"Our laboratory is the floor of the glass factory!" – This was a famous slogan of a former director of HVG and DGG. What did he mean to say? HVG e.V. was founded in 1920 and in the early days the activities of the association consisted of recording of heat-technical indexes by measuring techniques, preparation of heat balances and optimization of the glass melting. So we can look back on a long tradition of scientific work very close to the production lines. Today the glass industry puts forward topics of special interest to the HVG council. Such topics are then either processed directly by the HVG or jointly with the various universities. Even now the realization of these research projects occurs mainly as on-site experimental work. Thus, it is guaranteed that the requirements of industrial practice are considered adequately and the results can be applied as soon as possible. The main topics of the current research deal with optimization of combustion processes, the influence of gas composition changes, hot forming of glass, i.e. the influence of feeder, spout and delivery on the wall thickness distribution of hollow ware, surface corrosion of glass and its effects on the efficiency of photovoltaic systems up to tracking of enrichment processes in the melting unit. The presentation will give a brief look back to the history and will focus on some results of current activities.

Posters

Student Poster Competition

Room: Symphony Ballroom I

(GOMD-SP-P001-2015) Specialty optical fibers for temperature sensing based on spontaneous Raman scattering

D. Manzani*[1]; H. Ebendorff-Heidepriem[2]; S. J. Ribeiro[1]; T. M. Monro[2]; 1. Institute of Chemistry, Brazil; 2. Institute for Photonics and Advanced Sensing, Australia

Temperature sensing conducted using conventional electric temperature sensors have limitations for applications, and optical fibers based sensors show advantages. One widely used type of optical fibers sensor is based on Raman, where the ratio of anti-Stokes and Stokes backscattered from within the fiber is a function of the absolute temperature.In this paper we describe advances based on the use of microstructured optical fibers made from highly-nonlinear glass compositions and present a real-time temperature sensor using Raman as nonlinear optical effect to detect temperature changes along the fiber. Were investigated the impact of glass type (silica, silicate, lead-germanate and tellurite) and optical fiber structure on the sensitivity to temperature. We studied two different fiber structures (unstructured and suspended core fibers) and SMF28. The Raman light within the optical fibers was collected in 40cm fiber lengths pumped at 532 nm under heating. The microstructured fibers showed highest sensitivity due to high fiber nonlinearity, which results from both high material nonlinearity (tellurite) and high light confinement within the small core. Despite the higher optical loss, the Raman intensity of these fibers is 70 times higher than that found for SMF28, which demonstrates that tellurite and germanate fibers are promising candidate for highly precision temperature detection.

(GOMD-SP-P002-2015) Development Strategies for Fibre Glasses

K. Kölker*[1]; R. Conradt[1]; 1. RWTH Aachen University, Germany

The theoretical glass development on the basis of thermodynamic data is a powerful tool to estimate physical and chemical properties of a glass before the actual melting process. The replacement of the conventional empirical approach by a systematic one offers the opportunity of time and cost savings. In the course of the development of a novel fibre glass composition, a new theoretical strategy was introduced. It is based on a constitutional approach to the amorphous state. Since the properties of glass building systems are closely related to the properties of the phases occurring under equilibrium conditions, it is possible to make accurate predictions about the glassy state utilizing existing thermodynamic data of the crystalline reference system. By the means of the thermochemical software FactSage^{TM} constitutional ranges of the glass building system CaO-ZnO-Al_2O_3-SiO_2 (CZAS) were identified. In a second step, the oxide compositions and the liquidus temperatures of invariant points within the system were calculated. As a final result of this theoretical phase, a network describing ternary and quaternary invariant points of CZAS in addition to their melting temperatures and the corresponding saturation lines was derived. Starting out from suitable invariant points of this polythermic phase diagram, four oxide compositions were determined. The glasses were melted, processed, and their properties were verified by experiment.

(GOMD-SP-P003-2015) Na-based sulfide glasses for solid electrolyte

A. Bréhault*[1]; S. Cozic[1]; R. Boidin[2]; L. Calvez[1]; P. Masselin[3]; O. Bošák[4]; V. Labas[4]; E. Bychkov[3]; X. Zhang[1]; D. Le Coq[1]; 1. University of Rennes 1, France; 2. University of Pardubice, Czech Republic; 3. University of Littoral Côte d'Opale, France; 4. Slovak University of Technology, Slovakia

Our study aims to search new compositions of solid electrolytes among sodium based in sulfide glasses. Liquid electrolytes based on lithium are available since a long time, however due to several incidents the current research is directed on solid electrolytes. Nowadays, the best results were obtained with sulfide glasses based on lithium. In this work, Na-based sulfide glass compositions are investigated since Na is more abundant and less expensive than Li. The chalcogenide glasses in the NaX-GeS_2-Ga_2S_3 (X = Cl or I) system were synthesized. Different series in the NaX-GeS_2-Ga_2S_3 (X = Cl or I) system were studied in order to highlight the influence of the sodium halide addition on glass properties. The macroscopic properties including characteristic temperatures and density are given. Other parameters such as optical band-gap and chemical stability of these samples are also detailed. The evolution of conductivity parameters (conductivity at row temperature and activation energies) will be studied according to the atomic percentage and the salt nature allowing to evaluate the potential of some compositions as sulfide glasses solid electrolytes.

(GOMD-SP-P004-2015) Pressure-Induced Changes in Inter-Diffusivity, Compressive Stress, and Hardness in Chemically Strengthened Glass

M. N. Svenson*[1]; L. Thirion[2]; R. Youngman[2]; J. Mauro[2]; S. Rzoska[3]; M. Bockowski[3]; M. Smedskjær[1]; 1. Aalborg University, Denmark; 2. Corning Incorporated, USA; 3. Polish Academy of Sciences, Poland

The short- and intermediate-range structures of a glass are tunable through high-pressure treatment and may thus give rise to properties unattainable under ambient pressure. Moreover, chemical strengthening of glass through K^+-for-Na^+ ion exchange can be used to improve the damage resistance of glasses by introducing a compressive stress in the glass surface. However, the interplay among isostatic compression, pressure-induced changes in alkali diffusivity, compressive stress generated through ion exchange, and the resulting mechanical properties are poorly understood. In this work, we employ a specially designed gas pressure chamber to compress bulk glass samples isostatically up to 1 GPa at elevated temperature before or after the ion exchange treatment of an industrial sodium-magnesium aluminosilicate glass. Compression after the ion exchange treatment changes the shape of the potassium-sodium diffusion profiles and significantly increases glass hardness. Compression of the samples prior to ion exchange leads to a decreased Na^+-K^+ inter-diffusivity and increased compressive stress, and reveals a strong dependence of glass hardness on the compression temperature. We discuss these results in terms of the underlying structural changes in network-modifier environments and overall network densification.

(GOMD-SP-P005-2015) Phase Theoretical Development of Fiber Glasses

K. Hellmann*[1]; R. Conradt[1]; 1. RWTH Aachen Institute of Mineral Engineering, Germany

In a first step, compositions from the quaternary system $CaOMgOAl_2O_3SiO_2$ are generated theoretically with the help of a commercial software. Then, the suitability for continuous filaments drawing at the laboratory scale is tested. By thermodynamic calculations, the eutectic composition belonging to the given phase equilibria can be identified. Afterwards a melting test of the correspondent glass is performed and the liquidus temperature is determined with a gradient furnace. To test the fiberization ability the corresponding fiberization temperature is measured. Single filament fibers were drawn from suitable compositions. Young's Moduli of the bulk glass were determined using impulse excitation technique. In this study, eight glasses were melted; so far two of them were well applicable for continuous fiber drawing with promising Young's Modulus values.

(GOMD-SP-P006-2015) Red Mud Recycling for Reinforcement Glass Fibers

S. V. Krogel[1]; K. Hellmann*[1]; S. Bunk[1]; F. M. Kaussen[1]; R. Conradt[1]; B. Friedrich[1]; 1. RWTH Aachen University, Germany

Red mud is currently stored as hazardous waste on mono landfills. The possibility of a holistic recovery will be investigated through the production of glass fibers from the slag after iron removal. During the production of aluminum using the so-called Bayer process, the metal is extracted out of the bauxite ore in a high pressure alkaline leaching. The residue of this process is red mud, which is deposited as hazardous waste so far. As a variety of valuable materials are included, it is reasonable to investigate ways to reuse the red mud. Since the oxide composition is similar to glasses used for mineral fibers, it is an option worth investigating to utilize red mud as a raw material for the glass industry. Due to the too high iron content, it is necessary to extract the iron oxide as pig iron. Thermodynamic calculations confirm a possible ideal oxide composition by means of a low liquidus temperature when some aggregates are added. By processing the red mud with additives in an electric arc furnace it is possible to gain a pig iron and to obtain the desired slag composition for mineral fibers in one step. At lab scale, the emerged slag is remelted and quenched to gain an amorphous material. Afterwards the fiberization ability is tested and evaluated.

(GOMD-SP-P007-2015) Investigation of short range order and elastic properties of multicomponent oxide glasses

K. Philipps*[1]; R. P. Stoffel[1]; R. Conradt[1]; R. Dronskowski[1]; 1. RWTH Aachen University, Germany

Well-directed design of glasses with outstanding mechanical properties is still not possible. Understanding the mechanisms responsible for elastic moduli would lead to a systematic development of high modulus glasses, e.g. of novel glass fibres used for reinforcement. The present project aims to overcome the limitations of semi-empirical approaches by establishing a systematic approach deeply rooted in physical and chemical principles. By combining quantum mechanical calculations and thermodynamic methods, a predictive model for mechanical properties of glasses is presently developed. Electronic, vibrational and thermodynamic properties as well as elastic moduli of crystalline entities are calculated based on solid-state DFT. Structural changes invoked by a gradual increase of volume help not only to determine the structures and mechanical properties of crystalline polymorphs but also of their isochemical glasses. The influence of short range order (coordination polyhedra and their linkage) on elastic properties is studied in one-component glasses as well as mixing series between two end members in pseudo-binary systems such as anorthite-enstatite or diopside-jadeite, respectively. In all cases, special attention is given to atomic coordination, the nature of the linkage between adjacent coordination polyhedra, packing density, and bond percolation.

(GOMD-SP-P008-2015) New Bioactive Glass Fibers for Soft Tissue Regeneration

M. T. Souza*[1]; O. Peitl[1]; M. Puzzi[2]; E. Dutra Zanotto[1]; 1. Universidade Federal de São Carlos, Brazil; 2. State University of Campinas, Brazil

Bioactive glasses are widely known for their ability to regenerate hard and soft tissues. However, their low glass stability hinders most manufacture processes. This trait causes many problems in the manufacturing of shaped devices, fibers or scaffolds. To overcome this phenomenon, a new bioactive glass composition was developed at the Vitreous Materials Laboratory (UFSCar, Brazil) that shows high stability and bioactivity, thus allowing one to make fibers, meshes and 3D shapes. These fibers are bioresorbable and flexible, making this material a potential alternative for soft tissue regeneration. Therefore, the aim of this study was to characterize some properties and explore the effects of these new biomaterial on fibroblast proliferation. For that, SBF-K9 tests were performed from 4 to 48 h followed by FTIR and SEM analyses. ICP-OES was conducted to monitor the release of Ca, Na, P and Si. Fibroblasts viability was demonstrated using 65 year old patient cells, which were seeded in RPMI-1640 medium for 7 days. Results indicated a highly bioactive material, with the formation of the HCA layer in only 4 hours in SBF solution and with the dissolution of ions in a similar trend to Bioglass 45S5. Fibroblasts proliferated in a satisfactory rate, increasing their number from 510^4 to 310^5. Hence, this new biomaterial could be a potential alternative in applications that aim soft tissue regeneration.

(GOMD-SP-P009-2015) Atomic-Level Structure of Rare-Earth Doped (0.2 - 2 at%) Sodium Phosphate Glasses

F. Amir*[1]; C. Yoo[1]; E. S. Gunapala[1]; G. Marasinghe[1]; P. Akhter[4]; L. Skinner[2]; C. Benmore[2]; C. U. Segre[3]; K. Zhang[1]; T. Shibata[3]; R. K. Brow[5]; 1. University of North Dakota, USA; 2. Argonne National Laboratory, USA; 3. Illinois Institute of Technology, USA; 4. State University New york, USA; 5. Missouri University of Science and Technology, USA

Preliminary photoluminescence studies of a series of $(RE_2O_3)_x(Na_2O)_y(P_2O_5)_{1-x-y}$ glasses (RE $\equiv$ Pr, Nd, & Er, $0.005 \le x \le 0.05$ and $x+y = 0.3$ or 0.4) suggest that their optical gain may not be adversely affected by concentration quenching near the lower end of the above rare earth ion (RE^{3+}) concentration range (0.2 - 2 at%). The primary objective of this study is to investigate the coordination environment of RE^{3+} of these samples. Na_2O was use as a "filler oxide" simply to maintain the O/P ratio above approximately 2.7 in order to avoid having to deal with hygroscopic samples. High-energy X-ray diffraction and extended X-ray absorption spectroscopy (both carried out at the Advanced Photon Source, Argonne National Laboratory) were the main techniques used. Other supplementary techniques including FTIR, DTA/DSC, and NMR also were utilized. Near-neighbor RE-O coordination numbers ranging from 10 – 6.5 have been observed with a trend for this number to decrease with increasing RE^{3+} content, especially in the case of lighter rare earths. The first shell is surrounded by a loosely defined 2nd coordination shell of phosphorus atom which merges into a 3rd coordination shell of oxygens. Sodium atoms are found only beyond the 3rd shell. These findings predict a model in which rare earth ions are well separated and shielded from each other.

(GOMD-SP-P010-2015) Tellurite glasses for the near-IR: from material design to fiber fabrication

S. Danto*[1]; T. Billotte[1]; N. Lo[1]; F. Désévédavy[2]; C. Strutynski[2]; S. Chenu[3]; M. Dussauze[1]; V. Rodriguez[1]; G. Délaizir[3]; J. Duclere[3]; P. Thomas[3]; F. Smektala[2]; K. Richardson[4]; E. Fargin[1]; T. Cardinal[1]; 1. University of Bordeaux, France; 2. University of Burgundy, France; 3. University of Limoges, France; 4. College of Optics & Photonics-UCF, USA

Tellurite-based oxide glasses possess both a wide transparency in the near-IR region and excellent nonlinear optical properties. Beyond they exhibit interesting thermo-viscous ability making them potential candidates for optical fiber amplifiers. Building on their assets, methodology for the development of tellurite-based glass fibers as Raman amplifier is presented. The strategy consisted in establishing on a set of suitable materials the correlation between structure, vibrational response and nonlinear optical properties. As an illustration hyperpolarizability of tellurite glasses in the $TeO_2–TaO_{5/2}–ZnO$ system has been quantified. Combination of vibrational spectroscopies and hyper-Rayleigh scattering techniques emphasized a clear relationship between the linear optical polarizability, hyperpolarizability, Raman gain intensity and the level of polymerization of the TeO_4 chain-like structures in the glass system. Furthermore fiber drawings performed in the $TeO_2–TaO_{5/2}–ZnO$ system yield attenuation in the order of 5 $dB.m^{-1}$. We believe the results presented here will bring decisive insights for the development of customized tellurite-based glasses and glassceramics optical components.

(GOMD-SP-P011-2015) The Structure and Properties of Glasses in the $ZnO-B_2O_3-P_2O_5$ System

P. T. Freudenberger*[1]; 1. Missouri University of Science and Technology, USA

The glass forming region of the $ZnO-B_2O_3-P_2O_5$ (ZBP) system was expanded from previous studies and the effects of structure on properties were investigated. Three sets of compositions having constant O/P ratios of 3.0, 3.25, and 3.5, with ZnO contents ranging from 30mol% to 60mol% were prepared. The types and concentrations of phosphate anions that constitute the structures of these glasses were characterized by High Pressure Liquid Chromatography (HPLC), and additional structural information was obtained by Raman and Infrared (IR) spectroscopies. For glasses with similar O/P ratios, molar volume and glass transition temperature decrease as ZnO replaces B_2O_3, indicating a decrease in the strengths of the metal-oxygen bonds that tie together the phosphate anions and an increase in the packing efficiency of the various polyhedra. Phosphate anions become progressively smaller with increasing O/P ratio and the effects of these structural changes on properties will also be described.

(GOMD-SP-P012-2015) Rubidium Ion Conducting Glasses for Solid State Alkali Atom Sources

A. Whale*[1]; S. W. Martin[1]; J. Bernstein[2]; 1. Iowa State University, USA; 2. Charles Stark Draper Laboratory, USA

Specialty cold atom sensors have used technology which requires a high vacuum with specific atom restrictions. The proposed Solid State Alkali Atom Source (SSAAS) will become both a source and sink for rubidium ions and have more optimum operating conditions. The current glass systems under study for the alkali atom source are $xRbI + (1-x)[0.4GeSe_2+0.6Ga_2Se_3]$ and $xRbI + (1-x)[0.4GeSe_4+0.6Ga_2Se_3]$ with $0.4 \le x \le 0.55$. Since these glasses will be heavily ion conducting they will be characterized using Differential Scanning Calorimetry, Raman spectroscopy, and FTIR, with an emphasis on ionic conductivity.

(GOMD-SP-P013-2015) Dynamic Light Scattering in Aluminophosphate Glass-forming Melts

A. Keller[1]; D. Sidebottom*[1]; 1. Creighton University, USA

In previous work, our group has investigated a series of phosphate-rich aluminophosphate glasses along a tie line from $NaPO_3$ to $Al(PO_3)_3$ using dynamic light scattering and observed a systematic decrease in fragility with increasing network connectivity caused by the replacement of Q^2 phosphorus species by predominantly Q^6 alumina species. In that study, as well as in a study of alumina-free, sodium ultraphosphate melts, the Kohlrausch exponent (β) that characterizes the non-exponential decay of the dynamic structure factor exhibited compositional variations (at temperatures well above T_g) that seemed to be associated with the concentration of alkali ion. In the present study, dynamic light scattering has been preformed on low phosphate melts along the tie line between $NaPO_3$ and $NaAlO_2$ (for which the molar percentage of alkali remains fixed) in an effort to verify this behavior.

(GOMD-SP-P014-2015) The shape of diopside glass particles probed by crystallization kinetics and DSC

R. G. Fernandes*[1]; E. B. Ferreira[1]; 1. University of São Paulo, Brazil

An important problem in the modeling of sintering with concurrent crystallization of glasses is how to take into account the effect of particle shape. Currently an empirical correction factor relative to the particle shape is considered when using the Clusters Model, which is actually obtained by fitting the model itself to experimental data. Aiming at independently characterize the particle shape, we examined the sensitivity of DSC's crystallization peaks modelled considering the thickness of a crystalline shell growing from the surface, as the geometry contraction of the glass particle, and varying particle's size and shape. We compared the calculated peaks to experiments of heat flux DSC for a diopside (CaO.MgO.2SiO2) glass powder in narrow size ranges. The agreement between the experimental and theoretical curves was evaluated, constrained to the surface area of the powder samples measured by BET and the aspect ratio from microscopy and image analysis, to infer which regular parallelepiped shape best fits to the DSC signal.

(GOMD-SP-P015-2015) A Sampling Method for Semi-Quantitative and Quantitative Electron Microprobe Analysis of Glass Surfaces

J. L. Weaver*[1]; J. Reiser[1]; O. Neill[1]; J. McCloy[1]; N. Wall[1]; 1. Washington State University, USA

The determination of the long-term stability and corrosion of vitrified nuclear waste is an important aspect of research for the U.S. Department of Energy (DOE). It is necessary to understand the rate and mechanisms of Nuclear Waste Glass (NWG) corrosion to determine whether or not the glassy matrix will be able to retain radionuclides for the required repository performance time period. Glass corrosion and the rate of glass corrosion is determined by both chemical methods and microscopy. Combined scanning electron microscopy (SEM) and electron microprobe analysis (EPMA) is a common and powerful method utilized in the examination of the chemographic difference between corroded and uncorroded NGWs. In this work, two forms of quantitative and semi-quantitative EPMA methods are defined by the use of wavelength-dispersive X-ray spectroscopy, using primary and secondary standards to optimize and verify precision and accuracy for measurements of NWG. Data collected on both the planar and cross-sectioned surfaces of an unaltered simulated NWG by WDS was found to be comparable to the theoretical composition of the glass. Conventional "standardless" Energy Dispersive Spectroscopy (EDS) data collected on the same surfaces was not comparable. However, "comparative" based EDS analysis is shown to be able to discriminate between unaltered and corroded glass surfaces.

(GOMD-SP-P016-2015) Structure of S-rich Binary As-S Spin-Coated Thin Films

J. Cook*[3]; P. Xiong-Skiba[3]; M. Vlcek[1]; H. Jain[2]; A. Kovalskiy[3]; 1. University of Pardubice, Czech Republic; 2. Lehigh University, USA; 3. Austin Peay State University, USA

The structure of binary As-S spin coated thin films is investigated using X-Ray Photoelectron Spectroscopy (XPS) and Raman spectroscopy. The films of $As_{28}S_{72}$ and $As_{33}S_{67}$ were deposited from propylamine based solution. After solution processing, we have found that the As content of spin-coated films is lower relative to the original glass composition. We propose this loss of As is caused by volatilization of As containing units during post-deposition annealing. In addition, XPS results show a complete lack of As-As homopolar bonds in the spin-coated films. We have also found that the structure of various compositions of spin-coated films is not influenced by exposure to bandgap or super-bandgap light. This photostability is preferred for IR optical and photonic applications. To evaluate the structural stability, the thin layers were exposed to bandgap and super-bandgap light. It is confirmed by Raman spectroscopy that the bulk film structure is unchanged after illumination. The XPS analysis shows complete lack of As-As bonds on the film surface explaining the photostability. As known, these bonds are primarily responsible for photoinduced effects in chalcogenide glass layers. This work was supported by NSF Award No 1409160 and the grant CZ.1.07/2.3.00/30.0058 from the Czech Ministry of Education, Youth and Sports.

(GOMD-SP-P017-2015) Evolution of Sodium Borosilicate Glasses in Humid Environments

Y. Gong*[1]; C. Yatongchai[1]; A. W. Wren[1]; C. Durucan[2]; N. P. Mellott[1]; 1. Alfred University, USA; 2. Middle East Technical University, Turkey

Borosilicate glasses are internationally preferred containment for radionuclides under geological depository. Interaction between glass surfaces and water can be a key factor for the lifetime of disposed nuclear wastes. Phase separation is a well observed behavior in borosilicate glasses, and hence the effect of phase separation on glass dissolution is important. In this study, two distinct sodium borosilicate glasses and their phase separated counterparts were reacted in humid environments for various durations of time. Chemical composition, phase identification and morphology were measured by X-ray photoelectron spectroscopy, X-ray diffraction and scanning electron microscopy, respectively. Phase and compositional evolution of these glasses will be discussed as a function of time.

(GOMD-SP-P018-2015) The effect of heat treatment schedule on the composition and microstructure of aluminosilicate crystals in High-Alumina High-Level Nuclear Waste glasses

J. Marcial*[1]; J. S. McCloy[1]; O. K. Neill[1]; 1. Washington State University, USA

The Hanford site in southeastern Washington State serves as the largest United States nuclear waste repository. At this site 177 underground tanks store over 50 million gallons of waste. This waste will be mixed with glass-forming additives and vitrified at the Waste Treatment and Immobilization Plant. A major challenge for nuclear waste vitrification is understanding the crystallization of aluminosilicate phases in nuclear waste glasses. Crystallization has been previously shown to reduce glass durability due to the extraction of durable components from the glass-forming matrix. Robust studies on the compositional dependence of nepheline formation have focused on large compositional spaces with hundreds of glass compositions. However, there are clear benefits to obtaining complete descriptions of the conditions under which crystallization occurs for specific glasses, adding to the understanding of nucleation and growth kinetics and interfacial conditions. This work describes the investigation of the effect of crystallization under isothermal and continuous cooling schedules on the microstructure, crystal fraction, and composition of simulant high-level nuclear waste glass. It was observed that when subjected to low undercooling conditions, nepheline was the most abundant aluminosilicate phase.

(GOMD-SP-P019-2015) Characterization of Na_2S-P_2S_5 glassy electrolyte thin films preparesd by pulsed laser deposition

Y. Ito*[1]; A. Hayashi[1]; M. Tatsumisago[1]; 1. Osaka Prefecture University, Japan

Rechargeable Na^+ ion batteries with abundant sodium sources are more suitable for the wide prevalence than Li^+ ion batteries. In order to realize all-solid-state sodium batteries, the exploration of inorganic solid electrolytes with high Na^+ ion conductivity is indispensable. We have reported the preparation of Na_2S-P_2S_5 glass and glass-ceramic electrolytes by mechanical milling and crystallization processes. The glass-ceramic electrolytes with cubic-Na_3PS_4 showed Na^+ ion conductivity of over 10^{-4} S cm^{-1} at 25 ºC. Solid electrolyte thin films are useful for the formation of favourable electrode-electrolyte interfaces in bulk-type batteries. We have also reported the preparation of amorphous Li_2S-P_2S_5 solid electrolyte thin films for surface-coatings on electrode particles by pulsed laser deposition (PLD). In this study, $75Na_2S25P_2S_5$ (mol%) thin films were prepared using PLD. The film morphology, chemical compositions and ionic conductivities were investigated. Dense amorphous thin films with a smooth surface were obtained. The thin films showed glass transition phenomenon at about 160 ºC, suggesting that the obtained thin film were in a glassy state. In the XRD pattern of thin films with a heat treatment at 270 ºC, the diffraction peaks due to cubic-Na_3PS_4 crystal were observed. The ionic conductivity was increased from 4.4×10^{-6} S cm^{-1} to 3.0×10^{-5} S cm^{-1} after the heat treatment.

(GOMD-SP-P020-2015) Second Harmonic Generation stability in Chalcogenide glasses

A. Lepicard*[2]; V. Rodriguez[1]; K. Richardson[2]; M. Dussauze[1]; 1. University of Bordeaux, France; 2. University of Central Florida, USA

Glass substrates with controlled linear and non-linear optical properties are necessary for micro-photonic applications. Such platforms can be used for the design of novel devices suitable for active optical elements and detectors. Chalcogenide glasses offer a large window of transparency in the infrared region, where most organic compounds have their signatures, making them ideal for spectroscopic applications. They also exhibit a high third order optical susceptibility: $\chi^{(3)}$. Second order optical properties are forbidden in a centrosymmetric medium. Thermal poling can break this centrosymmetry and result in a strong second order optical response. Chalcogenide glasses with their high $\chi^{(3)}$ give potentially the highest second harmonic generation among glasses. However, it has been shown that the second order optical response of poled chalcogenide glasses is not stable in time. To avoid fast relaxation of the process and to enhance longer term stability, the effect of silver injection in sulfide glasses was investigated. Second harmonic generation has been studied as a function of thermal poling parameters such as atmosphere, type of electrodes, applied voltage and temperature. Resulting signals were evaluated for their magnitude and post-poling stability. We show that the origin of the resulting signal is due to several contributions: one from the electric field and another from induced structural rearrangement.

(GOMD-SP-P021-2015) Heterogeneous Nucleation on Palladium doped $Li_2O.2SiO_2$ glass by Differential Thermal Analysis

N. Roth*[1]; K. S. Ranasinghe[1]; 1. Southern Polytechnic State University, USA

The effect of concentration of palladium particles on nucleation was investigated for lithium disilicate glass. The heterogeneous nucleation rate for 440C, 450C, and 460C was calculated for different concentrations of palladium. The DTA method of measuring nucleation and crystallization was used in this calculation. Results shows a considerable increase in the number of nuclei and the nucleation rate and the heterogeneous nucleation is observed.

(GOMD-SP-P022-2015) Growth Mechanism of Amorphous Sb_2Te_3 Thin Films and Nanowires Prepared by Electrochemical Deposition

C. A. Ihalawela*[1]; M. Sundararajan[1]; X. Lin[2]; M. Kordesch[1]; G. Chen[1]; 1. Ohio University, USA; 2. Argonne National Lab, USA

Exhibiting a rapid phase transition triggered by an optical or electric pulse excitation and followed by significant changes in optical and electric properties is a key feature of phase change memory materials (PCMMs) and backbone of the non-volatile PCM devices. One of the challenges is however to downsize the materials to match the shrinking size of the devices. In this study, an electrochemical method has been employed, mainly because of its excellent void -filling capability, for the synthesis of amorphous Sb_2Te_3 PC thin films and nanowires. The contribution of main influential parameters, such as electrolyte depletion, mass transportation, E-field modification, restricted diffusion, and reduction-surface stability to the growth of the amorphous materials has been studied using chronoamperometry curves. Energy dispersive X-ray spectroscopy, X-ray diffraction and electron microscopy have been used to characterize the composition, structure and morphology of the materials. It has been found that the growth mechanism of amorphous nanowires is different from that of thin films and significantly different from that of metallic nanowires. It is hoped that our study will shed light on the growth mechanism of amorphous nanowires prepared by electrodeposition and benefit their device applications.

(GOMD-SP-P023-2015) Simulations of silver-doped germanium-selenide glasses and their response to radiation

K. Prasai*[1]; D. Drabold[1]; 1. Ohio University, USA

Chalcogenide glasses doped with silver have many applications including their use as a novel radiation sensor. We report the first atomistic simulation of radiation damage and healing in silver-doped Germanium-selenide glass. We jointly employ empirical potentials and *ab initio* methods to create and characterize new structural models and to show that they are in accord with many experimental observations. Next, we simulate a thermal spike and track the evolution of the radiation damage and its eventual healing by application of a simulated annealing process. The silver network is strongly affected by the rearrangements and its connectivity (and thus contribution to the electrical conductivity) change rapidly in time. The electronic structure of the material after annealing is essentially identical to that of the initial structure.

(GOMD-SP-P024-2015) Corrosion Study of a Glass Composite Material for Intermediate Level waste Disposal

C. Hutchison*[1]; 1. Imperial College London, United Kingdom

An asbestos based Glass Composite Material (GCM) prepared by plasma vitrification is considered as a candidate to immobilise intermediate level nuclear waste (ILW). The pristine wasteform was first characterised using SEM-EDX and XRD, revealing it to be mainly composed of a glass matrix with uniformly distributed iron-rich diopside crystals (few tens μm) and also of less than 5 vol.% of 5 micron Fe and Cr based metallic phases. Leach testing using MCC-1 and PCT protocols (90ºC deionised water) were performed up to 10 weeks to assess the durability of the wasteform and to observe the course of its corrosion. Inductively coupled plasma optical emission spectroscopy showed a near constant concentration for most elements in solution is quickly obtained. SEM observations on the solid proved this was due to micro-crystalline formation onto the surface. SEM also pointed towards the formation of iron hydroxide into fractures on the surface of the glass. Cross sectional EDX line scans and ToF SIMS also suggested an undesirable mode of corrosion for a wasteform since no protective layer forms leading to linear corrosion kinetics.

(GOMD-SP-P025-2015) Characterization of silicate bioactive glasses with combined polyvalent ions

F. Stölzel[2]; A. Lenhart[2]; R. detsch[1]; A. hoppe[1]; P. Balasubramanian*[1]; A. R. Boccaccini[1]; 1. University of Erlangen-Nuremberg, Germany; 2. Technische Hochschule Nürnberg Georg-Simon Ohm, Germany

Novel melt-derived bioactive silicate glass similar to the composition of 13-93 with Sr and combinations of the polyvalent elements Cu, Ce and Fe by substituting CaO were produced. The new compositions were assessed in terms of their glass-technological properties and cellular response in order to test the influence of the reaction of polyvalent elements and their redox state on the cell response. Differential scanning calorimetry was used to identify the glass transition temperature and crystallization onsets of the different bioactive glasses. Three-dimensional scaffolds were fabricated using the foam replica technique. Sintered pellets were used to evaluate the in vitro biocompatibility. For this study, human osteoblast-like cells (MG-63) were seeded on top of the sample surfaces for 48 hours. The analysis of cell viability and cell morphology showed in all cases that the glasses support cell attachment and cell growth. Thus, the quantitative effect of incorporation of Cu, Ce, and Fe and their combinations on MG63 cell activity was assessed.

Poster Session

Room: Symphony Ballroom I

(GOMD-S1-P001-2015) Preparation of Composite Positive Electrodes with Li_3PS_4 Glass as Active Material for All-Solid-State Lithium Secondary Batteries

T. Hakari*[1]; M. Nagao[1]; A. Hayashi[1]; M. Tatsumisago[1]; 1. Osaka Prefecture University, Japan

All-solid-state lithium secondary batteries with inorganic solid electrolytes (SE) have attracted much interest because of their safety. However, total energy densities per gram of positive electrodes for all-solid-state batteries are significantly small because contents of active materials in the electrodes are still small. It is difficult to retain high utilization of the active materials with an increase in the active material contents in the electrodes. The Li_3PS_4 glass is often used as SE for all-solid-state cells and the glass is electrochemically inactive. However, the glass has Li^+ ions and thus the glass itself has a potential utilization as an active material by adding carbon as conducting additives. The glass would show bifunctional properties as not only solid electrolyte (Li^+ ion conduction paths) but also active material, and total energy densities per gram of positive electrodes will thus increase by use of the glass in the electrode. In this study, the Li_3PS_4 glass was evaluated as an active material in all-solid-state lithium cells. Favorable electron conducting paths to the glass were formed by mechanical milling with acetylene black (AB) as the conductive additives. The prepared Li_3PS_4-AB composite electrodes were applied to all-solid-state cells and their electrochemical performance was investigated.

(GOMD-S1-P002-2015) Comparison of electrochemical performance between amorphous and crystalline TiS_3 positive electrodes in all-solid-state lithium batteries with sulfide solid electrolytes

T. Matsuyama*[1]; M. Deguchi[1]; A. Hayashi[1]; M. Tatsumisago[1]; T. Ozaki[2]; Y. Ishii[1]; Y. Togawa[1]; S. Mori[1]; 1. Osaka Prefecture University, Japan; 2. Technology Research Institute of Osaka Prefecture, Japan

All-solid-state lithium batteries using inorganic solid electrolytes are expected to be highly safe because of elimination of flammable components such as organic liquid electrolytes. We have found amorphous TiS_3 electrodes prepared by mechanical milling showed high capacity and good cyclability in all-solid-state batteries with Li_2S-P_2S_5 solid electrolytes. Amorphization of active materials is potentially capable of achieving higher capacity and cyclability because of open and random structure in amorphous materials. However, comparison of electrochemical performance between amorphous and crystalline electrodes in all-solid-state batteries has not been examined. In this study, amorphous and crystalline TiS_3 particles were applied as a positive electrode to all-solid-state lithium cells with Li_2S-P_2S_5 electrolytes. Electrochemical properties of amorphous TiS_3 were compared with those of crystalline TiS_3. The all-solid-state cell with the amorphous TiS_3 showed better cyclability than the cell with the crystalline TiS_3. Microstructures and morphologies of amorphous and crystalline TiS_3 electrodes before and after charge-discharge tests were analyzed by XRD, XPS and high-resolution transmission electron microscopy (HR-TEM). The cell performance will be discussed from the viewpoint of structure of TiS_3.

(GOMD-S1-P003-2015) Ion transport and atomic structure of rubidium chloride doped sulphide glasses

M. Bokova[1]; F. Hindle[1]; A. Cuisset[1]; E. Bychkov*[1]; I. Alekseeev[2]; A. M. Whale[3]; S. W. Martin[3]; 1. University of Littoral, France; 2. St Petersburg University, Russian Federation; 3. Iowa State University, USA

Caesium or rubidium halide doped sulphide and selenide glasses are promising functional materials for optical applications. Nevertheless, their ionic and electronic transport properties are hardly known in contrast to numerous studies of lithium and sodium chalcogenide glassy systems. We report here the conductivity and ^{86}Rb tracer diffusion measurements for the two sulphide glass families, RbCl-Ga_2S_3-GeS_2 and RbCl-Ga_2S_3, over a wide composition range changing between 0.01 and 70 mol.% RbCl. Different transport regimes have been observed in these glasses and will be discussed in comparison with their atomic structure studied using pulsed neutrons, hard x-rays and Raman spectroscopy. Additional structural information will also be obtained by DFT modelling of the Raman spectra and RMC/EPSR modelling of the diffraction data.

(GOMD-S2-P004-2015) Sol-gel preparation of calcium sulphate/bioglass composite and its in vitro evaluation

K. Cheng*[1]; Q. Lv[1]; X. He[1]; W. Weng[1]; 1. Zhejiang University, China

Bioglass has been regarded as one of the best candidate to bone regenerative biomaterials. It is reported that the release of Si ions from the bioglass could significantly improved the responses of osteoblastic cells. It is reported that the dissolution products are able to promote the formation of extracellular matrix, and up-regulated cell-cell and cell-matrix adhesion. On the other hand, calcium sulphate (CS) has been widely used as bone repairing materials. The main advantages of CS lie on its fast biodegradation rate and release of calcium ions, which may be very useful for fast bone regeneration. Therefore, if a composite between CS and bioglass could be used, both the stimulation of bioglass dissolution and fast biodegradation of CS could be utilized to generate synergetic effects to promote new bone formation. In this work, a sol-gel method was used to synthesize bioglass and calcium sulphate dihydrate was incorporated to form a composite. The phase composition of composite was characterized with X-ray diffractometer. The chemical groups were identified with Raman and FTIR. The microstructure was observed with scanning electron microscopy. Finally, the cellular responses of osteoblastic cells and protein adsorption behaviors were characterized.

(GOMD-S2-P005-2015) Bioactivity of $2Na_2O.1CaO.3SiO_2$-P_2O_5 glasses

I. C. Dechandt*[1]; G. D. Dogado[1]; F. C. Serbena[1]; 1. State University of Ponta Grossa, Brazil

This study investigates the bioactivity of the glass system 2Na2O.1CaO.3SiO2. This is one of the few glasses that crystallizes in the volume and its properties are not well established. Its composition is close to one of the most bioactive materials, the 45S5 glass. The volume crystallization allows the possibility of improving its mechanical properties such as hardness, elastic modulus, bending strength and fracture toughness by controlled crystallization. Glass samples in the $2Na_2O.1CaO.3SiO_2$-P_2O_5 system were prepared with different P_2O_5 concentrations (0%, 3% and 6% in weight) and soaked in SBF solution for different time intervals up to 4 weeks. Hydroxyapatite growth is observed after 3 weeks in all samples. This result reveals that this glass system is bioactive. The effect of crystallization on the bioactivity of this glass-ceramic is currently being investigated.

(GOMD-S3-P006-2015) Role of glass homogeneity in Ge-As-Se system

R. Wang*[1]; Z. Yang[1]; B. Luther-Davies[1]; 1. Australian National University, Australia

Homogeneity in glasses is important especially in chalcogenides since the properties of the chalcogenides can be easily tuned in a widely compositional range. Consequently, this leads to a difficulty in determining the exact values of some physical parameters of the glasses if they are inhomogeneous in terms of chemical compositions.We therefore prepared three groups of Ge-As-Se glasses with different rocking time to explore the effects of glass homogeneity on the structure and physical properties. It was found that, although well-defined glass network structure can be formed in the samples with short rocking time of 10 hours, physical properties do exhibit the difference with different rocking time. Examination of the homogeneity in the different spatial scale down to 1μm indicates that homogeneous glasses can be achieved with prolonged rocking time typically about 20-30 hours depending on the chemical compositions, and this time is longer for strong glass former. The present results verified that the reliable measurements of the physical parameters should be performed on the glasses with prolonged rocking time

(GOMD-S3-P007-2015) Exploring relaxation and the glass transition with sugar glasses and home-built apparatus

W. R. Heffner*[1]; K. E. Calay[1]; 1. Lehigh University, USA

We present a collection of experiments to measure the glass transition, relaxation and aging phenomena in simple, easy to prepare glasses made from sugars (hard candy) and other low T_g materials. These experiments complement a larger collection of low-cost experiments for exploring the science of glassy materials through hands-on activities presented earlier. Sugar based glasses, as well as the artificial sweetener isomalt (a sugar based alcohol) can be prepared in the kitchen or home laboratory at moderate temperatures and have glass transitions slightly above room temperature, around 40 C. These lower temperature glasses are convenient to prepare and show significant rheological effects such as aging even at room temperature. We include demonstrative experiments to examine the cracking of these glasses after cooling and the mitigating influence of annealing. The effect of aging on the glass transition and development of the post T_g endothermic peak are quantified using a commercial DSC as well as our home-built DTA. A simple spreadsheet model mimics the effect of cooling rate and subsequent annealing on the Tg and it's endotherm. Taken in part or as a collection these experiments can provide an interesting and intuitive path to the student's understanding of the relaxation phenomena in glasses.

(GOMD-S4-P008-2015) Teaching Nano-particle Fluorescence in Glass with Candy

W. R. Heffner*[1]; D. Wright III[2]; 1. Lehigh University, USA; 2. Oakwood University, USA

The brilliant colors of nano-metallic glasses are well known and provide a common "hook" for introducing students to the interesting field of nano-optics in glass. However, making such glasses requires both high temperature furnaces and skill in processing. We present an alternate example of nano-particle optics in glass, that of the fluorescence we observe in some sugar glasses (hard candy) with stove temperature processing. We characterized the emission using a homebuilt system consisting of high intensity LEDs for the excitation and the student grade Ocean Optics Red Tide Spectrometer to resolve the emission. The fluorescence was found to span between about 470 nm and 650 nm and the emission demonstrated a marked drop in intensity for LED excitation below green. The fluorescence also increased as the glass caramelized (browned) with further heat treatment (cooking). Recent literature has shown similar fluorescence in caramelized sugars to be due to the production of carbon nanoparticles and we propose the experiment as a cross-disciplinary and open-ended one for an undergraduate lab in physics, chemistry or material science.

(GOMD-S3-P009-2015) Crystallization versus temperature in an iron-rich lead aluminosilicate composition: a contribution to the understanding of French Renaissance glazes preparation

N. Capobianco[1]; G. Wallez[1]; A. Bouquillon[2]; D. Caurant*[1]; C. Doublet[2]; P. Lehuédé[2]; 1. CNRS, France; 2. C2RMF, France

During the Renaissance period in France, a well-known ceramist, Bernard Palissy, succeeded to create amazing lead glazed ceramics, but the raw materials, preparation and firing processes he used remained unknown. This study is a first step to try to understand how Palissy's glazes were fired by reconstructing them from a mixture of chemical reagents. For this, using the analyzed composition of a glaze fragment of an attested Palissy's production (24.3 SiO_2-63.7 PbO-4.3 Al_2O_3-5.4 Fe_2O_3-1.1 CaO-0.3 K_2O wt%), a mixture of SiO_2, $PbCO_3$, $Al(NO_3)_3$, Fe_2O_3, KCH_3CO_2, $CaCO_3$ was treated in three phases: 1) calcination at 350-500°C 2) heating under air 1 or 10h between 750-1170°C 3) rapid (5h) or slow (5°C/h) cooling. The obtained samples were characterized by XRD, SEM, EDX and Raman spectroscopy. Whereas the cooling rate has not important effect on the nature of the crystalline phases, it appears that their nature (quartz, hematite, (K,Pb)-rich feldspar, melanotekite ($Pb_2Fe_2Si_2O_9$), magnetoplumbite ($PbFe_{12}O_{19}$)), their abundance and microstructure strongly depend on heating temperature. Glazing tests on a kaolinitic clay body was also performed and characterized. Comparison of the results obtained for experimental glazes with authentic Palissy's glazes is still in progress and will help to better understand the artist technique.

(GOMD-S3-P010-2015) Evaluation of critical cooling rate of silicate melts by the guided random parameterization method

E. B. Ferreira*[1]; E. D. Zanotto[2]; 1. Engineering School of São Carlos/USP, Brazil; 2. UFSCar, Brazil

The critical cooling rate necessary to vitrify any liquid on cooling has been related to the glass-forming ability, which is a major issue for the glass industry and for the development new glasses. However, the critical cooling rate (CCR) is a complex function of several parameters, some of which very difficult to obtain. Alternatively, drawing random values for the key parameters and using the theory to examine probabilistic distributions of the critical cooling rates has been proposed and tested for metallic glasses. In this method (denominated Guided Random Parameterization – GRP) the resulting broad distributions of CCR are sharpened by guiding the random parameterization by calorimetric data. The results suggested the possibility of determination of critical cooling rates in absence of data for some parameters. However, the application of this method to silicate glasses has been criticized. Here we evaluate the critical cooling rates of two glass forming silicate melts using the Guided Random Parameterization method and Differential Scanning Calorimetry. The applicability of the GRP method is tested for a lithium disilicate glass (which has moderate internal nucleation rates) and a dibarium titanium silicate glass (which has very high internal nucleation rates, similar to metallic glasses). The results will be fully discussed.

(GOMD-S3-P011-2015) Thermooptical devices for the investigation of the properties of glass at high temperatures

M. Kilo[1]; A. Diegeler*[1]; F. Raether[2]; B. Durschang[1]; M. Krauss[1]; 1. Fraunhofer ISC, Germany; 2. Fraunhofer HTL, Germany

Using a specially developed thermo-optical measurement system (glass-TOM) thermal properties of glass and glass mixtures are investigated in situ. With thermo-optical measurements, glass batch melting can be monitored during the melting process and the behaviour can be described using sintering models. The thermal characteristics can be descibed in a wide temperature range, even in the only poorly accessible transformation zone. Among the detectable properties are thermal expansion and wetting, adhesion, gluing properties and contact angle of glass with different materials can be measured. Viscosity fixed points, such as Littleton temperature, softening point and Tg of glasses are also determined. These values are compared with results from conventional measuring devices. Futhermore, viscosity can be measured in-situ using the worldwide unique High-Throughput Screening System for the automated production of a large number of different glass types.

(GOMD-S3-P012-2015) Thermal analysis of novel multifunctional glasses and glass-ceramics for IR photonics

L. Saturday*[1]; C. Johnson[1]; Y. Shpotyuk[2]; R. Golovchak[1]; 1. Austin Peay State University, USA; 2. University of Rennes, France

Chalcogenide glasses (ChG) are considered as the most viable media for applications in modern photonics, combining high IR transparency, excellent fiber drawing capability, and the largest optical nonlinearities reported to date. Many tellurium- and selenium-based compositions are being studied to improve and optimize their performance. The nanoscale modification of ChG is intriguing, since nano-engineering opens the possibility to design hybrid materials combining multiple useful properties (mechanical, electronic, optical, magnetic) in a functional medium. In this regard, several chemical elements (Bi, rare earth, Ga) are found to modify ChG at the nanoscale. In this work we report thermal stability and crystallization kinetics studies for the complex glasses of Bi-Ga-($GeSe_4$)-($GeTe_4$) family, which are anticipated to be used as a host matrix having potential to combine the thermo-electric effect, rare earth solubility, different types of conductivity, and topological insulating behavior in one medium. Crystallization of five different phases is identified with differential scanning calorimetry (DSC) technique. The Dietzel criterion of glass stability is determined and the activation energies for each crystallization process are calculated. The applicability of Johnson-Mehl-Avrami (JMA) relation to describe the crystallization kinetics is verified in these glasses using J. Malek's approach.

(GOMD-S3-P013-2015) The effect of Li2O, Na2O, and ZnO on phase separation of TeO2 glass towards porous tellurite microsphere in vapor adsorption application

J. wang*[1]; 1. NSYSU University, Taiwan

The applications of porous glass microsphere have been known for years in various areas. It is also quite clear that the majority of the study is on silica-based glass microsphere, mostly because of its superiority of property in practical usage. However, other glass systems are not so much well studied, i.e. tellurite glass. Tellurite glass has few unique properties in comparison to silica-based glass, such as wider IR transmission window, lower processing temperature, and higher refractive index and dispersion, etc. In this study, I would like to study the processing of porous microsphere of tellurite through chemical etching technique of the phase-separated glass. Phase separation in tellurite glasses are made by varying the amount of Li2O, Na2O and ZnO constituents and the heat treatment temperatures and durations. A possible rationale of phase separation behavior between silica and tellurite glasses is discussed with respect to the constituent, the extent of composition and heat treatment temperature. The effect of etchant on the phase separated glasses is also studied in order to obtain various porous sizes and shapes of microsphere. Furthermore, the porous tellurite microsphere is used for vapor adsorption/absorption study for potential storage and catalytic applications.

(GOMD-S3-P015-2015) NMR Structural Investigation of Zinc Borophosphate Glasses

C. Bischoff*[1]; P. T. Freudenberger[1]; R. Brow[1]; 1. Missouri University of Science and Technology, USA

Glasses in the ZnO + B_2O_3 + P_2O_5 glass system are being developed to serve as substrates for waveguides created by femtosecond lasers. To this end, glasses have been synthesized to determine the composition dependence of glass structure at a given O/P ratio. Further, the glass forming region in this system was expanded from what has previously been reported by investigating compositions with a constant O/P ratio. O/P ratios investigated are 3, 3.25, and 3.5, which represent metaphosphate, polyphosphate, and pyrophosphate glasses, respectively. Local glass structures have been probed with ^{31}P and ^{11}B nuclear magnetic resonance (NMR) techniques and the results are compared with findings from vibrational spectra (Infrared and Raman) and high pressure liquid chromatography (HPLC) to identify the types, concentrations, and connectivity of phosphate and borate anionic species.

(GOMD-S3-P016-2015) Relaxation processes of densified silica glass: structural approach

A. Cornet[1]; C. Martinet[1]; B. Champagnon[1]; V. Martinez[1]; D. de Ligny*[2]; 1. Institut Lumière Matière, France; 2. Universität Erlangen-Nuremberg, Germany

Above the elastic deformation limit, SiO_2 glass samples recovered from high pressure are permanently densified. This densified state of silica glass evolves depending on the pressure and temperature conditions. Many experimental and theoretical studies have been already realized to describe densified silica glasses. Their structure were analyzed, in particular in terms of inter-tetrahedral angles and rings distribution evolutions under in-situ or ex-situ conditions. Nevertheless, to our knowledge, the relaxation process from densified silica glasses toward undensified samples were not already studied. Then, the aim of this study is to observe the structure evolution during relaxation following different isotherms. Samples permanently densified at different temperatures and pressures were studied. For that, in-situ Raman temperature relaxation experiments have been performed. Isothermal treatments allowed deducing the activation energy of this relaxation process. Depending on the macroscopic density and structure of silica glasses, the relaxation processes will be discussed in terms of small rings distribution evolution, nano-heterogeneities, stresses in glasses and polyamorphism.

(GOMD-S3-P017-2015) Study of Bi and Ga incorporation in glassy selenides and tellurides

A. Thai*[1]; R. Golovchak[1]; Y. Shpotyuk[2]; W. R. Heffner[3]; H. Jain[3]; 1. Austin Peay State University, USA; 2. Université de Rennes 1, France; 3. Lehigh University, USA

Bismuth is shown to be a unique dopant in chalcogenide glasses (ChG), leading to a number of interesting phenomena: conduction type reversal from *p*- to *n*-type, strong thermoelectric effect, topological insulating behaviour, etc. Gallium is usually added to ChG matrix in order to increase the solubility of rare-earth elements, which can significantly enhance their optical properties. So, understanding the impact of Bi and Ga on the electronic and atomic structure of ChG is a key to successful engineering of complex glassy materials, combining several useful properties in one functional medium. In this work, we have investigated structural features of As(Ge)-based selenides and tellurides with additions of Ga and Bi (including mixed Bi-Ga-Ge-Se-Te system), using X-ray photoelectron spectroscopy (XPS), Raman scattering and extended X-ray absorption fine structure (EXAFS) spectroscopy. The results show that Bi enters a glass network in the form of pyramidal units, most probably forming dispersed partially ordered nanophases. These nanodomains of trivalent Bi (III) may be a reason for the conductivity percolation and type reversal in these glasses as well as their thermoelectric behavior. The number of nearest neighbors for Ga atoms is determined to be four regardless of the chalcogen element. At higher concentrations, both Bi and Ga additions trigger crystallization of Se/Te-based ChG during quenching.

(GOMD-S3-P018-2015) Structure-Property Relationships in Chalcogenide Glasses: Novel Insights from 2D High-Resolution ^{77}Se NMR Spectroscopy

D. C. Kaseman*[1]; I. Hung[2]; Z. Gan[2]; B. Aitken[3]; S. Sen[1]; 1. University of California Davis, USA; 2. National High Magnetic Field Laboratory, USA; 3. Corning Inc, USA

The identification and quantitation of the Se-centered structural units and their connectivities in binary Ge_xSe_{100-x} and As_xSe_{100-x} glass systems was studied using a new ^{77}Se nuclear magnetic resonance (NMR) technique, known as two-dimensional (2D) Magic Angle Turning Phase Adjusted Spinning Sidebands (MATPASS) spectroscopy. This technique separates the chemical shift anisotropy (CSA) and isotropic chemical shift into correlated dimensions to yield high-resolution ^{77}Se NMR spectra free of CSA-related broadening. The compositional evolution of the Se sites is quantified in the isotropic dimension while simulation of the CSA dimension provides CSA tensor information to distinguish between Se sites with similar isotropic chemical shifts. The subsequent development of structural models of these systems were fully consistent with the compositional variation of a wide range of physical properties including T_g, elastic moduli, refractive index, density and optical band gap.

(GOMD-S3-P019-2015) Glass Transition and Reversibility in Silicate Glasses

Y. Yu*[1]; B. Wang[1]; Y. Lee[1]; M. Micoulaut[2]; M. Bauchy[1]; 1. UCLA, USA; 2. Université Pierre et Marie Curie, France

The knowledge of the glass transition temperature, in particular the relationship with the composition, is a critical issue in glass industry. It is directly correlated to the energy needed to produce glasses. In addition, it was recently reported that some glasses characterized by a reversible glass transition, show an optimal glass forming ability. This problem is investigated through molecular dynamics simulations of sodium silicate glasses, a base model for depolymerized silicate glasses used for ion-exchanging. Compositions with 0%-30%

soda are simulated with different cooling rates. The compositional trends of the glass transition temperature and the degree of reversibility are shown to be linked to the rigidity of the glasses and liquids networks. This study provides fundamental insights into the glass transition and how it is linked to the composition of the glass.

(GOMD-S3-P020-2015) Rigidity Theory Applied to Amorphization of Nano-Materials

B. Wang*[1]; Y. Yu[1]; M. Bauchy[1]; 1. University of California, Los Angeles, USA

Rapid advances in surface and nano-scale engineering during the past decade request in-depth understandings of the structural behavior of materials in these fine structures. Amorphization of crystalline materials that are beyond the traditional scope of glass-forming materials has become an important issue for many novel applications such as nanostructured battery cathode and catalysts. Based on recent understandings coming from irradiated silica samples, the amorphization in titanium dioxide induced by reduction and alkaline ion intercalations was studied with atomistic simulations. Rigidity theory, which was successfully used to understand the structural changes found in irradiated silica, was applied to establish the relationship between amorphization and structure modifications, such as defect and surface creation. The results showcase that the knowledge accumulated from decades of glass research has the potential to significantly advance the broader field of advanced material science and engineering.

(GOMD-S3-P021-2015) Structural Rigidity During Radiation-Induced Amorphization

B. Wang*[1]; Y. Yu[1]; M. Bauchy[1]; 1. University of California, Los Angeles, USA

Radiation damages in quartz and amorphous silica were studied with molecular dynamics simulations of high-energy ballistic events. Simulations showed that, as the structural damage accumulated, both materials converged to a similar structure that was substantially different from amorphous silica. More interestingly, anomalous behaviors were observed in quartz during the initial stage of damage. As the configurational energy continued to increase before eventually reaching a plateau, several important structurally related properties, such as the Si-O-Si bond angle and swelling, did not follow the same monotonic behavior. Structural analyses revealed that such behaviors were the result of an underlying rigidity transition induced by high concentrations of defects. The results presented would facilitate the design of materials resistant to the radiation damage, and provide insights into defect-induced amorphizations in other materials.

(GOMD-S3-P022-2015) Combining Ab-Initio GIPAW Calculations and Experimental ^{29}Si NMR Spectra to Analyze the Structure of Amorphous Silicon Oxycarbides

J. P. Nimmo[1]; P. Kroll*[1]; 1. UT Arlington, USA

Experimental data of ^{29}Si NMR chemical shifts of silicon oxycarbide (SiCO) ceramics show broad peaks for so-called mixed $\{Si\}C_nO_{(4-n)}$ (n=0-4) tetrahedra. To extend the analytical capabilities of NMR investigations, we provided extensive modeling and GIPAW calculations and derived relations between Si-O-Si angles and various bonding environments of C surrounding $\{Si\}C_xO_{(4-x)}$ tetrahedra on one side, and ^{29}Si NMR chemical shifts found at this center on the other side. These relations are now used to analyze in more detail several experimental ^{29}Si NMR spectra, from which we obtain additional structure information. Si-O-Si bond angle distributions of SiO2 nano-domains in SiCO indicate more local strain in the amorphous ceramics in comparison to silica glass. Furthermore, the average Si-O-Si angle in a ring of the SiCO network is smaller the more C atoms the ring contains. Common to SiCO materials with high content of “free” carbon is a pronounced signature 10-15 ppm lower than the typical chemical shift of $\{Si\}O_4$ units in silica. This is related to Si-O-Si bonds at internal SiO_2 surfaces or in large cages. Analyzing $\{Si\}CO_3$-peaks we find no evidence for bonding between Si of the glass matrix and embedded C of the “free” carbon phase. Thus, in SiCO ceramics “free” carbon units are incorporated into voids and cages surrounded by a glassy SiCO matrix.

(GOMD-S3-P023-2015) Mechanical properties and thermal history dependence of melt quenched glass in comparison to amorphized zeolite material

T. Palenta[1]; S. Fuhrmann*[1]; M. Mackovic[2]; E. Spiecker[2]; L. Wondraczek[1];
1. University Jena Otto-Schott Institute for Materials Research, Germany;
2. Friedrich-Alexander University Erlangen; Center for Nanoanalysis and Electron Microscopy, Germany

Crystalline zeolites are microporous aluminosilicates with large cages, where cations and molecules can be caught. By thermal, pressure or particle irradiation such zeolites can be collapsed to an x-ray amorphous phase. This phase is expected to be more ordered than normal melt-quenched glass of the same composition. This poster presents the comparison of mechanical properties of amorphized (Na,K)-LSX zeolite and a melt-quenched glass of the same chemical composition, as well as the structural evolution of the amorphous with varied thermal history.

(GOMD-S3-P024-2015) Strength of SiO_2-$A1_2O_3$-MgO glass fibers at high temperature

Q. Zu*[1]; Y. Zhang[1]; S. Huang[1]; W. Song[1]; 1. Sinoma Science & Technology Co.,Ltd., China

HS^{TM} high strength glass fiber bundles (without sizing) were heated from room temperature to 750, and then cooled to room temperature. The tensile strength and density of HS glass fibers were investigated before and after heat treatment with the difference of temperature, heating time and B_2O_3 content in glass composition. HS glass structure was analyzed by IR, XRD, and SEM was used to reveal the surface and fracture morphology of HS glass fiber before and after heating. Results indicated that the structure of HS high strength glass is mainly composed of tetrahedron [SiO4], tetrahedron [AlO4], octahedrons [AlO6], etc. The structure contained tetrahedron [BO4] and triangle [BO3] if the glass component contains B_2O_3. Fe^{3+}, Mg^{2+} and Li^+ being as modifiers filled in the space of glass network by the combination of silica, alumina and boron oxygen networks. The structure HS glass did not change much while the fiber density increased at high temperature. When the content of the glass network forming oxides was at the same value, tensile strength of glass fiber could be improved by reducing the amount of B_2O_3 at room and high temperature. The strength degradation after heat treatment was caused by larger micro cracks and devitrification phases on the glass fiber surface.

(GOMD-S4-P027-2015) Electrical Activity of Boron and Phosphorous in Hydrogenated Amorphous Silicon

A. Pandey*[1]; B. Cai[2]; D. Drabold[1]; 1. Ohio Univeristy, USA; 2. Washington University School of Medicine, USA

Using realistic models of hydrogenated amorphous silicon and density functional methods, we explore doping and transport with the most popular impurities: boron and phosphorous. We discuss conventional analogies of doping based upon shallow acceptors and donors in a crystalline matrix and highlight the limitations of such an approach. We show that B enters the network always with considerable strain, whereas P is much more “substitutional” in a tetrahedral site. We show that H is attracted to strained centers, especially for B, which increases the likelihood of H passivation effects on B impurities. We elucidate doping and nondoping static configurations in doped a-SiH, and the role of H passivation as a partial explanation for the well-known low doping efficiency the material exhibits. We show that thermal fluctuations (that induce both network motion and H hopping) can also significantly impact conduction. We draw comparisons to experimental work.

(GOMD-S4-P028-2015) Optical thermometry based on visible upconversion luminescence of Er^{3+} and Er^{3+}/Yb^{3+} co-doped tellurite glasses and optical fibers

D. Manzani*[1]; K. Nigoghossian[1]; V. A. Rivera[2]; S. J. Ribeiro[1]; 1. Institute of Chemistry, Brazil; 2. Instituto de Física de São Carlos, Brazil

Recent advances on glass chemistry have led to new multifunctional optical glasses with technological importance. Tellurite based glasses have been studied for potential applications in nonlinear optics, infrared amplifiers for telecommunication and visible emitters' devices. This work provides an optical thermometry study based on upconversion luminescent emission of Er^{3+} and Er^{3+}/Yb^{3+} co-doped tellurite glasses and optical fibers for application as optical temperature sensing platform. Infrared and red-green upconversion emissions were observed for glasses and both effects are enhanced for co-doped samples. The infrared emission was also explored, showing high quantum efficiency and large full width half maximum wavelength. The upconversion emissions are governed by two photons and described by excited state absorption, energy transfer and cross-relaxation processes. Er^{3+} concentration effect over the temperature dependence on luminescence was explored for a temperature range from room temperature up to 570K and the intensity ratio of green emissions assigned to the two transitions from the thermal coupled $^2H_{11/2}$ and $^4S_{3/2}$ levels to the fundamental level of Er^{3+} ions has been studied as function of temperature in bulk glasses samples and optical fibers.

(GOMD-S4-P029-2015) Ultraviolet transmission spectrum of synthetic fused silica containing molecular oxygen

M. Stamminger*[1]; 1. Heraeus, Germany

The ultraviolet transmission spectrum of synthetic fused silica containing dissolved oxygen was studied. Type III fused silica doped with oxygen at 600 bar partial pressure showed a large shift of the ultraviolet transmission edge of about 20 nm for a sample thickness of 1 mm. Ultraviolet irradiation of this oxygen-doped silica glass with a deuterium lamp led to a broad absorption band centered around 255 nm, assumed to be caused by ozone. When synthetic type IV fused silica containing molecularly-dissolved oxygen was irradiated with a 193 nm excimer laser, a similar absorption band centered around 255 nm appeared in the spectrum. Heat treatment of the type III fused silica sample at 300°C eliminated the ultraviolet absorption band at 255 nm. Presumably, the dissolved ozone dissociated during the thermal treatment of the glass.

(GOMD-S4-P030-2015) Precipitation of divalent Pd and metallic Pd nanostructures in glass for UV plasmonics

D. Bust[1]; S. Fuhrmann[1]; K. Wondraczek[4]; D. Möncke[1]; H. Ebendorff-Heidepriem[3]; E. Spiecker[2]; L. Wondraczek*[1]; 1. University of Jena, Germany; 2. University of Erlangen-Nuremberg, Germany; 3. University of Adelaide, Australia; 4. Leibniz Institute of Photonic Technologies, Germany

The plasmonic resonance of metallic nanostructures can be used to tailor light-matter interaction within a given range of wavelengths. For the ultraviolet spectral range, this means the use of metals with UV resonance, such as Pd. However, the optical properties which Pd ions and metallic Pd nanostructures exhibit within an inorganic glass matrix remain largely unknown. Here, we present a quantitative multi-method evaluation of the ligand-dependent optical extinction of divalent Pd, and of the plasmon resonance of metallic Pd particles with a size of up to 50 nm in UV-transparent glass matrices.

(GOMD-S4-P031-2015) Effect of oxide buffer layer and microstructure on the optical properties of VO$_2$ film deposited on soda lime silicate window glass

J. Cho*[1]; H. Koo[1]; C. Park[1]; 1. Seoul National University, Republic of Korea

Vanadium dioxide (VO$_2$) shows abrupt change in electrical and optical properties through reversible metal-to-insulator transition(MIT) near room temp. The attractive transition characteristics can make VO$_2$ to be used in fabricating thermochromic(TC) smart window For VO$_2$ to be used to fabricate TC window, it has to be deposited on soda lime glass(SLG). It, however, is difficult to deposit highly crystallized VO$_2$ film directly on SLG due to the diffusion of alkali ions during deposition. Moreover, TC properties, such as amplitude of transition or hysteresis width, of VO$_2$ films should be improved for practical use. In order to improve TC properties of VO$_2$ films deposited on SLG, buffer layers were introduced between SLG and film and the microstructure of VO$_2$ film was controlled. First, SiN$_x$ buffer layer was applied to prevent alkali ion diffusion from SLG. Secondly, various oxide buffer layers such as ZnO, TiO$_2$, SnO$_2$ and CeO$_2$ were used to investigate the effect of crystal structure and crystallinity of buffer layers on the properties of VO$_2$ film. The changes of microstructure were induced by controlling the film deposition parameters. Electrical/optical properties were measured, and microstructures were observed. The relation between alkali ion diffusion, buffer layer material, sputtering power and TC properties of VO$_2$ film will be discussed.

(GOMD-S4-P032-2015) Relaxation phenomena in fs-laser modified glass studied by μ-Raman-spectroscopy

T. Seuthe*[1]; A. Mermillod-Blondin[2]; M. Grehn[3]; J. Bonse[4]; M. Eberstein[1]; 1. Fraunhofer IKTS, Germany; 2. Max-Born-Institute for Nonlinear Optics and Short Pulse Spectroscopy, Germany; 3. Technische Universität Berlin, Germany; 4. BAM - Federal Institute for Materials Research and Testing, Germany

Structural relaxation processes after the permanent modification of the surface and the volume of a model-glass (consisting of Li$_2$O and SiO$_2$) and a glass with multicomponent composition (consisting of Li$_2$O, Na$_2$O, MgO and SiO$_2$) by single Femtosecond(fs)-laser pulses were investigated. The initial and modified glass structures were characterized using μRaman-spectroscopy. Refractive index changes in the glass bulk were measured quantitatively using a spatial light interference microscopy setup. Afterwards, the modified glasses were annealed at various temperatures below and above the glass transition temperature and Raman-spectra were taken after 10, 30, 60, 120 and 240 minutes. Below the glass transition temperature, only structural changes of the glasses' Q^n-structure are receding to their initial state before fslaser modification while changes of the silicate network require temperatures above the glass transition temperature to relax to their initial state. Therefore, it was possible to separate α- and βRelaxation behavior. Furthermore, it can be shown that the permanent positive refractive index change of a volume modification also vanishes after a temperature treatment below the glass transition temperature and can therefore be directly correlated to the structural changes of the glasses' Q^n-structure.

(GOMD-S4-P033-2015) Compressive Stress Profiles of Chemically Strengthened Glass After Exposure to High Voltage Electric Fields

L. Thirion*[1]; E. Streltsova[1]; M. He[1]; J. Mauro[1]; 1. Corning Incorporated, USA

Recent work has shown that chemically strengthened glass can be used as an effective substrate material for organic thin film transistors (TFTs), since the temperatures involved with organic TFT deposition are low enough to avoid any compromise in the compressive stress profile. This opens the possibility of fabricating high strength organic TFT displays. However, the question remains as to whether the exposure of the glass to an electric field may lead to diffusion of the alkali ions and a corresponding alteration of the stress profile, which could compromise the strength of the organic TFT device. In this poster, we demonstrate that there is no change in the stress profile of Corning® Gorilla® Glass 3 after subjecting the glass to much higher voltage dc fields compared to the maximum field that would be exhibited in an organic TFT device. The stress profile is modified only after treating the glass at sufficiently high temperature, where alkali migration becomes thermally activated.

(GOMD-S4-P034-2015) Impurity absorption of *d*-elements in tellurite-molybdate glasses

O. Zamyatin*[1]; A. Sibirkin[1]; M. Churbanov[1]; E. Torokhova[1]; 1. Lobachevsky State University of Nizhni Novgorod, Russian Federation

At present tellurite glasses are considered to be a promising material for optical applications. But their use is restricted by high optical losses due to transition element impurities. The purpose of this study was to ascertain the effect of Ni, Co, Cu, Cr and Fe atoms in TeO_2-MoO_3 glass on the optical transmission in the visible and near infrared spectral ranges. Melting of the batch with the specified impurity atom content was carried out at 800°C. The transmission spectra of glass were registered with Perkin Elmer Lambda 900 spectrophotometer. All impurity atoms involved have absorption bands in the visible and near infrared spectral ranges. Nickel impurity possesses two absorption bands with maxima at 810 and 1320 nm. Cobalt ions provide a single broad band with a maximum at 1380 nm. Chromium contaminants lead to a rather narrow band at 660 nm. Copper traces caused to a band at 830 nm. Iron dopants give two bands with maxima at 600 and 860 nm. The spectral dependences of the specific absorption coefficient of the impurity atoms listed are found. The regularities of *d*-element ion impurity absorption in the visible and near infrared spectral ranges are revealed. The specific requirements to the purity of initial materials using for preparation of tellurite glass with the preset level of optical losses are stated.

(GOMD-S4-P035-2015) Infrared-Transparent Glass Ceramics: an Exploratory Study

B. Riley*[2]; J. McCloy[1]; D. A. Pierce[2]; 1. Washington State University, USA; 2. Pacific Northwest National Laboratory, USA

In this work, the vision and need for a fully ceramized long-wave infrared (LWIR)-transmitting glass ceramic has been articulated. Three sulfide systems were explored including two with La_2S_3 in hopes of imparting strong bonds from this refractory sulfide, and two containing GeS_2 in hopes of widening the glass-forming region. Attempts were made to produce glasses in the Ga_2S_3-La_2S_3-(ZnS,CaS) system, the GeS_2-La_2S_3 system, and the GeS_2-Ga_2S_3-CdS system. Water quenching produced glasses of Ga_2S_3-La_2S_3-CaS and GeS_2-Ga_2S_3-CdS. Microstructural and thermal analyses were used to explore nucleation and growth in these systems and infrared transmission and mechanical hardness showed potential for LWIR window use. The GeS_2-Ga_2S_3-CdS system showed good LWIR transmission and pre-crystallized hardness superior to chemical vapor deposited ZnS. The Ga_2S_3-La_2S_3 glasses did not appear to be viable candidates at this time due to a small temperature window between crystallization and glass transition temperatures and problems with oxygen contamination in the La_2S_3 source. Suggestions are made for two alternative methods for producing fully ceramized LWIR-transmitting glass ceramics.

(GOMD-S5-P036-2015) Sintering of glasses with concurrent crystallization assisted by DC electric field

M. G. Bacha*[1]; E. B. Ferreira[1]; 1. University of São Paulo, Brazil

Electric field can strongly influence the sintering kinetics of crystalline ceramics, increasing the linear shrinkage and final relative density, decreasing grain growth, temperature and time for sintering compared to conventional techniques. The effects on glass, however, have been little studied. We thus studied the sintering of glasses with concurrent crystallization assisted by DC electric field, aiming at producing glass-ceramics. We distinguished the three stages of flash sintering, which is often reported in the literature of ionic conducting ceramics, also for glasses in the system Na_2O-CaO-SiO_2. In stage I the electric field is applied and ions can move and concentrate on the surface of particles in a compact. In the contact between particles, the ion concentration favors the passage of current, causing Joule effect and a resulting increase in temperature, reducing the resistivity of the material, which enhances the ionic current, further increasing the temperature, in an avalanche effect that characterizes the stage II. In stage III, the current and electric field are steady. The microstructure of the samples was characterized by microscopy.

(GOMD-S5-P037-2015) Insight into chemical reactivity during nuclear glass synthesis

E. Boué[1]; S. Schuller*[1]; A. Mesbah[2]; T. Charpentier[1]; S. Poissonnet[1]; M. Toplis[3]; 1. CEA, France; 2. ICSM, France; 3. CNRS, France

Nuclear glasses are produced by a succession of physical and chemical interactions between a solid waste (calcine) and a glassy precursor (glass frit) through a vitrification process. Under non-optimal process parameters, these reactions can lead to the formation of crystalline phases, such as yellow phase. From a microstructural scale to an atomic scale, mechanisms are studied to determine the transformation kinetics and key parameters responsible for the formation and dissolution of yellow phase (as Na_2MoO_4) during glass synthesis. The effect of molybdenum oxide is considered in the case of simplified borosilicate glass frit and calcine (Na_2O-Al_2O_3-MoO_3). The influence of time and temperature on the formation and dissolution of Na_2MoO_4 and sodium aluminate phases ($NaAl_6O_{9.5}$ and $NaAlO_2$) was studied by in-situ X-ray diffraction and Rietveld analysis. Results are correlated with the structural changes of borosilicate network determined by NMR spectroscopy (^{27}Al, ^{11}B) and the evolution of Al_2O_3 and MoO_3 concentrations in the glass measured by microprobe. It has been shown that Na_2MoO_4 dissolution is controlled by the thermodynamic solubility of MoO_3. Na_2MoO_4, formed in the calcine, dissolves in the glass melt independently of the aluminates dissolution. These results give new insights on yellow phase and lead to describe a kinetic empirical law of Na_2MoO_4 and aluminates dissolutions during nuclear glass synthesis.

(GOMD-S5-P038-2015) Advanced Nuclear Waste Glass Development for the DOE Hanford Site

K. M. Fox*[1]; D. K. Peeler[1]; A. A. Kruger[2]; 1. Savannah River National Laboratory, USA; 2. U.S. Department of Energy Office of River Protection, USA

The U.S. Department of Energy Office of River Protection is developing advanced glasses for the immobilization of low and high level nuclear wastes at the Hanford site in Washington. The program is developing new models for the prediction of glass properties, such as chemical durability and viscosity, as a function of composition over the broad range of feeds to be processed at Hanford. Alternative methods for the avoidance of nepheline crystallization are being studied. Crystal tolerant glasses are being formulated, where the volume fraction and size of spinel crystals are controlled. Methods of operating a Joule heated melters with an acceptable amount of crystals are being developed, with provisions for responding to off-normal events. The overall objective is to allow for higher waste loadings in glass, which will significantly reduce the mission life and cost for immobilizing nuclear waste at DOE sites. This presentation will detail recent advancements at Savannah River National Laboratory in support of these programs.

(GOMD-S5-P039-2015) Comparison of corrosion of rare earth oxides containing borophosphate and borosilicate glasses

M. Wang[1]; W. Deng[2]; R. Dongol*[2]; B. Clark[2]; P. Tumurugoti[2]; N. Mellott[2]; S. Sundaram[2]; 1. Inner Mongolia University of Science and Technology, China; 2. New York State College of Ceramics, Alfred University, USA

The investigation on chemical durability of borophosphate and borosilicate glasses containing rare earths elements prepared with traditional melt-quenching methods has been carried out in a closed system by means of solution and solid analysis, to compare their corrosion behavior under identical testing conditions. A modified product consistency (PCT) test is used. The concentration of constituents and pH of the leachate in the deionized water are determined with inductively coupled plasma atomic emission spectroscopy (ICP-AES) and a temperature corrected pH meter, and the normalized releases are calculated. Characterization of the surface of glasses after corrosion experiments is performed using the scanning electron microscopy (SEM) equipped with energy dispersive spectroscopy (EDS), and x-ray photoelectron spectroscopy (XPS). The resistance against acid and alkaline attacking is also characterized by the weight losses, variation of surface morphology, and chemical composition of glasses samples. The results will be reported in terms of the relative leachability of these glasses and mechanisms of corrosion.

Tuesday, May 19, 2015

George W. Morey Award Lecture

Room: Symphony Ballroom IV

8:00 AM

(GOMD-AL-001-2015) Control of the metastable state of glasses (Invited)

J. Qiu*[1]; 1. South China University of Technology, China

Materials science deals with relationships between synthesis, structure, properties and performance of the materials. Glass is a special material featuring good homogeneity, variable composition, easy shaping and doping, owing to its meta-stable state and topological network structure. It is considered that the nature of glass and glass transition are among the most important problems in the field of condensed matter. We have focused our research on the change and enhancement of the properties of glass by manipulation of the metastable nature of glasses. In this talk, I will highlight our recent research developments on the design and control of the optical properties of glass through fast-cooling, crystallization and phase separation. We have demonstrated the realization of ultra-broadband near-infrared emission via control of valence state of Bi ion, ligand field around transition metal ions and energy transfer between two active ions for broadband optical amplification and tunable laser. I will also introduce our results on the printing of three-dimensional nano- or microstructures and multiple functions inside glasses by fs laser based on multiphoton absorption assisted control of excited state of dopants and nanostructures. These studies are not only helpful for understanding the nature of glass, but also valuable for the fabrication of optical devices.

Symposium 1: Energy and Environmental Aspects - Fundamentals and Applications

Session 2: Glassy Solid Electrolytes I

Room: Concerto B

Session Chair: Steve Martin, Iowa State University

9:20 AM

(GOMD-S1-001-2015) Ion conducting borophosphate glasses and development of all solid state batteries (Invited)

A. Pradel*[1]; M. Ribes[1]; A. Piarristeguy[1]; G. Silly[1]; 1. Université Montpellier 2, France

The present success of lithium batteries is somewhat lessened by their dependence on liquid electrolytes which can suffer from leakage, volatilization or flammability. An alternative to these batteries is an all-solid-state battery which would be much safer as it would employ solid electrolytes rather than liquid organic electrolytes. Ion conducting glasses are potential candidates for use as solid electrolytes. As a matter of fact, thanks to the property of a glass to soften at its vitreous transition temperature, the elaboration of a monolithic device at low temperature (~300°C compared to 900°C when ceramics are considered) could be facilitated. As a first step and in order to test the feasibility of such devices, lithium and sodium borophosphate glasses which present the so-called mixed glass former effect have been selected as solid electrolytes. The choice of an optimized composition will be justified on the basis of thermal, electrical and structural properties of the materials. The development electrochemical and characterization of all solid state batteries comprising these materials as electrolytes will be described.

9:50 AM

(GOMD-S1-002-2015) Silicon-based Lihium Superionic Conductor for Solid-State Lithium Metal Battery (Invited)

S. Lee*[1]; 1. University of Colorado Boulder, USA

Replacing the liquid electrolyte in a lithium battery with a solid electrolyte can resolve many inherent safety issues as well as enable the use of next generation electrode materials. Recent research in solid electrolytes, however, has mainly focused on improving ionic conductivity while neglecting compatibility with energy dense anodes such as lithium metal. In this talk, a new crystalline solid electrolyte will be discussed in terms of its cost, ionic conductivity and compatibility with lithium metal. This study presents and characterizes an analog to $Li_{10}GeP_2S_{12}$ using the isovalent ion of silicon to displace germanium as a cost effective constituent. The crystal $Li_{10}SiP_2S_{12}$ displays a conductivity of 2.3×10^{-3} S cm^{-1}, the highest reported conductivity for an unsintered silicon-based solid electrolyte. Impedance spectroscopy is used to probe interactions between the new superionic conductor and lithium metal revealing a more favorable decomposition than previous metal containing electrolytes. Due to the enhanced compatibility of $Li_{10}SiP_2S_{12}$ with lithium metal, we present one of the longest cycling bulk solid-state lithium metal batteries to date.

10:20 AM

(GOMD-S1-003-2015) ^{7}Li NMR studies of lithium ion dynamics in ceramics (Invited)

M. Haaks*[1]; R. Riedel[1]; S. Martin[2]; M. Vogel[1]; 1. TU Darmstadt, Germany; 2. Iowa State University of Science & Technology, USA

Rising energy demand makes it important to improve the performance of lithium ion batteries. For this purpose it is important to understand the dynamics of lithium ions, in particular, in heterogeneous materials, which are used in modern strategies for material optimization. Combining spin-lattice relaxation, solid-echo, and stimulated-echo experiments, ^{7}Li NMR allows us to expand the accessible time scale of ion dynamics to about 10 orders of magnitude. We exploit this potential to study ion dynamics in mixed network former glasses and in complex ceramics. Investigations of the mixed network former glass $0.5Li_2S$-$0.5(xGeS_2$-$(1-x)GeO_2)$ reveal the importance of a broad distribution of correlation times and, consequently, activation energies of the lithium ionic jump motion. Studies of $0.7Li_2S$-$0.3P_2S_5$ show that not only the electric conductivity, but also the ionic jump rates are enhanced by ceramization. For a polymer-derived silicon oxycarbide ceramic, a promising anode material for lithium ion batteries, we reveal substancial difference of the average lithium dynamics in lithiated and delithiated states of the material, which are most probably due to different lithium distributions among regions with distinguishable carbon fractions.

10:50 AM

(GOMD-S1-004-2015) The Mixed Glass Former Effect in Glassy Solid State Electrolytes: Structural Properties, Physical Properties and Ionic Conductivities of the $0.5Na_2S + 0.5[xSiS_2 + (1-x) PS_{5/2}]$ glass system

D. Watson*[1]; B. Curtis[1]; S. Martin[1]; 1. Iowa State University, USA

The Mixed Glass Former Effect (MGFE) in solid glassy electrolytes is a phenomena in which the ionic conductivity of a ternary glass system is a nonlinear and non-additive change as the composition is varied from one glass former to another while holding the modifier concentration constant over the series. The MGFE is not limited to the ionic conductivities, but can be also observed in the glass transition temperatures, densities, and molar volumes across the system. To investigate the MGFE in these glasses, the short range structures were characterized for the glass system $0.5Na_2S + 0.5[xSiS_2+ (1-x) PS_{5/2}]$ by ^{29}Si and ^{31}P MAS NMR, Raman and IR spectroscopies and the Na ion conductivities were measured by impedance spectroscopy, glass transition temperatures by differential scanning calorimetry and the densities by Archimedes method. In this report we will review the results of these experiments to develop an understanding of the relationship that exists between the physical properties of mixed glass former glasses and the atomic network structure to advance understanding of the MGFE in glass and fast ion conducting glasses for solid state batteries.

11:10 AM

(GOMD-S1-005-2015) Glass formation and fast Ag ion conduction in the system $Ag_2Se-Ga_2Se_3-GeSe_2$

M. A. Marple*[1]; S. Kim[1]; B. Aitken[2]; S. Sen[1]; 1. University of California Davis, USA; 2. Corning Incorporated, USA

Ag-chalcogenide glasses are potential candidate materials for solid electrolyte and ionic switch applications where the high mobility of Ag ions gives rise to large ionic conductivity. Although significant work has been done on Ag-Ge-Se glasses to develop fast ion conducting glasses, compositions with high Ag content and correspondingly high conductivity are also unstable towards phase separation and eventual deterioration with thermal cycling. We have synthesized glasses in the stochiometric $Ag_2Se-Ga_2Se_3-GeSe_2$ ternary system with improved stability against phase separation and remarkably large electrical conductivity on the order of $\sim10^{-4}$ ohm^{-1}cm^{-1} at ambient temperature. ^{109}Ag NMR spectroscopy and dc polarization studies indicate that the conductivity is ionic and results from fast Ag ion dynamics. Compositional evolution of the structure of these glasses has been studied using Raman and ^{71}Ga and ^{77}Se NMR spectroscopy. These results will be discussed and related back to the trends observed in conductivity.

11:30 AM

(GOMD-S1-006-2015) Physical and Structural Properties of Glassy Solid State Electrolytes of the $0.2Na_2O+ 0.8[xB_2O_3+ (1-x) GeO_2]$ Series

B. Curtis*[1]; S. Keizer[2]; J. Wang[2]; M. Dettman[2]; D. Hynek[2]; S. Feller[2]; S. Martin[1]; 1. Iowa State University, USA; 2. Coe College, USA

Solid state batteries have been of particular interest due being safer, having a higher energy density, and lifetime. Glassy solid electrolytes prove to be an advantageous application to solid state batteries since they are cheaper and safer to manufacture. These types of electrolytes allow modification of the ionic conductivity by varying the ratio of glass formers leading to the mixed glass former effect. This effect is observed when the composition moves from one binary system to another through a ternary system. The physical, electrochemical, and structural properties of the glass change due to the different compositions. The glass transition temperature, density and ionic conductivity have been measured using differential scanning calorimetry, Archimedes method and impedance spectroscopy, respectfully. Structural properties have been measured through nuclear magnetic resonance, infrared spectroscopy and Raman spectroscopy. In this talk, these properties will be interpreted in terms of the short range order structural models developed from the structural nature of the glass.

Symposium 2: Glasses in Healthcare - Fundamentals and Applications

Borate-based Bioactive Glass

Room: Symphony Ballroom IV
Session Chairs: Steven Jung, Mo-Sci Corporation; Qiang Fu, Corning Incorporated

9:20 AM

(GOMD-S2-016-2015) Angiogenic Response of Bioactive Borate Glass Beads and Microfibers in "Hairless" Mice (Invited)

R. Watters[1]; R. Brown[1]; D. Day*[1]; 1. Missouri University of Science and Technology, USA

Angiogenesis, the formation of new blood vessels, is known to be important to the healing of chronic wounds, especially those seen in diabetic patients. The angiogenic behavior of three borate and two silicate glass compositions were evaluated in hairless mice by two techniques for three weeks. The first consisted of taking optical photographs of the microvasculature in dorsal skin windows and the second used quantitative histomorphometry of tissue sections from the hairless mouse. Live imaging of the dorsal skin window showed the presence of a halo-like region infused with microvessels, in the soft tissue that surrounded the borate 13-93B3 and 13-93B3Cu (0.4wt% Cu) glass beads, two weeks after implantation. No halo was observed in the region surrounding the 13-93 silicate glass beads. Quantitative histomorphometry of soft tissue surrounding the 13-93, 13-93B3, and 13-93B3Cu beads indicated that the microvascular density was 1.3, 1.6 and 2.5 times higher, respectively, than the untreated controls. The microvascular density of soft tissue surrounding 45S5, 13-93B3, and 13-93B3Cu microfibers was 1.6, 2.3 and 2.7 times higher, respectively, than the untreated controls. These results show that the two, faster reacting borate glasses produce a larger anginogenic response than the slower reacting silicate (13-93) glass and that the presence of 0.4 wt% CuO increases the angiogenic response.

9:50 AM

(GOMD-S2-017-2015) In Vitro and In Vivo Evaluation of Borate Bioactive Glass Microfibers for Soft Tissue Repair

M. N. Rahaman*[1]; W. Huang[2]; C. Zhang[3]; 1. Missouri S&T, USA; 2. Tongji University, China; 3. Shanghai Jiaotong University, China

Borate bioactive glass microfibers are showing a remarkable ability to heal soft tissue wounds in humans and animals but little is known about the process and mechanisms of healing. In the present study, melt-derived borate bioactive glass microfibers doped with single or multiple metals (such as Cu and Zn) were evaluated in vitro and in vivo. When immersed in simulated body fluid, the Cu-doped microfibers released Cu^{2+} and other ions into the medium and converted to hydroxyapatite. Cell culture studies showed that the ionic dissolution product of the Cu-doped microfibers (<3.0 wt. % CuO) was not toxic to fibroblasts, promoted the secretion of vascular endothelial growth factor and stimulated the expression levels of angiogenic-related genes of the fibroblasts. The use of Cu-doped microfibers to treat full-thickness skin wounds in rodents in vivo resulted in significantly enhanced blood vessel formation and faster wound size reduction. These results could provide clues for understanding the remarkable ability of Cu-doped borate bioactive glass microfibers to heal soft tissue wounds in humans and animals.

10:10 AM

(GOMD-S2-018-2015) Gel-Derived Borate Glasses for Bone Tissue Engineering

W. C. Lepry*[1]; M. James-Bhasin[1]; S. Nazhat[1]; 1. McGill University, Canada

Bioactive glasses have long been used as bone repair materials attributable to their ability to bond to bone. Compared to traditional silicate based glasses, and owing to their lower chemical durability, borate glasses degrade more rapidly in their conversion to bone-like mineral (hydroxy-carbonated apatite, HCA). To further increase bioactivity, the sol-gel process is often used as it can produce glasses with greater porosity and surface area. Herein we demonstrate a novel method for producing a wide range of bioactive borate glasses (36 – 61 mol% B_2O_3) using the sol-gel process and examine their *in vitro* bioactivity. The sol-gel process produced glasses with surface areas and porosities at least an order of magnitude higher than melt derived borate glasses. When submersed in simulated body fluid, HCA conversion took place as early as 6 hours, according to infrared spectroscopy and x-ray diffraction. This rapid conversion was verified through ion chromatography which showed rapid ion release rates that were dependent on glass composition. Cell viability studies using mesenchymal stem cells demonstrated no toxicity. To the best of our knowledge, this is the first report demonstrating the potential use of sol-gel derived bioactive borate glasses for bone tissue engineering and regenerative medicine applications.

10:30 AM

(GOMD-S2-019-2015) Dissolution Kinetics and Conversion to Hydroxyapatite of Bioactive Borate Glasses (Invited)

R. Brow*[1]; J. George[1]; K. Goetschius[1]; 1. Missouri S&T, USA

Borate glasses have been developed as scaffolds for tissue engineering applications [Rahaman, 2011] and used to promote soft tissue repair [Jung, 2012]. In this paper, recent studies on the interactions between borate glasses and aqueous solutions, including simulated physiological environments, will be reviewed and how those reactions promote desired physiological responses will be discussed. Borate glasses are more reactive than silicate glasses, dissolving by orders of magnitude faster in aqueous environments. Borate glasses dissolve congruently,forming borate species that depend on solution pH: $B(OH)_3$ for pH<8, $B(OH)_4^-$ for pH>8. Dissolution rates are dependent on the O/B ratio which determines the fraction of four-coordinated borate species that constitute the glass structure, and on the nature of other metal cations in the glass. Calcium ions released from borate glasses will react with phosphate anions in solution to form calcium phosphate phases (amorphous and hydroxyapatite) on the glass surfaces, and these phases can change the dissolution kinetics from linear to parabolic with time. Doping glasses with certain ions can stimulate cells to secrete growth factors that are associated with the wound healing process. MN Rahaman, et al., Acta Biomat., 7, 2355–2373 (2011); SB Jung, “Bioactive Borate Glasses,” in Bio-Glasses: An Introduction, J.R. Jones, A.C. Clare, eds., John Wiley & Sons, 2012

11:00 AM

(GOMD-S2-020-2015) Development, Characterization and In Vitro Bioactivity Study of Boron-containing Silicate, Borosilicate and Borate Bioactive Glass Scaffolds

P. Balasubramanian*[1]; B. Jokić[2]; A. Malchere[3]; L. Gremillard[3]; J. Jones[4]; J. Chevalier[3]; A. Boccaccini[1]; 1. University of Erlangen-Nuremberg, Germany; 2. University of Belgrade, Serbia; 3. INSA Lyon, France; 4. Imperial College London, United Kingdom

Bioactive glasses (BGs) attract research interest as promising materials for bone regeneration. In this study, we report the development of boron-containing silicate, borosilicate & borate BG scaffolds. BGs of the system SiO_2-CaO-Na_2O-P_2O_5-K_2O-MgO-B_2O_3 denominated as B1, B2 and B3 with 12.5%, 25% & 56.6% B_2O_3 & 37.5%, 25% & 0% SiO_2 (wt%) respectively, were used for the fabrication of scaffolds by the polymer replica technique. In situ experiments in an environmental scanning electron microscope (SEM) were performed to investigate the morphology of the BG particles during sintering. High temperature X-ray diffraction (XRD) measurements were carried out to investigate possible crystalline phases formed during heat treatment. The release of B ions and Si species under quasi-dynamic conditions from scaffolds soaked in SBF was measured. The compressive strength of these scaffolds was found to be significantly higher than that of standard 45S5 Bioglass® scaffolds which is related to the relatively high densification of struts achieved by viscous flow. *Invitro* bioactivity studies in SBF were carried out and hydroxyapatite formation was confirmed by SEM and XRD. A correlation between chemical composition, B ion release kinetics and mechanical properties was established to select suitable BG compositions for bone tissue engineering applications.

11:20 AM

(GOMD-S2-021-2015) *In-vitro* dissolution of a bioactive borate glass under dynamic conditions

J. George*[1]; R. K. Brow[1]; 1. Missouri University of Science and Technology, USA

Single-pass flow-through experiments were employed to study the dynamic dissolution kinetics of a borate bioactive glass 13-93B3 in water, simulated body fluid (SBF), and other solutions. Glasses dissolved faster under faster flow rates and smaller glass-to-solution volume ratios. The borate ion release rate ranged from $1x10^{-5}$ $g/m^2/s$ for slow flow rates to $2x10^{-4}$ $g/m^2/s$ for faster flow rates. As the glass particles dissolved, a calcium phosphate phase precipitated on the particle surfaces. For the slow flow rates, amorphous calcium phosphate was present after 43 days of dissolution, whereas nanocrystalline (12-23nm) hydroxyapatite formed for faster flow rate experiments. The formation of crystalline hydroxyapatite was favored with faster flow rates, longer reaction times, and increased phosphate concentration in solution.

Symposium 3: Fundamentals of the Glassy State

Session 3: Structural Characterization of Glasses IV

Room: Symphony Ballroom II
Session Chair: Gang Chen, Ohio University

9:20 AM

(GOMD-S3-034-2015) Identifying and characterising the different structural length scales in glassy materials (Invited)

P. Salmon*[1]; A. Zeidler[1]; 1. University of Bath, United Kingdom

The structure of several network-forming glasses and liquids is considered, where a focus is placed on the detailed information that is made available by using the method of neutron diffraction with isotope substitution. In the case of binary network glass-forming materials with the MX_2 stoichiometry (e.g. GeO_2, $GeSe_2$, $ZnCl_2$), two different length scales at distances greater than the nearest-neighbour distance manifest themselves by peaks in the measured diffraction patterns. The network properties are influenced by a competition between the ordering on these “intermediate” and “extended” length scales, which can be manipulated by changing the chemical identity of the atomic constituents or by varying state parameters such as the temperature and pressure. The extended-range ordering, which describes the decay of the pair-correlation functions at large-r, can be represented by making a pole analysis of the Ornstein–Zernike equations, an approach that can also be used to describe the large-r behaviour of the pair-correlation functions for liquid and amorphous metals where packing constraints are important.

9:50 AM

(GOMD-S3-035-2015) Isotope Substitution Neutron Diffraction Study of the Lithium and Tellurium Environments in Binary Li_2O-TeO_2 Glasses

F. Mohd-Noor*[1]; D. Holland[1]; A. Hannon[2]; E. R. Barney[3]; 1. University of Warwick, United Kingdom; 2. Rutherford Appleton Laboratory, United Kingdom; 3. University of Nottingham, United Kingdom

The advantageous optoeletronic properties of tellurite glasses are influenced by glass structure, particularly the coordination of Te^{IV}. Thus, a study of the structure of tellurite glasses is crucial to understanding and controlling their behavior. Isotope substitution neutron diffraction has been used to study binary TeO_2 glasses modified with 10 to 30 mol% of Li_2O. Use of the null-scattering isotope composition of lithium, combined with difference experiments using the natural lithium isotope, allowed determination of the tellurium-oxygen and lithium-oxygen coordinations, n_{TeO} and n_{LiO}, as a function of glass composition. The value of n_{LiO} remains constant at approximately 4.0 over the entire composition range whilst the average value of n_{TeO} remains constant at 3.66(7) until x = 15 mol% before decreasing linearly as more modifier is added. This is in accord with the recent model of alkali tellurite glasses in which the Te coordination change is explained by the presence of terminal oxygens in amorphous TeO_2.

10:10 AM

(GOMD-S3-036-2015) The Structure of Arsenic Sulphide Glasses: Evidence for Tetrahedral Units?

A. C. Hannon*[1]; A. Cuisset[2]; E. Bychkov[2]; 1. ISIS Facility, United Kingdom; 2. Université du Littoral, France

Structural studies of arsenic sulphide glasses are described, with emphasis on the evidence for the presence of quasi-tetrahedral (QT) units, $S{=}As(S_{½})_3$, as has been proposed in studies of the intermediate phase in these glasses. A series of As_xS_{1-x} glasses (from 5 to 43% As) has been studied using neutron diffraction (ND) and Raman scattering. The ND results are interpreted using fitting and simulation methods, supported by DFT calculations. The interpretation of the Raman spectra is also supported by the DFT calculations, and comparison with the Raman spectra of Ge-S glasses. The coordination numbers derived from ND are consistent with the conventional model for the structure of these glasses, in which all sulphur atoms are 2-coordinated, and all arsenic atoms are 3-coordinated, with a trigonal pyramid geometry, and with a strong preference for heteropolar As–S bonds. The observed neutron correlation functions are not consistent with a structure that involves a significant proportion of QT units. A Raman line at 495 cm^{-1} has been interpreted as arising from the stretch mode of As=S double bonds, but the DFT calculations show that this mode arises from S-S dimers. This is supported by the presence of the same line in the Raman spectra of Ge-S glasses, which do not contain double bonds to sulphur. It is concluded that there is no experimental evidence for the presence of QT units in As-S glasses.

10:30 AM

(GOMD-S3-037-2015) Structural investigations on glasses belonging to the SiO_2-B_2O_3-La_2O_3 system

D. Caurant*[1]; H. Trégouët[1]; O. Majérus[1]; T. Lerouge[1]; L. Cormier[2]; T. Charpentier[3]; H. Vezin[4]; 1. CNRS, France; 2. UPMC, France; 3. CEA, France; 4. Université de Lille1, France

Rare earths (RE) are present in glasses frequently for their optical properties but also as fission products in borosilicate nuclear waste glasses. Because of the beneficial effect of B_2O_3 on RE solubility in nuclear waste glasses, it is interesting to understand the interactions that could exist between boron and RE in simpler glasses. Whereas binary B_2O_3-RE_2O_3 glasses can be prepared with compositions close to metaborate ($RE_2O_3.3B_2O_3$), RE are only very slightly soluble in glassy SiO_2. In this work, we studied the extension of the glass formation region in the ternary SiO_2-B_2O_3-La_2O_3 system with La_2O_3 as only modifier, by rapid quenching melts at 1550°C. The presence of crystals or separated amorphous phases was checked by XRD, SEM and Raman spectroscopy. Inside the glassy region, the structural evolution with increasing B_2O_3 or La_2O_3 content was followed using a multispectroscopic approach by investigating both the borosilicate network (^{11}B, ^{29}Si, ^{17}O NMR, Raman spectroscopy, X-ray and neutron scattering) and the RE environment (optical absorption and luminescence, pulsed-EPR, for RE = Nd or Eu). We present results on the structural units found in these glasses, average bond lengths, depolymerization of the network and environment of RE, which give some clues on the glass structure in this system in comparison with the crystalline phases belonging to this system and other RE-bearing borate glasses .

10:50 AM

(GOMD-S3-038-2015) Study of Fluorophlogopite Crystallization using *in-situ* X-ray Diffraction and Pair Distribution Function

B. S. Johnson*[1]; C. Chung[1]; J. L. Jones[1]; 1. North Carolina State University, USA

Glass-ceramics are materials that exhibit properties that are unique from their glass and ceramic components. These materials are created by the controlled crystallization of a base glass and depending on their properties they can be used in many applications including, electrical insulators and medical components. One such material of interest is Fluorophlogopite glass-ceramics. The purpose of this research is to develop an understanding of the crystallization mechanisms and phase evolution processes during the heat treatment of Fluorophlogopite glass-ceramics. This is accomplished through the use of time-resolved *in-situ* X-ray diffraction (XRD) and pair distribution function (PDF) studies. Both experimental techniques are needed to understand the crystallization phase evolution because glass-ceramics exhibit short and long range order. Peaks corresponding to Fluorophlogopite and Enstatite phases were observed from the results of the *in-situ* XRD data. PDF data shows near-neighbor peaks consistent with the SiO_2 network from 0-5Å and higher r peaks corresponding to Fluorophlogopite. The PDF data was also used to calculate changes in amorphous phase fraction (APF) as a function of temperature and shows a linear decrease in APF with increasing temperature. These results provide fundamental knowledge needed to control crystallization to reach desired phases and phase fractions.

11:10 AM

(GOMD-S3-039-2015) Local structure of molten borates: testing the temperature dependent predictions of thermodynamic models

O. Alderman*[1]; C. Benmore[2]; L. Skinner[2]; M. Liška[3]; J. Macháček[4]; A. Tamalonis[1]; A. Lin[5]; R. Weber[1]; 1. Materials Development Inc., USA; 2. Advanced Photon Source, Argonne National Laboratory, USA; 3. Vitrum Laugaricio – Joint Glass Center of IIC SAS, TnUAD, and FChPT STU, Slovakia; 4. Institute of Chemical Technology, Czech Republic; 5. Northwestern University, USA

Thermodynamic models, such as the model of ideal associated solutions, have shown quantitative agreement with measurements for many room-temperature properties of glasses. On the other hand, very few, if any, tests of the structural predictions for melts and their temperature (T) dependencies have been made. Here we use high-energy synchrotron x-ray diffraction to monitor the structure of aerodynamically levitated sodium and calcium borate melts as a function of T for direct comparison to model predictions. We find quantitative agreement in the boron-oxygen coordination number, CN, which may increase, decrease or not change at all with T, depending upon the melt composition. We argue that using bond length, BL, as a proxy for CN leads to more accurate results in the present case, and this method can be corrected for BL thermal expansion using our direct measurement of this quantity for pure liquid B_2O_3. We discuss problems, such as with the completeness of sets of thermodynamic data, and compare to limited relevant measurements in the literature made by neutron diffraction, Raman and nuclear magnetic resonance spectroscopies. As well as demonstrating a deep connection between crystalline and melt chemistries, the present results suggest that predictive power may be greatly enhanced by combining thermodynamic modelling with modern versions of constraint theory.

11:30 AM

(GOMD-S3-040-2015) Advances in high energy x-ray scattering from glasses (Invited)

C. J. Benmore*[1]; L. Skinner[2]; O. Alderman[3]; R. Weber[3]; 1. Argonne National Laboratory, USA; 2. Stony Brook University, USA; 3. Materials Development Inc., USA

Structure factor, S(Q), measurements and Pair Distribution Function, PDF, analysis provides a direct probe of both the intermediate and short range order in disordered materials. Recently the Advanced Photon Source established a glass, liquid, amorphous materials and extreme conditions program on beamline 6-ID-D. Here the worlds first superconducting high-energy undulator provides a high photon flux and the monochromator allows the incident x-ray energy to be tuned anywhere between 50 keV and 130 keV. Combined with the use of silicon-based area detectors and careful dark current and gain corrections, enables accurate x-ray S(Q) measurements out to unprecedented high Q-values >30 $Å^{-1}$. Using typical beam sizes of 0.5x0.5 mm, down to ~20x20 mm^2, time resolved structural studies of liquids and glasses above and below the glass transition temperature are possible in as little as ~100 ms time steps. The x-ray PDF results are complementary to and are often combined with neutron diffraction measurements. The x-ray S(Q) and PDF data are also directly comparable to the results of atomistic simulations or modeling tools. Plans to implement focusing optics as well as SAXS/WAXS capabilities on the beamline for extended range PDF measurements will also be discussed.

Session 5: Mechanical Properties of Glasses III

Room: Symphony Ballroom III
Session Chair: Satoshi Yoshida, The University of Shiga Prefecture

9:20 AM

(GOMD-S3-041-2015) The Crack Tip in SLS and FS Glass from a Fracture Mechanics Perspective (Invited)

R. C. Bradt*[1]; 1. University of Alabama, USA

The immediate crack tip region in both soda lime silica (SLS) and in fused silica (FS) glasses is examined. First the extended Dugdale model of the flowed region about the crack tip is examined as presented initially by Broek. Using measured values of the hardness of the glasses, accounting for the indentation size effect, the size of the flowed region is estimated. The two glasses are compared. Next the effective mass of the crack tip region is estimated by a kinetic energy balance of the stored elastic strain energy released. It is a conservative estimate of the crack's effective mass. It is then extended to estimate the size of the flowed crack tips in the two glasses. The effective mass strongly suggested that any flow about the crack tip is these glasses is extremely limited.

9:50 AM

(GOMD-S3-042-2015) Glass-water interactions – lessons from surface-sensitive spectroscopy, indentation, and scratch tests

N. Surdyka[1]; H. He[1]; J. Luo[1]; L. Bradley[1]; N. Sheth[1]; C. Pantano[1]; S. H. Kim*[1]; 1. Pennsylvania State University, USA

Although multicomponent silicate glasses are involved in a variety of advanced technical applications, little is known for its surface chemistry in humid ambience. Thus, researchers, engineers and manufacturers rely on literature and analytical methods relevant to amorphous silica to understand their complex glasses even though it is well known that that the surface chemistry of multicomponent silicate is quite different than silica. We studied a hypothesis that the structure and reaction of water films on silicate glasses are a function of the glass surface composition as well as the process through which the surface is created and the presence of applied or residual surface stress. To test this hypothesis, a number of surface-sensitive spectroscopy techniques (XPS, IR, SFG) as well as mechanical tests (indentation, scratch) were employed for various types of commercial glass surfaces (soda lime, borosilicate, aluminosilicate, boroaluminosilicate) and melt-derived glass surfaces (bottle and fiber glasses). The comparison of test results revealed the unique roles of leachable sodium ions in mechanical properties of glass surfaces in humid environments, and also raised many new questions that have not been studied extensively. This work was supported by the National Science Foundation (DMR-1207328) and the Usable Glass Strength Coalition (UGSC).

10:10 AM

(GOMD-S3-043-2015) Chemical-mechanical characteristics & the formation of the Bielby layer on polished glass surfaces

T. Suratwala*[1]; N. Shen[1]; R. Steele[1]; M. Feit[1]; L. Wong[1]; R. Dylla-Spears[1]; R. Desjardin[1]; P. Miller[1]; 1. Lawrence Livermore Nat'l Lab, USA

The mechanical & chemical characteristics and proposed formation mechanisms of the polishing-induced Bielby surface layer are described. Fused silica, borosilicate, and phosphate glasses were polished using different slurries, polyurethane pads, and rotation rates. The mechanical properties were measured using ultra-low load nanoscratching, and the surface concentration profiles for key contaminants were measured using SIMS. Using load ranges expected on particles during polishing, plastic type scratches were observed with depths in the nm range. The load dependence of the removal depth was consistent with that expected from Hertzian mechanics for the phosphate glass. However, for fused silica and borosilicate glass, the deformation depth showed a weak dependence with load. Using a sub-T_g annealing technique, significant material relaxation was observed on the scratches suggesting as significant fraction of the plastic deformation was due to densification. The SIMS results show that K penetration *decreased* with increase in material removal rate during polishing. In contrast, Ce penetration *increased* with the material removal rate. K penetration is explained using a two-step diffusion process. On the other hand, Ce penetration is proposed to be governed by the hydrolysis rate ratio between Ce-O-Si and Si-O-Si.

10:30 AM

(GOMD-S3-044-2015) Modeling Crack Growth Behavior of Glass Strengthened by a Sub-Critical Tensile Stress

J. H. Seaman*[1]; T. A. Blanchet[1]; P. J. Lezzi[1]; M. Tomozawa[1]; 1. Rensselaer Polytechnic Institute, USA

Glasses exhibit slow crack growth under stress intensities below the fracture toughness in the presence of water vapor or liquid water. It has been observed by several authors (T.A. Michalske, E. Gehrke et al., S.M. Wiederhorn) that when an oxide glass sample with a large crack is held under a subcritical stress intensity in water vapor or liquid water (where no slow crack growth occurs), upon loading to a higher stress intensity, a 'finite restart time' is observed prior to measurable crack extension. This phenomenon has traditionally been attributed to concepts such as corrosive dissolution of the crack tip, crack tip blunting, and water diffusion and subsequent swelling of the material around the crack tip. A newly observed surface stress relaxation process that is aided by molecular water diffusion has been used to strengthen glass fibers and to explain the subsurface stress peak in ion-exchanged strengthened glasses. The same phenomenon is now used to explain these interesting experimental slow crack growth data. A rigorous mathematical model has been developed utilizing concepts such as water diffusion and fracture mechanics. Predictions of restart times using the model agreed well with the published experimental data. Additionally, this novel model may be used to explain the fatigue limit, which is observed as non-propagation of a crack under low stress intensity.

10:50 AM

(GOMD-S3-045-2015) Sub-critical crack growth in hydrous borate and silicate glasses

C. Rössler*[1]; U. Bauer[2]; A. Pönitzsch[1]; J. Deubener[1]; H. Behrens[2]; S. Reinsch[3]; R. Müller[3]; 1. TU Clausthal, Germany; 2. Leibnitz University of Hannover, Germany; 3. Federal Institute for Materials Research and Testing, Germany

C. Rößler[1], U. Bauer[2], A. Pönitzsch[1], J. Deubener[1], H. Behrens[2], S. Reinsch[3], R. Müller[3] 1)Institute of Non-Metallic Materials, Clausthal University of Technology, Germany 2) Institute of Mineralogy, Leibniz University of Hannover, Germany 3) BAM Federal Institute for Materials Research and Testing, Berlin, Germany In order to study the effect of dissolved water on crack initiation and sub-critical crack growth the mechanical response to sharp contact loading (Vickers diamond) of hydrous (up to 6 wt%) and nominal dry soda lime borate glasses and soda lime silica glasses have been studied. Indentation experiments were conducted at 300 K in dry nitrogen gas and under humid conditions (RH » 40%). These measurements were supported by studying the elasticity of the same glasses using ultrasonic transverse and longitudinal wave propagation. Furthermore, the water speciation in the respective glasses was determined. We show that both glass families show a different behaviour with respect to increasing water content. While for the borate glasses water decreases the Young's modulus but increases the crack initiation probability and crack growth dynamics, the silica glass data are more complex. The reasons for these differences are to be found in the structural changes induced by the hydration of the glasses. We discuss this especially with respect to the different water speciation in borate and silicate glasses.

11:10 AM

(GOMD-S3-046-2015) Volume Expansion caused by Water Penetration into Silica Glass

S. Wiederhorn*[2]; F. Yi[2]; D. Lavan[2]; T. Fett[1]; L. Richter[2]; 1. Karlsruhe Institute of Technology, Germany; 2. NIST, USA

By measuring the curvature of thin disks of vitreous silica that have been penetrated by water from one side only, we determined the volume expansion of the silica and the effect of this volume expansion on its strength. We found that the water-strengthening process depended on cracksize, temperature and the amount of swelling of the silica. We also evaluated the diffusivity of water in vitreous silica, using the swelling stresses as the diffusion metric. Diffusivity values, so obtained, are close to the accepted values for the diffusion of water in vitreous silica, as is the activation energy for the diffusion process. Our data suggests that swelling and the consequent bending of the disks is caused by silanol group formation in the silica structure; molecular water plays little role in the swelling process.

11:30 AM

(GOMD-S3-047-2015) Mechanical spectroscopy studies on hydrous borate and silicate glasses

S. Reinsch*[1]; U. Bauer[2]; C. Rössler[3]; R. Müller[1]; H. Behrens[2]; J. Deubener[3]; 1. BAM Federal Institute for Materials Research and Testing, Germany; 2. Leibniz University of Hannover, Germany; 3. Clausthal University of Technology, Germany

Sub-T_g relaxation phenomena have crucial impact on aging and fatigue of glass. For multi-component glasses they were reported to cause compaction and sub-critical crack growth at room temperature, where these relaxation modes are much faster (τ » 10^0-10^8 s) and decoupled from the cooperative rearrangements of the glassy network ($\tau > 10^{27}$ s). To get insights into fast relaxation processes internal friction measurements can be used. In this work, a forced oscillation method (dynamic mechanical thermal analysis) is used to study the internal friction of hydrated oxide glasses with total water content up to 5 wt. % using temperature-frequency sweeps from near T_g to 273 K and from 1 to 55 Hz. Several relaxation modes below the glass transition T_g can be measured. The correlation of these measured internal friction peaks to e.g. the low-temperature motion of alkali ions or the cooperative movement of equal or dissimilar mobile species such as alkali or alkali alkaline earth ions as well as the influence of OH or H_2O in the structure of hydrated glasses on the relaxation modes will be discussed.

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 3: Laser Processing and Photostructuring

Room: Concerto A
Session Chair: Juejun Hu, MIT

9:20 AM

(GOMD-S4-028-2015) Point by point direct laser writing of waveguide in chalcogenide glass (Invited)

P. Masselin*[1]; D. Le Coq[2]; E. Bychkov[1]; 1. Université du Littoral Côte d'Opale, France; 2. Université de Rennes 1, France

Direct laser writing technique is now widely used in particular in glass, to produce both passive and active photonic devices. We report the results of femtosecond writing of buried waveguide in chalcogenide glass by point by point method. This method consists in irradiating the sample by a femtosecond laser pulse burst and translating the sample to modify the next zone. This is in contrast of traditional experiments where the sample is translated continuously but however it produces similarly homogeneous structure. The glass composition used in the experiments is 90 (80 GeS_2 - 20 Ga_2S_3) - 10 CsCl. A static irradiation of this glass results in a local positive refractive index variation whose magnitude depends on the duration of the pulse burst but with a diameter being independent over all the experimental parameters. Therefore, in order to vary the diameter of the waveguide, cylinders of positive refractive index are written closely pack to each other, with their axis parallel to the beam propagation direction. An example of single mode waveguide at a wavelength of 1.5 μm will be shown. In conclusion direct laser writing using a point by point method enables the production of homogeneous waveguide of controllable diameter and numerical aperture on a wide range of values. Therefore this technique is suitable for the design of single mode waveguide for wavelength ranging from the visible up to the infrared.

9:50 AM

(GOMD-S4-029-2015) Rotatory laser-induced single crystal growth of Sb_2S_3 on the surface of Sb-S-I glass

D. Savytskyy*[1]; N. Tamura[2]; V. Dierolf[1]; H. Jain[1]; 1. Lehigh University, USA; 2. Lawrence Berkeley National Laboratory, USA

Laser-induced glass → crystal transformation can be realized by two different paths: 1) heating the glass from ambient to crystallization temperature (Tx), or 2) cooling the melt to Tx. In general, the first approach leads to the formation of polycrystalline glass-ceramics, whereas the latter can produce single crystals. Here we report the first successful fabrication of Sb_2S_3 single crystal dots, lines and 2D architectures on the surface on Sb-S-I glasses by the first process. EBSD mapping indicates that the 1D crystal grows in a straight line, while simultaneously rotating gradually around a direction parallel to glass surface and normal to laser scanning direction, e.g. the crystal rotates by ~50^O over a length of 100 mm. The scanning X-ray microdiffraction Laue patterns obtained at the LBNL synchrotron show split spots surrounded by narrow streaks along laser scanning direction, which is similar to the observation of plastic deformation in nanoindented Cu single crystal. So laser-grown Sb_2S_3 single crystal is "plastically deformed", with unpaired dislocations and small-angle tilt boundaries. The growing crystal accommodates its structural mismatch with glass matrix by introducing unpaired dislocations, which then order to form tilt dislocation walls. These dislocations compensate mismatch and cause rotation along the direction of growth, which coincides with the laser scanning direction.

10:10 AM

(GOMD-S4-030-2015) Direct Laser Writing surface microstructuring of silver-doped phosphate glasses for new functionalities

J. Desmoulin*[1]; T. Cardinal[1]; S. Danto[1]; M. Vangheluwe[2]; Y. Petit[1]; M. Dussauze[1]; M. Lahaye[1]; L. Canioni[1]; V. Rodriguez[1]; R. Vallée[2]; 1. University of Bordeaux, France; 2. University of Laval, Canada

Direct Laser Writing (DLW) relies on femtosecond pulse laser interaction with materials. It enables accessing original designs and functionalities in glasses hardly reachable otherwise. This approach applied to silver-containing tailored phosphate glasses yields a variety of photo-induced species or nanoparticles. The understanding of the relationship between the physico-chemical modifications following the laser-material interaction remains essential for the tailoring of local properties. The characterization of the material at the micro and nano-scale is crucial to master the laser interaction for the precise structuration of the glass surface and/or volume. Indeed, thanks to nonlinear absorption phenomena, the energy of the laser beam is confined in a voxel of interaction and leads to local material modifications. Elementary analysis allows evidencing the migration of the silver species from the center of the voxel towards its edges, correlatively to the production of fluorescence. A selective chemical treatment of the surface enables revealing the inscribed patterns via the non-homogeneous silver distribution. Correlations have been established between the local photo-chemistry and the resulting luminescence, the refractive index and the nonlinear optical properties. The DLW method enables designing complex surface topology combined with innovative optical properties.

10:30 AM

(GOMD-S4-031-2015) Features of Photostructural Response in Spin-Coated Chalcogenide Glass Thin Films

A. Kovalskiy*[1]; J. Cook[1]; R. Golovchak[1]; S. Slang[3]; K. Palka[3]; L. Loghina[3]; M. Vlcek[3]; H. Jain[2]; 1. Austin Peay State University, USA; 2. Lehigh University, USA; 3. University of Pardubice, Czech Republic

Spin-coated chalcogenide glass thin films are known to be photostable, i. e. insensitive to photon irradiation, contrary to traditional thermally deposited layers. The structure of the spin coated films in stoichiometric and S-rich arsenic sulphide system was studied before and after irradiation with UV and band gap light. X-ray photoelectron spectroscopy (XPS) was the primary method to explore photostructural transformations on the surface of the films and Raman spectroscopy/microscopy was used to study structure inside the layers. It was found that for all chemical compositions except S-rich As30S70 the spin-coating technology results in As-poor films in comparison with composition of the dissolved glass. It is concluded that the lack of photostructural response to the band gap light is associated with absence of As-As bond in glass matrix and lack of voids which are filled with organic residual. It was revealed that UV radiation damage the surface of the film leading to the fluorescence-based background in Raman spectra. Isolation of organic residuals in the structure is confirmed by XPS data which do not show any sign of formation of As-O bonds. This work was supported by NSF Award No 1409160 and the grant CZ.1.07/2.3.00/30.0058 from the Czech Ministry of Education, Youth and Sports.

10:50 AM

(GOMD-S4-032-2015) Optical damage performance of widegap semiconductor transparent electrodes

S. Elhadj*[1]; J. Bude[1]; J. Adams[1]; M. Menor[1]; J. Yoo[1]; T. Olson[1]; J. Lee[1]; A. Samanta[1]; C. Stolz[1]; 1. Lawrence Livermore National Laboratory, USA

In this study we seek to describe how transparent conductive electrodes properties such as microstructures, defects, conductivity, and carrier mobility contribute to optical damage performance in high power laser applications, and how these parameters relate to specific materials, fabrication processes, and to enhanced laser annealing. Specifically, our initial focus is on ITO and doped ZnO thin films on fused silica substrates exposed to a nanoseconds pulsed laser at 1064nm wavelength. Similar results on other widegap semiconductors are also described. We use large aperture, high power optical damage tests techniques on exit surfaces to probe optical damage mechanisms up to 20 J/cm^2 characterized by microscopy. In turn, microstructural and electrical thin film measurements are related to the apparent optical damage mechanisms and properties of the films. In general, we find that 1) the optical damage performance is strongly dependent on the number of test cycles performed, affecting lifetime performance, and 2) evidence that suggests the presence of single defects in amorphous ITO films, which will be discussed. The optical damage performance can be affected by pre-exposure laser processing of the films under controlled conditions to minimize precursor related damage events

11:10 AM

(GOMD-S4-033-2015) Glass surface texturing by demixing under CO_2-laser irradiation

A. Veber*[1]; M. R. Cicconi[1]; N. Travitzky[1]; D. de Ligny[1]; 1. Universität Erlangen-Nürnberg, Germany

Different ways are proposed today to increase efficiency of light emitting and receiving devices, including light-emitting diodes and solar cells. Light management by means of a structured design can significantly increase in/out coupling efficiency and improve the performance. Among other possible techniques good results could be obtained by proper texturizing of a device surface. Laser processing is a powerful technique allowing to create various textures on glass surface with a desired design, e.g. controllable microlenses or nanostructures. Furthermore it can be easily implemented on a production line. In the present work texturing of borate and borosilicate glasses under CO_2 laser radiation is considered. Using of 10 μm radiation allows to effect on the near-surface layer of a pure glass directly, without need of any additional doping element. Despite the fact that laser spot radius is limited by the diffraction limit, sub wavelength structures were obtained on the surface by means of decomposition of the initial glass. The characteristic sizes of the structures can be controlled both by laser treatment mode as well as initial glass parameters. The optical features obtained make this new family of texturized glasses promising devices for in/out light coupling applications.

11:30 AM

(GOMD-S4-034-2015) Implantation of gold into pure and silver containing glass by means of ArF-excimer laser irradiation

M. Dubiel*[1]; M. Heinz[1]; J. Meinertz[2]; J. Ihlemann[2]; 1. Martin Luther University Halle-Wittenberg, Germany; 2. Laser-Laboratorium Göttingen e.V., Germany

The generation of plasmonic Au/Ag nanostructures in glass surfaces showing a tunable surface plasmon resonance in a wide range of wavelengths should be realized by laser implantation of gold by means of excimer laser irradiation. These are promising materials for optoelectronics and nanoplasmonics. Thin films of Au were applied to the glass surface and then Au species were incorporated by means of intense UV radiation using fluences below the ablation threshold of the glass. The formation of Au and Au/Ag nanoparticles with surface plasmon resonances between 500 and 620 nm could be verified by optical spectroscopy. These results demonstrate that such procedures enables the space-selected generation of plasmonic Au/Ag structures in glass surfaces by excimer laser irradiation.

11:50 AM

(GOMD-S4-035-2015) Structural changes and relaxation phenomena responsible for the permanent refractive index change of glasses after fs-laser modification

T. Seuthe*[1]; A. Mermillod-Blondin[2]; M. Grehn[3]; J. Bonse[4]; M. Eberstein[1]; 1. Fraunhofer IKTS, Germany; 2. Max-Born-Institute for Nonlinear Optics and Short Pulse Spectroscopy, Germany; 3. Technische Universität Berlin, Germany; 4. BAM - Federal Institute for Materials Research and Testing, Germany

The processes leading to the permanent structural changes of model-glasses and glasses with multicomponent compositions after irradiation with a single Femtosecond(fs)-laser pulse were investigated. Initial glass structures and structural changes after modification were examined using µRaman-spectroscopy. Composition dependent reactions of the silicate network and structures containing network-modifiers, the so-called Q^n-structure, were found and could be related to the laser-energy used for modification. Investigation of the molar fraction of the Q^n-structural elements reveals a temperature increase of the modified area above the glass transition temperature. The permanent refractive index change of the glass volume was quantitatively measured using spatial light interference microscopy. The change in refractive index was used to evaluate the isostructural temperature of the modified glass. An isostructural temperature is similar to the fictive temperature, but considering a possible pressure-induced influence to the frozen-in structural state. It can be shown that the permanent refractive index change of a glass after fs-laser modification is a result of the maximum transient refractive index change after absorption of the fslaser pulse and the following cooling process, which is mainly dominated by the thermal conductivity of the glass.

Symposium 5: Glass Technology and Cross-cutting Topics

Session 4: Waste Glass Corrosion I

Room: Concerto C
Session Chair: James Marra, SRNL

9:20 AM

(GOMD-S5-020-2015) Hydration-induced morphological evolution at glass-liquid interfaces: a new model of long-term glass corrosion (Invited)

J. V. Ryan*[1]; 1. Pacific Northwest National Laboratory, USA

For decades, there has been general agreement that corrosion is due to the combined contributions of two broad categories of mechanisms: reaction control (solution affinity, local solution changes due to secondary phase precipitation, and kinetic limitations) and transport control (ion exchange, pore tortuosity, and diffusion of rate-limiting ions). Existing models based on these mechanisms predict the resultant solution concentrations with reasonable accuracy, given good parameterization. They do not, however, predict (or attempt to predict) the formation of many of the structures observed at the surface of corroding glasses. Recent advanced characterization of these structures has led to a new model of the dominant corrosion-controlling mechanism. Like other models, this model suggests that the glass quickly alters to form a dense material that then provides the controlling interface between the dissolving solution and the glass. Unlike others, it is suggested that this layer is effectively non-reactive (in static conditions) and impervious to any consequential diffusion of reactive species. In this talk, we show how the morphological evolution of this interfacial region can account for the dynamic behaviors and structures seen in the study of glass corrosion. Mathematical fits to disparate long-term corrosion datasets are also presented.

9:50 AM

(GOMD-S5-021-2015) How nanoporous alteration layers can make borosilicate glasses very durable?

S. Gin*[1]; P. Jollivet[1]; 1. CEA, France

During aqueous corrosion of silicate glasses and minerals, it is observed that a succession of layers form and, under certain conditions, these layers affect the corrosion rate by several orders of magnitude. Until now, the underpinning mechanisms remained unclear, and commonly-accepted models based on thermodynamics only, failed to predict the long-term corrosion of such materials in natural environments. Here, isotopically-tagged experiments were performed on a model borosilicate glass, and by correlating the results of our multi-scale characterization approach, we show how the different glass constituents interact and how the related processes affect the long-term dissolution rate of the glass. One of the outcomes of the study, we show for the first time that, under silica saturation conditions, the surface layer becomes passivating after in-situ reorganization, leading to a thermodynamic equilibrium with the bulk solution, thereby greatly slowing the material's degradation. We demonstrate that passivation can make the glass very durable. We eventually come up with original suggestions to improve the design of geological repository for nuclear glasses.

10:10 AM

(GOMD-S5-022-2015) Stage III Dissolution of High Level Waste (HLW) and Low Activity Waste (LAW) Glasses Triggered by Leachate Interactions

C. M. Jantzen*[1]; C. Crawford[1]; 1. Savannah River National Laboratory, USA

The necessity to a priori predict the durability of HLW and LAW glasses on extended time scales has led to a variety of modeling approaches based primarily on the solution (leachate) evolution with time. These durability models, used for geologic repository Performance Assessments (PA) for HLW glass and for land disposal of LAW glass, do not consider the impact of the interaction between the glass gel that evolves with time on the glass surface and the evolving leachate. A database, entitled Accelerated Leach Testing of GLASS (ALTGLASS), was developed in 2013. ALTGLASS contains 218 glasses of which 79 are HLW glasses and 139 LAW glasses: some known to resume leaching at an accelerated rate and some continue at a steady state rate. A statistical approach was used to compare the glasses which resume accelerated leaching to those that do not resume. The "trigger" for the Stage III dissolution was found to be related to the acid base equilibrium in the maturing leachates and how that equilibrium interacts with the evolving gel. The specific acid base equilibrium is expressed as strong base minus weak acid or [SB]-[WA] and glasses that return to an accelerated rate have [SB]-[WA]>>0.

10:30 AM

(GOMD-S5-023-2015) Preparation of an Information Basis for Development of Practical Performance Assessment Models on Waste Glass Corrosion in Geological Disposal

S. Mitsui*[1]; T. Ohe[2]; Y. Inagaki[3]; T. Ohkubo[4]; S. Kurosawa[5]; T. Goto[5]; M. Inagaki[5]; K. Ishiguro[5]; H. Takase[6]; H. Takahashi[6]; 1. Japan Atomic Energy Agency, Japan; 2. Tokai University, Japan; 3. Kyushu University, Japan; 4. Chiba University, Japan; 5. Nuclear Waste Management Organization of Japan, Japan; 6. Quintessa Japan, Japan

In geological disposal of high-level radioactive waste, vitrified waste will function as the first engineered component of a multi-barrier system. The glass is expected to retain radionuclides for long time periods by limiting radionuclide release from its own structure. A more realistic understanding and modeling of the glass corrosion processes can improve reliability of the radionuclide migration analyses. Therefore, we need to develop practical performance assessment models of the glass corrosion coupled with various near-field processes to be applied to an open system relevant for disposal conditions. In order to develop robust performance assessment models on waste glass corrosion, we have been preparing an information basis regarding glass properties and corrosion processes under disposal conditions as a part of NUMO-JAEA joint project. Our iterative working process for the preparation of the information basis comprises five steps: (1)integration of current knowledge; (2) development of glass corrosion scenarios based on current knowledge; (3)development of conceptual model; (4)sensitivity analyses to evaluate relative importance of relevant processes and associated uncertainties; and (5)identification of future R&D issues towards further improvement of the information basis. The current status will be presented in this talk.

10:50 AM

(GOMD-S5-024-2015) Formulation and durability testing of glass ceramics for immobilization of waste products from used fuel reprocessing

C. Crawford*[1]; J. Crum[2]; J. Marra[1]; 1. SRNL, USA; 2. PNNL, USA

The use of glass ceramics has been studied for nuclear waste immobilization in Australia, France and the USA. Glasses containing pyrochlore, zirconolite and insoluble residues from used fuel reprocessing have been considered. This study examines the crucible formulation of glass ceramics designed for incorporation of large volumes of fission products separated from nuclear fuel by aqueous reprocessing that contain Mo, Sr/Y, Cs/Ba, Ce, Nd, La and Zr. The glass ceramic was designed to be a single-phase borosilicate glass at melting temperature and undergo bulk recrystallization into targeted powellite, oxyapatite and lanthanide borosilicate phases upon slow cooling. An initial statistical design formulation matrix used fixed ratios of waste components while a latter design varied these ratios. Waste component oxides are in the range of 40 to 50 wt%. Powdered glass ceramic leach tests were used to assess the waste form durability as compared to glass used for HLW immobilization in the USA. Glass ceramic fabrication, analyzed chemical composition of the matrix and leach tests results for glass and waste components spanning > 1 year will be presented.

11:10 AM

(GOMD-S5-025-2015) Structure and diffusion properties of boroaluminosilicate nuclear waste glasses

J. Du*[1]; L. deng[1]; M. Ren[1]; 1. University of North Texas, USA

The knowledge of detailed atomic structures for nuclear waste glasses is critical to the understanding of chemical and radiation stability, diffusion and corrosion resistance, and the optimization of composition and waste loading. The understanding of the structure of nuclear waste glasses is complicated by their multicomponent nature, especially the existence of several glass formers and their composition dependent structure features. In this paper, we present the development of effective empirical potentials that are capable of simulating the structures of boroaluminosilicate nuclear waste glasses. After initial testing and validating of the potentials, they are used to study the International Standard Glass (ISG) model system. Results of short and medium range structure features of the glasses from detailed structural analysis will be presented. In addition, diffusion behaviors of the glass modifier and former cations of ISG are studied and diffusion coefficients and diffusion energy barriers will be reported in comparison with available experimental data.

11:30 AM

(GOMD-S5-026-2015) First-Principles Based Modeling Of Borosilicate Glass Hydrolysis

D. C. Ford*[1]; H. He[2]; P. Zapol[1]; 1. Argonne National Laboratory, USA;
2. Valparaiso University, USA

Long-term predictions of the dissolution behavior of glass waste forms in aqueous environments can potentially have reduced uncertainties by utilizing first-principles informed models. Subcontinuum approaches based on first-principles theory develop understanding of reaction mechanisms at the atomic scale and provide estimates of reaction rates. We used density functional calculations to evaluate reaction energies and reaction barriers of hydrolysis reactions on model sodium borosilicate glasses, which are used as input to a kinetic model. Development of kinetic approaches based on first-principles calculations of barriers for water reactions and comparison of the dissolution rate far from equilibrium to experiments provides insights into the molecular-level mechanisms of glass dissolution and can then be used for a coarser scale modeling and for building predictive models of the dissolution behavior for glass waste form.

Norbert J. Kreidl Award Lecture

Room: Symphony Ballroom IV

12:00 PM

(GOMD-AL-002-2015) Structure and Nonlinear Elasticity of Silica Glass Fiber under High Strains

M. J. Guerette*[1]; 1. Rensselaer Polytechnic Institute, USA

In-situ Raman and Brillouin light scattering techniques with a spatial resolution of 1 mm have been developed to study structural signatures and elastic moduli of silica glass fiber under tensile and compressive strains in a two-point bend test. By traversing the cross-section at the apex, a convenient way to determine the neutral axis of a bent fiber was established. Resulting from the nonlinear elastic behavior of silica glass, the predicted neutral axis shift was directly observed for the first time in our experiments. The verified neutral axis shift will allow for more accurate calculations of both strain and stress of a bent fiber. An expression for elastic modulus is generated which includes the 5th order term that is required to capture both the minimum in compression and the maximum in tension for silica glass in bend. Raman spectra show polarization-dependent structural signatures of silica glass in tension and compression. Our studies contribute to a fundamental understanding of the structure and elastic properties of glasses under high strain conditions, which is of critical importance for developing strong glasses.

Symposium 1: Energy and Environmental Aspects - Fundamentals and Applications

Session 2: Glassy Solid Electrolytes II

Room: Concerto B
Session Chair: Annie Pradel, Université Montpellier 2

1:20 PM

(GOMD-S1-007-2015) Glass-Based Na_3PS_4 Solid Electrolytes for All-Solid-State Sodium Batteries (Invited)

A. Hayashi*[1]; M. Tatsumisago[1]; 1. Osaka Prefecture University, Japan

Development of rechargeable batteries with high energy density is important for storage of the renewable energies and power supply to eco-cars such as BEV and plug-in HEV. Solidification of rechargeable batteries has several advantages such as long cycle lives and versatile geometries. Solid electrolytes with high Na^+ ion conductivity is needed to fabricate all-solid-state sodium batteries having a strong merit of using ubiquitous sodium sources. We have found that cubic Na_3PS_4 phase precipitated from the mother glass increased conductivity from 10^{-6} to 10^{-4} S cm^{-1} at 25°C. Furthermore, all-solid-state Na-Sn/TiS_2 cells with the prepared Na_3PS_4 glass-ceramic electrolytes operated as a secondary battery. The partial substitution of Si for P in Na_3PS_4 further increased conductivity to $7.4x10^{-4}$ S cm^{-1}. Conductivity enhancement for glass-based electrolytes is a priority issue for developing solid-state sodium batteries. In this study, Na_3PS_4 glass-based electrolytes were prepared by a mechanochemical technique and consecutive heat treatment. The preparation conditions and glass compositions for achieving high conductivity will be reported. Electrochemical performance of all-solid-state cells with a developed electrolyte will be demonstrated.

1:50 PM

(GOMD-S1-008-2015) Heavy vs. Light Cation Chalcogenide Glasses: Ion transport and Structural Features (Invited)

E. Bychkov*[1]; 1. University of Littoral, France

Light alkali (Li^+, Na^+) and d^{10} (Cu^+, Ag^+) cation chalcogenide and chalcohalide glasses were extensively studied over the last twenty years giving rise to numerous applications (batteries, non-volatile memory, sensors, etc.) and fundamental findings related to ion diffusion mechanisms and specific structural features of the glass network. Much less is known about heavy cation glassy chalcogenides whose ionic conductivity is far below the requested transport parameters for a vast majority of electrochemical applications. Nevertheless, a recent need in portable ion sources for mass-spectroscopy analysis at the ppb level and reliable chemical sensors for heavy-metal detection has renewed the interest to heavy alkali, mercury and thallium chalcogenide glasses. Caesium or rubidium halide doped sulphide and selenide glasses are also promising functional materials for optical applications. We will compare the ion transport properties of heavy and light cation chalcogenide glasses over a wide composition range studied using conductivity measurements and ^{22}Na, ^{64}Cu, ^{86}Rb, ^{108m,110m}Ag and ^{204}Tl tracers. The changes in the conductivity nature and ion transport mechanism will be related to the structural features in the glass network revealed by pulsed neutron diffraction, high-energy x-ray scattering and Raman spectroscopy associated with the DFT calculations and RMC modelling of the diffraction data.

2:20 PM

(GOMD-S1-009-2015) Rare-earth aluminosilicate glasses as solders for joining of silicon carbide components via laser supported process

S. Ahmad*[1]; M. Herrmann[2]; W. Lippmann[2]; M. M. Ahmed[1]; M. Steinbrück[1]; H. J. Seifert[1]; 1. Karlsruhe Institute of Technology, Germany; 2. Technical University of Dresden, Germany

The structural applications of silicon carbide (SiC) materials have increased tremendously during the past decade in different fields of engineering especially in aerospace industry and nuclear industry. The joining of SiC based components for assembling complex structures is a scientific challenge. The conventional welding processes cannot join SiC assemblies due to their non-wetting nature. The high temperature stability of rare-earth aluminosilicate glasses combined with their low coefficient of thermal expansion, high glass transition temperatures and good mechanical properties make these glasses interesting to be used as solder for the joining of SiC materials. Different rare-earth aluminosilicate glasses (RE_2O_3, RE: Sc, Yb, Ho, Dy, Y, Nd) were prepared by melt-quench technique. The quantitative and qualitative studies of the produced glasses were conducted to determine their properties and to establish a structure-property relationship. These prepared glasses were used to join the SiC assemblies via laser supported joining method. The properties and the chemistry of the joints were evaluated by examining the interface between solders and SiC. This study supports the development of high temperature resistant glasses for the hermetic sealing of SiC-based devices during short-time laser process.

2:40 PM

(GOMD-S1-010-2015) Development of Flexible Glass Capacitors for Power Inverters in Electric Drive Vehicles

B. Balachandran*[1]; B. Ma[1]; M. Pyrz[2]; M. Lanagan[2]; S. Garner[3]; P. Cimo[3]; 1. Argonne National Laboratory, USA; 2. Pennsylvania State University, USA; 3. Corning, Inc, USA

Advanced power inverters in electric drive vehicles require capacitors that operate under high-voltage at under-hood conditions and have minimal footprint. Due to the low dielectric constant (k ≈2.5) of polymer films, the currently used polymer film capacitors are very bulky, occupying ≈ 35% of the inverter volume. Polymer film capacitors are limited to operating temperature of ≈75°C and do not have sufficient high temperature performance for future automotive applications. New flexible dielectric materials for capacitors are needed for advanced power inverters. Glass capacitors are good candidates for advanced power inverters because of their flexibility, good insulation resistance, high-temperature capability, and high dielectric constant. We are exploring the potential of flexible glass substrates for this application. We have deposited ≈200-nm-thick platinum electrodes on 100-μm-thick Corning® Willow™ Glass substrates and evaluated their dielectric properties. We measured k of ≈6 and low dielectric loss of ≈0.001 (0.1%) in the frequency range of 1-100 KHz. Polarization-electric field measurements showed recoverable energy density of ≈60 mJ/cm^3. The dielectric properties of the Willow Glass samples and targeted performance goals for capacitors will be presented in this talk. Work at Argonne National Laboratory is supported by the U.S. Department of Energy, Vehicle Technologies Program.

3:00 PM

(GOMD-S1-011-2015) Porous Vycor®-Glass: Alternative leaching techniques for new applications

F. N. Somorowsky*[1]; B. R. Durschang[1]; M. Kilo[1]; G. Sextl[1]; 1. Fraunhofer Institute for Silicate Research ISC, Germany

Vycor®-glass is known for its spinodal demixing into a SiO_2-rich and a $NaBO_3$-rich phase after heat treatment. The latter phase is soluble in a wide range of acids and the remaining structure is a porous SiO_2-glass. The conditions during the phase separation and the subsequential leaching process influence its porosity, pore size and the surface area. Porous Vycor® Glass (PVG) shows a high chemical, mechanical, and thermal stability giving rise to various applications in research and industry. In order to prepare PVG for applications in large quantities, e. g. in the building industry, the production process has to be more ecologically friendly. One starting point is the reduction of the acid concentration and temperature. Furthermore the leaching was performed in an autoclave with weak acids and water as the leaching medium with temperatures up to 200 °C and at pressures up to 25 bar. The PVG was investigated by SEM, N_2-sorption isotherms, and water sorption tests. The structure of the PVG, produced under hydrothermic conditions, differs significantly in comparison to normally leached glass. A partial dissolution of the silica network causes a bimodal pore structure. The pore size and the size distribution depend on the temperature and duration of the treatment. PVG with this a pore structure can be interesting e. g. as support in applications.

Session 3: Thin Film Technologies

Room: Concerto B
Session Chair: B.G. Potter, University of Arizona

3:40 PM

(GOMD-S1-012-2015) Helping to optimize Solar Energy-Conversion Devices with Soft X-Ray and Electron Spectroscopies (Invited)

C. Heske*[1]; 1. University of Nevada, Las Vegas (UNLV) and Karlsruhe Institute of Technology (KIT), USA

In order to maximize the contribution of *solar* energy to the future global energy portfolio, it is important to optimize the performance (up!) and cost (down!) of the devices involved in solar energy conversion. The purpose of this talk is to demonstrate how a tool chest of soft x-ray and electron spectroscopies (in particular using high-brilliance synchrotron radiation) is uniquely suited to unravel the electronic and chemical properties of surfaces and interfaces, and how an understanding of solar devices on that level can lead to increased performance. It will be shown how photoelectron spectroscopy (PES), x-ray-excited Auger electron spectroscopy

(XAES), inverse photoemission (IPES), x-ray emission spectroscopy (XES), and x-ray absorption spectroscopy (XAS) can be suitably combined to derive band gaps, study local chemical bonding and electronic level alignment, and obtain insights into chemical stability (illustrating why we need so many abbreviations). As examples, Cu(In,Ga)(S,Se)$_2$ and CdTe thin film solar cells as well as GaInP$_2$- and WO$_3$-based solar water-splitting devices will be discussed.

4:10 PM

(GOMD-S1-013-2015) CdTe-ZnO Nanocomposite Thin-Film Spectral Sensitizers in Hybrid Photovoltaic

W. Huang*[1]; S. De Valle[1]; K. Simmon-Potter[1]; B. Potter[1]; 1. University of Arizona, USA

CdTe nanocrystals embedded in an electrically active ZnO matrix are integrated into thin film photovoltaic heterojunction devices as spectral sensitizers. The CdTe-ZnO nanocomposite film offers control of both spectral absorption and photocarrier transport behavior through the manipulation of nanophase assembly. A sequential RF-magnetron sputter deposition technique affords the control of semiconductor nanophase spatial distribution relative to the heterojunction plane in a hybrid, ZnO-P3HT test structure. Energy conversion performance, (including current-voltage and quantum efficiency (QE) response) was examined as a function of the location of the CdTe nanophase absorber region using both 1-D device modeling and the experimental examination of analogous P3HT-ZnO based thin film devices. Enhancement in simulated QE over a spectral range consistent with the absorption region of the CdTe nanophase (i.e. 400 – 475 nm) is confirmed in the experimentally determined external quantum efficiency collected from the hybrid devices. Trends in spectral response of the experimental devices in this wavelength range and, moreover, outside the primary absorption range for the CdTe nanocrystals, are interpreted in terms nanostructural variation in the thin films and the effect of carrier scattering/recombination to mitigate the successful transport of photocarriers across the junction.

4:30 PM

(GOMD-S1-014-2015) High temperature effects on AR-coated silica glass for solar tower receivers

G. Helsch[1]; R. Uhlig[2]; H. Bornhöft[1]; J. Deubener*[1]; 1. Clausthal University of Technology, Germany; 2. Institute of Solar Research, DLR, Germany

In solar tower power plants the incident sunlight is focused by heliostats to the receiver in the top of the tower, where temperatures up to 1000 °C are reached. For preventing convection losses, the receiver is covered with silica glass, which however leads to a loss in solar transmittance of about 7 %, caused by reflection. An antireflective (AR) coating from porous silica increases solar transmittance of the silica glass from 93 to 97 %. The AR-coated silica cover glass will reach operating temperatures up to 900 °C. Unfortunately, in combination with organic and inorganic contaminants, crystallization and sintering processes will be induced during operating temperatures. The paper aims in providing operating conditions for preventing these processes, which lead to a reduced transmittance and an increased safety risk. Therefore longtime experiments in a gradient furnace as well as cleaning and heating cycles were performed. These investigations led to the result, that a specific cleaning procedure is necessary to support continuous operation of the solar tower power plant.

4:50 PM

(GOMD-S1-015-2015) Sol-gel Derived Materials for Yb Disk Lasers

T. Ribeiro[1]; L. F. Santos[1]; M. Goncalves[1]; R. M. Almeida*[1]; 1. Instituto Superior Técnico / UL, Portugal

Many industrial and scientific applications require high-power diode-pumped solid state lasers with good beam quality. The key challenge is how to manage the generation and removal of waste heat in the pumping process. The thin disk laser concept offers high optical efficiency, good output beam quality and good thermal management. Due to the small disk thickness, the absorption efficiency has to be increased by re-imaging the unabsorbed pump power onto the disk several times in a multi-pass scheme. For the fabrication of the active material, low cost alternatives to Yb:YAG single crystal have been investigated using Sol-Gel processing. Yb-doped thick films have been prepared in glassy phospho-silicate (SiO$_2$-P$_2$O$_5$), alumino-silicate (SiO$_2$-Al$_2$O$_3$) and polycrystalline YAG (3 Y$_2$O$_3$.5 Al$_2$O$_3$) matrices by multilayer spin-coating. Results of their structural (XRD, FTIR / Raman spectroscopies, SEM) and optical characterization (ellipsometry and photoluminescence at ~ 1 μm) will be presented as a function of the Yb concentration (0 – 30 mol%). Evidence of good Yb dispersion was obtained and both the alumino-silicate and YAG matrices appear especially promising as SG-derived materials for Yb disk lasers.

5:10 PM

(GOMD-S1-016-2015) Exceptional Kinetic Stability of Vapor Deposited As$_2$S$_3$ Films

P. Thapar*[1]; D. Savytskii[1]; W. R. Heffner[1]; H. Jain[1]; 1. Lehigh University, USA

The general notion about glass is that vapor deposited films are kinetically and thermodynamically less stable than the bulk form. However, Swallen et al. (Science, 2007) observed that organic glass films vapor deposited onto a substrate at temperature $T_s=T_g-50$ were more stable than those deposited at lower T_s. Here we report on the stability of As$_2$S$_3$ films, vapor deposited at various T_s. In this first study of kinetic stability of inorganic glass films by varying T_s, we also find from DSC, an increase of the onset temperature of glass transition (T_{onset}) by 13°C for films deposited at $T_s=T_g-50=163$°C vs. Ts = room temperature (RT). The glass forming at a high T_s can be thought of as a simultaneous deposition and annealing process, which allows for enhanced mobility of molecules during deposition without crystallization. A large overshoot in the glass transition endothermic peak occurs for films deposited at $T_s=163$°C, compared to the glass transition endothermic peak for films deposited at lower T_s. This overshoot shows that the films behave as aged glass on the DSC curve. The higher T_{onset} and the increase in the T_g overshoot suggest that contrary to general notion, the films prepared at $T_s=163$°C are kinetically more stable than films deposited at RT, as they require a higher temperature to cause rearrangement of molecules.

5:30 PM

(GOMD-S1-017-2015) Density dependence of refractive index of nanoparticle-derived titania films on glass

A. Matthias*[1]; N. Raicevic[2]; R. D. Tchana[1]; J. Deubener[1]; D. Kip[2]; 1. Clausthal University of Technology, Germany; 2. Helmut Schmidt University, Germany

In order to investigate the relationship of refractive index to porosity, titania films up to 800 nm were prepared from particular anatase sols with a primary particle size below 7 nm, on silica glass by dip-coating. If the curing temperature was increased from 100 °C to 1000 °C profilometry showed a decrease in film thickness and an increase in refractive index of up to 50 %. The decrease in film thickness was related to an increase in mass density, which directly acts on the optical polarizability and thus determined the effective refractive index of the film. In particular, mass density-refractive index calculations were performed using linear (Arago-Biot, Gladstone-Dale) and nonlinear mixture models (Drude, Lorentz-Lorenz), assuming either air- or water-filled pores, while anatase and rutile fractions were determined by X-ray diffraction. The investigations were verified using refractive index and mass density data from literature. For each effective medium theory noticeable deviations from the expected trend were evident. We show that an empirical power law expression holds for Lorentz-Lorenz theory and permits to calculate effective density and porosity of titania films from effective refractive index with high accuracy.

Symposium 2: Glasses in Healthcare - Fundamentals and Applications

Bioactive Glass in Dental and Medical Applications

Room: Symphony Ballroom IV
Session Chair: Delia Brauer, Friedrich-Schiller-Universität

1:20 PM

(GOMD-S2-022-2015) Influence of Mg and Zn substitution on bioactive glass dissolution at neutral and acidic pH (Invited)

D. S. Brauer*[1]; M. Blochberger[1]; 1. Friedrich-Schiller-Universität, Germany

Glass ionomer cements (GIC) are used in dentistry as fillers or luting cements; however, they contain aluminum ions in the glass, which is a neurotoxin (thereby precluding orthopedic uses) but plays an important role in both glass degradation (hydrolysis of Si–O–Al bonds) and GIC stability (crosslinking by Al^{3+} ions). Bioactive glasses (BG), which readily degrade in aqueous solution and release ions, may be an alternative for use in orthopedic GIC. We studied the dissolution of Bioglass® 45S5 (where either zinc or magnesium were substituted for calcium on a molar base; 0 to 100%), at a physiological pH of 7.4 and an acidic pH of 4. At pH 7.4 Mg-substituted glasses showed ion release profiles and pH changes similar to those of 45S5, while Zn-substituted glasses showed very low ion release (less than 10%) and no pH changes over 7 days. At pH 4, by contrast, the ion release behavior was more similar, with 40% of ions being released at 15 min and 80% at 3 hours for all glasses. Despite similar field strength of Zn^{2+} and Mg^{2+} ions, the dissolution behavior of the BG differed significantly. Mg acted like a typical modifier, with ions being released in exchange for protons. Zn-substitution, by contrast, seemed to prevent ion exchange at neutral pH, while the release at acidic pH may involve hydrolysis of Si-O-Zn bonds, in analogy to alumina-containing glasses used in dental GIC.

1:50 PM

(GOMD-S2-023-2015) Glass-fibers with antimicrobial properties for bone defects restoration

L. Esteban*[1]; B. Cabal[2]; R. Torrecillas[2]; C. Prado[2]; R. López[2]; F. Quintero[3]; J. Pou[3]; J. Panide[3]; J. Moya[1]; 1. Consejo Superior de Investigaciones Científicas, Spain; 2. Nanomaterials and Nanotechnology Research Center, Spain; 3. Universidad de Vigo, Spain

Two types of antimicrobial glass nanofibers with diameters ranging from tens of nanometers to 1 micrometer, containing ZnO and CaO respectively were fabricated by laser spinning technique. Pellets of glasses containing ZnO or CaO were used as precursors. These fibers were found to be highly biocide against gram+, gram-bacteria and yeast (>3log of reduction). In the present work the biocompatibility and the capability to prevent infections of these glass nanofibers were stablished. This is the first time that glass nanofibers free of metal nanoparticles and free of toxicity for living beings but with a high antimicrobial activity have been fabricated following a different process from electrospinning. These nanofibers have been used as filler in different dental commercial composites and they have demonstrated to improve the composites mechanical properties and adding a specific antimicrobial activity. Therefore they have an extensive field of applications, especially in dental care.

2:10 PM

(GOMD-S2-024-2015) Twofold internal crystallization of lithium disilicate and fluorapatite in the SiO_2-Li_2O-Al_2O_3-CaO/SrO-K_2O-P_2O_5-F system for dental restorations

M. Rampf*[1]; C. Ritzberger[1]; M. Schweiger[1]; W. Höland[1]; 1. Ivoclar Vivadent AG, Liechtenstein

Controlled two-fold crystallization widens the range of attainable material properties as well as opens up new fields of applications and processing technologies for glass-ceramics. Targeting apatite, materials such as machineable bioactive mica-apatite glass-ceramics or leucite-apatite glass-ceramics with an optical appearance interesting for prosthodontics have been engineered so far. In the latter case fluorapatite, $Ca_5(PO_4)_3F$, was precipitated in form of needlelike submicron sized crystals. While these former investigations made use of internal nucleation combined with surface nucleation, the present study is to outline the possibilities and potential of precipitating apatite in lithium disilicate glass-ceramics from bulk glasses. Therefore, the crystallization in glasses of different compositions derived from the non-stoichiometric lithium disilicate glass system was studied by means of DSC, XRD combined with Rietveld analysis and REM. Basic and dentistry relevant material properties including biaxial fracture strength, fracture toughness, translucency and chemical durability were determined. The experiments revealed the precipitation of sub-micrometer scaled fluorapatite crystals within the microstructure dominated by lithium disilicate. Phase separations in the base glass could be observed. The systematic variation of CaO, P_2O_5 and F^- as well as the substitution of CaO by SrO yielded different glass crystallization phenomena. Besides their impact on the qualitative and quantitative composition of crystal phases, an influence of glass phase separation on crystallization will be considered. Together with microstructure properties relationships, the potential of the material for dental applications will be discussed.

2:30 PM

(GOMD-S2-025-2015) Influence of bioactive glasses on self-restoring potential of dentin adhesive systems

J. Brandt*[1]; R. Göbel[2]; A. Rzanny[2]; D. S. Brauer[1]; 1. Friedrich-Schiller-University, Germany; 2. University Hospital Jena, Germany

Dental adhesives are used to fix and integrate composite dental fillings in line with caries treatment. A strong and tight bond is desirable to prevent the occurrence of gaps which would lead to infiltration of microorganisms and to secondary caries. Bioactive glasses (BG) dissolve in aqueous media like saliva and release ions, leading to crystallization of hydroxyapatite. The aim of this study was to evaluate the influence of two BG on compression shear strength and microleakage of a dental adhesive system. Two BG (Bioglass® 45S5 and a strontium-substituted version of 45S5) were mixed into the adhesive system; BG-free systems were used as controls. The in vitro dissolution behavior of the two glasses was investigated in Tris-buffer solution for 1 or 3 days, and apatite formation confirmed by FTIR. Dentin of extracted human teeth was ground, etched, primed and bonded. For microleakage tests conditioned glass plates were attached to the prepared surface using a thin layer of composite. The prepared samples were stored in TRIS-buffered solution (pH 7.4) at 37°C for 1 day or 29 days. Subsequently, microleakage samples were stored in methylene blue solution for 14 days. No differences were observed between compression shear strength of BG-containing samples and controls. By contrast, microleakage at 29 days was reduced significantly in the BG-containing samples.

2:50 PM

(GOMD-S2-026-2015) Development of mica-based glass-ceramics for dental applications

D. Chaysuwan*[1]; T. Srichumpong[1]; K. Suputtamongkol[2]; 1. Kasetsart University, Thailand; 2. Mahidol University, Thailand

This research focused on development of a machinable glass-ceramic in order to utilize as a restorative dental material. The glass system of SiO_2-Al_2O_3-MgO-MgF_2-$SrCO_3$-$CaCO_3$-CaF_2 and P_2O_5 was prepared with 4.0 mol % fluorapatite called GCF4. Then glass chemicals were melted at 1420°C and quenched in cold water to form frits. Glass frits would be remelted and poured in the carbon mould at the same temperature, then annealed at 580°C (Tg-50 °C) and cooled to room temperature to obtain a glass rod. Because of DTA results and Marotta's paper, it was elucidated that the optimum nucleation and the crystallization temperatures were 643°C and 872°C, respectively. The coefficient of thermal expansion (CTE) of GCF4 by dilatometer was analyzed and found that close to those of human enamel and dentin. In addition, the results of the biaxial flexural strength, fracture toughness and chemical solubility values were reported and suitable to exploit as a substructure (core ceramics) for dental restorations according to ISO 6872:2008 (E). Furthermore, the glass-ceramic was able to fabricate by CNC with CAD/CAM technology due to its machinability, however, its appearance was rather opaque and white.

3:10 PM

(GOMD-S2-027-2015) Manufacturing of highly porous, anisotropic glass monoliths with a honeycomb-like structure

S. Krenkel*[1]; H. Uhlig[2]; D. Enke[2]; E. Rädlein[1]; 1. Ilmenau University of Technology, Germany; 2. University of Leipzig, Germany

Porous glasses provide nano-porous support materials with high mechanical, chemical and temperature stability as well as a high specific surface area up to 500 m^2/g. These materials are suitable as catalyst support as well as carrier for biologically active materials such as enzymes or microorganisms. Porous glasses offer the possibility to immobilize nano-materials without losing their desired properties but reducing the toxicology. Currently porous glasses are produced predominantly as membranes, flakes, micro-encapsulate or particles. The disadvantages of these products are increased pressure losses as well as a decreased flow rate. These disadvantages can be avoided through the production of honeycomb-like structures. Compared to the conventional method of honeycomb structure made of ceramic, carbon or glass, these structures are produced by the draw-down process from tube bundles. This allows the generation of transport pores in the range of micrometers. Applying internal pressure the wall thickness can be controlled. By this process, honeycomb structures with a total diameter of 4 cm and a total length of 1 m are generated. Subsequently, the production of nanometer pores is carried out by a heat treatment followed by extractions. The combination of honeycomb construction principles with self-organized porous material leads to a hierarchical pore structure similar to a lung.

Symposium 3: Fundamentals of the Glassy State

Session 3: Structural Characterization of Glasses V

Room: Symphony Ballroom II
Session Chair: Philip Salmon, University of Bath

1:20 PM

(GOMD-S3-048-2015) Oxide glasses under extreme compression and 2 dimensional confinement (Invited)

S. Lee*[1]; 1. Seoul National University, Republic of Korea

Upon compression, oxide glasses and melts are subject to successive structural transitions with multiple densification mechanisms that are distinct from those of their crystalline analogues. Experimental verification of this phenomenon remains a major target of glass-melt studies. Recent breakthroughs in element-specific experimental probes of local structures including synchrotron inelastic x-ray scattering (IXS) and multi-dimensional solid-state nuclear magnetic resonance (NMR) reveal previously unknown structural details of the pressure-induced changes in the diverse multi-component network glasses under static and dynamic compression. Here, we provide an overview of the recent progress and insights by IXS and NMR into electronic structures of oxide glasses under both static and dynamic compression. Contrary to an expected complexity in densification for multi-component oxide glasses, the pressure-induced changes in melt structures show a simplicity where the effect composition can be somewhat predicted and quantified. Finally, the structure of the surface/interface of amorphous oxide glasses under spatial confinement has remained illusive. Here, we also report the first high-resolution solid-state NMR results for the amorphous oxides under 2-dimensional confinement where the degree of structural disorder tends to decrease with increasing degree of confinement.

1:50 PM

(GOMD-S3-049-2015) Structure and Mechanical Properties of Nanoporous Glasses Characterized by X-ray Scattering

M. Sundararajan[1]; C. A. Ihalawela[1]; G. Chen*[1]; 1. Ohio University, USA

Nanoporous glasses have very interesting structure and properties due to their large specific surface area that can easily exceed 1000 m^2/g. The large surface area leads to a high fraction (as high as one third) of atoms on the surface. Therefore, nanoporous glasses are prototypical materials for studying structure and properties of ultra-thin glasses. In this talk, we report an application of small-angle and wide-angle X-ray scattering to the study of structure and mechanical properties of periodic mesoporous silica. The short-range, medium-range, and nanoscale structure of the nanoporous glasses have been characterized. It has been found that pore walls of the nanoporous glasses are highly strained, which originates from the anisotropic structure between the surface and bulk of the glasses. Mechanical properties such as Young's modulus and Poisson's ratio have also been characterized using small-angle and wide-angle X-ray scattering in conjunction with in situ capillary condensation. A significant enhance of the Young's modulus of the nanoporous glasses has been observed after an increase of thermal annealing temperature by merely 100 Celsius degrees. The structure-property relationship behind this observation will be discussed.

2:10 PM

(GOMD-S3-050-2015) Usable Strength of Glass—Surface Chemistry Perspective

N. Sheth*[1]; N. Surdyka[1]; J. Luo[1]; J. Barnerjee[1]; C. Pantano[1]; S. Kim[1]; 1. Pennsylvania State University, USA

Although theoretically strong, surface defects significantly reduce the usable strength of glass. Modern theory views strength-compromising defect formation as a series of chemical bond dissociation events creating thermodynamically unstable sites on the glass surface. Limited research has been done to understand the relation between surface chemical reactivity and the glass network structure, such as the hydrolysis of Si-O-Si network, which forms silanols that are preferential water absorption sites. By understanding the parameters that affect the density of surface silanol groups, its effects on the structure of interfacial water, and the surface mechanical properties of glass, the nucleation of strength-compromising defects can be better understood. Surface sensitive spectroscopy techniques (SFG, XPS, IR) were used to study the structure of the water interfacial layers formed at ambient conditions on multicomponent silicate glass. These findings were then related to the glass surface strength using indentation and scratch tests under subcritical loads. This study revealed critical parameters that effect glass surface chemistry and network structure which limits the usable strength of multicomponent silicate glass. This work was supported by the Usable Glass Strength Coalition (UGSC).

2:30 PM

(GOMD-S3-051-2015) Surface Studies of Calcium Aluminosilicate Glasses

D. Kramer*[1]; C. Pantano[1]; C. Trivelpiece[1]; 1. Pennsylvania State University, USA

The purpose of this work to understand the surface chemistry of glass in response to a variety of surface preparation methods using analysis techniques such as x-ray photoelectron spectroscopy and infrared spectroscopy. The calcium aluminosilicate system is an ideal model for understanding the surface chemistry of alkali-free glass because it is structurally simple, contains two different modifier sites and is relevant display glasses whose processing exposes the surface to a variety of aqueous chemistries. The surfaces being prepared and studied include fracture surfaces, melt surfaces, polished surfaces, and surfaces produced from various corrosion processes across a range of acidic, neutral, and basic conditions. The XPS and FTIR/ATR data provide information about surface composition and structure relative to the bulk. The effects of non-bridging oxygen versus aluminate sites in the hydration, leaching and dissolution of the glass are of particular interest.

2:50 PM

(GOMD-S3-052-2015) Atomic scale investigation of dopant in glass using aberration corrected STEM-EELS

T. Mizoguchi*[1]; A. Masuno[1]; H. Inoue[1]; 1. University of Tokyo, Japan

Heavy elements doped glasses have been known to show various kinds of optical properties, and thus various dopants are added in commercially available optical glasses. To achieve high performance optical properties, control of the dopant distribution in the glass is crucial. Some studies have been performed to capture evidence of the local structure around the heavy elements. However, spectroscopic methods, such as extended X-ray absorption fine structures (EXAFS), have yet to show us the atomic environment around single dopant atom because the information obtained through these methods is essentially averaged across multiple dopants. For understanding the role of dopants on the optical properties, atomic scale identification of the lanthanide dopants in the optical fiber is crucial. Here, individual lanthanide dopants, such as Er, buried in the optical glass are visualized using aberration corrected STEM. Molecular dynamics and image simulations are used to interpret the experimental images and draw quantitative conclusions. The visibility of the buried dopants in the amorphous glass is strongly dependent on the defocus and specimen thickness, and only dopants in very thin regions can be reliably identified [1]. Further results using aberration corrected STEM and EELS will be discussed in this presentation. [1] T. Mizoguchi et al. ACS Nano, 7 (2013) 5058-5063.

Session 3: Structural Characterization of Glasses VI

Room: Symphony Ballroom II
Session Chair: Steve Martin, Iowa State University

3:40 PM

(GOMD-S3-053-2015) Combining optical and x-ray absorption spectroscopies: application to medieval stained glasse

M. Hunault*[1]; F. Bauchau[2]; C. Loisel[2]; M. Hérold[3]; G. Calas[1]; 1. University Pierre and Marie Curie, France; 2. Laboratoiry of Research on Historical Monuments, France; 3. Centre André Chastel, France

The coloring properties of transition metal (TM) elements rely on their redox state and their local geometry. Optical and x-ray absorption (XANES) spectroscopies are powerful complementary methods to quantify the speciation of TM ions and their coloring properties in glasses. As an example, the blue color of Middle Age glasses may come from the presence of Co^{2+}, Fe^{2+} and Cu^{2+}. The main blue colorant is Co^{2+}, which only occurs in this oxidation state in the glass. On the contrary, Fe, Cu and Mn can occur in several oxidation states and the mutual interaction of their redox equilibria influences the glass color. The oxidation state is also sensitive to the temperature and to the oxygen partial pressure of the furnace. We have combined the data obtained on glasses by XANES and optical absorption spectroscopies, with data on crystalline references with 4-, 5- and 6-coordinated ions and numerical modeling of some of spectroscopic properties. This enables to determine the speciation of coloring ions in medieval stained glasses. This was applied to the analysis of binary glasses as well to 13th century blue glasses (Sainte Chapelle of Paris). These results revealed the extent of the compositional dependence of the spectroscopic properties of Co^{2+} in glasses and also demonstrate the use of peculiar melting conditions for these 13th century glasses .

4:00 PM

(GOMD-S3-054-2015) Structure and properties of strontium aluminosilicate glasses and melts

D. R. Neuville*[1]; A. Novikov[2]; P. Florian[2]; L. Hennet[2]; 1. CNRS-IPGP, France; 2. CNRS-CEMHTI, France

The chemical and structural role of strontium in silicate and aluminosilicates glasses and melts is of interest with regard to the vitrification of high-level radioactive waste, glass ceramic and ceramic material. The configurational properties of melts and glasses provide fundamental information needed to characterize industrial processes. A main difficulty is to link the "macroscopic" configurational entropy with the structure of melts. This has been done by combining viscometry with Raman and X-ray absorption/diffraction spectroscopic studies. From the viscosity measurements, we have obtained the configurational entropy, *Sconf* and the Raman spectra and X-ray diffraction give structural information on the middle range order and on the connected rings and X-ray absorption spectroscopy give structural information on the short range order. The structural information, which is related to the aluminosilicate network, can be affected by the presence and nature of non network former cations. Indeed, strontium can play a different structural role: either as a modifier that participates to the network depolymerization or as a charge compensator at the proximity of $(AlO_4)^-$ tetrahedra.

4:20 PM

(GOMD-S3-055-2015) Structure in Surface Depletion Layers formed on Sodium Aluminosilicate Glasses by Thermal Poling

N. J. Smith*[1]; I. Dutta[1]; C. W. Ponader[1]; 1. Corning Incorporated, USA

Thermal poling processes can be used to form modified surface layers on glass with induced second-order nonlinear optical activity, and under some conditions results in structurally-altered layers depleted of electrically-mobile, network-modifying cations on the anodic surface. An outstanding question in this realm is how different "parent" glass structures reform in such a way so as to satisfy the bonding and charge requirements of network-forming elements inside such modifier-depleted surface layers. This phenomenon is particularly not well understood in aluminosilicate glass compositions, where aluminum ions in the parent glass are predominantly present as charge-compensated $[AlO_4]^-$ tetrahedra prior to poling. In this talk, we summarize results of an investigation into the structure of such layers for a range of simple sodium aluminosilicate glasses, using surface-sensitive methods such as IR ellipsometry, TEM-ELNES, and Al K-edge XANES to directly interrogate the atomic structure.

Session 4: Modeling and Simulations of Glasses I

Room: Symphony Ballroom IV
Session Chairs: Jincheng Du, University of North Texas; Walter Kob, Universite Montpellier 2

3:40 PM

(GOMD-S3-056-2015) Molecular dynamics simulations of borate and borosilicate glasse

L. deng*[1]; J. Du[1]; 1. University of North Texas, USA

Borosilicate glasses find wide industrial and technological applications. Their atomic structures are critical to understand the properties and behaviors of these glasses but structural understanding is usually complicated by the compositional dependence of boron coordination change and possibly larger boron containing structure units. In this paper, we present development of potentials that are capable of describing the coordination change and other structure features of borosilicate glasses and the application of these potentials to study the structure and properties of several sodium borate and borosilicate glasses using molecular dynamics simulations.

4:00 PM

(GOMD-S3-057-2015) Physicochemical properties of nuclear glasses (SiO_2-B_2O_3-Na_2O-La_2O_3) by Molecular Dynamics simulations

F. Pacaud*[1]; M. Salanne[1]; J. Delaye[2]; 1. Phenix Laboratory, France; 2. CEA Marcoule, France

Physicochemical properties of nuclear glasses (SiO_2-B_2O_3-Na_2O-La_2O_3) by Molecular Dynamics simulations. Silicon (SiO_2), boron (B_2O_3) and sodium (Na_2O) oxides are the main components of the industrial radioactive waste confinement glass (French R7T7 glass). The proposed study is about the simulations by Molecular Dynamics of sodo-borosilicate glasses (SiO_2-B_2O_3-Na_2O) to determine physical properties like density, electrical conductivity, viscosity and the structure for several compositions. A polarizable force field is developed to perform the simulations with different compositions. This force field is fitted with systems which are equilibrated by *ab initio* calculations (DFT). The force field has been validated by comparing the densities, the electrical conductivities, the viscosities and the boron coordinations to the experimental results. Moreover, the coexistence of threefold-coordinated and fourfold-coordinated boron atoms is reproduced for the first time in such borosilicate systems with this kind of force field. The studies of several sodo-borosilicate glass compositions allowed analyzing the impact of every component on the physicochemical properties. The same study is performed on SiO_2-B_2O_3-Na_2O-La_2O_3 with a force field based on the previous one including new terms describing the interactions with La.

4:20 PM

(GOMD-S3-058-2015) Transport anomalies, structure and ring structure in densified liquid B_2O_3

A. Baroni*[1]; G. Ferlat[1]; M. Salanne[1]; M. Micoulaut[1]; 1. Paris Sorbonne Universités, France

While there has been many studies devoted to densified tetrahedral liquids (silica, water, germania), little has been performed numerically on systems having a different local geometry (here BO3 planar triangles) such as in B_2O_3. Furthermore, the B_2O_3 system is one of the best known examples for which supra-molecular units are detected, and these consist of six-membered boroxol rings. The dynamical and structural properties of densified liquid B_2O_3 are investigated using Molecular Dynamics simulations based on a Aspherical Ion Model taking into account the increased effect of polarization with pressure. Results lead to an agreement of unprecedented quality with neutron determined structure functions under pressure (static structure factor, pair correlation function). The evolution of the local structure (from three-fold to four-fold boron) and intermediate range structure (boroxol rings) is followed with pressure and compared with neutron diffraction experiments Reference: A. Zeigler and al. Phys. Rev.B **90**, 024206 (2014).

4:40 PM

(GOMD-S3-059-2015) The role of oxygen packing in the structural transformations of oxide glasses (Invited)

A. Zeidler*[1]; P. S. Salmon[1]; 1. University of Bath, United Kingdom

Liquid and glassy oxide materials play a vital role in multiple scientific and technological disciplines. Here we investigate the structural transformations in silica, a building block of geophysically relevant silicates, as well as germania and B_2O_3. We show that an interplay between experiment and simulation leads to a new understanding of the pressure induced changes within these materials. A new structural map is devised for predicting the likely regimes of topological change. It is shown that this can be applied to a range of oxide materials. The information obtained can be used to forecast when changes may occur to the transport properties and compressibility of, e.g., fluids in planetary interiors, and is a prerequisite for the preparation of new materials following the principles of rational design.

Session 5: Mechanical Properties of Glasses IV

Room: Symphony Ballroom III

Session Chairs: Richard Bradt, University of Alabama; Morten Smedskjaer, Aalborg University; Stefan Karlsson, Glafo - the Glass Research Institute

1:20 PM

(GOMD-S3-060-2015) Mechanical Property and Nanostructure of Anisotropic Glass (Invited)

S. Ito*[1]; S. Inaba[1]; H. Hosono[2]; J. Endo[1]; 1. Asahi Glass Co., Ltd., Japan; 2. Tokyo Institute of Technology, Japan

Glass has generally isotropic structure, but it has anisotropic structure with birefringence when its structure is frozen under stress. We investigated the relation between mechanical property and anisotropy of alkali phosphate glasses. Thin rod-like samples of 0.05-0.5 mm in diameter were prepared by being drawn directly from melt near Tg and cooled to room temperature under tension. It was confirmed that the multi alkali metaphosphate glass of (Li, Na, K, Cs)PO_3 had a highly oriented P-O-P chain structure and a large birefringence, compared to single alkali metaphosphate glasses. The anisotropic glass showed the increase in strength and Young's modulus parallel to the tensile direction with increasing birefringence. It showed also a huge lengthwise shrinkage of about 35 % via an endothermic process without volume change upon heating above Tg and relaxing its anisotropic structure. This shrinkage was induced due to entropic elasticity. The unusual and unique mechanical properties in the anisotropic glass will be discussed in terms of the structure and interaction of the -P-O-P- chain in glass.

1:50 PM

(GOMD-S3-061-2015) Silica deformation under a uniaxial stress: a non-isotropic material behavior

B. Champagnon*[1]; S. Degioanni[1]; C. Martinet[1]; 1. Université Lyon1, France

Under a uniaxial stress silica deformation is not isotropic. This behavior was first observed for silica glass fibers in which "the existence of asymmetric hollows in the open silica glass structure deformed and oriented by the fiber drawing process was shown". This anisotropy was quenched by the rapid cooling of the silica fibers(1). In permanently densified silica a differential stress and a residual anisotropy were also observed for uniaxial stress compressions at room temperature above the elastic limit(2). Very recently Brillouin scattering measurements have shown that this anisotropy exist even in the elastic domain(3).These results will be discussed and compared with Molecular Dynamics Simulations and related to the deformation of the atomic silica structure under stress. 1. J.Murach and R.Bruckner Journal of Non-Crystalline solids 21 (1997)250 2. T.Sato, N.Funamori, T.Yagi J.Appl.Phys.114 (2013)103509 3 B.Champagnon, S.Degioanni, C.Martinet J.Appl. Phys.116(2014)123509

2:10 PM

(GOMD-S3-062-2015) Unit polarizability as a predictor of stress-optic response

J. Galbraith[1]; J. Zwanziger*[1]; 1. Dalhousie University, Canada

In an effort to understand the physical basis of the empirical model we proposed relating bond length and cation coordination number to stress optic response, we have discovered that unit polarizability is at least as effective in predicting the response. This new approach, which quantifies and extends an earlier model of Weyl, involves relating the polarizability of cation-based polyhedra to the stress-optic response. This quantity includes we believe the essential information in the earlier bond length/coordination number model, in a way much closer to the physics of light-atom interactions, and furthermore provides a more accurate correlation with both the stress-optic and elasto-optic responses. This new approach will be outlined as well as its extension to understanding dispersion of the stress-optic response.

2:30 PM

(GOMD-S3-063-2015) Mechanical Properties of Densified Silica Glass (Invited)

L. Huang*[1]; 1. RPI, USA

Molecular dynamics (MD) simulations were carried out to study densified silica glass prepared by pressure-quenching from the non-rigid state. Density and elastic moduli including the Poisson's ratio of silica glass increases with the increase of the quenching pressure. Uniaxial tension, nano-indentation and fracture tests all show a brittle-to-ductile transition with increasing density and Poisson's ratio of silica glass. In densified silica glass, more and more silicon atoms become five coordinated with oxygen atoms with the increase of density. These five-coordinated silicon atoms create additional energy dissipation pathway and facilitate shear flow during mechanical tests and play a critical role in the mechanical behaviors of densified silica glass. In addition, the correlation between densification, shear flow and Poisson's ratio is examined and a qualitative explanation is proposed.

3:20 PM

(GOMD-S3-064-2015) Thermodynamics of the Dilation Anomaly in Ion Exchange Strengthening

P. Gupta*[1]; P. Kreski[1]; A. Varshneya[1]; 1. Saxon Glass Technologies, Inc, USA

Recent experimental and simulation studies of ion-exchange stresses have revealed a discrepancy between the experimentally measured residual surface compression values and those expected from theory. We attribute the source of this discrepancy – known as the dilation anomaly – to a fast secondary relaxation taking place on a time scale of nanoseconds. A thermodynamic analysis of the secondary relaxation is formulated to rationalize the dilation anomaly.

3:40 PM

(GOMD-S3-065-2015) Mechanical models for viscoelastic relaxation during ion exchange in glass

A. Varshneya*[1]; P. K. Kreski[1]; G. A. Olson[1]; P. K. Gupta[1]; 1. Saxon Glass Technologies, Inc., USA

Measured surface compression in a soda-lime silicate glass as a function of immersion time from a few minutes to several days in molten KNO_3 bath is presented. The difference between these data and those from Cooper-Krohn argument is analyzed. MD simulations suggest that, after a fraction of a picosecond buildup, the stress rapidly relaxes to a polyamorphic structure which is unattainable on a V-T (P=1) diagram. Over the next few nanoseconds, the structure further relaxes to reduce the stress even in a topologically constrained constant volume condition. The next relaxation allows swelling in a biaxial plate where shape is no longer preserved. The final step to stress release is the volume and shape relaxation due to viscous flow to approach the compositionally-equivalent as-melted ("CEAM") structure with changed topology. The viscoelastic relaxation behavior of glass is simulated using springs and dashpots in series and parallel configurations.

4:00 PM

(GOMD-S3-066-2015) Warp reduction during chemical strengthening of float-produced thin flat soda lime silicate glasses: I, Thermal treatment

A. Varshneya*[1]; P. Kreski[1]; G. Olson[1]; 1. Saxon Glass Technologies, Inc., USA

Float-produced flat soda lime silicate glasses have chemically asymmetric surfaces. Presence of tin on the underside impedes the penetration of K ions relative to the upper side ("air surface"), hence, the air side usually develops a convex shape in substrates thinner than ~1 mm after immersion in a molten KNO_3 bath for chemical strengthening. This is a deterrent to their use in personal electronic communication devices. By a careful short exposure to heat in air, the disparity in surface chemistry of the two surfaces is reduced resulting in reduced warp during the chemical strengthening treatment. These then represent a cost-effective alternative to the traditional aluminosilicate glasses manufactured using non-float technology. (Patent application US 2014/0178663 A1).

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(GOMD-S3-067-2015) Warp reduction during chemical strengthening of float-produced thin flat soda lime silicate glasses: II, Differential methods

P. Kreski[1]; T. Goldberg[1]; A. Varshneya*[1]; 1. Saxon Glass Technologies, Inc., USA

Warp in thin chemically strengthened float-produced flat soda lime silicate glasses due to differential surface chemistry of the two surfaces is compensated by three different differential paste-based methods. Our methods utilize: (1) different time exposure, (2) different salt chemistry and (3) different areal density on the two surfaces. Each method represents a competitive commercializable option to the usual immersion-based chemical strengthening method. Paste-based methods have the distinct advantage that they avoid expensive molten salt bath maintenance. (Patent applications US2014/0178689, US2014/0178690, and US2014/0178691).

4:40 PM

(GOMD-S3-068-2015) Electric field assisted ion exchange of soda lime silicate and borosilicate glass tubes

A. Talimian*[1]; V. M. Sglavo[1]; 1. Universitá degli Studio di Trento, Italy

In this study, soda lime silicate and borosilicate glass tubes were subjected to electric field assisted sodium-potassium ion exchange process. Electric fields with intensities of 500, 1000 and 2000 V/cm were applied to test tubes immersed in a molten potassium nitrate. The current was controlled to avoid arc formation during the process. The mechanical properties were checked by four point bending and the Vickers indentation; the potassium concentration profiles was studied by energy dispersive x-ray spectroscopy. Monitoring the current demonstrates it increases at first, reaches a maximum, and then decreases continuously; the soda lime silicate tubes break apart after a certain time due to the stress build up. The decreasing rate and the saturation point are depended to the field intensity. The bending strength reveals that introducing residual stress layers on both inner and outer sides of tubes by changing the polarization of the applied field is more efficient than applying the field only in one direction. Vickers indentation demonstrates that the residual stress prevents formation of radial cracks. The potassium concentration profiles demonstrate there is a layer with high potassium concentration below the surface. In conclusion, the electric field can be used to accelerate the chemical tempering of soda lime silicate and borosilicate glass; however, more studied are recommended.

5:00 PM

(GOMD-S3-069-2015) Effect of KNO_3 molten bath Na enrichment on the mechanical performances of ion-exchanged soda-lime-silicate float glass

V. M. Sglavo*[1]; H. Hassani[1]; 1. University of Trento, Italy

Chemical tempering of glass by ion-exchange process has gained notable interest during the last years because of its flexibility in reinforcing components of different geometries and the possibility to obtain strengths much higher than in thermal tempering. In a typical industrial process, sodium atoms in the glass are substituted by potassium ions diffusing from the molten salt. An interesting aspect regards the poisoning of the bath after each process and its enrichment in sodium. In the present work, a systematic analysis of the effect of the sodium concentration in the bath on the performances of the strengthened glass has been carried out. Soda-lime-silicate float glass samples were subjected to ion-exchange in KNO_3 baths containing controlled limited amount of $NaNO_3$. The flexural strength was measured by a ring-on-ring test method, the compressive stress was determined by optical methods and the surface chemical composition of the glass was analyzed by Energy Dispersion X-ray Spectroscopy (EDXS). The results point out that the residual stress decreases in a non linear and monothonic fashion as a function of the sodium concentration within the bath; the same is for the potassium surface concentration and the flexural strength. A threshold for the Na cotamination within the molten KNO3 which guarantees elevated performances can therefore be identified.

Session 7: Response of Glass to Extreme Conditions

Room: Symphony Ballroom I
Session Chair: Mario Affatigato, Coe College

3:40 PM

(GOMD-S3-070-2015) Surface interactions on glass optics during fabrication, post-processing & laser operation (Invited)

T. Suratwala*[1]; 1. Lawrence Livermore Nat'l Lab, USA

Glass optics have a variety of uses in commercial and fusion energy laser systems. The glass surface quality typically limits fluence operation of many high-peak-power laser systems. During the fabrication, post-processing, and laser operation, numerous and complex surface interactions occur which can create, modify, and/or remove surface precursors which can cause localized laser damage via direct absorption & heating or downstream modulation of the incoming laser light. The progress for understanding these interactions, the resulting surface precursors, and the methods to mitigate them are reviewed. During optical fabrication, complex interactions between grinding or polishing particles, liquid medium, and lap material with the glass surface create many of these surface precursors. In particular, the creation and managing fractures during various grinding steps, the creation and prevention of polishing microfractures during polishing due to rogue particles are reviewed. During post-processing, various treatments (chemical or laser) can be used to modify the surface. Some of these process technologies, including a novel etch process (called AMP) on fused silica optics, a CO_2 laser ablation process to repair damage sites, and a laser conditioning process on glass optics with multi-layer dielectric coatings, have greatly improved the survivability of such optics to high laser fluence.

4:10 PM

(GOMD-S3-071-2015) Extreme-condition response of glass under moderate electric field, temperature and stress

C. McLaren*[1]; W. Heffner[1]; H. Jain[1]; 1. Lehigh University, USA

Recently, field-assisted viscous flow of glass was reported, indicating that application of DC field significantly lowers the softening temperature. Field-induced softening (FIS) occurs with application of moderate external electric fields and pressures. Under these parameters individually, the FIS effect should not be dramatic. However, when moderate external electric field and pressure are applied with increasing temperature, the glass behaves similar to dielectric breakdown that is known to occur only under extreme conditions. There appears to be a synergistic response from the combined effect of ohmic heating, electrolysis and finally dielectric breakdown, creating a complex mechanical response as seen under extreme conditions. We have expanded the scope of these observations, focusing on the mechanisms of FIS by exploiting the mixed-alkali effect. Samples of lithium-sodium silicate and sodium aluminosilicate glasses were prepared and tested mechanically in situ under compression (10 MPa) in external electric field ranging from 0 to 300 V/cm. The role of ohmic heating from alkali diffusion, that appears to be the major cause of FIS, is delineated from other field-induced effects. Just before field-induced softening, photoemission occurs near the anode with a broad band and several characteristic wavelengths of light, believed to be related to dielectric breakdown mechanisms.

4:30 PM

(GOMD-S3-072-2015) High Temperature Infrared Glasses for Optical Fiber Sensing

J. Roth*[1]; S. Martin[1]; J. Ballato[2]; 1. Iowa State University, USA; 2. Clemson University, USA

Non-oxide glasses are being developed for infrared fiber-based sensor assemblies. Many of these compositions are resistant to radiation-induced darkening, but their relatively weak chemical bonding limits their thermal stability, as seen in systems like As_2Se_3. In this study, a different family of ionic rather than covalent non-oxide infrared transparent glasses, based on the BaS + La_2S_3 + GeS_2 ternary system, is being explored. Glass compositions are melted in silica ampoules at 1175°C for 24 hours then quenched in air. These glasses are found to have some of the highest Tg's for chalcoginide based glasses. As the amount of modifer is added to the base GeS_2 glass the Tg was found to increase as expected. The Tg for GeS_2 glass is around 400°C but with the addition of 5 mol% BaS and 5 mol% La_2S_3 the Tg is raised to about 610°C. Infrared transmitting glasses of selected composition ratios have been made and the infrared transmission and glass transition temperatures have been measured. Future plans are presented to advance the glass optical and radiation-resistance properties.

4:50 PM

(GOMD-S3-073-2015) Chemical durability of 'forbidden' glasses

R. A. Schaut*[1]; S. A. Tietje[1]; 1. Corning Incorporated, USA

The chemical durability of glass is heavily influenced by both glass composition and structure. For example, despite having very similar network structures, melt-derived potassium silicates are known to have substantially degraded chemical durability relative to their sodium silicate analogs. As ion-exchanged glasses (i.e. K for Na) gain popularity and application space, the chemical durability of the surface produced could be driven by the change in chemistry (poor durability resulting from potassium-rich surface), the parent structure of the glass (good durability driven by melt-derived network structure), or the presence of stress. Here we separate the role of glass chemistry from structural effects through the use of ion exchange and heat treatments. The durability of melt-derived glasses is compared to ion-exchanged glasses with the same chemical composition. We discuss dissolution rate as of function of glass composition in strong acid and base solutions in relation to the influence of alkali identity, stress, molar volume and network structure.

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 3: Optical Thin Film and Planar Devices

Room: Concerto A
Session Chair: Juejun Hu, MIT

1:20 PM

(GOMD-S4-037-2015) Nanophotonic chalcogenide glass device fabrication using electron beam lithography

Q. Du*[1]; H. Lin[2]; C. Smith[3]; K. Richardson[3]; J. Hu[1]; 1. MIT, USA; 2. University of Delaware, USA; 3. University of Central Florida, USA

Chalcogenide glasses stands out as an important material for phonics due to its wide transparency window in the IR region and high refractive indices. Thin film chalcogenides are typically patterned using photolithography followed by plasma etching or lift-off process. Here we report the fabrication and characterization of chalcogenide glass waveguides and optical resonators using electron beam lithography followed by reactive ion etching or lift-off. Compared to optical lithography, the new fabrication protocol offers significantly enhanced pattern resolution and fidelity.The relation between device performance and material processing is examined in the context of optical loss and sidewall roughness in the fabricated photonic structures.

1:40 PM

(GOMD-S4-038-2015) Flexible chalcogenide glass waveguide-integrated photodetectors

L. Li*[1]; H. Lin[1]; Q. Du[2]; C. Smith[3]; K. Richardson[3]; J. Hu[1]; 1. University of Delaware, USA; 2. Massachusetts Institute of Technology, USA; 3. University of Central Florida, USA

Photodetectors or light receivers are important components for imaging, communications and sensing applications. Traditional photodetectors are typically made on rigid semiconductor substrates and couple to incident light via free space. Here we present the experimental demonstration of waveguide-coupled flexible photodetectors. The devices are fabricated by combining our glass photonic integration technology on flexible substrates (Nat. Photonics **8**, 643-649) with an alignment-free adhesive bonding approach to incorporate InP multi-quantum-well active layers. Optical performance at 1550 nm wavelength and mechanical properties of the flexible photodetectors will be presented.

2:00 PM

(GOMD-S4-039-2015) Hydrogenated amorphous silicon for nonlinear optic applications

D. Choi*[1]; X. Gai[1]; B. Luther-Davies[1]; 1. Australian National University, Australia

Recently, hydrogenated amorphous silicon (a-Si:H) attracts a significant interest from photonics community due to its CMOS-compatibility, low-temperature deposition facilitating back-end integration with CMOS electronic chips. It also proves to be a highly promising nonlinear material for power efficient photonic devices due to its ultra-high optical nonlinearity and low nonlinear loss relative to crystalline silicon. In this work we optimized the deposition of a-Si:H thin films, developed the fabrication of photonic wires and micro-ring resonators, and characterized the produced devices. We deposited the films by plasma-enhanced chemical vapour deposition using silane as a dominant precursor gas, mixed with helium. By investigating the effect of deposition parameters - substrate temperature, input rf power, gas flow rates, chamber pressure, etc. upon the film properties, we obtained high quality a-Si:H film with smooth surface and low optical attenuation around 0.3 dB/cm. Electron beam lithography and plasma dry etching were employed to fabricate sub-micron wide waveguides. The measured propagation loss from 500 nm wide, 200 nm tall wire was 5-6 dB/cm in TE mode. We also designed, fabricated, and characterized a-Si:H micro-ring resonators.

2:20 PM

(GOMD-S4-040-2015) Deposition of luminescent quantum dot doped chalcogenide glass films from solution

S. Novak*[1]; W. Liyanage[2]; C. Li[3]; H. Hodei[3]; C. Smith[3]; N. McClenaghan[4]; M. Khajavikhan[3]; M. Nath[2]; W. Deng[3]; K. Richardson[3]; 1. Clemson University, USA; 2. Missouri S&T, USA; 3. University of Central Florida, USA; 4. Universite Bordeaux, France

The incorporation of luminescent quantum dots (QDs) into chalcogenide glass (ChG) films provides the potential to fabricate an integrated light source for microphotonic chemical sensing devices. In contrast with physical vapor deposition methods, solution-based methods allow doping by simple mixing of the ChG solution with QDs prior to film deposition. Two methods of solution-based film deposition were used, including traditional spin-coating, and electrospraying, which we have applied to ChGs for the first time. Dispersion of the QDs continues to be the main challenge, as the high surface energy of the QDs makes them prone to aggregation. Potential solutions to this problem include tuning the surface energy to reduce the thermodynamic driving force of aggregation, or kinetically trapping the QDs within the film before aggregation can occur. This study compares the deposition of $Ge_{23}Sb_7S_{70}$ films by spin-coating and electrospray, and evaluates them with the aim of optimizing QD dispersion within the film matrix. Transmission electron microscopy was used to analyze the dispersion of QDs, and the luminescent properties of the doped films were also measured.

Session 2: Optical Fibers I

Room: Concerto A
Session Chair: Frederic Smektala, Universite de Bourgogne

3:40 PM

(GOMD-S4-041-2015) Advances in infrared fibers (Invited)

G. Tao*[1]; A. F. Abouraddy[1]; 1. University of Central Florida, USA

Infrared fibers offer a versatile approach to guiding and manipulating light in the infrared spectrum, which is becoming increasingly more prominent in a variety of scientific disciplines and technological applications. Despite well-established efforts on the fabrication of infrared fibers over the past decades, a number of remarkable breakthroughs have recently rejuvenated the field – just as related areas in infrared optical technology are reaching maturation. In this review, we describe both the history and recent developments in the design and fabrication of infrared fibers including infrared glass and single-crystal fibers, multimaterial fibers, and fibers that exploit the transparency window of traditional crystalline semiconductors. This interdisciplinary review will be of interest to researchers in optics and photonics, materials science, and electrical engineering.

4:20 PM

(GOMD-S4-042-2015) All-solid chalcogenide microstructured optical fibers exhibiting photonic bandgap propagation

C. Caillaud*[1]; G. Renversez[3]; L. Brilland[2]; D. Mechin[2]; J. Adam[1]; J. Troles[1]; 1. Institut des Sciences Chimiques de Rennes - University of Rennes 1, France; 2. PERFOS - R&D Platform of Photonics Bretagne, France; 3. Aix-Marseille Université - CNRS - Centrale Marseille - Institut Fresnel UMR 7249, France

Light propagation with single-mode regime in infrared has been demonstrated in all-solid chalcogenide microstructured optical fibers, theoretically and experimentally. An original way to obtain single-mode fibers is to design microstructured optical fibers (MOFs). In this study, two configurations of all-solid chalcogenide microstructured optical fibers were obtained and characterized. These configurations consist of replacing the air holes of the microstructured optical fiber by another chalcogenide glass. The first category of fibers is made of $As_{40}S_{60}$ low refractive index inclusions (n=2.4) embedded in an $As_{38}Se_{62}$ glass matrix (n=2.8). The second type of fiber consists of the same $As_{38}Se_{62}$ glass matrix with inclusions of high refractive index glass based on $Te_{20}As_{30}Se_{50}$ (n=2.9). Concerning the first category of fibers, refractive index contrast between the $As_{38}Se_{62}$ and As_2S_3 is sufficient to allow a confinement of the light in the core of the fiber. The single-mode guiding of the fiber has been shown theoretically and experimentally. In the second case, several transmission bands have been observed in the mid-infrared depending on the geometry. This behavior is typical of a photonic bandgap guiding. For the first time, single-mode propagation by photonic bandgap effect in a chalcogenide microstructured optical fiber has been observed at 3.39 μm.

4:40 PM

(GOMD-S4-043-2015) Photo-inscriptible silver-containing phosphate glass fibers

S. Danto*[1]; J. Desmoulin[1]; F. Désévédavy[2]; F. Smektala[2]; Y. Petit[1]; L. Canioni[1]; M. Dussauze[1]; V. Rodriguez[1]; E. Fargin[1]; T. Cardinal[1]; 1. University of Bordeaux, France; 2. University of Burgundy, France

Here we propose silver-containing phosphate glass fibers with new or improved functionalities that stem from altering both the materials composition and the fiber arrangement. Tailored silver-containing phosphate glass materials possess excellent thermo-viscous ability and linear/non-linear optical properties. Beyond they have proven to offer a promising matrix for the direct femto-laser-induced structuring of fluorescent patterns. Building on their properties, methodology for the fabrication of photo-sensitive, photo-inscriptible silver-containing phosphate glass fibers is presented. The strategy consists in selecting the most suitable materials for the targeted application, to develop the fiberization technique, to test and adopt innovative fiber geometry and to establish correlation between fiber architectures, materials chemistry and properties. We believe these results could lead to a decisive breakthrough in the field of photosensitive fiber. Direct laser-writing on fiber could offer a powerful alternative to bottom-up synthesis methods for producing multi-scale structured patterns with photo-luminescent, nonlinear or innovative plasmonic effects.

5:00 PM

(GOMD-S4-044-2015) Cladded single crystal fibers for high power single frequency fiber lasers

W. Kim*[1]; B. Shaw[1]; C. Askins[1]; J. Peele[2]; D. Gibson[1]; S. Bowman[1]; S. Bayya[1]; J. Sanghera[1]; 1. Naval Research Laboratory, USA; 2. Sotera Defense Solutions, USA

Crystal fibers are advantageous over glass fibers for single frequency fiber lasers due to their higher thermal conductivity, high SBS threshold, excellent environmental stability, and higher doping concentrations. These crystal fiber lasers would pave the way forward for very high-power single frequency fiber lasers; each Yb:YAG crystal fiber potentially capable of ~17 kW output power [1], which significantly exceeding the capabilities of existing Yb doped silica glass fiber lasers (<2kW). In this paper, we present our recent efforts on developing single-mode cladded single crystal fibers. Results on the growth of various single crystal fibers, the application of cladding materials on the core crystal fibers, and the laser, optical and physical properties of these cladded single crystal fibers are presented. [1] J. W. Dawson, M. J. Messerly, J. E. Heebner, P. H. Pax, A. K. Sridharan, A. L. Bullington, R. J. Beach, C. W. Siders, C. P. J. Barty, M. Dubinskii., “Power scaling analysis of fiber lasers and amplifiers base on non-silica materials,” Proc. SPIE 7686 (2010).

Symposium 5: Glass Technology and Cross-cutting Topics

Session 4: Waste Glass Corrosion II

Room: Concerto C
Session Chair: Stephane Gin, CEA

1:20 PM

(GOMD-S5-027-2015) The effect of high sodium waste streams on the product quality of UK vitrified high level waste

M. Harrison*[1]; C. Steele[2]; 1. National Nuclear Lab (UK), United Kingdom; 2. Sellafield Ltd, United Kingdom

Sodium carbonate is currently being considered as a wash-out reagent for the unagitated Highly Active Liquor (HAL) storage tanks at Sellafield. This will result in a feed to the Waste Vitrification Plant (WVP) containing high concentrations of sodium as well as the high molybdenum expected to be present in any settled tank solids. In a previous study, it was shown that at high molybdenum incorporations (10–12 wt% on an oxide basis) there was very little tolerance in the new Ca/Zn-containing base glass for extra sodium before the formation of significant yellow phase. Hence, it was concluded that the waste loading in the glass was limited by the high sodium in the wash-out liquor rather than the molybdenum. The work reported here extends the previous study to include; the use of lower wash-out waste loadings in order to increase the amount of sodium that can be accommodated in borosilicate glasses, a broadening of the waste envelope to include higher proportions of reprocessing waste, and the use of base glass compositions other than borosilicates, e.g. phosphates. In these experiments, small scale melts (50 g) were initially carried out in order to determine incorporation limits, followed by a fuller product quality assessment on larger batches at these limits. The characterisations included bulk density, crystallinity, durability, glass transition temperature, and viscosity.

1:40 PM

(GOMD-S5-028-2015) Dissolution of UK high level nuclear waste glass under conditions relevant to geological disposal

C. L. Corkhill*[1]; N. Cassingham[1]; C. Mann[1]; D. J. Backhouse[1]; R. Hand[1]; N. Hyatt[1]; 1. The University of Sheffield, United Kingdom

We present recent results obtained from static and flow-through dissolution experiments performed on simulant UK Magnox – Thorp blended high level waste (HLW) glass. A range of alkaline pH values were chosen to represent a geological disposal scenario where clay backfill buffers ground water to pH 7.0 - 11.0, while cementitious pore water was used as the dissolution medium to represent conditions of a co-located intermediate level waste and HLW repository. Dissolution data derived from single-pass flow-through techniques were applied to the TST kinetic rate law to determine the fundamental parameters necessary to model the dissolution kinetics of UK HLW glass: activation energy ($_{Ea}$), pH power law coefficient () and the intrinsic rate constant (k_0). Forward dissolution rates suggested that the dissolution mechanism was not sensitive to composition as defined by the wt% loading of Magnox waste. Dissolution in the presence of cementitious pore water, with high concentrations of Ca (> 200 mg L^{-1}), was found to be an order of magnitude lower than dissolution in water. This mechanism of dissolution was found to be controlled by the incorporation of Ca into the hydrated surface and subsequent precipitation of C-S-H phases, characterised using surface analytical techniques and thermodynamic modelling.

2:00 PM

(GOMD-S5-029-2015) Characterisation of Corroded Simulant UK Magnox HLW Glass using ToF-SIMS

N. Ahmad*[1]; S. Fearn[1]; J. R. Jones[1]; W. E. Lee[1]; 1. Imperial College London, United Kingdom

UK high level nuclear waste (HLW) glass from Magnox fuels has higher magnesium and aluminium contents than HLW glasses from other countries, which renders it more reactive. As the glass wasteform has to retain radioelements for thousands of years during geological disposal, understanding of the UK HLW glass corrosion mechanism is of great importance. In this project, a non-radioactive UK HLW simulant glass was subjected to aqueous corrosion in a static mode at 90 °C in deionised water for a period of one to four weeks. These glasses were then assessed using Ion ToF-Secondary Ion Mass Spectrometry (SIMS) to observe the elemental distribution via ion mapping and the data obtained were extrapolated as a function of depth. Cross-sectional images of the glass were captured using Transmission Electron Microscopy (TEM) and the composition of layers observed after leaching were assessed using Energy Dispersive X-ray spectroscopy (EDX). This innovative sample preparation for characterization allowed evidencing phenomena such as ion exchange and hydrolysis at the initial stage of corrosion process. At longer leaching times, re-precipitation of leached ions led to the formation of an ‘alteration layer’ on the glass surface.

2:20 PM

(GOMD-S5-030-2015) Effect of Ca and Mg Addition on the Aqueous Durability of Glasses in High-pH Environments

R. Hand[1]; D. J. Backhouse*[1]; C. L. Corkhill[1]; N. Hyatt[1]; 1. University of Sheffield, United Kingdom

The unique role of Ca and Mg in forming surface alteration layers on HLW glass under high-pH conditions, as are possible within a proposed UK geological disposal facility (GDF), was investigated. Long-term durability experiments were conducted on a range of borosilicate glasses using the PCT-B protocol at 50 °C, representative of the likely temperatures within a GDF. These glasses contained varying CaO and MgO contents, ranging from 0 to 10 mol.%, with $Ca(OH)_2$ and KOH/KCl solutions (pH 11.6) used as leachants. Aqueous analytical data up to 112 days show increased dissolution of all glasses in KOH/KCl, and a decrease in dissolution with increasing CaO and MgO contents. ^{11}B, ^{27}Al and ^{29}Si NMR analysis suggests that the compositions which exhibit lower dissolution have higher network connectivity. SEM-EDX of altered samples suggests that an alteration layer is only formed in the presence of Ca or Mg. The presence of Ca or Mg at high-pH, whether in solution or within the glass matrix, leads to a reduced level of glass dissolution due to the formation of a protective alteration layer on the glass surface, which impedes further leaching.

2:40 PM

(GOMD-S5-031-2015) Glass alteration in alkaline conditions: comparison between SON68 and ISG

K. Ferrand*[1]; S. Liu[1]; K. Lemmens[1]; 1. sck-cen, Belgium

In Belgium, the *Supercontainer design* with Ordinary Portland Cement (OPC) was selected by ONDRAF/NIRAS as reference design for geological disposal of vitrified nuclear waste and Spent Fuel in the Boom Clay formation. Based on the general knowledge about the glass alteration in aqueous conditions at neutral pH, experiments were performed, allowing to determine the glass alteration rate, and to identify the key mechanisms responsible for the glass alteration in such alkaline conditions. Tests were conducted with the inactive French SON68 glass and the International Simplified Glass (ISG) at 30°C or 70°C and pH ranging from 9 to 13.5 using either a KOH solution or synthetic cementitious waters simulating the pore water in contact with OPC at different ages of degradation. For both glasses, the positive effect of Ca on glass dissolution was highlighted as already described by several authors. The evolution of the main constituents concentrations was similar for SON68 and ISG altered in the same conditions. The main discrepancy was noticed for tests at the higher temperature and pH. Geochemical modeling coupling diffusion and secondary phases formation can give a consistent explanation of both experimental data.

3:00 PM

(GOMD-S5-032-2015) Simulating Stage II → Stage III Dissolution with Saturated Glass Solutions

C. L. Trivelpiece*[1]; C. Pantano[1]; Y. Zhang[1]; 1. Pennsylvania State University, USA

The dissolution rate of silicate glass is usually observed to decrease upon reaching silica saturation in the contacting solution. But in complex multicomponent systems, a resumption of high rate dissolution can occur after long times. This phenomenon is usually coincident with crystallization of one or more phases in solution. We are using ‘saturated glass solutions’ (SGS) to simulate, accelerate and model this phenomena for simplified sodium borosilicate compositions. Here, we report the effects of lithium, aluminum and calcium on the equilibrium pH, solubility and precipitation of crystals. The glasses are crushed into powder and aged in water at 900C to produce the SGS. Aliquots of the SGS are periodically sampled, and the concentration of glass species in solution are measured via ICP-AES. Likewise, the solids in the digestion vessel are also sampled for detection and identification of crystalline phases. The precipitation of crystals is often accompanied by an abrupt decrease in the solution concentration of one or more species to a steady-state level, especially in simple binary systems. Presumably, this drives an increase in the dissolution rate of the glass. Thermodynamic modeling of the reactions using Geochemist Workbench is also reported.

Session 4: Waste Glass Corrosion III

Room: Concerto C

Session Chair: Mike Harrison, National Nuclear Lab (UK)

3:40 PM

(GOMD-S5-033-2015) Low-Temperature Alkali Diffusion in Boroaluminosilicate Nuclear Waste Glasses

S. Kerisit*[1]; J. J. Neeway[1]; Z. Zhu[1]; J. V. Ryan[1]; 1. Pacific Northwest National Laboratory, USA

Ion exchange is recognized as an integral mechanism influencing the corrosion of nuclear waste glasses. Corrosion experiments performed at 90 °C using isotopically tagged Li demonstrated that Li diffuses farther into the glass than H. This result is counter to previous understandings of glass corrosion, where water was believed to be at the forefront of any interactions within the glass structure. Due to the formation of alteration layers in aqueous conditions, it is difficult to conclusively deconvolute the mechanisms of ion exchange from other processes. Therefore, alkali diffusion was isolated by conducting a series of experiments in which glass coupons were contacted with a solution of ^{6}LiCl dissolved in DMSO at temperatures ranging from 25 to 150 °C for various periods of time and for two separate HLW simulant glasses (SON68 and CJ-6) and quartz. An interdiffusion model was developed to model the alkali depth profiles measured using tof-SIMS and to derive diffusion coefficients and their activation energies. The results show that Li from the non-aqueous solution exchanges with both Li and Na from the glass. Additionally, diffusion coefficients were found to vary significantly with depth due to changes in alkali concentrations and structural changes that occur during the exchange process. Implications for the long-term durability of nuclear waste glasses will also be discussed.

4:00 PM

(GOMD-S5-034-2015) The Effects of Lithium Ion Counter-Diffusion on Glass Dissolution

C. L. Trivelpiece*[1]; C. Pantano[1]; 1. Pennsylvania State University, USA

The purpose of this study was to investigate the counter-diffusion of lithium ions from an aqueous solution into a glass surface and how this phenomenon might affect the dissolution of nuclear waste glasses. Monolithic samples of two different simplified nuclear waste glass compositions based on SON68 were prepared by remelting cut pieces of the annealed glasses to obtain flat/smooth melt surfaces for neutron depth profiling (NDP). The monoliths were corroded in pH 9 and 10 NaOH and LiOH solutions, as well as pH 9 and 10 saturated glass solutions, which were prepared by dissolving lithium disilicate and sodium disilicate glasses in water. The NDP data for the corroded samples revealed that Li^+ ions did diffuse into the glass surfaces under some conditions as evidenced by measured lithium concentration depth profiles that were higher than that of the nominal composition. This was accompanied by a reduction in the thickness of the boron leached layer at the surface, suggesting that Li^+ ions counter-diffuse into the glass surface from solution and compete with protons for sites in the leached layer, thereby retarding the boron leaching reaction.

4:20 PM

(GOMD-S5-035-2015) Dissolution Rate of Borosilicate Glass SON68: A Method of Quantification Based upon Interferometry

J. P. Icenhower*[1]; 1. Sandia National Laboratory, USA

The dissolution rate of SON68 glass was determined in a single-pass flow-through (SPFT) system at 90 °C and pH 9 over a silica-saturation interval. Dissolution rates were determined on both powdered and monolithic specimens conducted at the same flow-rate (q) to surface area (S) ratio by assaying the concentration of elements released from glass to effluent solution by ICP methods. In addition, rates of twelve monolithic specimens were quantified using a Vertical Scanning Interferometry (VSI) method. The method entails measuring the difference in height between the surface that reacted with solution and a reference surface preserved by masking a small area on the monolith that prevented water from interacting with the affected area. The height difference is proportional to the dissolution rate. Values of the dissolution rate, based upon chemical assay on the one hand, and VSI methods on the other, were compared. Rates in experiments with dilute solutions were within experimental uncertainty to rates determined by the VSI method on monoliths, but rates determined by VSI on samples in Si-rich solutions were faster than rates determined by chemical assay (up to a factor of 3.5×). BSE images of the glasses contacted with Si-rich solutions indicate the presence of a secondary layer that causes the VSI method to underdetermine the true depth of chemical reaction.

4:40 PM

(GOMD-S5-036-2015) Evaluation of Glass Melt Surfaces with Aqueous Corrosion: An Atomic Force Microscopy Approach

Y. Gong*[1]; N. P. Mellott[1]; 1. Alfred University, USA

The aqueous corrosion of borosilicate glasses are of considerable scientific and engineering interest given potential applications including radionuclide containment. Prior to major scale usage of these glasses for nuclear waste storage, their aqueous corrosion behavior must be understood in detail. The majority of reported corrosion studies of borosilicate glasses rely heavily on elemental release from powdered glasses into solution. It has been shown however that to understand the corrosion behavior fully one must also examine the reacted glass composition, structure, and morphology. In fact, previous work in our group shows that initial surface morphology of glasses can impact the dissolution behavior. In this study, we examine the evolution of surface morphology prior to and throughout corrosion in basic solutions at ambient temperatures. Furthermore an attempt to measure the dissolution rate using atomic force microscopy will be described.

5:00 PM

(GOMD-S5-037-2015) Study of Composition Effects on Stage III Dissolution Using Glass Fiber

J. Rice*[1]; C. Trivelpiece[1]; C. Pantano[1]; 1. The Pennsylvania State University, USA

Vitrification is a common practice to immobilize radioactive waste for long-term storage in stable geological formations. Models for the initial stages of glass corrosion have been well developed. But little is known about the recent phenomena known as Stage III dissolution: an abrupt increase in the dissolution rate driven by the precipitation of one or more crystalline phases in the contacting solution. We are using glass fibers, a glass form with a high specific surface area and reproducible uniform surface, to simulate and accelerate the onset of this transition. Of particular interest is the glass composition dependence. Glass fibers have been fabricated with pure and various combinations/blends of both complex nuclear waste glasses (SON68 and AFCI) and a simplified 7-component glass (ISG). The fibers are corroded under static or flow conditions in various (high) pH and/or pre-saturated glass solutions. Under these conditions, the time dependent dissolution, crystallization, and physical alteration of the fibers can be observed at reasonable time scales. A common observation is transformation of the fibers into amorphous or crystalline tubes. The time and temperature dependence of this transformation is characterized using FESEM, TEM, and XRD to provide a physical model that can be related to the corresponding solution chemistry.

5:20 PM

(GOMD-S5-038-2015) An Interlaboratory Study on the Precision of ASTM C1285 Tests

W. Ebert*[1]; 1. Argonne National Lab, USA

The ASTM C1285 product consistency test (PCT) is routinely conducted to evaluate the durabilities of glasses being developed as potential waste forms based on the measured solution concentrations of soluble glass components. The PCT-A response is used as a characteristic measure that is compared with responses of other glasses (or a benchmark) and the PCT-B responses are commonly used to quantify dissolution rates under a range of test conditions. The current version of ASTM C1285 calls for removing fines from crushed glass prior to testing because the rapid dissolution of fines dominates the test response and greatly affects the values and precisions of the PCT-A and PCT-B measurements. An interlaboratory study was conducted to measure the precision of PCT conducted with ARM-1 and SRM 623 glasses that were carefully washed to remove fines. Sized and washed ARM-1 and SRM 623 glasses were prepared at ANL and provided to five participating laboratories to conduct triplicate tests under PCT-A conditions. The results and statistical analyses will be presented to show the precision of tests with each glass and compared with results from previous studies to show the impact of removing the fines on the test response and precision. These results will be used to up-date the test precisions reported for these glasses in ASTM C1285-14.

5:40 PM

(GOMD-S5-039-2015) Sr ion implantation in the obsidian glass for its performance assessment as a waste form under hydrothermal-like conditions in geological repository

N. Rani*[1]; P. Kumar[2]; R. Sharma[2]; S. Chopra[2]; G. Roonwal[2]; J. Shrivastava[1]; 1. UNIVERSITY OF DELHI, India; 2. IUAC, India

Naturally occurring obsidian is considered as potential natural analogue for radioactive waste form. However, Sr ion implantation and its alteration studies have not been carried out in details. Using SRIM code, the stopping range of Sr ions in obsidian glass were calculated and determined by RBS. The depth of penetration was determined by TRIM code calculations that helped to simulate trajectories and sputtering effects of ions in the obsidian. Present study mainly focussed on implantation of Sr ions in specimens using Negative Ion Implanter. To quantify retention of long lived ions in glass surface, pre and post ion implanted specimens were studied under hydrothermal-like conditions. It has been found that implanted Sr ions were retained in the matrix even in the high P, T conditions for a longer period and results have been discussed.

Wednesday, May 20, 2015

Varshneya Frontiers of Glass Science Lecture

Room: Symphony Ballroom IV

8:00 AM

(GOMD-AL-003-2015) Structural aspects of relaxational dynamics in glasses and supercooled liquids (Invited)

S. Sen*[1]; 1. University of California, Davis, USA

The structure of a liquid in equilibrium undergoes rapid rearrangement with time. The structural rearrangement processes, however, drastically slow down with decreasing temperature in a glass-forming liquid as the glass transition temperature T_g is approached from above and the liquid falls out of thermodynamic equilibrium. This kinetic slowdown is typically exemplified by the variation in the transport properties such as viscosity (or diffusivity) that can easily increase (or decrease) by ~ 15 orders of magnitude on cooling the liquid from T » 3*T_g to T » T_g. It is also at the very heart of nucleation and crystallization of a supercooled liquid and control the technological utility of glass and glass-ceramics. The dynamical processes associated with the viscous/diffusive transport have been treated in the literature principally as macroscopic phenomena within the framework of phenomenological models and often interrogated using bulk relaxation (volume, enthalpy, shear, dielectric, photon echo) experiments that typically lack a *direct* microscopic understanding of the atomic scale processes that accompany structural relaxation. On the other hand, the unique combination of the timescale associated with dynamical NMR spectroscopic techniques (ms to s) and the accompanying structural information, is ideally suited

*Denotes Presenter

for probing the mechanistic aspects of the relaxational dynamics at atomic/molecular level in glasses and viscous liquids. In this talk I will present an overview of the work from our laboratory in the recent years involving the application of such spectroscopic techniques to address the nature and timescales of the various thermally driven configurational changes in a wide variety of inorganic and organic glasses and supercooled liquids and their relationship to macroscopic relaxation and transport processes.

Symposium 1: Energy and Environmental Aspects - Fundamentals and Applications

Session 1: Flat Glasses, Capillaries, Foams and Enamels

Room: Concerto B
Session Chair: Joachim Deubener, Clausthal Univeristy of Technology

9:20 AM

(GOMD-S1-018-2015) Evidence for self-healing effect in a multilayer glass / vanadium boride coating

L. Montagne*[1]; T. Carlier[1]; F. Méar[1]; R. Podor[2]; S. Saitzek[1]; R. Desfeux[1]; J. Blach[1]; 1. University of Lille, France; 2. ICSM, France

Glasses and glass-ceramics are a technological solution to achieve efficient materials able to operate at high temperatures, such as for enamel protective coatings applications. To overcome cracking when subjected to thermal cycles, self-healing is a promising solution. The self-healing property is defined as the capacity of a material to recover its mechanical integrity and initial properties after destructive actions of external environment or under internal stresses. We report an innovative approach based on self-healing glassy thin films. They are based on a heterostructure made of alternating layers of glass-ceramics and active particles, deposited by pulsed laser ablation. The properties of the deposited films are optimized according to the number of pulse and laser power, atmosphere, temperature of the substrate, target-substrate distance. The characterization of the films has been carried out with ellipsometry, ToF-SIMS, AFM, microprobe and XPS, and ATR-FTIR spectroscopy. We also developed an original characterization based on DNP-NMR, which induces a substantial increase of NMR sensitivity, and thus enables analysis of thin films. Finally, the efficiency of the self-healing effect on nanometric scale thin-layers is demonstrated by an *in-situ* experiment performed into an environmental scanning electron microscope (HT-ESEM).

9:40 AM

(GOMD-S1-019-2015) Compositional Dependence of Alkali Resistance in $CaO–Al_2O_3–SiO_2$ Glasses

H. Takebe*[1]; S. Takahashi[1]; 1. Ehime University, Japan

The alkali resistance of $CaO–Al_2O_3–SiO_2$ (CAS) glasses was studied by MCC-2 static leaching method. CAS plate samples with a size of 9×9×2 mm were immersed in 1.3 mol/L NaOH aqueous solution at 180 0C for 72 h. The weight loss increased with increasing $[Al_2O_3]/[CaO]$ molar ratio for CAS glasses. Especially CAS glasses with $[Al_2O_3]/[CaO] \geq 0.8$ had relatively poor alkali resistance. After alkali resistance tests, a white-color layer appeared on the surface of glass samples. The results of SEM-EDX and XRD analyses revealed that an alumina-depleted intermediate layer with a main phase of tobermorite was formed between surface layer and glass part. IR spectra indicated that the CAS glasses with $[Al_2O_3]/[CaO] \geq 0.8$ contained mainly mixed-anion structures of SiO_4 and AlO_4 tetrahedra with ring-type morphology and the intermediated layer consisted of a similar mixed-anion structure and –OH, H_2O, and CO_3^{2-} absorption bands. The formation conditions of alumina tobermorite in the intermediate layer were discussed in terms of glass and crystalline structures.

10:00 AM

(GOMD-S1-020-2015) Influence of network modifiers on the glass system $ZnO-Al_2O_3-B_2O_3-SiO_2$

A. Deinhardt*[1]; M. Kilo[1]; S. Senger[1]; G. Sextl[1]; 1. Fraunhofer Institute for Silicate Research ISC, Germany

The decorative graphics and fonts that are emblazoned on laboratory and household glassware as well as medical vials really make an impression, but they contain up to 50 wt% of lead oxide and are therefore considered to be toxic. It was the aim of this research project to develop a low-melting lead-free glass decor, which can be applied as a coating on both, borosilicate and soda-lime silicate glass. The new glass system is based on $ZnO - Al_2O_3 - B_2O_3 - SiO_2$. Glass systems with melting temperatures between 540 - 600 °C could be developed, by adding additional alkali and earth alkali elements. The thermal expansion, the melting and the wetting behavior of the glass on soda lime glass and borosilicate glass were tested. Furthermore, the chemical stabilities both towards water as well as under high and low pH were investigated. The melting behavior of the coatings on borosilicate and soda-lime silicate glass were investigated in a temperature gradient furnace, which made it possible to assess the properties of the glass coating visually in dependence of the temperature. Potential crystallization can be also easily assessed by this method. Finally, the optical properties of the base glass and of glass, containing inorganic color pigments were tested. The most promising glass has a melting temperature of 530 °C and excellent hydrolytic stability, making it an ideal candidate for decorative imprints.

10:20 AM

(GOMD-S1-021-2015) Large-area fluidic windows (Invited)

L. Wondraczek*[1]; 1. University of Jena, Germany

Integration of micofluidics with window and facade elements enables various routes for improving the energy efficiency of buildings. As a prerequisite, however, such microfludic elements must be provided in large area and at low cost. In the present talk, a technology roadmap, exemplary applications and a status report on the recently established consortium "LaWin" will be presented. Possible solutions for active and adaptive windows, based on microfluidic glass sheet, will be discussed.

10:50 AM

(GOMD-S1-022-2015) Improving the thermal insulation properties of the foam glasses (Invited)

J. König*[1]; R. R. Petersen[1]; Y. Yue[1]; 1. Aalborg University, Denmark

Foam glass is a lightweight material used for thermal and acoustic insulation applications in the construction and other industries. It exhibits several advantages in comparison to insulation materials such as organic foams and mineral wool, e.g., water and steam resistance, freeze-thaw cycle tolerance, excellent chemical and thermal stability, and superior mechanical properties. In the last decade, the possibility of recycling different glass cullets and waste glassy materials into this high value added product has been presented. The main drawbacks of foam glass are its high unit price and somewhat higher thermal conductivity. These issues, however, are not addressed in the scientific community. Here, we present the background of the drawbacks of the foam glass and show our work for improvements. The improvements are based on the understanding of the foaming mechanism (this includes chemical reactions between glass and foaming agent(s), actual foaming reaction, physical and chemical properties of the glass and their changes, etc.), which leads to a foam glass product with preferable density, pore structure and pore gas. We investigate the dependence of the thermal conductivity of the developed foams on both chemical and processing conditions and finally describe the perspectives for further improvements of the foam glass.

11:20 AM

(GOMD-S1-023-2015) New Glass-Seal-Type for Solid Oxide Fuel Cells

B. R. Durschang*[1]; M. Kilo[1]; M. Müller[2]; S. Hornauer[2]; 1. Fraunhofer ISC, Germany; 2. ElringKlinger AG, Germany

High-temperature glass-seals for Solid Oxide Fuel Cells (SOFC) are well known. The specifications to be fulfilled by a glass seal are numerous: besides the chemical and mechanical stability for long times at operation temperatures above 800 °C, the thermal properties are important like thermal expansion coefficient and viscosity behavior. Up to now, seals were developed, where the glass show a good flowing behavior to ensure gas tightness. During the thermal assembling of up to 50 single cells to a stack, the whole stack or single cells are usually settled to significantly lower height. The relative displacement induced thereby inside the stack lead to high mechanical stress. At Fraunhofer ISC a new glass-seal-type was developed, where a gas tight sealing could be combined without a significant decrease in height starting from a screen printed paste having almost the final geometrical dimension of the joint. The new glass, a demixing borosilicate glass containing high amount of earth-alkaline oxides, sinters to a gas tight body before crystallization starts. The glasses were examined by thermo optical measurements, X-ray diffraction, SEM, mechanical, chemical and resistivity tests. The non-settling glass-seal show high mechanical strength, good chemical compatibility to the contact materials and excellent electrical resistivity.

11:40 AM

(GOMD-S1-024-2015) Glass capillaries for hydrogen storage (Invited)

M. Prewitz*[1]; P. Ried[1]; M. Gaber[1]; R. Müller[1]; K. Holtappels[1]; C. Marotzke[1]; 1. Federal Institute for Materials Research and Testing, Germany

Glass capillaries for hydrogen storage must provide low hydrogen permeability, excellent workability, high strength, and corrosion resistance. Burst pressure tests on fused silica, borosilicate glass, and barium alumosilicate glass capillaries showed that burst pressures up to 1 kbar can be achieved easily. This correlates with a circumferential strength of ≈ 275 MPa as estimated with FEM simulations. Safe handling of storage modules, however, requires further increase of strength as a safety factor. In this context, it is important to utilize the high strength of juvenile glass capillaries protected by polymer coating. FEM simulations revealed that, among various complex implications resulting from this concept, glass - polymer adhesive strength is most crucial for mechanical reliability. Thus, different elastic moduli can cause delamination and coated capillaries glued into steel valve caps can be pushed out below the burst pressure for non-adequate sealing lengths. Compared to this difficulty, hydrogen permeation measurements indicate that gas leakage is not significant if sealing length is above several millimeters. As being essential for storage systems, hydrogen permeability of the glasses was measured by means of EGA techniques. Lowest permeability was found for the alumosilicate glasses wherein the powder method turned out to be most sensitive.

Symposium 3: Fundamentals of the Glassy State

Session 2: Glass-ceramics

Room: Symphony Ballroom III
Session Chair: Mark Davis, SCHOTT North America, Inc.

9:20 AM

(GOMD-S3-074-2015) Don Stookey (1915-2014): Pioneering Researcher and Adventurer (Invited)

G. H. Beall*[1]; 1. Corning Incorporated, USA

Don Stookey, the father of glass-ceramics, was a pioneer in inducing and understanding nucleation in glass. His early work on opal glasses and photosensitive gold glasses led to an amazing series of inventions: Fotalite®, a photosensitive opal, chemically machined Fotoform® and Fotoceram®, and TiO_2-nucleated Pyroceram™ products including missile nosecones and oven-proof cookware. He received a basic patent on glass-ceramics that was affirmed in court. Don went on to demonstrate a clear photochromic glass that showed reversible darkening for thousands of cycles. This material became a fixture in the ophthalmic industry. He later invented a full-color polychromatic glass capable of yielding a permanent patterned and monolithic stained glass. In his life outside science, Don chaired an interfaith group that founded a home for the elderly in Corning. He was also a wilderness enthusiast, surviving a plane crash in the Arctic and two boat capsizings. Even in his later years he continued fishing off Florida and on Lake Ontario, and went solo on a trip to the Patagonian Andes. Don Stookey was a special person by any measure: an unassuming optimist, eminent scientist and inventor, adventurer, and beloved family man.

9:50 AM

(GOMD-S3-075-2015) Current topics in glass-ceramics R&D - an industrial perspective (Invited)

I. Mitra*[1]; 1. SCHOTT AG, Germany

Partly-crystalline materials are available in industrial scale fabricated by a two-step procedure. A base glass produced first subsequently undergoes a thermal treatment to provoke controlled crystallization. These glass-ceramics provide the advantages of conventional glass production, such as high homogeneity and lack of porosity, with specific properties of the embedded crystal phase. LAS–based glass-ceramics are established products, e.g. cooktop panels and oven windows, due to their outstanding performance of extremely low expansion. ZERODUR® is nowadays widely used in high-precision applications, e.g. metrology and microlithography, facing increasing demands in respect to thermal expansion. Among the broad field of emerging R&D topics, emphasis is given to glass-ceramics with electrically active crystals enabling the development of new electronic functional materials: Novel dielectric materials allow passive components such as capacitors for high voltage applications. Ferroelectric and varieties of nonferroelectric (polar) glass-ceramics revealed piezoelectricity up to elevated temperatures. Lithium-conducting glass-ceramics have received much interest as here described oxidic systems are chemically stable. Interesting high-temperature performance is demonstrated by lead-free glass-ceramics as oxide thermoelectrics, qualifying these new material classes as key-components for future energy management systems.

10:20 AM

(GOMD-S3-076-2015) Recent research in low thermal expansion glass-ceramics for new application (Invited)

S. Nakane*[1]; 1. Nippon Electric Glass, Japan

Transparent low-expansion glass-ceramics, traditional material with nanophase β-quarts solid solution crystals, have been used in the heat-resistant field like a cookware. The glass ceramics was first developed by Dr. Stookey more than 50 years ago, but still,

*Denotes Presenter

R&D is active and prospective. In recent years, the application of the glass-ceramics has been extended into electronic and optical devices and production process equipment. In conjunction with the appearance of new application, research of the glass ceramics from new perspective is necessary, for example, large sheet forming process, high thermal stability in inhomogeneous heating, and toxic substance free composition. Recently, we have developed forming process for producing large sheets by precise control of molten glass flow on the forming roller. This product created a market of setter and furnace lining for firing electronic parts. Some our research in the glass ceramics with approaching to new application will be demonstrated.

10:50 AM

(GOMD-S3-077-2015) Characterization of Pd-doped CMAS-TiO_2 Glass-Ceramics

M. J. Davis*[1]; P. Vullo[1]; M. Reich[2]; R. Golovchak[3]; C. Saiyasombat[4]; H. Jain[4]; 1. SCHOTT North America, Inc., USA; 2. SCHOTT AG, Germany; 3. Austin Peay State University, USA; 4. Lehigh University, USA

Electrical and microstructural characterization was performed on Pd-bearing and Pd-free, electrically-conductive glass-ceramics in the CMAS-TiO_2 system. AC impedance plots clearly revealed both grain-core and grain-boundary semicircles. Grain-boundaries had a lower magnitude of conductivity but a similar activation energy to grain-core conduction except when Pd was present, for which much lower activation energies were indicated. The lack of any frequency dependence of conductivity for $f < 100$ Hz while using noble-metal electrodes, suggests the conduction was dominantly electronic in origin in these glass-ceramics. Time-dependent polarization measurements showed no change in electrical current over several days, consistent with this conclusion. The temperature dependence of the conductivity was relatively low over a very large temperature range, but quite complex. The appearance of a sharp minimum in conduction seen near 600 °C suggests some type of transition occurred with our glass-ceramics, possibly related to semiconductor-to-metal transitions seen with some transition-metal crystals. The available data suggests that Pd did have some effect on grain-boundary conduction, but that a percolating Pd network was not formed. Attempts using SEM and TEM to identify where Pd resides in our glass-ceramics were only moderately successful.

11:10 AM

(GOMD-S3-078-2015) Element Partitioning and Residual Glass in Beta-Spodumene Glass-Ceramics

R. Youngman*[1]; C. Smith[1]; Q. Fu[1]; M. Comte[1]; 1. Corning Incorporated, USA

Glass-ceramics have been deployed in a variety of technological applications, capitalizing on the formability provided by the parent glass, as well as the resulting physical and optical properties of the crystalline phases grown during careful heat treatment of the glass. Understanding the development of crystal phases, composition and the residual glass structure and properties, is critical for exploration into new materials and applications involving glass-ceramics. Nuclear magnetic resonance (NMR) spectroscopy is uniquely suited for study of the short-range structure in a wide range of glass-ceramic compositions. This technique has proven useful in characterizing glass network structure, and in the case of glass-ceramics, can provide similar details on both the glass and crystalline phase(s). In this work, we make use of multi-nuclear NMR methods to examine the structure of precursor aluminosilicate glasses and the resulting b-spodumene glass-ceramic. In particular, these NMR data allow for determination of partitioning of different network former and modifier cations between the glass and lithium aluminosilicate crystallites, yielding details on the residual glass composition, amount of residual glass, and crystallite stoichiometry.

11:30 AM

(GOMD-S3-079-2015) Crystallization Toughening in Lithium Disilicate Glass-Ceramic

F. C. Serbena*[1]; I. Mathias[1]; C. E. Foerster[1]; E. D. Zanotto[2]; 1. State University of Ponta Grossa, Brazil; 2. Federal University of São Carlos, Brazil

Lithium disilicate glass-ceramics have an important and increasing share in dental restorative applications. They are also one of the most studied and characterized glass-ceramic systems, but their toughening mechanism (and of most glass-ceramics) are still unknown. In this work, stoichiometric lithium disilicate glasses were crystallized using two-stage heat treatments to obtain different crystallized volume fractions while keeping a constant grain size of about 12 μm. Hardness, elastic modulus, 4-point bending strength, indentation fracture toughness, fracture toughness and residual stresses were measured for samples having different crystallized volume fractions, spanning from the parent glass to a fully crystallized sample. The bending strength and fracture toughness measured by double torsion increases continuously with crystallization. The mechanisms that contribute to toughening - crack deflection, crack bowing and trapping, and crack bridging - were modeled. A simple model - incorporating the elastic modulus, precipitate fracture toughness and crystallized volume fraction - was proposed and successfully tested to explain the evolution of fracture toughness with crystallized volume fraction.

11:50 AM

(GOMD-S3-080-2015) Nepheline glass-ceramics

C. Smith*[1]; G. H. Beall[1]; S. A. Tietje[1]; A. Ellison[1]; 1. Corning Incorporated, USA

Nepheline containing glass-ceramics (natural nepheline having the composition $Na_6K_2Al_8Si_8O_{32}$) can be ion-exchanged in a potassium-containing bath. With the proper stoichiometry of the starting glass-ceramic, the K+ for Na+ exchange induces a phase change from the starting nepheline phase to a kalsilite phase (KAlSiO4). Accompanying this phase change is a large volume change, resulting in high compressive stresses. Nepheline glass-ceramics are typically made with the use of TiO_2 as a nucleating agent, producing opaque materials. Alternatively, highly transparent nepheline glass-ceramics can produced through the use of phosphate as a nucleating agent. Using the latter, grain sizes on the order of 30nm yield can be achieved. The chemistry of nepheline glass-ceramics and ion-exchange behavior will be presented.

Session 3: Structural Characterization of Glasses VII

Room: Symphony Ballroom II
Session Chair: John McCloy, Washington State University

9:20 AM

(GOMD-S3-081-2015) Pure network former SiO_2-P_2O_5 glass Topological aspects of $[PO_4]^{4-}$ incorporation and nanoscale homogeneity of the glassy network

S. Fuhrmann*[1]; C. Domscheit[1]; S. Unger[2]; K. Schuster[2]; L. Wondraczek[1]; 1. University Jena Otto-Schott Institute for Materials Research, Germany; 2. Leibnitz Institute of Photonic Technology, Germany

Low concentration P_2O_5 doped SiO_2 glass is technologically relevant for telecommunication and in optical applications such as e.g. Raman fiber lasers. Usually, such high temperature melting glasses with high purity requirements are prepared by Modified Chemical Vapor Deposition (MCVD). With this method, the glass is deposited layer by layer from the gaseous phase. Finally, the substrate tube is collapsed and the respective binary glass composition, which is controlled by the composition of the reactants, is formed in the core of the final preform. In the presented study the structure of MCVD synthesized binary SiO_2-P_2O_5 glasses with up to 9.5 mol% P_2O_5 are characterized by ^{29}Si and ^{31}P MAS NMR as well as Raman and IR spectroscopy. As expected from network forming oxides, the SiO_2

glass network remains fully polymerized. The intensity of the P-O double bond scales linear with P_2O_5 concentration and the phosphorous is mainly incorporated as double phosphorous centers. The structural study is accomplished by low temperature calorimetry, monitoring the position of the caloric boson peak in dependency of P_2O_5 concentration. Combining all assessed structural length scales and statistical considerations, the consequence of P_2O_5 incorporation on the homogeneity of the glassy network will be discussed.

9:40 AM

(GOMD-S3-082-2015) Elastic Properties of Mixed-Network Former Glasses

W. Wang*[1]; R. Christensen[2]; J. Byer[2]; G. Olson[2]; S. Martin[2]; J. Kieffer[1]; 1. University of Michigan, USA; 2. Iowa State University of Science & Technology, USA

The key properties of a solid-state electrolyte are high stiffness, needed to suppress dendrite growth on the anode, a large redox potential difference to provide electrochemical stability, and high ionic conductivity for the rapid charge and discharge of electrochemical energy. In this respect, oxide glasses are promising candidates, especially in light of the ease with which one can control the structure and properties of these materials via compositional changes. Indeed, since elastic modulus and ionic mobility typically exhibit opposing trends, careful materials design optimization is required. To identify the principal design criteria, we systematically investigated the mechanical properties of two systems: $0.33Na_2O + 0.67[xB_2O_3 + (1-x)2SiO_2]$ and $0.35Na_2O + 0.65[xB_2O_3 + (1 - x)P_2O_5]$. We use concurrent Raman and Brillouin light scattering, and IR spectroscopy, to simultaneously measure the complex mechanical modulus at the nano-scale, infer the degree of network connectivity, and reveal structural characteristics of the glasses. We discuss the role of atomic packing and the mixed-network former effect on the elastic properties. For the mixed network-former glasses, most properties depend nonlinearly on composition. Furthermore, by comparing these results with the ionic conductivity and activation energy data for the same systems, we can derive consistent criteria for materials design optimization.

10:00 AM

(GOMD-S3-083-2015) Composition Effects on Ionic Transport in Alkali - Alkaline-Earth - Aluminosilicate Glass

S. Amma*[1]; M. T. Lanagan[2]; S. H. Kim[2]; C. G. Pantano[2]; 1. Asahi Glass co. ltd, Japan; 2. The Pennsylvania State University, USA

The alkali - alkaline-earth - aluminosilicate glass system is important for glass substrates requiring high temperature durability, low production cost and/or a high ion-exchange rate. In sodium silicate glasses without aluminum oxide, incorporation of larger alkaline earth ions is known to decrease the Na mobility. Also, it is generally accepted that alkali modifier ions associated with AlO_4^- sites in the glass structure show higher mobility than those coordinated with non-bridging oxygen. But it is unknown how these trends are influenced by the presence of alkaline-earths in aluminosilicate glasses, especially since their coordination with aluminum can vary with the size/field strength of the alkaline-earth ion. Impedance spectroscopy can provide insight about ion transport phenomena in glassy materials. We prepared Na_2O-Al_2O_3-SiO_2 and Na_2O-RO-Al_2O_3-SiO_2 glasses (R = Mg, Ca, Sr, Ba), and determined the ionic conductivity and its activation energy from analysis of the impedance data. Our analysis shows that for the glasses with $[Al_2O_3] = [Na_2O] + [RO]$, the presence of larger alkaline-earth ions increases the activation energy for Na diffusion slightly, while there is no effect on the dielectric constant. The results for glasses with $[Al_2O_3] < [Na_2O] + [RO]$ will also be reported.

10:20 AM

(GOMD-S3-084-2015) Statistical deconvolution of soda-lime glasses Raman spectra

W. Woelffel*[1]; C. Claireaux[1]; E. Burov[1]; É. Barthel[2]; M. Toplis[2]; E. Gouillart[1]; 1. Saint-Gobain Recherche/CNRS, France; 2. CNRS, France

Over the course of our study of partially melted soda-lime glass, the need for a quick, non-destructive analytical tool arose. Raman spectroscopy meets all these requirements, but commonly used deconvolution techniques fail to provide a reliable chemical analysis of the glass. To avoid the heavy assumptions usually encountered, such as Gaussian bands and arbitrarily fixed-number of components, we use statistical methods to extract components and mixing information from a collection of spectra. Samples were obtained by heating stacked discs of soda-lime glasses for 1 h at 1000°C. Diffusion profiles from transverse slices were then probed by a Raman confocal spectrometer and an electron microprobe analyzer. The resulting spectra were treated by a combination of algorithms hinged on Principal Component Analysis and Non-negative Matrix Factorization. Our analysis of 170 spectra yields 4 components and a mixing matrix. In the so called Q band, this deconvolution supports and extends classic band shape interpretations, as the mixing matrix can be correlated with the EMPA profiles. Deeper insights can be reached by a multilinear regression from the mixing coefficients to the actual glass composition. The deconvolution of the main band reveals correlation between localized vibrations and medium-range order. Statistical exploitation of Raman data thus opens the path for a rigorous chemical and structural glass analysis.

10:40 AM

(GOMD-S3-085-2015) Transition and Post-Transition Metal-Borate Glasses: Structure-Property Correlation, Cluster Formation and Borate Ligand Speciation

D. Möncke*[1]; D. Palles[2]; E. I. Kamitsos[2]; L. Wondraczek[1]; 1. Friedrich-Schiller University Jena, Germany; 2. National Hellenic Research Foundation, Greece

In borate glasses the type of modifier oxides influences the borate network by different processes. Structural variations were studied by IR and Raman spectroscopy in transition and post-transition metal oxide containing borate glasses with varying metal oxide contents (MnO, ZnO, PbO, SrO, Bi_2O_3, Eu_2O_3). The M-O bond strengths, evaluated from cation-motion bands measured in the far infrared, were correlated to glass properties such as T_g. 1. CN and EN of the metal cations determine the degree and strength of cross-linking. 2. Charge balancing cations influence the equilibrium between trigonal (BØ$_2$O$^-$) and tetrahedral groups [BØ$_4$]$^-$ at the metaborate composition (O: non-bridging, Ø bridging O-ions). 3. The disproportionation of metaborate units into overmodified pyro- and undermodifed polyborate units is strongly supported in the ZnO-B_2O_3 glass system. 4. In lead-borates, a PbO-pseudophase forms and reduces the number of O-atoms available for the modification of the borate network. 5. B_2O_3 levels well-below the orthoborate composition are realized in (1-2x)MnO-x(SrO-B_2O_3), and (1-2x)Eu_2O_3-x(SrO-B_2O_3) glasses. For O:B$\geq$3, Mn^{2+} and Eu^{3+} ions show a strong preference to coordinate to tetrahedral borate groups with 2 bridging and 2 non-bridging O-atoms, [BØ$_2$O$_2$]^3, instead of the more common trigonal orthoborate $(BO_3)^{3-}$ species.

11:00 AM

(GOMD-S3-086-2015) Investigation of the Glass Transition Widths in Alkali and Alkaline-Earth Germanate and Borate Glass Systems at Low Modifier Loading

A. Potter*[1]; J. Bainbridge[1]; D. Starkenburg[1]; B. Perez[1]; D. Hynek[1]; C. Wilkinson[1]; D. Shadle[1]; M. Franke[1]; M. Affatigato[1]; S. Feller[1]; 1. Coe College, USA

We have found that glass transition widths vary across different alkali and alkaline-earth loadings in glass systems with low amounts of modifier. The glasses studied include JM_2OGeO_2, $JM_2OB_2O_3$, and

JNOB_2O_3, with J being the molar ratio of modifier to glass former, M being an alkali modifier, and N being an alkaline-earth modifier. Differential scanning calorimetry (DSC) and simultaneous thermal analysis (STA) were employed to determine the onset glass transition temperature, T_g, the end of the glass transition, T_f, and the glass transition width ($\Delta T_g = T_f - T_g$). Analysis of germanate glasses yielded identical glass transition width trends for each modifier. However, alkali and alkaline-earth borate glasses yielded widely disparate ΔT_gs. This suggests that glass transition widths may offer insight into structure that might not otherwise be found using T_g alone. **Acknowledgments** The National Science Foundation is acknowledged for their support under NSF grant DMR 1407404. Coe College is also thanked for their ongoing support of glass research programs

11:20 AM

(GOMD-S3-087-2015) Transition elements in glasses at dilute levels

M. Cicconi*[1]; D. de Ligny[1]; 1. University of Erlangen-Nürnberg, Germany

The vitreous state has been known for millennia and most of the actual technology uses glasses, since they offer optical transparency and environmental sustainability. However, after decades of glass research, the influence of basic parameters, such as temperature, alkali, alkali-earth and multivalent elements, still are not fully understood. Fundamental researches are critical for enabling future breakthroughs in glass science and technology and primarily, we need a deeper knowledge of structure–property relationships. Most of the commercial glasses contain impurities, such as Mn, Fe, Ti, Mg, K, Al. Especially important are the transition elements (TE) since they exhibit different valence states and coordination geometries and, moreover, they control the fining processes and the final colors of glasses. Hence, TE play a key role in glass production. Moreover, since TE are present at dilute levels and are more likely to be incorporated around point defect sites, the study of their distribution and speciation in glasses will be useful to track defects, and to enhance our understanding in important physical properties. Our goals are to better understand i) the local structure of TE in glasses for different concentrations and at dilute levels, ii) the effects of glass composition upon them (because this can influence several physical properties) and iii) to enhance our understanding of the short- and medium-range ordering of glasses

11:40 AM

(GOMD-S3-088-2015) Structure of molten $ZnCl_2$ salts: a combined theoretical and experimental study.

P. Lucas*[1]; A. Al Sayoud[1]; A. Edwards[1]; K. Muralidharan[1]; V. Manga[1]; P. deymier[1]; 1. University of Arizona, USA

Molten $ZnCl_2$ salts exhibit a prototypical ionic network forming behavior which leads to atypical transport properties such as ionic diffusion or viscosity in comparison to conventional ionic liquids. Moreover, $ZnCl_2$ is the only known single component glass-forming halide salt in addition to BeF_2. Most recently $ZnCl_2$ salts have also been considered for high temperature fluid and shown to exhibit very low corrosion kinetics, a behavior which is most likely related to its network character. In this presentation, we report on a combined experiment/modeling effort aimed at clarifying the nature of the $ZnCl_2$ network in the melt and glass. First principle quantum mechanical calculations were performed with CASTEP to establish reliable assignment of Raman modes for various structural units such as edge- and corner-sharing tetrahedral chains. High temperature Raman spectroscopy was then conducted on ultra-dry molten $ZnCl_2$ to characterize the temperature dependence of the melt structure. A complex mixture of edge and corner sharing tetrahedral is observed.

Session 7: Glass under Extreme Conditions I

Room: Symphony Ballroom I
Session Chair: Benoit Ruffle, Montpellier University

9:20 AM

(GOMD-S3-089-2015) Network glass-forming materials at high pressures and temperatures (Invited)

P. Salmon*[1]; A. Zeidler[1]; 1. University of Bath, United Kingdom

The structural changes in glasses and liquids induced by high-pressure and/or high-temperature conditions can alter substantially their dynamical and transport properties. A notable example is provided by so-called polyamorphic transitions where the variation of a state parameter such as pressure or temperature leads to an abrupt transformation between two phases having the same composition but different densities. Unravelling the mechanisms by which these transformations occur is, however, a formidable task owing to the nature of structural disorder and the experimental difficulties associated with the investigation of materials under extreme conditions. This talk will focus on recent advances to measure the structure of network glass-forming materials with neutron diffraction at pressures up to 17.5 GPa using a Paris-Edinburgh press and at temperatures up to 2000 K using aerodynamic levitation. Topics to be considered are (i) the mechanisms of density-driven structural collapse in glasses such as GeO_2 and $GeSe_2$ and (ii) the structural transformations on quenching in fragile glass-formers such as $CaAl_2O_4$. In both cases, detailed information is obtained from pioneering applications of the method of neutron diffraction with isotope substitution. The diffraction data are complemented by the results obtained from molecular-dynamics simulations.

9:50 AM

(GOMD-S3-090-2015) High energy x-ray measurements at extreme conditions (Invited)

C. J. Benmore*[1]; L. Skinner[2]; O. Alderman[3]; R. Weber[3]; R. Mayanovic[4]; A. Anderson[5]; L. Lazareva[2]; J. Parise[2]; 1. Argonne National Laboratory, USA; 2. Stony Brook University, USA; 3. Materials Development Inc., USA; 4. Missouri State University, USA; 5. St. F.X. University, Canada

Current and near future capabilities for glass science at extreme conditions at the Advanced Photon Source using high energy x-rays will be presented. A newly built aerodynamic levitator has achieved temperatures >3000 °C by laser heating, allowing the structural studies of ceramics over a wide temperature range. Time resolved x-ray studies also provide access to structural information on metastable, intermediate or transient states. The ability to mix levitation gases allows the exploration of different oxidation states and their associated structures in the liquid state as well as through the glass transition. In addition, an acoustic levitator serves as an ideal screening tool for the synthesis of amorphous pharmaceuticals, analogous to products made by industrial spray drying processes. High pressure experiments on glass (several tens of GPa) have been shown to be feasible using Diamond Anvil Cells. Also, the development of a Hydrothermal Diamond Anvil Cell has opened the investigation of glass corrosion studies and the dissolution of glass in aqueous environments at lower pressures (~ 1GPa and 800 ºC). Gas pressure cell experiments on glassy mesoporous materials are under development and plans to build a radioactive container for future x-ray pair distribution function studies of nuclear waste glasses will also be discussed.

10:20 AM

(GOMD-S3-091-2015) Using Prince Rupert's drops to induce extreme tensile stress in glasses, a Raman spectroscopy study (Invited)

D. de Ligny*[1]; A. Posch[2]; F. Kalkowski[1]; J. Ernst[3]; A. Nowak[3]; D. R. Neuville[4]; A. Lenhart[2]; 1. University Erlangen-Nürnberg, Germany; 2. Georg-Simon-Ohm-Hochschule Nürnberg, Germany; 3. Fraunhofer Institute for Integrated Circuits IIS, Germany; 4. Institut de Physique du Globe CNRS, France

Prince Rupert became famous in the 17th century by touring the European Royal Societies with his glass drops. First reported in Holland, these glass drops, also called Dutch tears, are obtained by pouring glass into water. The very strong difference of cooling rate between the external and central part of the drop associated with strong thermal expansion coefficient induces a very high tensile stress in the center of the drop. Until now, most of the structural studies of glass under pressure were performed at high pressure. Studies at negative pressure are however very difficult due to brittleness of glass. The Prince Rupert drops allow us to work on a pressure profile between compressive stress on the surface and tensile stress in the core. We will report attempt to perform Prince Rupert drops with a large range of composition from soda lime to borosilicate glasses. The drops prepared are then analyzed with polarized light. Pictures obtained will be interpreted in term of photoelasticity and some attempt to determine local stress presented. Using confocal Raman spectroscopy depth profiles were performed throw out the drops. The structural modifications in the short and medium range order could then be evaluated.

10:50 AM

(GOMD-S3-092-2015) Experimental investigations at high temperature of the glass / melt structures (Invited)

L. Cormier*[1]; G. Lelong[1]; L. Hennet[2]; 1. CNRS - UPMC, France; 2. CNRS, France

Measuring the structure of oxide liquids is still technically difficult due to the necessity to reach temperatures around 1000 K. However, the comparison of the glass/liquid structures reveals significant changes that can now be detected and quantified. Structural changes induced by temperature can be determined with X-ray or neutron diffraction, showing different behaviors: silicate systems are dominated by modifications at intermediate range order and are related to the silicate network relaxations, while borate systems present important short range order reorganization, associated with the conversion of BO_3 to BO_4 units as the temperature decreases. Alternatively, inelastic X-ray scattering (IXS) have been recently developed to probe the liquid state of lights elements (Li, B or O). This technique has also the unique advantage to characterize the environment of the most abundant elements in these oxide samples, *i.e.* the O surrounding. These studies address key questions to understand disordered structures: the importance to investigate a broad range of compositions, the usefulness to use crystalline references as benchmark to identify specific structural features, the necessity to couple experiments with simulations (Reverse Monte Carlo, Molecular Dynamics, ab initio calculations), the possibility to correlate the structural information to thermodynamics values.

11:20 AM

(GOMD-S3-093-2015) Impact of extreme forming conditions on glass properties (Invited)

Y. Yue*[1]; 1. Aalborg University, Denmark

By applying extreme thermal or mechanical conditions to a supercooled liquid, one can get glass states with extraordinary structure and properties. Studies of such glass states will be crucial for a deep understanding of nature of glass and glass transition. Here we present our recent studies dealing with the effect of extreme glass-forming conditions (e.g. hyperquenching, extremely high force drawing and milling) on glass properties. First, we show the severe consequences of hyperquenching to glass transition, atomic vibrational dynamics, microstructure and physical properties of glasses. For such studies, both poor oxide and non-oxide glass formers are used as objects. Second, we explore the impact of extremely large drawing force on the structure and mechanical properties of oxide glass fibers. Finally, we show the strong influence of extreme crushing conditions on the vitrification process of several selected non-oxide materials and on some physical properties of the derived glasses. This study sheds light on the glass transition and formation mechanism of the mechanically derived glasses.

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 2: Optical Fibers II

Room: Concerto A
Session Chair: Johann Troles, University de Rennes I

9:20 AM

(GOMD-S4-045-2015) Entering the mid-infrared with supercontinuum generated in chalcogenide fibers (Invited)

U. Møller*[1]; C. Petersen[1]; I. Kubat[1]; O. Bang[1]; 1. Technical University of Denmark, Denmark

Supercontinuum generation (SCG) is one of the most dramatic effects in nonlinear optics where severe spectral broadening up to several octaves of the monochromatic laser pump beam is obtained. Silica-fiber based supercontinuum (SC) light sources covering the visible and near-infrared have been widely explored and are commercially available. However, the infrared material loss edge of silica at 2μm precludes further broadening into the mid-infrared (MIR). As-Se chalcogenide glass, on the other hand, is transparent up to 15um and has a high Kerr nonlinearity making it a promising candidate as a fiber material for MIR SCG. We show two different cases of MIR SCG in As-Se fibers: (1) Pumping with intense 100fs pulses at 6.3um an SC spanning from 1.4 to 13.3μm was generated in a step-index fiber with a core diameter of 16μm. (2) Pumping with 320fs pulses an SC spanning from 1.7 to 7.5μm with an average output power of more than 15mW was generated in a suspended core microstructured fiber with a core diameter of 4.5μm. The MIR region is of great interest because many fundamental molecular vibrations are to be found in this region. The demonstrated MIR SC light sources open the door for a number of applications such as early cancer diagnostics, gas sensing, and food quality control, where thee spatial coherence, broad bandwidth, high brightness and portability of a SC light source is needed.

10:00 AM

(GOMD-S4-046-2015) Atmospheric Aging of As_2S_3 Microstructured Fibers: Optical, Structural, Surface Issues and their Impact on Mid-Infrared Supercontinuum Generation

O. Mouawad[1]; F. Desevedavy[1]; J. Jules[1]; G. Gadret[1]; F. Amrani[1]; B. Kibler[1]; J. Fatome[1]; O. Heintz[1]; E. Lesniewska[1]; F. Smektala*[1]; 1. Universite de Bourgogne, France

A significant alteration of optical transparency is pointed out for the core of high-purity As_2S_3 Microstructured Optical Fibers (MOFs) stored in atmospheric conditions, through a Fourier Transform Infrared Spectrometry (FTIR) study. The surface evolution followed by Atomic Force Microscopy (AFM) and inherent deviation of corresponding chemical composition analyzed by X-ray Photoelectron Spectroscopy (XPS) confirm that the physico-chemical properties of MOFs core degrade upon exposure to ambient conditions because of counteractive surface process. This phenomenon substantially reduces the optical quality of the MOFs core and therefore restrains the spectral expansion of generated supercontinuum (SC). The good matching between SC experimental results and numerical simulations based on the generalized nonlinear Schrödinger equation confirms this aging process.

10:20 AM

(GOMD-S4-047-2015) Optical fiber fabrication of zero photoelastic ZnO–SnO–P_2O_5–B_2O_3 glasses

A. Saitoh*[1]; Y. Oba[1]; G. Tricot[2]; H. Takebe[1]; 1. Ehime University, Japan; 2. Université de Lille 1, France

We have developed water durable ZnO-SnO-P_2O_5-B_2O_3 glasses possessing zero photoelastic constant that requires to realizing an optical fiber current sensor based on the Faraday effect for monitoring the electric current in conductor. Since the lead-free zero photoelastic glass has an advantage of high sensitive current sensing due to very small stress induced birefringence. In this contribution, we will show thermal and optical properties aiming for optical fiber fabrication using the zero photoelastic composition. The optical fibers were obtained by pulling of the preform providing core and cladding structure. Isothermal heating time and temperature of crystallization on the glasses were estimated by a time-temperature-transformation diagram for preventing devitrification. Actual drawing temperature of the preform was taken into consideration as an equivalent temperature of viscosity with ~10^6 Pas estimated by a fiber elongation method. The network structures of the glass and fiber were evaluated by spectroscopic methods to discuss the photoelastic and water durable properties.

10:40 AM

(GOMD-S4-036-2015) Innovative fabricaiton approaches of multi-material nanostructured glass-based photonic systems (Invited)

F. Sorin*[1]; 1. Ecole Polytechnique Federale de Lausanne, Switzerland

Chalcogenide glasses are an increasingly important component in a variety of photonic systems owing to heir high refractive indexes, strong nonlinear properties, transparency in the infrared as well as their tunable optoelectronic properties. The transition towards large area, flexible and stretchable configurations have further increased the interest in this class of materials owing to their compatibility with simple and scalable processing approaches, In this talk we will review emerging processing schemes that enable the fabrication of a variety of nanostructured glass-based photonic architectures over a variety of substrates. We will show in particular how thermal drawing can lead to one-dimensional fiber devices with optical but also optoelectronic functionalities, and present a novel combination of conventional two-dimensional fabrication approaches that utilizes lithography and thin-film deposition techniques to realize nanostructured photonic devices. The challenges and opportunities of these approaches will be discussed.

Symposium 5: Glass Technology and Cross-cutting Topics

Session 4: Waste Glass Corrosion IV

Room: Concerto C

Session Chair: Joseph Ryan, Pacific Northwest National Laboratory

9:20 AM

(GOMD-S5-040-2015) Dissolution Behavior of High-Sodium and High-Sulfate Glasses Designed for Immobilization of Hanford Low-Activity Waste

J. J. Neeway*[1]; J. V. Ryan[1]; R. M. Asmussen[1]; N. P. Qafoku[1]; 1. Pacific Northwest National Laboratory, USA

Cleanup plans for Hanford site high-level radioactive mixed tank wastecall for separating the waste into high-level waste (HLW) and low-activity waste (LAW) fractions, which will be vitrified at the Hanford Tank Waste Treatment and Immobilization Plant (WTP). In general, the HLW and LAW glass compositions are expected to differ significantly in alkali and sulfate content, with baseline LAW glass Na_2O content up to 21 wt% and SO_3 up to 0.77 wt%. Previously, a number of studies have been performed to understand the corrosion behavior of baseline LAW glasses. Experimentally determined dissolution rate law parameters were obtained experimentally and used as inputs to models designed to describe the impacts of on-site LAW glass disposal. Recently, however, there has been an effort to develop glasses with increased waste loading. These higher-loaded glasses have alkali and sulfate contents that are much higher than the baseline glasses (Na_2O up to 26 wt% and SO_3 up to 1.5 wt%). Here we report on the corrosion behavior of the higher-loaded glass formulations under development. We present measured rate law parameters on a select number of the higher-loaded glasses and compare their dissolution behavior to the baseline LAW glass compositions. Insight on the effects of other glass additives used to increase waste loading, such as SnO_2 and V_2O_5, will also be provided.

9:40 AM

(GOMD-S5-041-2015) Corrosion in Surface and Bulk Cracks of an ILW Glass Composite Material

R. Chinnam*[1]; B. Lee[1]; 1. Imperial College London, United Kingdom

Glass Composite Materials (GCM) containing intermediate level nuclear wastes (ILW) are currently being designed for disposal in repositories. The conditions in deep repositories are hostile and the glass composite can experience stresses due to temperature and pressure differences. Such conditions may eventually lead to cracks on the surface and in the bulk of the material. When ground water comes in contact with the cracks in glass, the rate of corrosion increases because of greater surface area. Studying corrosion inside a crack is difficult and there is no standardized test to replicate cracks in glass. This study is considered as an attempt to simulate surface and bulk cracks in a GCM with access to reaction products. To start with, a Borosilicate glass (BS) system was chosen as a prototype because of its simple composition and the level of understanding reported in the literature. BS glass with thickness of ~100μm (A) and ~2mm (B) was subjected to corrosion tests at 90°C. These tests were performed on A and B and on stacks of A-A, B-B and A-B. The interface between the two layers of a stack simulates a crack. The surface cracks are simulated by stacking A-A and bulk cracks by stacking B-B. The resulting corrosion behaviour will be studied using different characterization techniques and compare to literature.

10:00 AM

(GOMD-S5-042-2015) Effect of hematite, solution compositions, and surface/volume ratio on the alteration of SON68 and ISG glasses

N. A. Wall*[1]; T. Lemesle[1]; J. Neeway[2]; J. V. Ryan[2]; Q. Nikolla[2]; J. McCloy[1]; 1. Washington State University, USA; 2. Pacific Northwest National Laboratory, USA

High level wastes vitrification consists of conditionment in a borosilicate glass matrix that is then placed in an iron canister for permanent storage in a long-term repository. This work aims at understanding the alteration of the International Simple Glass (ISG) (simplified glass composition with only 6 oxydes based on SON68 composition) and SON 68 glass (French borosilicate glass composition used for high level waste storage) in iron bearing environment. This work focused on the influence of different parameters on glass alteration at 90°C over 9 months: the presence of hematite (Fe_2O_3), the solution compositions (water, NaCl, $CaCl_2$, and $MgCl_2$); and the Surface/Volume ratio of 40 cm-1 or 60 cm-1 (surface area measured by BET). For most systems, calculated normalized mass loss (NL) of each element and dissolution rates showed that the presence of hematite lead to little or no glass alteration modification. However, SON68 alteration in $MgCl_2$ solution demonstrated a lower NL in presence of hematite. Furthermore, data indicate an interaction between salt and hematite. A lower normalized loss was observed for sample in 5 M NaCl compared to 0.01 M, interpreted as the formation of a NaCl dense layer at the surface of the glass that limites the release of elements in solution. Finally, the normalized mass loss is higher for 40 cm^{-1} than for 60 cm^{-1} experiments.

10:20 AM

(GOMD-S5-043-2015) Glass Corrosion in the Presence of Iron-Bearing Materials and Potential Corrosion Suppressors

J. Reiser*[1]; L. Neill[1]; J. Weaver[1]; B. Parruzot[1]; C. Musa[1]; J. Neeway[2]; J. Ryan[2]; N. Qafoku[2]; S. Gin[3]; N. Wall[1]; 1. Washington State University, Chemistry Department, USA; 2. Pacific Northwest National Lab, Energy and Environment Directorate, USA; 3. CEA Marcoule DTCD SECM LCLT, F-30207, France

A complete understanding of radioactive waste glass interactions with near-field materials is essential for appropriate nuclear waste repository performance assessment. In many geologic repository designs, Fe is present in both the natural environment and in the containers that will hold the waste glasses. In this paper we discuss investigations of the alteration of International Simple Glass (ISG) in the presence of Fe^0 foil and hematite (Fe_2O_3). ISG alteration is more pronounced in the presence of Fe^0 than with hematite. Additionally, minimal glass corrosion is observed for distances of 5 mm between Fe materials and ISG, but substantial glass corrosion is observed for systems exhibiting full contact between Fe^0 material and ISG. Diatomaceous earth appears to better minimize corrosion than silica does when present with iron and ISG.

10:40 AM

(GOMD-S5-044-2015) Structure and chemical durability of molybdenum-bearing sodium borosilicate glass

E. Nicoleau[1]; F. Angeli*[1]; P. jollivet[1]; S. Schuller[1]; A. Le Gac[1]; M. Fournier[1]; T. Charpentier[2]; 1. CEA Marcoule, France; 2. CEA Saclay, France

Due to their low solubility, some high-level waste elements contained in nuclear glasses, such as lanthanides, noble metals or molybdenum, could lead to the formation of crystalline or separated phases in the vitreous matrix. These phases depend on glass composition and waste loading. It is thus necessary to gain more insight into their influence on the glass matrix chemical durability during aqueous alteration. The impact of molybdenum content on the structure and chemical durability of a sodium borosilicate glass is highlighted here. Glass structural characterizations were carried out by ^{29}Si, ^{11}B, ^{23}Na and ^{95}Mo MAS NMR and crystal phases were quantified by the XRD-Rietveld refinement method. Glasses were leached at 90°C in various short to long term alteration regimes. Molybdenum oxide addition beyond 1.5 mol% lead to the formation of macroscopic crystalline phases. Despite alkaline molybdenum phase solubility, the higher the molybdenum content, the lower the alteration rate. Our results point out that the alteration rates for these partially crystallized matrixes are controlled by the composition and structure of the surrounding glass. Indeed, correlations between chemical durability and structural changes were obtained. These changes are mainly due to the boron and silicon coordination, and the resulting proportion of non-bridging oxygens.

11:00 AM

(GOMD-S5-045-2015) Surface Alternation of Cr_2O_3-CoO-Al_2O_3-doped Iron-Phosphate Glasses Containing Fission Products During Immersion in Water and Heating in Vacuum

T. Yano*[1]; H. Tateno[1]; T. Kishi[1]; K. Matsuyama[2]; T. Okita[2]; S. Miyamoto[2]; H. Kofuji[3]; M. Myochin[3]; 1. Tokyo Institute of Technology, Japan; 2. Toshiba Corporation, Japan; 3. Japan Atomic Energy Agency, Japan

Surface alternations of Cr_2O_3-CoO-Al_2O_3-doped Iron-Phosphate Glasses containing simulated fission products on heating after water immersion test are investigated. Iron-phosphate glasses doped with Cr_2O_3-CoO-Al_2O_3 show quite high chemical durability. Valences of iron and doped Chromium ions have been found to play important roles to form water-resistant glass surface from the analysis of X-ray photoelectron spectroscopy (XPS). In this study, glass surfaces of Cr_2O_3-CoO-Al_2O_3-doped iron-phosphate glasses containing simulated fission products after 1 week-chemical durability test are analyzed using XPS. Surface compositions and chemical bonding are monitored with increasing temperature up to their glass transition temperature in vacuum. Unique alternations with the compositional relations P_2O_5-Fe_2O_3-(Al_2O_3+Cr_2O_3) are found; the recovery of the atomic ratio of Fe/P of the surface to the initial ones after heating with valence changes of iron and chromium ions. Nature of the surface of Cr_2O_3-CoO-Al_2O_3-doped iron-phosphate glasses are discussed from the points of view of the origin of high chemical durability.

11:20 AM

(GOMD-S5-046-2015) Dissolution behavior of Na_2O–FeO–Fe_2O_3–P_2O_5 glasses

L. Ma*[1]; R. K. Brow[1]; M. E. Schlesinger[1]; 1. Missouri University of Science and Technology, USA

The dissolution behavior of five series of $Na_2OFeOFe_2O_3P_2O_5$ glasses with ranges of O/P (3.03.5) and Fe/P (0.130.67) ratios were investigated in water using static and semi-dynamic tests. Glass composition, which determines the average phosphate chain length, affects the dissolution mechanism and kinetics. Initial dissolution is described by a 3D diffusion model (DM), whereas a contracting volume model (CVM) describes later dissolution kinetics. Temperature dependent rate parameters, K_{DM} and K_{CVM}, increase by several orders of magnitude with increasing Fe/P ratio, but are less dependent on the O/P ratio. The surface morphology and composition of the corroded glasses are characterized by analytical electron microscopy, which provides information about the change from DM to CVM kinetics.

Symposium 3: Fundamentals of the Glassy State

Session 2: Nucleation, Growth and Overall Crystallization

Room: Symphony Ballroom III
Session Chair: Edgar Zanotto, Federal University of São Carlos

1:20 PM

(GOMD-S3-094-2015) Formation and Coexistence of Crystalline Motifs in Supercooled Liquids and Glasses (Invited)

J. Kieffer*[1]; 1. University Of Michigan, USA

Cooling rates attainable in molecular dynamics simulations are still several orders of magnitude higher than can be achieved in experiments, especially, considering that to obtain reasonable statistics on nucleation phenomena, the simulated systems must contain several tens or hundreds of thousand atoms. Direct observation of nucleation and crystallization phenomena using simulations is therefore difficult, and to make progress we need to resort to simplified glass-forming model systems. For example, in simple alkali halide compounds, crystallization cannot be suppressed, no matter how fast they are quenched. By adding relatively small amounts of a structurally incompatible second compound, we can frustrate the mixture into glass formation. Systematic study of such as system reveals important aspects about crystal nucleation, visualized by reversing the temporal evolution of the simulation. We discuss the characteristics of structural fluctuations that occur during nucleation, what may constitute a critical nucleus, and what factors control the nucleation process. Alternatively, in strongly networked glasses, we can identify crystalline structural motifs based on how they affect glass properties, such as causing anomalous thermo-mechanical behaviors. We illustrate this for silica glass and discuss the consequences it may have for crystallization or the suppression thereof.

1:50 PM

(GOMD-S3-095-2015) Problems in simulations of crystal nucleation in glass-forming liquids: a review (Invited)

M. Micoulaut*[1]; 1. Universite Pierre-et-Marie Curie, France

In this talk, we will review the current computational efforts made in the understanding and characterization of crystallization in glass-forming liquids using either classical or ab initio simulations. This issue is a problem of considerable complexity and, to a large extent, still outside the capability of direct simulation owing to the relatively low temperatures encountered in most of the crystallization experiments. We will provide recent examples from metallic, chalcogenide and oxide glass-forming liquids where structural as well as dynamic properties have been used to understand the general behavior.

2:20 PM

(GOMD-S3-096-2015) Tammann curves of crystallization: from textbook to current research in multi-component glass-ceramics

S. Krüger[1]; M. Dressler[1]; J. Deubener*[1]; 1. Clausthal University of Technology, Germany

Temperature-dependent crystal nucleation and growth rate curves were pioneered by Tammann in the beginning of the last century, quickly become textbook knowledge and provided the basis for manufacturing glass-ceramics by controlled crystallization of glasses using his two-stage development method.However, for the commercially most successful system, i.e. lithium alumosilicate (LAS) glass-ceramics, the stationary nucleation rate curve is still lacking. Thus, the paper aims in addressing this problem. Thermoanalytical data as well as results from microscopy and X-ray diffraction studies were analyzed to show new paths, which allow the detection of fast crystal nucleation in LAS glasses catalyzed by different nucleation agents. In conclusion, it can be seen that Tammann curves of LAS glasses show a relative strong overlap typical for the heterogeneous nature of the involved nucleation process. The shift of nucleation rate maximum towards the liquidus temperature is connected with a spread of nucleation temperatures, which allows to measure induction times with statistical relevance at relative low degrees of supercooling. First results in glass ceramic model systems show an lag-time distribution, as predicted by classical nucleation theory, even when heterogeneous nucleation is occurring at the same favourable site.

2:40 PM

(GOMD-S3-097-2015) Heterogeneous surface nucleation of lithium disilicate: An isothermal DSC study

S. Krüger*[1]; J. Deubener[1]; 1. Clausthal University of Technology, Germany

Isochronal DSC experiments to determine crystallization parameters using Johnson-Mehl-Avrami-Kolmogorov (JMAK) formalism has been critically discussed in the last 20 years due to the erroneous assumptions in the dependence of temperature. So far only little efforts have been made to bypass these problems. Therefore this paper aims in correlating isothermal DSC signals to the actual nucleation and crystallization processes in a lithium disilicate glass as determined by optical microscopy. The results show that in the overlap of Tammann's rate curves the DSC signal reflects the change from an initial surface nucleation to a site saturation regime (constant number of crystals) leading to a coast-island microstructure of monolithic samples. The isothermal JMAK analysis revealed a maximum of the local Avrami coefficient at the onset time of saturation. Onset times were used to approximate heterogeneous nucleation rates, which were found to correlate positively with temperature in the range 0.6 - 0.7 T_m.

3:00 PM

(GOMD-S3-098-2015) Nucleating agents: is there any specific site for nucleation?

L. Cormier*[3]; O. Dargaud[1]; G. Calas[3]; C. Jousseaume[2]; S. Papin[2]; 1. Cité de la céramique – Sèvres et Limoges, France; 2. Saint-Gobain Recherche, France; 3. UPMC - CNRS, France

Different explanations have been proposed about the structural origin of the role played by nucleating agents in glasses. The environment around most nucleating agents can be selectively investigated by X-ray absorption spectroscopy (XAS), giving structural information on site geometry and the topology of the linkage of these sites to the glassy network [1]. We have investigated the role of ZrO_2 on the nucleation/crystallization properties of aluminosilicate glasses [2]. A comparison between Zr-free and Zr-bearing glasses shows that adding ZrO_2 favors nucleation in Li-, Mg-, Ca- and Zn-bearing glasses and has no effects in Na-bearing glasses. The Zr environment corresponds to six-fold coordinated sites (Li and Na glasses) and seven-fold coordinated sites (Mg, Ca and Zn glasses), indicating the coordination number has little influence on the ability to crystallize. Direct Zr-Zr polyhedral linkages are observed for all glasses except the Na-bearing one. Since no correlation between the local Zr site and its ability to promote nucleation can be observed, the origin of the nucleating role of Zr has been interpreted as resulting from the Zr distribution with the aluminosilicate matrix. Medium range ordering appears as a key parameter to explain properties of Zr-bearing glasses. [1] Cormier et al., Int. J. Appl. Glass Sci., 5(2014)126-135. [2] Cormier et al., Mater. Chem. Phys. (2015)

3:40 PM

(GOMD-S3-099-2015) The Effects of Phase Morphology on Nucleation and Growth Behavior in $GeSe_2$-As_2Se_3-PbSe Glasses

A. K. Buff*[1]; C. Smith[1]; A. Swisher[2]; A. Pogrebnyakov[2]; M. Kang[2]; T. Mayer[2]; K. Richardson[1]; 1. University of Central Florida, USA; 2. The Pennsylvania State University, USA

Chalcogenide glasses (ChG) are known for their wide transmission ranges in the infrared and for their high refractive indices. However, applications for ChG are often limited by their poor thermal/mechanical properties. Precipitating a secondary crystalline phase in the glass matrix can improve these properties, but too much crystallization and/or large or multiple phase crystallites can lead to a loss in transmission. Controlled crystallization can be used to tune the properties of these glasses. Previous work has shown how crystallization behavior can be characterized through the creation of nucleation and growth curves. This work aims to expand this understanding, by characterizing how nanoscale changes in phase separation affect the nucleation and growth rates in $GeSe_2$-As_2Se_3-PbSe glass and the corresponding physical properties of the resulting glasses. The type, size, and degree of phase separation is quantified using transmission electron microscopy. The crystallization behavior of various phase morphologies and the corresponding structural implications of such, is analyzed through thermal analysis and other spectroscopic techniques.

4:00 PM

(GOMD-S3-100-2015) Crystallization kinetics of a non-stoichiometric glass monitored by electrical conductivity measurements

T. S. Bello[1]; A. M. Rodrigues*[1]; E. D. Zanotto[1]; V. M. Fokin[2]; 1. Federal University of São Carlos, Brazil; 2. S.I. Vavilov State Optical Institute, Russian Federation

Changes of the residual glass composition always occur during crystallization of non-stoichiometric glass-forming liquids, but this phenomenon has been scarcely investigated. The aim of this work was to use electrical conductivity measurements to monitor the composition of the residual glass after volume crystallization of the $65(Li_2O{\times}SiO_2)$-$35(CaO{\times}SiO_2)$ glass composition which belongs to the lithium metasilicate (LS)-calcium metasilicate (CS) joint. To this end, this glass composition was partially crystallized at 560°C (Tg=450°C) for different periods of time. X-ray analysis confirmed the presence of LS as the only crystal phase in all samples. Thus, crystallization of LS consumes lithium ions from the glass matrix and the residual glass phase becomes progressively depleted in lithium as crystallization proceeds, which changes its ionic conductivity. The conductivity of glasses with different compositions belonging to the LS-CS joint were measured as a function of temperature and employed as a standard to estimate the residual melt composition in the investigated glass. After correction of the sample's geometric factor, taking into account the new pathway for ion conduction due to the presence of the crystals, the lithium content in the residual melt estimated via conductivity measurements matches that estimated from the change of glass transition temperature.

4:20 PM

(GOMD-S3-101-2015) Investigations towards an automated detection of the crystallization of high-performance glasses using thermooptical methods

M. Kilo[1]; A. Diegeler*[1]; I. Göbel[1]; G. Maas-Diegeler[1]; F. Raether[2]; M. Straub[1]; 1. Fraunhofer ISC, Germany; 2. Fraunhofer HTL, Germany

Glass is thermodynamically not stable in the amorphous state. Depending on the thermal treatment, there are at least two different crystallisation temperatures, the upper and the lower crystallisation temperature. In order to measure these temperatures, different methods are applicable. For the lower crystallisation temperature, usually thermochemical methods like DTA can be used, while for the upper crystallization temperature, optical detection methods can be used. In this paper, we present first results towards an automated detection of the upper crystallisation using an automated thermooptical detection method. In order to do that, a robot-controlled setup was established, which consists of an TOMMI-system, which is operated by a robot. This robot handles also the sampling system and a further -driven analysis tool. The system takes automatically samples from a glass melt using optimised platinum nets and transfers them to the measuring device, where the samples can be analysed. The crystallisation is detected by monitoring the opacity of the sample. Also for this, an automatic routine is defined. After the measurement, the samples are removed by the robot from the analysis system. The sensitivity and the reproducibility of the method are discussed.

4:40 PM

(GOMD-S3-102-2015) Non-Isothermal Crystallization and Glass Stability on Heating in some Silicate Systems

G. M. Melo[1]; A. A. Cabral*[1]; 1. FEDERAL INSTITUTE OF MARANHÃO, Brazil

Depending on the thermal history and specimens form (i.e. powder or slabs), it is well known that volume crystallization can occur by growth from a fixed number of nuclei or from simultaneous nucleation and crystal growth. On the other hand, the glass forming ability (GFA) can be inferred by some glass stability parameters (GS), such as those ones proposed by Hruby (K_H), Weinberg (K_W) and Lu and Liu (K_{LL}). In this paper, regular samples of two silicate glasses that nucleate internally, $BaO.2SiO_2$ (BS_2), 2BaO.TiO2.2SiO2 (B2TS2) and $Li_2O.2SiO_2$ (LS_2), were non-isothermally heat treated in a DSC furnace using two different routes in order to privilege one of those crystallization mechanisms. The corresponding crystallization activation energies were calculated using the Kissinger (K) and Matusita & Sakka (MS) models. Then, these values were compared with the corresponding GS parameters. A possible correlation between the activation energy and glass stability parameters is discussed.

5:00 PM

(GOMD-S3-103-2015) Hydrodynamic coarsening observed by in-situ tomography in barium borosilicate melts

E. Gouillart*[1]; D. Bouttes[2]; O. Lambert[1]; W. Woelffel[1]; D. Vandembroucq[2]; E. Boller[3]; 1. Joint Unit CNRS/Saint-Gobain, France; 2. PMMH, France; 3. ESRF, France

Liquid-liquid phase separation in silicate melts is an appealing mechanism for building glasses with tailored microstructure. Understanding and controlling coarsening kinetics is paramount for tuning the typical size of the microstructure. We investigate in-situ the coarsening stage of a barium borosilicate glass-forming melt, far above its glass transition in the range 1000-1300°C. Using in-situ microtomography imaging and a dedicated furnace on the ID19 beamline of the ESRF synchrotron, we follow the 3-D geometry of the two phases during isothermal treatments. Quantitative geometrical measurements and direct observations demonstrate that viscous coarsening is the dominant mechanism governing the evolution of the bicontinuous structure [1]. This mechanism results in a linear growth of domain size with time, much faster than the t^1/3 growth associated to diffusive mechanisms, that have been observed so far in silicates. The activation energy for domain growth is consistent with the one of viscosity. Furthermore, we observe a progressive fragmentation of one of the percolating phases, that we relate to the important viscosity contrast between phases. The rate of fragmentation is found to depend strongly on the volume fraction of the less viscous phase. [1] Bouttes, D., Gouillart, E., Boller, E., Dalmas, D., & Vandembroucq, D. (2014). Physical review letters, 112(24), 245701.

5:20 PM

(GOMD-S3-104-2015) The breakdown of the Stokes-Einstein-Eyring equation versus fragility of oxide glasses

D. R. Cassar[1]; M. L. Nascimento[1]; V. M. Fokin[1]; N. Natalia Vedishcheva[2]; E. D. Zanotto*[1]; 1. Federal University of São Carlos, Brazil; 2. Institute of Silicate Chemistry, Russian Federation

We show for approximately 20 stoichiometric oxide glass-formers that the inability of the viscosity in describing crystal growth rates below T_b~1.25 - 1.10T_g - owing to the breakdown of the Stokes-Einstein-Eyring equation - scales with the glass fragility, m. The more fragile the liquid, the more the crystal growth rates depart from the values calculated using viscosity. It has been suggested that this breakdown is caused by *dynamic heterogeneities* (which are quite difficult to detect) in the liquid. In order to dig deeper into this problem, we tentatively ascribe this relationship with fragility to structural changes of the undercooled liquid with temperature, which is stronger for more fragile liquids (simulations of the Q^n distributions in several of these liquids as a function of temperature are underway). Hence, below a certain temperature T_b, the viscosity can no longer describe the effective diffusivity controlling the crystal growth kinetics because structural modifications of the liquid change the transport process that determines crystal growth.

Session 4: Modeling and Simulations of Glasses III

Room: Symphony Ballroom IV

Session Chairs: Walter Kob, Universite Montpellier 2; Carlo Massobrio, Institut de Physique de Chimie des Matériaux

1:20 PM

(GOMD-S3-105-2015) A new method to model heat transfers at the atomic scale: the approach-to-equilibrium molecular dynamics (Invited)

E. Lampin*[1]; P. Palla[1]; F. Cleri[1]; 1. IEMN, France

Thermal properties of materials at the nanoscale deviate from macroscopic laws. Therefore, atomic-scale approaches are ideally suited to address these phenomena. None of the available MD methods appear as fully satisfactory and prone to be employed efficiently, in order to model heat transfer between a poor and a good thermal conductor, as in the case of a crystal/glass interface. We devised a new method that is based on a transient approach and proves to be an an efficient alternative to what has been used so far when modelling thermal transfer via MD. In our approach, a hot region and a cold one are first topologically defined. Then, the approach-to-equilibrium is simulated by releasing the thermal constraint. The temperature difference between the two regions is monitored and interpreted by means of exact solutions of the Fourier heat equation. Bulk and interface properties can be easily obtained as a function of the system size and of the atomic structure, as will be illustrated on several cases. The computational cost is lower when compared to previous methods, with the accessible length scale ranging in between the nm to the μm. When referring to peculiar examples of application, we shall emphasize the challenging issue of a small resistance between a good and a poor thermal conductor, representative of the crystal/glass interface physical situation.

2:00 PM

(GOMD-S3-106-2015) Molecular Dynamics Simulations of Ion-Exchanged Glass

K. D. Vargheese*[1]; A. Tandia[1]; J. Mauro[1]; 1. Corning Inc, USA

Chemically strengthened glass is one of the key enablers of the modern consumer electronics industry. Molecular dynamics simulations offer an opportunity to build enhanced fundamental understanding of the ion exchange process used for chemical strengthening. In this work, we apply molecular modeling techniques to investigate several aspects of ion-exchanged glasses that are either inaccessible through experiment or too difficult to probe through experiments alone. In particular, we use atomistic modeling to study the dependence of the linear network dilation coefficient on the concentration of alkali ions exchanged. We also calculate the evolution of elastic moduli as a result of the ion exchange process. Both of these quantities—the network dilation coefficient and the Young's modulus—are critical parameters for determining the final compressive stress profile of the chemically strengthened glass. Finally, we revisit the issue of structural differences between as-melted and ion-exchanged glasses in terms of local atomic number density around alkali ions. The results of this work point to the unique structures attainable through ion exchange that cannot be achieved through melt-quenching alone.

2:20 PM

(GOMD-S3-107-2015) Simulation of Ion Implantation into Fractal Aerogel Structures

W. Wu*[1]; J. Kieffer[1]; 1. University of Michigan, USA

Optical waveguides are prepared by ion implantation due to the photoluminescence properties of ions such as Er^{3+}. However, ion implantation into conventional silicate glass samples results in limited concentrations and penetration depths. One alternative is to implant ions initially into an aerogel. The fractal pore structure can potentially provide for an increase in the range of stopping lengths that would be advantageous, even when taking the shrinkage during densification heat treatment into account. To verify this hypothesis, and to predict the extent of spatial dispersion that can be expected for various pore structures, we carried out simulations of the implantation process. To this end, we wrote C++ code that generates a spatial arrangement of massive objects so as to represent materials with specific pore structures. By comparing the behavior of regular and fractal patterns of the pores, we find that the fractal aerogel structures facilitate a spatially well-dispersed arrangement of implanted ions. Thus, using aerogels as precursors in which to implant rare-earth ions is a possible manufacturing route for optical waveguides with increased the of lasing ion concentrations, and hence, superior the emission intensity efficiencies.

2:40 PM

(GOMD-S3-108-2015) Anomalous transport and shear bands in glass-forming systems under shear (Invited)

J. Horbach*[1]; P. Chaudhuri[2]; G. P. Shrivastav[1]; 1. Heinrich Heine University of Duesseldorf, Germany; 2. Institute of Mathematical Sciences, India

An important mechanical property of amorphous solids is the existence of a yield stress: only when the applied stress exceeds the yield stress, the system starts to display a steady-state flow. Around the yield stress, creep flow is observed, associated with a very slow deformation of the system. We consider model glass formers (Yukawa, Lennard-Jones), and study the onset of Couette and Poiseuille flow under an externally applied constant stress as well as under a constant shear rate. In the Couette flow case under constant stress, the timescale for the onset of steady flow diverges, when the imposed stresses is gradually decreased toward the yield stress. Around the yield stress, persistent creep in the form of shear-banded structures is observed. Creep flow is also seen for the Poiseuille flow; however, different from the Couette flow, creep is observed even in regions where the local stress is larger than the bulk yielding threshold. We analyze the nucleation of the shear-banded structures in the creep flow regimes and investigate how the shear-banding depends on the history of the initial glass states from which the shear simulations are started. Morover, we compare the shear bands observed at constant stress to those obtained in simulations at constant shear rate. In the latter case, we see transient shear bands and analyze their growth as a function of time.

Session 4: Modeling and Simulations of Glasses IV

Room: Symphony Ballroom IV

Session Chairs: Jincheng Du, University of North Texas; Walter Kob, Universite Montpellier 2

3:40 PM

(GOMD-S3-109-2015) Structural properties of As-Se glasses and melts: insight from ab initio simulations

M. Bauchy[2]; A. Kachmar[3]; M. Micoulaut*[1]; 1. Universite Pierre-et-Marie Curie, France; 2. University of California, USA; 3. Qatar Fundation, Qatar

The structural, vibrational, electronic and dynamic properties of amorphous and liquid As_xSe_1-x (0.10 < x <0.45) are studied by First Principles Molecular Dynamics. Within the above range of compositions, thresholds and anomalies are found in the behavior of reciprocal and real space properties that can be correlated to the experimental location of the so-called Boolchand intermediate phase in these glassy networks, observed at 0.29< x < 0.37. These findings are associated with diffusion anomalies for the parent liquid phase, thereby linking structural and dynamical atomic-scale fingerprints for the onset of rigidity within the network, while also providing a much more complex picture than the one derived from mean-field approaches of stiffness transitions. Ref. *Structural, dynamic, electronic and vibrational properties of flexible, intermediate and stressed rigid As-Se glasses and liquids from First Principles Molecular Dynamics simulations,* M. Bauchy, A. Kachmar, M. Micoulaut, Journal of Chemical Physics **141**, (2014). .

4:00 PM

(GOMD-S3-110-2015) Challenges in glass property prediction

A. Priven*[1]; 1. Corning Korea, Republic of Korea

The final goal of any simulation and modeling is prediction. Glass industry needs new models for prediction of glass properties from chemical composition, temperature and (in a less degree) other factors. Fundamental glass science suggests multiple approaches to such predictions, such as molecular dynamics, Monte-Carlo, thermodynamics. However, these approaches are mostly applied in fundamental research, not in the industry. Like 120 years ago, the only practical approach to glass property prediction is empirical modeling. During the last 20-30 years, new empirical approaches were suggested basing on big data arrays available via the electronic databases. However, even nowadays, the methods developed 50-70-90 years ago - without any computers - often remain the best practical tools. In other words, huge growth of knowledge, available data and computer power has caused only little progress in this direction during nearly half a century. Why the known theoretical approaches virtually do not work with most of industrial glasses? Why the empirical methods evolve so slowly? What the (real) obstacles are, and why they remain unrepaired for so long time? How to efficiently use the new resources that became available within the recent decades? In this presentation, the author describes his vision basing on his own experience in glass property prediction and general trends of the evolution of scientific knowledge.

4:20 PM

(GOMD-S3-111-2015) Bond constraint modelling of the mixed-alkali-effect on the Tg of ternary metaphosphates

B. Poletto Rodrigues*[1]; L. Wondraczek[1]; 1. Otto Schott Institute of Materials Research, Germany

Recently the bond constraint theory has been successfully used to understand the compositional dependence of the glass transition temperature of chalcogenide, alkali borate and alkali phosphate glasses and also the surface hardness of alkali borate glasses. Its application to phosphate glasses is particularly interesting due to the general reliability of the structural models and data found on the literature, which is needed to test the theory. In past years the Bond constraint theory has been successfully applied to model the glass transition temperature of single modifier ultraphosphates. In this work we extended the theory to model the departure from the law of mixtures in the glass transition temperature of metaphosphates containing a mixture of two monovalent cations. We find that the mixed-alkali-effect can be modelled with only one parameter and that its physical meaning is closely related to the observed structural distortions found in these mixed metaphosphates.

4:40 PM

(GOMD-S3-112-2015) Topological Origin of the Fracture Toughness of Silicate Glasses

M. Bauchy*[1]; Y. Yu[1]; B. Wang[1]; J. Mauro[2]; 1. University of California, Los Angeles, USA; 2. Corning Inc., USA

Brittleness is the main limitation of glasses, as impacts, scratching, or vibrations can result in undesirable or even dangerous fracture. As such, increasing the intrinsic ductility of glasses would allow designing tougher yet transparent materials, which is one of the *Grand Challenges* in glass science. Here, based on molecular dynamics simulations, the structure of calcium aluminosilicate glasses of different composition is investigated and coupled to computed and experimental measurements of their respective fracture toughness. We show that glasses characterized by an isostatic network, rigid but unstressed, present an optimal resistance to fracture. This relationship between atomic-scale structure and fracture toughness allows us to predict the compositions of new intrinsically tougher glasses.

5:00 PM

(GOMD-S3-113-2015) Thermodynamic Optimization and Experimental Study of the K_2O-Na_2O-CaO-MgO-Al_2O_3-SiO_2 System

D. Kim*[1]; M. Van Ende[1]; I. Jung[1]; 1. McGill University, Canada

The aim of this study is to develop a self-consistent thermodynamic database of the K_2O-Na_2O-CaO-MgO-Al_2O_3-SiO_2 system, which contains key components for the glassmaking industry. All available experimental data in the literature were critically reviewed regarding the phase stabilities, thermodynamic properties as well as the melt structures. Because of remaining uncertainties and discrepancies in the data assessment, key experiments were performed using thermal analysis (DSC/DTA/TG) and equilibration/quenching method with EPMA and XRD phase characterization techniques. Thermodynamic optimization was conducted using the Modified Quasichemical Model (MQM) to reproduce the thermodynamic properties of the liquid phase. In particular, the charge compensation effect of the aluminosilicate melts was taken into account by the introduction of $KAlO_2$ and $NaAlO_2$ associates in the MQM. An accurate thermodynamic database with high predictability was developed and uncertainties in the experimental data from literature were successfully resolved. The effect of K_2O on the silicate network structure (Q-species) and crystallization behavior of the melt were well reproduced for various glass and glass-ceramic applications. The overview of the thermodynamic database development and the applications of the database to the glassmaking industry will be presented.

5:20 PM

(GOMD-S3-114-2015) Benchmarking the Cation-Interlinking Network Cluster Approach (CINCA) with larger calculations

J. R. Oelgoetz*[1]; L. Judy[1]; R. Golovchak[1]; A. Kovalskiy[1]; 1. Austin Peay State University, USA

The Cation-Interlinking Network Cluster Approach (CINCA) approach to modeling glass networks is based on looking at the glass network as a series of interconnected network forming clusters (NFCs). Calculations using this approach begin with detailed quantum chemistry calculations modeling the NFCs, and then proceed to look at the energetics of linking the various NFCs together using the stoichiometry of the glass as a restriction. The thermodynamics of the overall networks can be used to estimate the relative compositions of the various NFCs considered. This approach has been used with low levels of theory (Hartree Fock) with substantial basis sets (such as 6-311G*) for small numbers of NFCs (2-3) but has not been examined for larger networks or for methodologies which would do a better job at predicting the thermochemistry of the networks (such as hybrid density functional theory methods, quantum chemistry composite methods [such as G2, G3, & G4], Møller–Plesset perturbation theory, or coupled cluster methods). This talk will present results exploring the extension of CINCA to larger networks using both semi-empirical methods (PM6 & PM7) and density functional theory as well as results looking at the effect of using more accurate methods (such as those listed above) on small clusters of NFCs.

5:40 PM

(GOMD-S3-115-2015) Prediction of Long Term Mechanical Reliability of Curved Display Panels considering Glass Fatigue

S. Kim*[1]; H. Lee[1]; 1. Samsung Display Co. Ltd., Republic of Korea

Curved display panels which can provide clear images with enlarged immersion of viewers have been actively and competitively developed by display set makers. However, curvature of display panel is set by bending it from flat configuration, which inevitably imposes permanent tensile stress conditions on the back side of panels. Therefore, fracture of panels after several months or years could be occurred because of very slow crack propagation due to those permanent stresses on curved panels, which is called fatigue or stress-corrosion of ceramic materials. Until now, mechanical reliability of display panels could be achieved by adding safety factors to maximum practicable load, which can be applied only to very short term failure of panels. In this paper, two new evaluation methods are proposed to predict and estimate long term mechanical reliability of curved display panels. The one is by finite element modeling combined with glass strength and fatigue data. The other is by predicting panel failure from bending test of panels considering glass fatigue characteristics. Long term reliability of curved panels are estimated in order to investigate performances as well as to provide limit radius of curvature with respect to panel sizes and glass thickness. It is expected that robust design of curved panels could be obtained in short time with suggested estimation methods.

Session 6: Non-Oxide and Metallic Glasses I

Room: Symphony Ballroom II
Session Chair: Pierre Lucas, Univ of AZ-Harshbarger Rm 224B

1:20 PM

(GOMD-S3-116-2015) Liquid-liquid transition in metallic melts (Invited)

R. Busch*[1]; 1. Saarland University, Germany

Polymorphic transitions are very common in crystalline materials and can be first order transitions like e.g. from austenite to ferrite or second order like in the case of the ordering transition from BCC to B2. Recently polymorphic transitions within the liquid state termed polyamorphisms have been observed or proposed. In this contribution experiments on kinetics, thermodynamics and structure of molten Zr based alloys in the equilibrium state as well as in the undercooled state are presented. In particular the two alloys $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10.0}Be_{22.5}$ (Vit1) and $Zr_{58.5}Cu_{15.6}Ni_{12.8}Al_{10.3}Nb_{2.8}$ (Vit106$_a$) can be investigated in the entire supercooled liquid region. In the case of Vit1 we observe sudden changes of viscosity of 2 orders of magnitude that are associated with a latent heat in the absence of crystalline reflexes under synchrotron radiation. These effects are observed upon cooling and heating and exhibit a pronounced hysteresis. The results suggest that the Vit 1 liquid alloy undergoes a weak first order phase transformation likely from a short range ordered fragile state at high temperatures to a medium range ordered strong state at low temperatures. This behavior is compared with other Zr-based alloys and discussed in a bigger picture that can be drawn when comparing fragile –strong transitions in different material classes.

1:50 PM

(GOMD-S3-117-2015) Connection Between Structure and Fragility of Metallic Glass-forming Liquids

S. Wei*[1]; O. Gross[1]; M. Stolpe[1]; Z. Evenson[1]; I. Gallino[1]; W. Hembree[1]; J. Bednarcik[2]; J. Kruzic[3]; R. Busch[1]; 1. Saarland University, Germany; 2. Deutsches Elektronen-Synchrotron DESY, Germany; 3. Oregon State University, USA

We investigate the structural evolution of various metallic glass-forming liquids and quantitatively connect the structural changes to their viscosity behavior in the supercooled liquid region near Tg. Using in-situ synchrotron X-ray scattering, we find a common signature of thermally-induced structural changes on the short and medium range order length scale, which are consistently correlated with liquid's fragility. These experimental findings suggest that the fragility of metallic glass-forming liquids is strongly affected by the changes in nearest neighbour atomic environment and the temperature dependence of atomic spatial correlations on a length scale of about 1 nm. The structural changes associated with fragility is consequently linked to temperature dependence of configurational entropy as well as mechanical properties of the glassy state. The present work provides new insight into the relation between liquid's structure and their kinetic properties.

2:10 PM

(GOMD-S3-118-2015) Microscopic origin of the fragile-to-strong transition in glass-forming liquids (Invited)

Y. Yue*[1]; L. Hu[2]; 1. Aalborg University, Denmark; 2. Shandong University, China

The fragile-to-strong transition (FST) occurs in many glass-forming liquids during cooling from above liquidus (T_{liq}) towards glass transition temperature (T_g). Some liquids exhibit FST above T_{liq} (e.g. silica), while other show FST in the supercooled regime (e.g., water, metals). FST is a fascinating dynamic phenomenon accompanied with a thermodynamic transition. FST must be associated with a structural transition within medium range. However, this structural transition is extremely difficult to be probed due to severe crystallization during FST. Recently we have obtained some implications on the structural transition by sub-T_g relaxation and diffraction studies. Here we describe our understanding about the microscopic origin of FST based on our recent findings. We propose a structural model to explain why FST can occur. We also point out major challenges and perspectives in attaining an overall picture of FST. This picture will be crucial for understanding general glass dynamics and glass transition, and also helpful for studying physical properties of the glasses derived from FST liquids, and hence for designing new glassy materials.

2:40 PM

(GOMD-S3-119-2015) On the Modelling of the Transient Flow Behaviour of Metallic Glasses: Analogy with Portevin–Le Chatelier effect

N. Alrasheedi*[1]; K. Hajlaoui[1]; 1. IMAM University, Saudi Arabia

The serrated flow has been extensively studied in order to control the yielding and plasticity of metallic glasses at room temperature. However, so far the underlying physical origin and its connection with the shear banding process are insufficiently understood. This work provide a new approach to analyze and model the serrated flow in BMGs. This approach comes from the phenomenological similarities elements between the serrated flow in BMGs and the PLC effect even though the underlying physical processes are different. A macroscopic constitutive model is presented that includes a time-varying state variable which represents the local degree of relaxation in the shear band after a shear event has taken place. The model is based on the transient behaviour of shear banding resulting from the time dependence of the flow defect concentration C_f. The transition from high to low C_f at a shear zone can be described by the "relaxation–saturation" process. The proposed elasto-viscoplastic model has been implemented in a finite element program and the non linear equations have been integrated using a Runge–Kutta method. The simulated results of stress-strain curves show a good agreement with the experimental data. The main features of the serrated flow effects have been also exhibited by the model.

3:00 PM

(GOMD-S3-120-2015) Effects of nitrogen on glass properties

S. Ali*[1]; 1. Linnæus University,, Sweden

It has been widely established that the incorporation of a relatively small amount of nitrogen leads to a significant change of the glass network, and therefore to a strong change of the properties. The objective of present work was to evaluate the effects of nitrogen content on the properties of M-Si-O-N glasses (where M= Ca, Sr and Ba). Nitrogen rich glasses in the M-Si-O-N systems were prepared by using a novel glass-synthesis route, wherein mixtures containing hydrides or metals of the modifiers CaH2, SrH2/Sr, BaH2, together with SiO2 and Si3N4, were heated at 1550-1750oC under a nitrogen atmosphere. A large glass forming region was found for the M-Si-O-N systems, with glasses retaining up to 58 e/o N and 42 e/o M. Physical property measurements for the these glasses showed that glass transition temperature (1050 C) and crystallization temperature (1230 C), viscosity, hardness (12 GPa), Young's modulus (140GPa), shear modulus and refractive index (2), depend strongly on the nitrogen content and that these properties increase approximately linearly with increasing nitrogen content. .

Session 6: Non-Oxide and Metallic Glasses II

Room: Symphony Ballroom II
Session Chair: Lothar Wondraczek, University of Jena

3:40 PM

(GOMD-S3-121-2015) Compositional homogeneity during synthesis of chalcogneide glasses

P. Lucas*[1]; B. Bureau[3]; S. Sen[2]; G. Coleman[1]; 1. University of Arizona, USA; 2. UC Davis, USA; 3. University of Rennes, France

Chalcogenide glasses have been synthesized by melt rocking for more than fifty years by scientists over six continents and they are currently produced industrially in the same manner. Indeed melt rocking is broadly used to achieve complete mixing of the component elements and to obtain the homogeneous glass structures that are critical to the development of fine optical components such as double index optical fibers. However, recent studies have suggested that melt-rocking is not an effective method for achieving melt homogenization. This claim is of tremendous significance since it cast doubt over five decades of chalcogenide glass research and consequently calls for closer inspection. We therefore present a comprehensive investigation of chalcogenide glass structural homogeneity involving multiple experimental techniques such as Raman spectroscopy, Energy Dispersive Spectroscopy, Nuclear Magnetic Resonance, as well as a characterization of optical components such as fibers, and a review of viscous process in chalcogenide melts, which as a whole unambiguously establish that melt-rocking is an effective method for the synthesis of compositionally homogenous glasses.

4:00 PM

(GOMD-S3-122-2015) Direct Observation of Sequential Lifting of Rotational Constraints in a Molecular Glass-Forming Liquid

D. C. Kaseman*[1]; B. G. Aitken[2]; S. Sen[1]; 1. University of California Davis, USA; 2. Corning Inc, USA

The temperature dependence of the rotational dynamics of van der Waals bonded P_4Se_3 molecules associated with shear relaxation of a glass-forming liquid is studied using two-dimensional ^{31}P nuclear magnetic resonance spectroscopy. In the low temperature regime between T_g and 1.13*T_g the molecules display characteristics of a dynamically constrained liquid (DCL) and perform uniaxial rotation without significant translational diffusion. Further increase in temperature results in a dynamical transition into isotropic rotational reorientation expected in a regular liquid (RL). Corroborating evidence in favor of this transition is obtained from differential scanning calorimetry experiments. While the timescales of both rotational processes follow that of α-relaxation of the liquid, the DCL→RL transition corresponds to sequential lifting of rotational constraints imposed by caging and reveals the dynamical nature of glass transition.

4:20 PM

(GOMD-S3-123-2015) Heat Capacity Spectroscopy Analysis of Structural Heterogeneity in As-Se and Ge-Se Glasses

O. Gulbiten*[1]; P. Lucas[2]; B. Aitken[1]; 1. Corning Incorporated, USA; 2. University of Arizona, USA

In this study, molecular clusters in As-Se glasses and structural heterogeneity in Ge-Se glasses were investigated by heat capacity spectroscopy. Molecular clusters in arsenic rich As-Se glasses were shown to respond peculiarly as a function of frequency in modulated differential scanning calorimetry measurements. The distinct dynamic responses of network backbone and molecular units can be correlated with the varying network dimensionality of the glass structure. The frequency dependency of two separate structural modes was found to be in a very good agreement with previous NMR and Raman studies. Distinct structural motifs in the Ge-Se system were identified by de-convoluting the out of phase heat capacity in the temperature spectrum. Aggregated tetrahedral units and long selenium chains were found to have little or no connectivity. Increasing structural heterogeneity was indicated by the non-Gaussian distribution of the out of phase heat capacity, and the contribution from selenium chains and tetrahedral units was quantified as a function of selenium content. These results clearly demonstrate the overall versatility of the interpretation of complex heat capacity in temperature and frequency spectra as well as the utility of heat capacity spectroscopy as a complementary technique to conventional structural analysis methods.

4:40 PM

(GOMD-S3-124-2015) Structural anisotropy in supercooled Ge_5Se_{95} liquid under uniaxial loading

S. Sen*[1]; D. C. Kaseman[1]; 1. University of California, Davis, USA

It is well known that inorganic glass-forming liquids behave like Newtonian fluids for moderate deformation rates. However, high strain rates that are quite typical of several forming techniques including extrusion, injection molding or fiberization, may result in shear thinning or viscosity reduction. Shear thinning in these liquids has typically been attributed in the literature to the formation of structural anisotropy through directional flow at high strain, although the exact nature of such anisotropy has remained elusive. We will present the results of a combined ^{77}Se NMR and Raman spectroscopic study of the structural changes induced in a supercooled Ge_5Se_{95} liquid, when subjected to uniaxial stress and strain rate. The results indicate strong alignment of Se chains in the glass/liquid structure in a plane perpendicular to the stress axis which controls the optical birefringence in the resulting glass. The relationship between such structural alignment and shear thinning will be discussed.

5:00 PM

(GOMD-S3-125-2015) First-principles modelling of chalcogenide glasses: how to achieve a quantitative structural characterization

C. Massobrio*[1]; A. Bouzid[1]; M. Boero[1]; G. Ori[1]; E. Lampin[2]; 1. Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), 23 rue du Loess, F-67034, France; 2. Institut d'Electronique, de Microélectronique et de Nanotechnologies, Avenue Poincaré, BP 60069, F - 59652, France

Chalcogenide glasses have proved to be a challenging playground for both experimental and theoretical efforts. On the experimental side, a precise structural characterization has become possible by combining pieces of evidence collected by several techniques such as neutron diffraction, Raman spectroscopy or NMR. The increased availability of reliable first-principles molecular dynamics results has conferred to atomic-scale modelling an unambiguous role in predicting the nature and the relative percentages of structural units for these disordered networks, by highlighting the interplay between structural and electronic properties. In this contribution, we focus on the most recent achievements for the $Ge_xSe_{(1-x)}$ and $Ge_xS_{(1-x)}$ families of chalcogenides, with special emphasis on the role played by the theoretical description adopted (i.e. exchange-correlation functionals within DFT). We demonstrate that, from the standpoint of modelling, these familes of non-oxide glasses are not only extremely sensitive to changes in the composition but also to the accuracy of the underlying statistical mechanics description.

5:20 PM

(GOMD-S3-126-2015) Structure of chalcogenide glasses in the system BaSe-Ga_2Se_3-$GeSe_2$: Role of Stoichiometry

A. Mao*[1]; B. Aitken[2]; S. Sen[1]; 1. University of California at Davis, USA; 2. Corning Incorporated, USA

Multicomponent chalcogenide glasses (ChGs) are primarily sulfides, selenides or tellurides of group IV and/or V elements, namely Ge, As, P and Si. However, relatively little is known about the structures of ChGs with modified or charge-compensated networks containing alkali and alkaline-earth modifiers. Here, we present the results from a comparative structural study of ChGs in the stoichiometric $BaSeGa_2Se_3GeSe_2$ (BGGS) ternary system and those that contain between +20% and -40% Se over/under-stoichiometry, using Raman and multinuclear (^{71}Ga and ^{77}Se) NMR spectroscopy. The stoichiometric glass structure consists primarily of a corner- and edge-sharing network of $(Ge/Ga)Se_4$ tetrahedra where addition of BaSe in excess of Ga_2Se_3 is accommodated via the formation of non-bridging Se environments, while glasses with Ga_2Se_3/BaSe >1 contain Ge-Ge homopolar bonds. In contrast, for off-stoichiometric glasses, the addition of Se in excess of stoichiometry is accommodated by the formation of Se chains, while Se deficiency forms metal-metal bonds. When taken together, these results suggest that the structure of glasses in the BGGS system exhibits attributes of both charge-compensated oxide networks and the continuous alloying model of ChGs.

Session 7: Glass under Extreme Conditions II

Room: Symphony Ballroom I
Session Chair: Morten Smedskjaer, Aalborg University

1:20 PM

(GOMD-S3-127-2015) Pressure effects in borosilicate glasses (Invited)

L. Wondraczek*[1]; 1. University of Jena, Germany

This talk will discuss the effects of isostatic and localized compression on the structure and properties of borosilicate glasses. For this, the various routes of compression, *i.e.*, room-temperature compaction, variations in fictive pressure, sharp contact loading and shock-wave compaction will be introduced. Depending on glass composition and structural homogeneity, compressive strain may be driven by a multitude of material interactions, including congruent compaction, distinct changes in short-range structure, structural and elastic ordering, and plastic flow. It will be argued as to how these various effects individually act on the overall deformation behaviour of glasses, and how they can be tailored in borosilicates.

1:50 PM

(GOMD-S3-128-2015) A-thermal and a-tensile silicate glasses obtained from high pressure experiments (Invited)

B. Champagnon*[1]; S. Degioanni[1]; C. Sonneville[1]; M. Heili[1]; C. Martinet[1]; V. Martinez[1]; D. Vouagner[1]; J. Le Brusq[1]; M. Rabia[2]; D. de Ligny[3]; 1. Université Lyon1, France; 2. Laboratoire de Physique des Rayonnements, Algeria; 3. Universitat Erlangen-Nurnberg, Germany

High pressure experiments on glasses above the elastic limit induce permanent changes of the density and of the atomic structure on the samples recovered at atmospheric pressure. These “densified glasses” have new mechanical and thermal properties which are dependent of the maximum pressure which has been applied on the sample. Applying different pressure makes it possible to monitor mechanical or thermal properties. Silica and some silicate glasses are characterized by the abnormal behavior of the elastic moduli which decrease when the pressure increases and increase when the temperature increases. This elastic anomaly progressively vanishes when the glass is compressed above the elastic limit. It is possible by application of high pressures to obtain a-thermal or a-tensile samples where the elastic moduli are independent of pressure or temperature. These high pressure effects will be shown and compared with composition effects which also modify the elastic behavior.

2:20 PM

(GOMD-S3-129-2015) Pressure induced changes to titanium phosphate glass

N. Lonnroth*[1]; R. Youngman[1]; M. N. Svenson[2]; B. Aitken[1]; M. M. Smedskjaer[2]; 1. Corning Incorporated, USA; 2. Aalborg University, Denmark

Titanium phosphate (TiO_2-P_2O_5) glasses are interesting materials due to their unusual glass forming range with high (65-75%) TiO_2 content, making them fascinating subjects to study from a structural point of view. The as-made glasses are dark due to the presence of a small amount of Ti^{3+}. They can be bleached to colorless glass when held in air for extended time at a temperature around Tg, resulting in pure Ti^{4+}-glasses as confirmed by EPR. We have subjected an Al-doped (5 Al_2O_3:67.5TiO_2:27.5P_2O_5) glass sample at T_g to a moderate pressure of 1GPa. Physical properties, including density, hardness and crack probability have been measured on both non-pressurized and pressurized samples. In addition, structural information has been obtained from Raman and MAS NMR spectroscopy. After pressurization a density increase of 6% is observed as well as an increase in hardness and crack probability. ^{31}P MAS NMR indicates that the uncompressed glass consists mainly of Q^1 and Q^0 phosphate groups. The glass appears to become more depolymerized after the pressure treatment. A corresponding increase in both the proportion of 6-fold coordinated Ti and the fraction of higher coordinated Al species is also observed. These structural modifications can be correlated with the measured changes in physical properties.

2:40 PM

(GOMD-S3-130-2015) Aluminum and boron coordination changes and densification of high pressure aluminosilicate and aluminoborosilicate glasses

S. Bista*[1]; J. F. Stebbins[1]; W. B. Hankins[2]; T. W. Sisson[2]; 1. Stanford University, USA; 2. USGS, USA

In this study, we compare the densification and Al-coordination of glasses with excess modifier (Na, Ca- aluminosilicates, Y- aluminoborosilicate) and no excess modifier ($NaAlSi_2O_6$ glass) recovered from piston cylinder experiments carried out at 1-3 GPa. In all of the compositions except the $NaAlSi_2O_6$ glass, Al-coordination and also boron coordination (in aluminoborosilicate) increased significantly up to 3 GPa. Structural changes in the Y-aluminoborosilicate are especially dramatic, going from mostly AlO_4 at low pressure to mostly AlO_6 at 3 GPa. The difference in Al-coordination changes between glasses with no excess modifier and excess modifier suggests the significance of non-bridging oxygen in the network cation coordination changes. For our aluminosilicate glasses, samples were quenched from two different temperatures (above liquidus and near to ambient Tg) at high pressure. Samples quenched from high T showed lower Al-coordination and densification compared to the samples quenched from near Tg at high pressure. The fictive T difference was not large enough to account for these differences. Their most likely cause is therefore the pressure drop during quenching from above the liquidus as the pressure medium does not respond quickly to the thermal contraction of the liquid and furnace parts.

3:00 PM

(GOMD-S3-131-2015) Elasticity of vitreous silica under fluid pressure

B. Coasne[3]; C. Weigel[1]; A. Polian[2]; M. Kint[1]; J. Rouquette[4]; J. Haines[4]; M. Foret[1]; R. Vacher[1]; B. Ruffle*[1]; 1. Montpellier University, France; 2. Université P. et M. Curie, France; 3. Massachusetts Institute of Technology, USA; 4. Université Montpellier 2, France

When vitreous silica is submitted to high pressures under helium or neon atmosphere, the change in volume observed is much smaller than expected from its elastic properties. It results from gas-atom penetration into the interstitial free volume of the glass network. We present here the results of Brillouin scattering experiments and molecular simulations relating the amount of gas adsorbed to the strain of the network. We show that a generalized poromechanical approach, describing the elastic properties of microporous materials upon adsorption, can be applied successfully to a glass in which the free volume exists only at the sub-nanometer scale. In that picture, the adsorptioninduced deformation accounts for the small apparent compressibility of silica observed in experiments.

Session 7: Modeling of Glass under Extreme Conditions

Room: Symphony Ballroom I
Session Chair: Liping Huang, Rensselaer Polytechnic Institute

3:40 PM

(GOMD-S3-132-2015) Constitutive Laws and Raman Spectroscopy of Silica Glasses submitted to High Mechanical Stresses (Invited)

A. Tanguy*[1]; E. Barthel[2]; N. Shcheblanov[1]; B. Mantisi[3]; G. Kermouche[4]; 1. Institut Lumière Matière, France; 2. ESPCI, France; 3. université Paris 6, France; 4. Ecole des Mines de St Etienne, France

Silica Glasses are known for their apparent non-monotonous elastic response under pressure. In this talk, we investigate the elasto-plastic response of silica glasses under compression and shear, with the help of high performance atomistic simulations. We show that the apparent non-monotonous behaviour of the elastic response of pure silica glasses under pressure can be related to micro-plastic events occuring at the nanometer scale. The plastic behaviour at low pressure is dominated by local shear transformations, while the high pressure behaviour is dominated by the densification of the sample. Moreover, we show with the help of semi-classical simulations of Raman spectra compared to experimental data, that the structural changes induced by the irreversible plasticity have a clear Raman signature, to which we can give a doubtless atomistic interpretation. .

4:10 PM

(GOMD-S3-133-2015) Amorphous $GeSe_2$ and $GeSe_4$ under high pressure: A first principles study (Invited)

A. Bouzid*[1]; S. Le Roux[1]; C. Tugène[1]; M. Boero[1]; C. Massobrio[1]; 1. Institut de physique et chimie des matériaux de Strasbourg, France

The evolution in structure of the prototypical network-forming glasses $GeSe_2$ and $GeSe_4$ is investigated at pressures up to ~16 GPa by first-principles molecular dynamics (FPMD) simulations. The densification of amorphous $GeSe_2$ occurs in two steps. For pressures lower than 8.5 GPa, edge-sharing tetrahedra persist as the dominant structural motif and the chemical order is preserved. When increasing the pressures for values higher than 8.5 GPa, a conversion from CS to ES configurations takes place in conjunction with a steady increase of the mean coordination number leading to the formation of a pseudo-cubic network. At the transition pressure, most of the higher coordinated Ge-centered polyhedral contain homopolar bonds. Therefore, the homopolar bonds play a mediating role in the occurrence of the transition. This mechanism of network collapse is likely to be generic for the class of glass-forming materials where homopolar bonds and ES motifs are prevalent in the ambient pressure network. In the case of $GeSe_4$, no structural change has been recorded. In agreement with X-ray experiment, ambient pressure network and chemical order are preserved upon compression. This behavior is due to the Se chains. By twisting and reducing the Se–Se–Se internal bond angles, Se chains fill the inter-tetrahedral space and prevent the system from undergoing any structural transition when high pressures are applied.

4:40 PM

(GOMD-S3-134-2015) Relaxation and thermodynamic reversibility in glasses and liquids under pressure (Invited)

M. Micoulaut*[1]; M. Bauchy[2]; 1. Universite Pierre-et-Marie Curie, France; 2. University of California, USA

If crystallization can be avoided during cooling, a liquid will display a substantial increase of its viscosity, and will form a glass that behaves as a solid with a relaxation time that grows exponentially with decreasing temperature. Given this “off-equilibrium” nature, a hysteresis loop appears when a cooling/heating cycle is performed across the glass transition. Here we report on Molecular Dynamics simulations of densified glass-forming liquids that follow this kind of cycle. Over a finite pressure interval, minuscule thermal changes are found, revealing glasses of “thermally reversible” character with optimal volumetric or enthalpic recovery. By analyzing the topology of the atomic network structure, we find that such liquids adapt under the pressure-induced increasing stress by experiencing larger bond-angle excursions. Ultimately, the results substantiate the notion of stress-free (Maxwell isostatic) rigidity in disordered molecular systems, while also revealing new implications for the anomalous relaxation in glass-forming liquids.

5:10 PM

(GOMD-S3-135-2015) Structural properties of densified Ge_xSe_{1-x} glasses (Invited)

C. Yildirim*[1]; M. Micoulaut[1]; J. Raty[2]; 1. Universite Pierre-et-Marie Curie, France; 2. Université de Liège, Belgium

The evolution in structural properties of liquid and densified glassy Ge_xSe_{1-x} is investigated by use of First Principles Molecular Dynamics (FPMD) combined with X-ray absorption (XAS) experiments for the glassy state. Four different compositions (x=10%, 16%, 18% and 33%) representing the flexible and stressed rigid sides of the reversibility window are the focus of the study. The target systems were studied at pressures up to ~ 11 GPa under both annealed and cold compression conditions. We examine the structure factors, pair distribution functions, bond angle distributions, coordination numbers and neighbor distributions. The results show that the real and reciprocal space properties are in very good agreement with the experimental findings. The structural evolution during densification reveals the edge sharing tetrahedra is maintained upon compression whereas Ge-Ge homopolar bonds tend to increase in number. Ge-Se-Ge bond angular distributions show a transformation from tetrahedral octahedral geometry. We discuss the effect of thermal history on structural properties during densification.

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 4: Optical Ceramics I

Room: Concerto A
Session Chair: Yiquan Wu, Alfred University

1:20 PM

(GOMD-S4-048-2015) Hot-Pressed ZnS Infrared Ceramics: Correlating Precursor Synthesis Method To Sinterability and Transparency (Invited)

O. Merdrignac-Conanec*[1]; N. Hakmeh[1]; X. Zhang[1]; J. Adam[1]; 1. University of Rennes 1, France

Chalcogenide ceramics exhibit the best trade-off between infrared optical transmission and thermal and mechanical considerations that are required in a number of diverse applications ranging from infrared lenses and related optical components, to windows and domes. Zinc sulphide, a commonly broad band infrared window material, is currently available at a relatively high cost as Chemical Vapor Deposited (CVD) polycrystalline material. Additional Hot Isostatic Pressing (HIP) process is often required to eliminate microscopic voids and defects which occur in CVD parts. An alternative route to reduce the overall costs associated with the ZnS optics production while increasing their erosion-resistance and mechanical strength is through hot pressing ZnS nanoparticles into small-grain material. To meet this need, we have developed low temperature, low cost, scalable processes for high purity precursor ZnS nanoparticles using wet chemical methods. The correlation of processing variables with respect to X-ray diffraction, purity, morphology of both, ZnS powders and sintered specimens, as well as densities and IR transmission of the sintered parts is presented. Hot pressing of ZnS powders produced transparent ceramics of CVD-HIP quality, with, depending on precursor method, maximum transmission

greater than 73% at 12μm or with the theoretical maximum transmission of 75% at 10μm.

1:50 PM

(GOMD-S4-049-2015) Cr^{2+} doped ZnS polycrystalline transparent ceramics

Y. Li*[1]; Y. Wu[1]; 1. Alfred University, USA

Cr^{2+} doped ZnS is an ideal candidate for the gain media of solid state lasers in the mid-infrared (IR) applications. In this present study, Cr^{2+} doped zinc sulfide ceramics was processed by using vacuum hot-press sintering of Cr^{2+} doped ZnS powders synthesized through a colloidal processing method. X-ray diffraction and scanning electron microscopy were employed to correlate the Cr^{2+} dopants with different concentrations to the phase configuration and microstructure features for the synthesized powders and ceramics. The sintering behavior during vacuum hot pressing was studied to better understand the densification mechanism. The characterization of optical properties for the Cr^{2+} doped ZnS ceramics was performed to the relationship between processing and properties.

2:10 PM

(GOMD-S4-050-2015) Optical ceramics for high power solid state lasers

W. Kim*[1]; C. Baker[1]; G. Villalobos[1]; J. Frantz[1]; B. Shaw[1]; M. Hunt[2]; S. Bayya[1]; B. Sadowski[3]; I. Aggarwal[3]; J. S. Sanghera[1]; 1. Naval Research Laboratory, USA; 2. Unversity Research Foundation, USA; 3. Sotera Defense Solutions, USA

We report our recent research progress to develop optical ceramics for high power solid state lasers. A rugged exit aperture window with low optical loss and a laser gain medium with high efficiency and power are the essential components for realization of high power solid state lasers. We have developed transparent magnesium aluminate spinel ($MgAl_2O_4$) ceramic as a rugged window material operating from the UV to the mid-IR. Here, we report various methods to lower the concentration of impurity elements that absorb in the 1-2 μm range in commercially available spinel powders. A dramatic improvement in the absorption loss is seen from the spinel ceramics fabricated by these novel techniques. In the second part of this paper, we present our recent results in the development of rare-earth doped sesquioxide ceramic gain media for high power solid state lasers. Synthesis, purification and post-process techniques to prepare high purity powders suitable for high power laser applications are discussed. The optical, spectral and morphological properties as well as the lasing performance from highly transparent rare-earth doped sesquioxide ceramics fabricated from these powders are also presented.

2:30 PM

(GOMD-S4-051-2015) Processing and characterization of Eu: $Ba_2Zr_2Si_3O_{12}$ optical ceramics

Y. Yang*[1]; Y. Wu[1]; 1. Alfred University, USA

Rare earth elements are important candidates for luminescence centers for of laser, phosphor, and scintillator applications. The energy transition of divalent europium (Eu^{2+}) [$4f^65d^1$ to $4f^7(^8S_{7/2})$] is characterized by a broad emission band, which is useful as efficient luminescence center for ionizing radiation detection. $Ba_2Zr_2Si_3O_{12}$ possesses cubic crystal structure with the space group P_{213}(198), and consists of SiO_4 tetrahedras and ZrO_6 octahedras in the framework. Eu^{2+}:$Ba_2Zr_2Si_3O_{12}$ optical ceramics were synthesized by a solid-state reaction sintering process. Scanning electron microscopy and X-ray diffraction were utilized to characterize microstructure and determine phase constitution. The optical properties of Eu: $Ba_2Zr_2Si_3O_{12}$ were examined by infrared and ultraviolet-visible spectroscopy. The photoluminescence properties and decay time were also investigated to understand the mechanisms for the luminescence behaviors.

2:50 PM

(GOMD-S4-052-2015) Scintillation and luminescence in transparent colorless single and polycrystalline bulk ceramic ZnS

J. McCloy*[1]; M. Bliss[2]; B. W. Miller[2]; Z. Wang[2]; S. Stave[2]; 1. Washington State University, USA; 2. Pacific Northwest National Laboratory, USA

ZnS:Ag is a well-known, extremely bright scintillator used in powder form for α-particle detection and, mixed with powdered LiF, for thermal neutron detection. Recently, we discovered some colorless and transparent commercial bulk single-crystal and polycrystalline (chemical vapor-deposited) ZnS forms that scintillate in response to α-particles. The scintillation light transmits through the sample thickness (millimeters), challenging the commonly held assumption that ZnS is opaque to its own scintillation light. Individual α-particle events were imaged in space and time using a charged-particle camera originally developed for medical imaging applications. Photoluminescence (PL) and PL excitation show that scintillating bulk ZnS likely depends on different electronic defects than commercial ZnS powder scintillators. These defects, associated with copper and oxygen, are discussed in relation to PL results and extensive literature assessment. Commercial transparent ZnS is routinely produced by chemical vapor deposition to sizes larger than square meters, enabling potentially novel radiation detection applications requiring large, thick apertures.

Session 4: Optical Ceramics II

Room: Concerto A

Session Chair: Yiquan Wu, Alfred University

3:40 PM

(GOMD-S4-053-2015) Spectroscopic and electrical properties of $CuAlO_2$ optical ceramics

Y. Liu*[1]; Y. Wu[1]; 1. Alfred University, USA

The wide band-gap $CuAlO_2$ has received an increase in interest due to its combined properties of p-type conductivity and Vis-IR transmittance. Although various studies have been focused on $CuAlO_2$ films and particles regarding their optoelectronic and photoluminescent properties, there are few reports on sintering bulk $CuAlO_2$ to investigate its potential application in optical or electronic ceramics. Due to the anisotropic crystal structure of $CuAlO_2$, high-efficiency sintering is needed to obtain ceramics with small grain sizes in order to improve the transparency. Field-assisted sintering was employed to consolidate the $CuAlO_2$ powders and the effects of sintering parameters on the densification were investigated in this work. With the improved bulk density, the related electrical properties could be simultaneously enhanced. In addition, the room-temperature luminescence of the $CuAlO_2$ was characterized and compared with that of the nanostructured $CuAlO_2$ films. It was demonstrated that bulk $CuAlO_2$ ceramics with high density could be developed as promising IR optical materials with semiconductor-like features.

4:00 PM

(GOMD-S4-054-2015) Compaction of Barium Chloride Transparent Ceramics at Low Temperature and High Pressure

T. Shoulders*[1]; M. Gascon[2]; G. Bizarri[2]; E. Bourret[2]; R. Gaume[1]; 1. University of Central Florida, USA; 2. Lawrence Berkeley National Laboratory, USA

Rare earth doped alkaline earth halides have demonstrated great potential as high light output scintillators. The use of some halide ceramics in the form of compressed discs for spectroscopy has peaked our interest in the application of similar preparation methods for these novel scintillators. In this talk we show the results of low-temperature (0-500°C) and high-pressure (0-150MPa) compaction studies on spray-dried Eu:$BaCl_2$. Spray-drying is an effective method to produce dispersed, dense, spherical aggregates on the order of micrometers in size. A house-built hot press, consisting of a removable vacuum-tight pressing chamber for loading powders inside the glove box, is used to sinter the spray-dried powders. Parameters of temperature, pressure, and pressure application rate are varied to study densification behavior. Our results show the threshold for onset of plastic deformation, as determined from densification curves, and the conditions suitable for minimizing porosity and maximizing transparency once within the plastic deformation regime. Scanning electron microscopy and UV-Visible spectrophotometry are used to characterize residual porosity and sample transparency respectively. The low-temperature and high-pressure compaction method is presented as a viable method for the production of fully dense and transparent alkaline earth halide ceramics.

4:20 PM

(GOMD-S4-055-2015) Combustion synthesis of lead oxide nanopowders for the preparation of PMN-PT transparent ceramics

X. Chen*[1]; S. Chen[2]; P. Clequin[2]; W. T. Shoulders[1]; R. Gaume[2]; 1. University of Central Florida, USA; 2. CREOL, USA

We describe the preparation of lead oxide nanopowders by a combustion synthesis process in which nitric acid and glycine are used as oxidant and fuel reagents respectively. We observe that the fuel-to-oxidant ratio affects the phase information, valence, yield, particle shape and size of lead oxide powders. 60 nm-diameter lead oxide particles, with a yield of 86%, were obtained for a 1.7 glycine-to-nitrate molar ratio. This process produces powders with greater uniformity and smaller particle size than commercially available and we illustrate the improvement that these nanopowders offer in the synthesis of $(1-x)Pb(Mg_{1/3}Nb_{2/3})O_3$-$xPbTiO_3$ (called PMN-PT) transparent ceramics by solid-state reaction.

Symposium 5: Glass Technology and Cross-cutting Topics

Session 3: Liquid Synthesis and Sol-gel-derived Materials

Room: Concerto B

Session Chairs: Rui Almeida, Instituto Superior Técnico; Alicia Duran, CSIC

1:20 PM

(GOMD-S5-047-2015) Sol-Gel Materials For Energy Applications (Invited)

B. Dunn*[1]; 1. UCLA, USA

Sol-gel chemistry has played a significant role in the development of materials used in batteries and electrochemical capacitors. The sol-gel derived pore-solid architectures in xerogels, aerogels and template-directed mesoporous materials have been successfully applied to a wide range of metal oxide compositions. By designing pore morphologies to incorporate liquid electrolytes, it is now possible to create materials that serve as electrolytes or electrodes depending upon the properties of the inorganic framework and the confined liquid phase. The emergence of sol-gel derived electrochemical materials has led to the development of three-dimensional electrode architectures that exhibit new energy storage mechanisms and state-of-the-art energy and power densities. Interconnected pore networks facilitate electrolyte access to redox-active frameworks and lead to the formation of local electrolyte reservoirs, thus avoiding ion starvation effects at high power. A number of future opportunities for sol-gel derived electrode materials are envisioned as new designs for battery architectures are just emerging and sol-gel methods for producing non-planar electrode structures are expected to develop.

1:50 PM

(GOMD-S5-048-2015) $BaTiO_3$/Low Melting Glass Core-Shell Nanocomposite for High Energy Storage Capacitor Applications

X. Su*[1]; B. Riggs[2]; M. Tomozawa[1]; J. K. Nelson[1]; D. Chrisey[2]; 1. Rensselaer Polytechnic Institute, USA; 2. Tulane University, USA

The dielectric and ferroelectric properties of barium titanate show a strong dependence on grain size. Nanocrystalline $BaTiO_3$ exhibits linear polarization response and high dielectric breakdown strength, which make it suitable for high energy storage capacitor applications. In order to obtain dense bulk nanocrystalline $BaTiO_3$, glass was added to promote densification by liquid phase sintering while suppressing grain growth. A core-shell nano-scale mixing technique was employed to fabricate $BaTiO_3$/low melting bismuth borosilicate glass nanocomposite using the sol-precipitation method in order to preserve the nano-grain $BaTiO_3$ after sintering. The resulting nanocomposite attained a high densification (~99%) under low sintering temperature (900°C) while maintaining $BaTiO_3$ grain size on the nanometer scale. This nanocomposite showed high dielectric breakdown strength (>1000 kV/cm), postponed polarization saturation, and low remnant polarization, which contributed to a high energy storage density of ~10 J/cm^3 at 1 MV/cm.

2:10 PM

(GOMD-S5-049-2015) Soft chemistry route to nanostructured GeS_2 hybrid materials

L. Courtheoux*[1]; R. Mathiaud[1]; G. Silly[1]; H. Albadri[2]; J. Levillain[2]; A. Gaumont[2]; M. Ribes[1]; A. Pradel[1]; 1. University of Montpellier, France; 2. ENSICAEN, France

The preparation of structured chalcogenides, and especially GeS_2, with adjustable properties in terms of surface chemistry and morphology with highly polarizable atoms is a very interesting challenge as it may lead to breakthrough in various fields such as electrochemistry, gas phase separation, etc. With this purpose in mind, the synthesis of GeS_2 by soft chemistry route has been investigated with tetraethoxygermanium as germanium precursor and thioacetamide as sulfur source in acetonitrile. An originality of this work lies in the fact that the structuration of the material is carried out by ionic liquids (IL). Without IL, the synthesis leads to an agglomeration of nanospheres, whereas the introduction of IL leads either to microspheres or to gypsum rosettes like particles. Raman, NMR, TGA and chemical analysis experiments clearly indicate that when an IL is used, a hybrid material is synthesized. The inorganic part corresponds to GeS_2 and the organic part corresponds to the cation of the IL with around 20 mol.% of organic phase. The morphology of the hybrid organic-GeS_2 particles strongly depend on the nature of the cationic moiety of the IL. The hybrid compounds do not show any long range order; however, some kind of nano-organisation of the GeS_2 part of the hybrid materials are evidenced by Raman experiments. Thus, nanostructured GeS_2 hybrid materials have been successfully prepared by soft chemistry routes.

2:30 PM

(GOMD-S5-050-2015) Effect of Tetraethoxy- and Tetramethoxysilane (TEOS/TMOS) on Melting Gel Behavior

L. C. Klein*[1]; K. Al-Marzoki[1]; A. Jitianu[2]; 1. Rutgers University, USA; 2. Lehman College-CUNY, USA

A characteristic of so-called melting gels is that, while they are rigid at room temperature, they are able to soften at temperatures around 110°C. However, after consolidation at temperatures higher than 150°C, the gels no longer re-soften. In general, mixing a di-substituted alkoxysilane and a mono-substituted alkoxysilane results in a melting gel. However, when a mono-substituted alkoxysilane is mixed with tetraethoxysilane (TEOS), the gel does not soften. To determine the limit of the melting gel behavior, 3 component mixtures were prepared containing phenyltrimethoxysilane (PhTMS)-diphenyldimethoxysilane (DPhDMS) with TMOS or phenyltriethoxysilane (PhTES)-diphenyldiethoxysilane (PhDES) with TEOS. The amount of the tetrafunctional silane was 0.02, 0.05 or 0.10 moles for 1 mole of the mono-substituted alkoxysilane. It was expected that the addition of the tetrafunctional alkoxysilane would make the gels stiffer, because of the ability of the TEOS/TMOS to form three-dimensional networks. In the case of the methoxy gels, the rigidity of the gels increased with increasing TMOS. However, the gels became more fluid with increasing TEOS addition. In all cases, the gels continued to show melting gel behavior. It appears that larger additions of TMOS and TEOS are needed to reach 3-dimensional connectivity.

2:50 PM

(GOMD-S5-051-2015) Chemical Solution-Processed Ferroelectric Thin Films and Nanostructure (Invited)

N. Bassiri-Gharb*[1]; 1. Georgia Institute of Technology, USA

Ferroelectric thin films and nanostructures find applications in capacitive elements, non-volatile memories, micro- and nano-electromechanical system sensors, actuators and transducers, actively tunable photonic and phononic crystals, and energy harvesting nano- and micro-generators. Chemical solution deposition provides a flexible approach for processing of ferroelectric nanostructures, and thin films with controlled crystallographic orientation and enhanced dielectric and piezoelectric response on a variety of substrates. Low aspect ratio ferroelectric nanostructures were processed by local crystallization of precursor sol-gel films via an AFM with heated cantilever tip. High aspect ratio ferroelectric nanostructures were processed through soft-template infiltration of precursor sol-gel solutions, followed by thermal treatment leading to removal of organic template and crystallization of the 3D ferroelectric nanostructures. Both methods allow a high-resolution control of the created shapes in terms of location and dimensions. Superlattice-like ferroelectric thin films were processed on Si substrates by leveraging the thermodynamic drive for the B-site cation gradient formation in $PbTiO_3$-based solid solutions, leading to an enhancement of the dielectric and piezoelectric response. Extrinsic ferroelectric size effects and impact of lateral and substrate-induced constraints will also be discussed.

3:40 PM

(GOMD-S5-052-2015) Novel nanostructured phosphate glasses derived by sol-gel route: from optical to environmental applications (Invited)

L. Zhang*[1]; J. He[1]; Y. Wang[1]; J. Ren[1]; 1. Shanghai Institute of Optics and Fine Mechanics, CAS, China

Novel phosphate nanostructure glasses with larger surface area and controlled pore sizes ranging from 2nm to 15 nm, composited with various functional species, have been developed by sol-gel method recently. The incorporation of various photo-active, bio-active, and environ-active species in nanoscale porous structure is currently attracting great attentions as for many significant applications, including solar cells, laser sources, optical amplifiers, catalyst, biomedical and pollution processing, etc. In this talk, we will report the successful preparations of series of phosphate glasses by a novel sol-gel route. The structure and structural evolutions of these glasses by investigated and monitored by advanced NMR spectroscopic. Some of these glasses exhibited the larger surface area and controlled pore sizes ranging from 2 nm to 15 nm. Various functional species, including laser dyes, rare earth and quantum dots, have been separately incorporated by different processing methods into mesoporous phosphate glass to achieve optical functionalities. Controllable emissions (e.g. intensity, broad bandwidth, bimodal Luminescence, etc.) were realized, showing the excellent fluorescence-tailoring properties. The excellent pollution-processing capability, as well as good bioactive properties, was observed in the prepared nanostructure phosphate glasses.

4:10 PM

(GOMD-S5-053-2015) Stress Manipulation of Mesoporous Titanium Phosphate Glass

M. Sundararajan*[1]; G. Chen[1]; 1. Ohio University, USA

Titanium Phosphate ($TiPO_4$) is a known photocatalyst with an optical band gap in the visible light region. One possible way to modify the optical band gap of a material is through stress manipulation. In our previous study, we have demonstrated that the pore walls of mesoporous glasses are highly stressed, which opens a way to manipulate optical properties of such materials. In this study, we synthesized mesoporous $TiPO_4$ through a sol-gel method. The atomic and nanoscale structure of the mesoporous glass was characterized by small and wide angle X-ray scattering as well as N_2 gas-sorption. The effect of thermal annealing on the structure and residual stresses of the material was examined, and its relation to the optical band gap of the material was established. Our study demonstrated a new physical method to modify the optical band gap of amorphous photocatalysts.

4:30 PM

(GOMD-S5-054-2015) Sol-Gel Derived Solid State Lithium Ion Conducting Organic-Inorganic Hybrid Electrolytes

W. Wang*[1]; J. Kieffer[1]; 1. University of Michigan, USA

Desired properties of solid electrolytes are high lithium conductivity and transference number, high shear modulus to prevent dendrite growth, chemical compatibility with electrodes, and ease of fabrication into thin films. We use sol-gel method to synthesize silica-based hybrid organic-inorganic materials for this application. The silica network provides chemical stability and mechanical rigidity. We use polyethene glycol (PEG), covalently grafted onto silica network, as the organic filler that provides the environment for ion conduction. The effects of PEG molecular weight, organic/inorganic ratio, lithium composition, and different grafting chemistries, on the degree of crystallinity, nano-mechanical properties, and ionic conductivity will be discussed. We use Brillouin light scattering(BLS), IR, DSC, impedance spectroscopy and X-ray diffraction to characterize these materials. BLS reveals the complex mechanical moduli and the degree of connectivity in the network at molecular level. The combination of experimental techniques allows us to find the optimal parameters and identify the underlying structural and chemical origins of particular electrolyte performances. We find that both the ionic conductivity and the mechanical modulus strongly depend on the molecular weight of PEG, as well as an optimum combination of polymer molecular weight and lithium concentration.

4:50 PM

(GOMD-S5-055-2015) Influence of surface pretreatment of magnesium alloy on the deposition of glass-like cerium coatings obtained by sol-gel

A. Duran*[1]; 1. CSIC, Spain

Magnesium alloys are presently used for many industrial applications due to their physical and mechanical properties such as high thermal conductivity, good machinability and high strength to weight ratio. They are used for electronic devices, aerospace and automobile industry or biodegradable implants. However, the high reactivity and poor corrosion resistance are main limitations to use the magnesium alloys in different environments, being so necessary to improve the corrosion resistance by the deposition of coating films. Sol-gel technique appears as a promising technology to obtain protective coatings. This technique is a cost-effective process, practical and "eco-friendly" method to deposit coating of different compositions. In this work, glass-like cerium-based coatings synthesized via sol-gel were deposited on AZ31B and AZ91D Mg alloys by dip-coating. Different cleaning pretreatments have been tested to evaluate their influence on the adhesion to the substrate and corrosion protective properties. The coatings were characterized by different techniques (thickness, contact angle, adhesion test, corrosion standard tests and electrochemical essays). The experimental results show that the cleaning pretreatments are a key factor to obtain homogenous and uniform coatings with excellent corrosion protective properties.

Session 4: Waste Glass Melting Processes - Experimental Studies and Modeling

Room: Concerto C
Session Chair: Vijay Jain, Savannah River Remediation LLC

1:20 PM

(GOMD-S5-056-2015) Laboratory-scale cold cap analysis for liquid-fed ceramic melter using high-temperature X-ray CT

T. Yano*[1]; K. Watanabe[1]; K. Mori[1]; T. Amagasa[1]; R. Nakata[1]; J. Ogata[1]; T. Kishi[1]; K. Takeshita[1]; Y. Miura[2]; N. Kanehira[2]; 1. Tokyo Institute of Technology, Japan; 2. Japan Nuclear Fuel Limited, Japan

Summary of research on the laboratory-scale pseudo-cold cap of liquid-fed ceramic melter (LFCM) using high-temperature X-ray computed tomography (CT) is reported. Vitrification of pseudo-liquid solution of high-level radio-active wates (HLW) and borosilicate glass beads are observed in situ by X-ray CT, and differences of the inner structure with/without dibutyl phosphate (DBP). LFCM has been employed for the vitrification of HLW from the reprocessing of spent nuclear fuel at Rokkasho. Cold cap is known as an important boundary for heat transportation, mass transportation and chemical reaction field of vitrification. Inner structure of cold cap at high temperature has been paid much attention to attain stable melter operation. Our group has investigated the cold cap in laboratory scale using pseudo-HLW solution and borosilicate glass beads, and applied X-ray CT technique to "in situ" observation at high temperature. We also paid attention to the effect of the small additive, dibutyl phosphate (DBP), in HLW solution on vitrification. 3D structural data from X-ray CT measurements are analyzed and characteristic features are picked up which are important for heat transfer and vitrification phenomena. In this paper, summarized results of this research project are presented.

1:40 PM

(GOMD-S5-057-2015) Non-Newtonian behavior of nuclear glass melts containing Platinum Group Metal particles

M. Neyret*[2]; J. Puig[2]; B. Penelon[2]; P. Marchal[1]; O. Pinet[2]; 1. CNRS, France; 2. CEA, France

High level radioactive wastes originated from nuclear fuel reprocessing are vitrified in a borosilicate matrix at 1100-1200°C. The optimization of such a vitrification process requires the knowledge of the rheological behavior of glasses at very high temperature. However, the presence of undissolved PGM particles (Platinum Group Metal) leads to complex phenomena such as non-Newtonian behavior of the glass melt, aggregation of particles and sedimentation. The aim of this work is to describe the influence of the PGM content on the rheological properties of nuclear glass melts during their elaboration. For this purpose, we have developed an original rheometer prototype, allowing to perform rheological tests at high temperature and at very low shear rates, which are representative of the shear sustained by the glass melt. Therefore, a scenario describing the particles motion in the melts has been proposed and confirmed using different characterization techniques. In particular, sedimentation speeds were determined under various experimental conditions. Finally, a rheological structural model, accounting for the physical phenomena occurring in the melts, was established on the basis of the experimental data. This model will represent a significant advance to the extent that the rheological data are lacking in the field of vitrification processes.

2:00 PM

(GOMD-S5-058-2015) Specific Surface Area Change of a High-Alumina HLW Melter Feed during Vitrification

K. Xu*[1]; P. Hrma[1]; M. Schweiger[1]; 1. Pacific Northwest National Laboratory, USA

Molten salt migration and drainage can result in a cold-cap in which accumulated refractory components reduce or even stop melt production during nuclear waste vitrification. This problem can be avoided if the amount of salt melt per area of solid components is low enough, so that spreading prevents salt migration and drainage. In this work, we investigated the effect of temperature on the specific surface area of a high-alumina HLW feed during heating up to ~700°C, a temperature by which the salts were nearly all decomposed. Feed samples were heated at 5 K/min from room temperature to 300–700°C in 100°C intervals and then air quenched. Crystalline phases were determined with X-ray diffraction. Salts were leached from heat-treated samples in deionized water. The specific surface area, pore size, and pore size distribution of leached and un-leached samples were measured by the BET method. The pore size (~3–~30 nm) was confirmed by transmission electron microscopy. Specific surface area in both leached (12.6 m^2/g for dry feed, 19.8 m^2/g at 500°C, and 5.4 m^2/g at 700°C) and un-leached (1.5 m^2/g for dry feed, 8.8 m^2/g at 500°C, and 0.8 m^2/g at 700°C) samples increased as temperature increased to 500°C and then decreased. As evidenced by elemental mapping, amorphous alumina provided an increased surface area (~10 m^2/g) that was wetted by salts.

2:20 PM

(GOMD-S5-059-2015) Thermal diffusivity of melter feed for a high-alumina high-level waste glass

C. P. Rodriguez*[1]; J. Chun[1]; M. J. Schweiger[1]; P. Hrma[1]; 1. Pacific Northwest National Lab, USA

In the nuclear waste vitrification, a mixture of radioactive waste and glass formers (melter feed) is charged into a continuous electrical glass-melting furnace (a melter). A cold-cap, a layer of unreacted feed, is formed on top of the molten glass pool covering 95 -100% of the melt surface. Heat flux must be transported from the molten pool to the cold cap for the feed- to-glass conversion process (i.e., melting), and thus thermal diffusivity within the cold-cap is one of the crucial parameters to determine the melting rate. In this work, we measured the heat conductivity of a high-alumina high-level simulated waste designed for the Waste Treatment and Immobilization plant at the Hanford Site in Washington State, USA. The measurements were conducted by using a large cylindrical clay crucible with an assembly of thermocouples which monitored the time evolution of the temperature field at specified horizontal positions at a designated depth in the feed while heated at a constant rate from room temperature up to 1100°C. The measured thermal diffusivity shows a clear signature of the evolution of foams as a function of temperature.

2:40 PM

(GOMD-S5-060-2015) Effects of Melter Processing Parameters on Technetium Retention in Glass during Waste Vitrification

D. Kim*[1]; A. A. Kruger[2]; 1. PNNL, USA; 2. Office of River Protection, USA

Technetium-99 is one of the major radionuclides of concern in Hanford low-activity wastes (LAW) because of its long half-life and high mobility. Processing the Tc-containing waste into a glass waste form is a challenge because of its extreme volatility. A series of studies is being performed to develop the methods to increase the retention of Tc-99 in the final glass product, which requires understanding the mechanism of Tc escape from, or incorporation into the glass melt. This study critically reviews the existing data on the retention of Tc and Re (surrogate for Tc) during processing of various glass feeds in the slurry-fed Joule-heated melters. The primary data sets include Tc-99 retention results obtained from the vitrification of actual high-level wastes at the Defense Waste Processing Facility and

Tc-99m and Re retention from the pilot tests of simulated wastes in the scaled melters at the Catholic University of America. These data from were evaluated to identify the parameters that affect the Tc retention and to help understand the mechanism of Tc incorporation into glass melt.

3:00 PM

(GOMD-S5-061-2015) Rhenium/Technetium Partitioning and Nitrate Decomposition during Melting of Simplified Low Activity Waste Glass Feeds

T. Jin*[1]; D. Kim[1]; M. J. Schweiger[1]; A. Kruger[2]; 1. Pacific Northwest National Laboratory, USA; 2. U.S. Dept of Energy, USA

According to the current cleanup plan for the U.S. Department of Energy's Hanford Site, a large volume of low-activity waste (LAW) will be vitrified into glass waste forms for long-term storage. The LAW is an aqueous solution containing predominantly nitrates with other salts/hydroxides. The high volatile loss of ^{99}Tc, a hazardous radionuclide in LAW, is a major concern during melting of LAW glass feeds. Previous crucible studies with simulated LAW feeds identified the plausible factors that are important for understanding the Re behavior during melting, i.e., partitioning into different phases and retention in the final glass. To examine the Re behavior (used as a nonradioactive surrogate) more closely, simplified feeds containing sodium nitrate spiked with Re and representative additives (SiO_2 and B_2O_3) were designed and tested in the temperature range from ~100 to 1100°C. This paper presents the results of thermal analysis (TG-DSC) of the dried feeds and microstructural/chemical analysis of heat treated samples performed to gain information on the nitrate decomposition or reaction and its effects on Re incorporation during feed-to-glass conversion.

Session 4: Vitrification Operations and Melter Studies

Room: Concerto C
Session Chair: John Vienna, PNNL

3:40 PM

(GOMD-S5-062-2015) Status of High-Level Radioactive Waste Vitrification in the United States (Invited)

V. Jain*[1]; 1. Savannah River Remediation LLC, USA

Since 1996, the United States has been successfully vitrifying high level radioactive wastes (HLW) generated from the reprocessing of the spent nuclear fuel. Vitrification of HLW has been successfully completed at the West Valley Demonstration Project (WVDP) in New York, is continuing at the Savannah River Site (SRS) in South Carolina, and construction of major vitrification facilities is underway at the Waste Treatment Plant (WTP) at the Hanford site in Washington. WVDP completed its processing campaign in 2003 which produced approximately 600 tons of glass poured in 275 stainless steel canisters while SRS has processed 15,140 tons of glass contained in 3,910 canisters as of 12/14/2014. Continued R&D and operational experience has led to many innovations to the baseline technologies that have improved overall efficiencies of the process. Crystal tolerant and higher sulfur solubility glass compositions now provide higher waste loadings allowing higher quantities of sludge to be incorporated in the glass, while introductions of bubbler technologies in the Joule-Heated Ceramic Melter at SRS resulted in a significant increase in production rate. This presentation will summarize the status of HLW vitrification programs and focus on ongoing innovations that have a potential to provide improvements in both waste loading and production rate.

4:10 PM

(GOMD-S5-063-2015) Technetium Behavior During Hanford LAW Vitrification

I. L. Pegg*[1]; K. S. Matlack[1]; H. Abramowitz[1]; M. Brandys[1]; 1. The Catholic University of America, USA

At the Hanford site, highlevel nuclear wastes (HLW) stored in aging underground tanks will be separated into low-activity waste (LAW) and HLW fractions that will be vitrified separately. The long half-life of ^{99}Tc and the high environmental mobility of the very soluble pertechnetate anion make ^{99}Tc one of the most significant risk contributors in performance assessments for the onsite disposal of the LAW glass. Characterizing the volatility of technetium in the high-temperature vitrification process and the effectiveness of its subsequent capture in the downstream off-gas treatment systems are important to the overall performance of the treatment and immobilization process and disposition of secondary wastes. In this work, the fate and retention in glass of technetium, and rhenium as a potential surrogate, were studied using three continuously fed joule-heated ceramic melters spanning a factor of 60 in scale-up. The test systems included off-gas treatment components that are prototypical of those under construction at the Hanford site and included submerged bed scrubbers, wet electrostatic precipitators, and a vacuum evaporator. Technetium removal efficiencies for each of these unit operations were measured and the effects of recycle of off-gas treatment system effluents back to the melter feed were quantified for the first time.

4:30 PM

(GOMD-S5-064-2015) Volume, density, and void fraction changes as glass batch converts to molten glass

P. Hrma*[1]; 1. PNNL, USA

Glass making efficiency largely depends on heat transfer to reacting glass batch (melter feed), which in turn is influenced by the bulk density (ρ_b) and void fraction (porosity, Φ) as functions of temperature (T). Neither $\rho_b(T)$ nor $\Phi(T)$ functions are readily accessible to direct measurement, but they can be determined based on monitoring the profile area of heated glass batch pellets and material density of batches quenched at various stages of conversion via pycometry. Typical curves representing batch volume versus temperature possess two maxima separated by a minimum, identifying three critical temperatures that are related to crucial stages of the batch-to-melt conversion progress. These critical temperatures are functions of the processing parameters, mainly the batch makeup variables (e.g., silica grain size) and the heating rate, thus presenting a possibility to optimize these parameters for maximum process efficiency.

4:50 PM

(GOMD-S5-065-2015) Investigation of Multiple Cold-Cap Temperature Profiles with Mathematical Modeling

D. Dixon*[1]; M. Schweiger[1]; B. Riley[1]; R. Pokorny[2]; P. Hrma[1]; 1. Pacific Northwest National Laboratory, USA; 2. Institue of Chemical Technology, Czech Republic

One option for the immobilization of nuclear waste is through vitrification into glass, which takes place in an electric melter. As liquid slurry is charged into a melter, the reacting waste feed floats on top of the molten glass and gases from the melt reactions and glass redox reaction accumulate and coalesce below the feed surface in a region called the cold cap. The foam layer in the cold cap limits the heat transferred to the reacting feed, which decreases the melting rate. A recently developed mathematical model describes the effect of the cold cap on the melting rate. To aid in the verification of the mathematical model, four cold caps were produced from a laboratory-scale melter using different feed charging conditions and their temperature profiles were characterized through correlation with feed heat treated to known temperatures. All of the cold caps demonstrated dry surface conditions, which lead to a buildup of feed around 400°C. The total height of the cold cap increased when a larger amount of base glass was used in the melter, but the fraction of the cold cap occupied by the foam layer was greater at the lower base glass level. Over the temperature range ~500°C – ~1100°C, the temperature gradients of the laboratory-made cold caps were comparable with those calculated in the mathematical model when corrections were applied for the changes in the foam layer upon glass cooling

5:10 PM

(GOMD-S5-066-2015) Integrated Heat Transfer Model of a Waste Glass Melter with Cold Cap Physics

D. P. Guillen*[1]; R. Pokorny[2]; P. Hrma[3]; 1. Idaho National Laboratory, USA; 2. Institute of Chemical Technology Prague, Czech Republic; 3. Pacific Northwest National Laboratory, USA

Jouleheated waste glass melters will be used for the vitrification of legacy radioactive tank waste at the Hanford site. This paper describes the development of a heat transfer model of the melter that couples the complex physicochemical processes occurring within the melt pool and the cold cap. Previous models of the glass melting process have not properly described the complex foamy region that lies on top of the molten glass called the "cold cap." This region, in which feedtoglass conversion reactions occur, is critical in determining the melting properties of any given glass melter. The computational fluid dynamics model of the melter includes convection of the melt due to forced air bubbling and ohmic heating supplied by the electrodes. An advanced cold cap model relates the melting rate to feed properties and melter conditions, such as molten glass temperature, foaminess of the melt and heat supplied to the cold cap from the plenum space. Videos of the cold cap during melter operation were studied to provide an understanding of the physical behavior of the cold cap. The ultimate goal of this integrated model is to guide the specification of melter parameters that improve glass quality and increase production rate.

5:30 PM

(GOMD-S5-067-2015) Immobilisation process for contaminated zeolitic ion exchangers from Fukushima

D. Pletser*[1]; B. Lee[1]; 1. Imperial College London, United Kingdom

The remediation of the Fukushima site in Japan has generated large volumes of contaminated zeolitic ion exchangers. These zeolitic adsorbents are currently stored on site but need to be immobilised in a solid wasteform before being permanently disposed of. The majority of the radionuclides in these adsorbents are Cs and Sr with relatively short half-lives so that the level of long-term performance of the wasteform is not as demanding as for usual High Level Waste immobilisation matrices. To preclude volatilising Cs and Sr species, a maximum immobilisation processing temperature of 800 °C is necessary. The requirement of developing low temperature processing conditions appropriate for treating nuclear waste using vitreous matrices has led to challenges in the design of a suitable process and durable wasteform. To accommodate these challenges a glass composite wasteform composed of a low melting temperature lead borosilicate glass frit sintered with a simulant waste zeolitic ion exchanger has been developed. The produced wasteforms are currently being submitted to mechanical testing and chemical durability testing in the form of MCC-type leach testing. Preliminary results notably show that producing a robust composite wasteform is possible at 550 °C, surpassing the initial requirement.

Symposium 3: Fundamentals of the Glassy State

Session 4: Modeling and Simulations of Glasses II

Room: Symphony Ballroom IV
Session Chairs: Carlo Massobrio, Institut de Physique de Chimie des Matériaux; Jincheng Du, University of North Texas

9:20 AM

(GOMD-S3-136-2015) New insights into oxide glass structure from a combined experimental and computational solid-state NMR approach (Invited)

T. Charpentier*[1]; F. Vasconcelos[1]; M. Salanne[2]; J. Delaye[3]; F. Pacaud[3]; F. Angeli[3]; S. Schuller[3]; 1. CEA, France; 2. UPMC Paris VI, France; 3. CEA, DEN, France

Recent years have seen many decisive methodological and technical progresses been made in Solid State NMR applications to the structural studies of glasses. Among them, the DFT GIPAW method enabled for the first time accurate computation of NMR parameters in solids, i.e. with the use of periodic boundary conditions. Thanks to its efficiency and robustness, GIPAW can now be combined with MD simulations with system size up to 1000 atoms (PAW-GIPAW as implemented in VASP), offering new promising means for addressing several NMR issues in Glass Science. Firstly, it can establish the missing relationships between the variations of the local environment associated with disorder and the NMR signatures. Secondly, it can improve the analysis and interpretation of the NMR experimental data, as the inhomogeneous broadening of spectra associated to disorder often leads to partial or complete overlap between the NMR resonances of the different sites. Finally, the computed NMR spectra from MD models can provide new constraints for assessments. In this respect, the development of force fields – offering better reproducible experimental NMR data – has now emerged as a new challenge. All these aspects will be illustrated through several applications to silicate and borosilicate glasses in the context of our studies on nuclear waste glasses.

10:00 AM

(GOMD-S3-137-2015) Development and analysis of amorphous calcium pyrophosphate structure models

J. M. Rimsza*[1]; J. Du[1]; C. Bonhomme[2]; C. Gervais[2]; C. Coelho Diogo[3]; C. Sassoye[2]; 1. The University of North Texas, USA; 2. UniversiteParis 06, France; 3. Universite Paris 06, France

Calcium pyrophosphates (CPP) are a classification of biomaterials which are of significant biological interest due their role in bone growth, water softening, and as a component in pseudogout (calcium pyrophosphate deposition disease). The pyrophosphate ion is of special interest in the bio mineralization process, where the hydrolysis of the pyrophosphate ions affects the growth rate of hydroxyapatite crystals. Therefore, amorphous calcium pyrophosphates (ACPP) structure models were created using Monte Carlo simulations followed by density functional theory (DFT) structural relaxations. The ACPP structure models were compared to experimental ACPP systems through the measurement and calculation of the NMR spectra of key elements (^{31}P, ^{43}Ca and ^{1}H) from MAS (magic angle spinning) NMR experimental techniques and GIPAW simulation methods. Calculated ^{31}P NMR isotropic chemical shifts for the amorphous $Ca_2P_2O_74H_2O$ systems were found to be in best agreement with experiments. The P-O-P bond angles and ^{31}P NMR isotropic chemical shift were found to be sensitive to hydration levels while the P-O pair distribution in the models remains unchanged.

10:20 AM

(GOMD-S3-138-2015) First-Principles Nuclear Magnetic Resonance of 29Si for Structural Analysis of Metal-Silicate Glasses

A. Dasmahapatra[1]; J. P. Nimmo[1]; P. Kroll*[1]; 1. UT Arlington, USA

We investigate mixed hafnia (HfO_2) - silica (SiO_2) glasses though network modeling and density functional calculations, providing a large data set for further analysis. Several 100 periodic models of glasses are generated and optimized, and subsequently ^{29}Si-NMR chemical shifts are computed within the gauge-including projector augmented wave (GIPAW) method. We derive angular correlation functions that related ^{29}Si-NMR chemical shifts to the angles at O surrounding the Si. There is a notable difference between {Si}-O-Si and {Si}-O-Hf units, indicating that the ^{29}Si signal is sensitive to neighbors in the 2nd coordination to the Si nucleus. The impact of 3-coordinated O atoms bonding to Si is also analyzed. We apply derived angular correlation functions to analyze a variety of experimental ^{29}Si spectra of HfO_2-containing silicate glasses and highlight that in previous literature some chemical shifts may have been attributed mistakenly to Si-OH bonds.

10:40 AM

(GOMD-S3-139-2015) Surface Reactivity of Silicate Glasses: New Insights from Reactive Potentials

Y. Yu*[1]; B. Wang[1]; Y. Lee[1]; M. Bauchy[1]; 1. UCLA, USA

Reactive potentials, which allow dynamical charge transfers between atoms during a chemical reaction, are appealing tools to simulate glass reactivity. However, their ability to model amorphous materials remains unknown thus far. Here, we use a reactive force-field (ReaxFF) to simulate the structure of various silicate glasses and their surface reactivity in the presence of water molecules. A computationally efficient method is developed to form a realistic glass structure with relatively low cooling rate. Three compositions, pure silica, sodium silicate, and calcium aluminosilicate are simulated for benchmarking. The outcomes are compared with classical potentials and validated by available experimental results. Based on the simulated structures, the ReaxFF potential is then used to study the surface reactivity of these silicate glasses with water. The analysis of the thermodynamical and structural properties of the glass-water interface provides insights and references to future studies of the chemical reaction of different amorphous materials.

11:00 AM

(GOMD-S3-140-2015) Clustering in Metal Silicate Glasses

A. Dasmahapatra*[1]; P. Kroll[1]; 1. UT Arlington, USA

We study mixtures of metal oxides, hafnia (HfO_2) and erbia (Er_2O_3), with silica in (quasi-) random and segregated model structures. We generate models using melt-quench approaches together with ab-initio molecular dynamic simulations as well as using network models with subsequent optimization with density functional theory. Our models comprise 100-200 atoms with up to 10 mol-% of metal oxide in the glass. Optimized melt-quench models indicate a strong trend to form metal oxide clusters in the glass. An statistical analysis clearly shows that the observed aggregation of M-O-M bonds is beyond that expected for a random mixture. On the contrary, network models indicate "avoidance" of M-O-M bonds and a (quasi-) homogeneous ditribution of metal cations in lowest energy structures. We compute signatures that may help to characterize small metal oxide nuclei in these glasses. For instance, vibrational spactra of segregated and (quasi-) random models show differences that relate to small nuclei, most natably a pinning of low-wave number vibrational modes. Another example are optical properties of erbia-doped silica glasses that differ depending on the degree of "dispersion" of Er atoms within the glass.

11:20 AM

(GOMD-S3-141-2015) Structural transitions in oxides at extreme temperatures: From Silica to molten Uranium dioxide (nuclear fuel) (Invited)

L. Skinner*[1]; C. Benmore[2]; R. J. Weber[3]; O. L. Alderman[3]; 1. stony brook university, USA; 2. Argonne Nat. Lab., USA; 3. Materials Development Inc., USA

Structural knowledge of many oxide melts above 2000K has been limited by softening and chemical reactions of the container with the sample. Uranium dioxide (UO_2), the major nuclear fuel component of power reactors, is one such example. A key concern during severe accidents is the melting and subsequent leakage of radioactive UO_2 as it corrodes through its Zr-cladding and steel containment. Yet, the very high temperatures have prevented structural studies of these melts. Recently we combined laser heating, sample levitation and synchrotron x-rays to obtain pair distribution function measurements of hot solid and molten UO_2 at temperatures up to 3300K (LB Skinner *et al.*, Science 2014). Molecular dynamics models consistent with these structure measurements are used to further investigate the structure and dynamics of this melt. These results will be discussed and placed into a broader context including results from other oxide melts, such as silica.

Thursday, May 21, 2015

Varshneya Frontiers of Glass Technology Lecture

Room: Symphony Ballroom IV

8:00 AM

(GOMD-AL-004-2015) The present and future of glass in medicine (Invited)

S. Jung*[1]; 1. Mo-Sci Corporation, USA

Glass is already being used in medical applications from cancer treatment to tissue regeneration. The future of glass in medicine will require advances in chemical composition, shape / form factor, and processing to continue to improve treatment options for clinicians. The beauty of glass is that it can be almost anything we want; durable or degradable, solid or porous, it can be manipulated into almost any shape, and the list goes on. The uniqueness of the material properties of glass ultimately makes way for truly unique medical devices. This talk will focus on present advances in hard and soft tissue regeneration and why it is believed glass materials will remain a viable and growing option for the future of healing.

Symposium 3: Fundamentals of the Glassy State

Session 1: Glass Heterogeneities and Structural Relaxation

Room: Symphony Ballroom III

Session Chair: Dominique de Ligny, University Erlangen-Nürnberg

9:20 AM

(GOMD-S3-142-2015) Structural heterogeneity in glass: Insight from relaxation studies (Invited)

Y. Yue*[1]; 1. Aalborg University, Denmark

As is known, dynamic and structural heterogeneities are present in suppercooled liquids and their glass states. Such heterogeneities are an important factor to be considered when designing nanostructured glasses. However it is still challenging to detect structural heterogeneity in macroscopically homogeneous inorganic glasses. Here we present our recent effort in detecting structural and energetic heterogeneity in several poor inorganic glass formers by considering medium range order. Based on calorimetric studies of relaxation in the hyperquenched and highly mechanically distorted glasses we have obtained strong indirect evidence for the existence of structural heterogeneity in those glasses. This evidence is supported by both nuclear magnetic resonance and high resolution transmission microscopy measurements. In this work, both the hyperquenched oxide glasses and the mechanically vitrified non-oxide glasses are chosen as the objects of our investigations. From the observed new relaxation phenomena we provide insight into the mechanism of the glass formation and glass transition of extremely poor glass formers.

9:50 AM

(GOMD-S3-143-2015) Viscosity of silicate melts: a key to understand the structure of melts: (Invited)

D. R. Neuville*[1]; 1. CNRS-IPGP, France

The configurational properties of melts and glasses provide fundamental information needed to characterize magmatic and industrial processes. A principal difficulty, however is to link the "macroscopic" configurational entropy with the structure of melts. This has been done by combining viscometry with NMR, XANES and Raman spectroscopic structural studies. From the viscosity measurements at low and high temperatures, we have obtained the configurational entropy, Sconf (log h = Ae + Be/TSconf, were h is the viscosity, T the temperature and Ae, Be two constants). And by using Raman spectroscopy allows the Q-species distribution and an idea of the polymerization of the melt, the short range order is determine by using NMR and XANES spectroscopies. It is now possible to establish some link between the variation of the viscosity, the configurational entropy as the function of chemical composition and the Q species obtained from the Raman spectroscopy and the short range order of the melts. These structural variations are related to the changes in configurational entropy.

10:20 AM

(GOMD-S3-144-2015) Atomic scale network relaxation observed in a silicate glass by XPCS (Invited)

B. Ruffle*[1]; 1. Montpellier University, France

Thanks to improved instrumentation for the collection of sparse scattering signals and to an increased flux and coherence of X-ray beams at beamline ID10 (ESRF, France), X-ray photon correlation spectroscopy (XPCS) has become a very powerful technique able to follow the evolution of the dynamics at the atomic length scale in crystalline and amorphous materials. The temporal and temperature evolution of the structural relaxation dynamics is followed in a prototypical network glass, sodium tetrasilicate (NS4), at both the mesoscopic and atomic length scales. The experiments show the existence of surprising fast collective atomic motions even deep in the glassy state, in contradiction with the common idea of an ultraslow arrested out-of-equilibrium state; the structural relaxation time is here several orders faster than expected from macroscopic measurements. These results are discussed in the light of existing microscopic theories and concepts of the glassy state.

10:50 AM

(GOMD-S3-145-2015) Two Complementary Approaches for the Quantification of Inhomogeneities in Glasses

S. Bartolomey*[1]; R. Conradt[1]; 1. RWTH Aachen University, Germany

Inhomogeneities in glasses can deal great damage to the manufacturing of high performance materials, as they affect their quality and accuracy of tailored properties. This work focuses on the quantitative evaluation of resolved thermally and chemically induced inhomogeneities in glasses. Two different approaches have been chosen: (i) a density titration procedure to monitor the density spread of a representative set of particles from the bulk sample and (ii) a thermo-analytical approach in a Calvet type calorimeter and a DSC for the determination of isobaric heat capacity. The measurements have been conducted on industrial fibre glass beads and homogenous lab samples of the same composition. In order to distinguish between both types of inhomogeneities a sub-T_g annealing step was introduced between two measurements. The density titrations show a shift of the mean density to higher values and a narrower density distribution. This density signature was traced back in the calorimetric measurements, where the density shift is reflected by the non-reversing enthalpy of configuration. The variation of density fluctuations ("structural heterogeneities") around the median may be explained by the width of the relaxation-time spectra. This comparison enables to estimate the order of magnitude of both types of inhomogeneities not only mirrored in macroscopic properties, but also in a structural context.

11:10 AM

(GOMD-S3-146-2015) Some Theoretical Approaches to Understanding a Universal Pattern in the Fragility of Network-forming Glasses

D. Sidebottom*[1]; T. Tran[1]; S. Schnell[1]; 1. Creighton University, USA

In a recent series of papers, we have demonstrated how a wide variety of network-forming glasses display a common, universal dependence of fragility on a relevant connectivity of the network. This connectivity is not defined identically in all cases, but instead is defined by the coarse-grained networks for which rigid features of short range and intermediate range order are encapsulated. In this talk, we briefly review the coarse-graining that produces the universal fragility pattern but focus more on possible theoretical interpretations for the specific pattern. We suggest that the fragility pattern is connected to changes in entropy associated with bond breaking that take two forms: one configurational and the other vibrational. We also demonstrate how the configurational part might be obtained from a direct enumeration of the possible self-avoiding walks of a chain on a simple cubic lattice.

11:30 AM

(GOMD-S3-147-2015) Structural relaxation in network glasses: do we need a new paradigm?

R. Golovchak*[1]; 1. Austin Peay State University, USA

Structural relaxation at below-T_g temperatures, also known as physical ageing (PhA), was firstly documented in the 19th century by J.P. Joule in silicate glasses. Today, the isothermal kinetics of changes in physical-chemical properties of many glasses have been studied on the timescales from several hours to several decades. The enthalpy recovery during PhA is thought to follow a sigmoidal time dependence, which is defined by a choice of ageing temperature T_a in respect to T_g. However, recently it was shown that in several glasses and polymers the enthalpy recovery proceeds via a step-wise process, showing kind of plateaus and steep regions in time dependence. Accepting this as a new paradigm, it is possible now to explain the dramatic deviations from extrapolated liquid-like behavior, observed in PhA of some glassy polymers. In this work, the long-term PhA kinetics in chalcogen-rich glasses are analyzed. The observed plateaus and steep regions in enthalpy recovery during isothermal structural relaxation well below T_g are related to Johari-Goldstein (JG) β-relaxation mechanism. It is shown that each of the individual steep regions can be described by a single exponent, while the overall kinetics can be fitted with a stretch-exponential Kohlrausch type function. The results support the possibility to develop a unified description of structural relaxation in disordered solids through the fractal theory.

Session 4: Modeling and Simulations of Glasses V

Room: Symphony Ballroom IV

Session Chairs: Carlo Massobrio, Institut de Physique de Chimie des Matériaux; Walter Kob, Universite Montpellier 2

9:20 AM

(GOMD-S3-148-2015) Atomic Scale Modeling of Amorphous Chalcogenide Surfaces (Invited)

G. Ori*[3]; B. Coasne[2]; M. Boero[1]; C. Massobrio[1]; 1. CNRS, France; 2. Massachusetts Institute of Technology, USA; 3. IPCMS-CNRS, France

Owing to their large surface area and tunable pore size, amorphous porous solids such as siliceous, carbonaceous and chalcogenide materials are at the heart of important applications: heterogeneous catalysis, energy (H_2 storage, lithium batteries) and environment (water treatment). Recently, nanoporous chalcogenides (chalcogels) have been demonstrated to be efficient sorbents for environmental remediation from waste media. From a computational point of view, producing glassy surface models capable of mimicking realistically the behavior of a chalcogel and its interface is mandatory in order to understand the structure and adsorption properties of such complex materials. In this work, I will show how atomistic simulations can be used to develop and investigate the properties of glassy chalcogenide surfaces. In a first step, first-principles modeling is used to develop a realistic model of these materials with special emphasis on their surface chemistry. A detailed account of the structure of the surface models is given in terms of pair correlation functions, structure factors, chemical order and bonding. The surface properties of these materials can then be assessed by simulating adsorption isotherms of various fluids using Monte Carlo simulations. I will show how the realistic details of the surface chemistry drastically affect the adsorption of various fluids such as N_2, CO_2, CH_4, H_2 and their mixtures.

10:00 AM

(GOMD-S3-149-2015) Glass surface properties enhancement with thermal poling: a molecular dynamics study

A. Tandia*[1]; K. Varghese[1]; 1. Corning Incorporated, USA

We have applied the process of thermal poling, with Molecular Dynamics simulations, on different glass compositions to achieve substantial modification of glass surface chemistry. Our simulation is based on a wide range of glass compositions with and without different types of alkalis and alkaline earth, under different poling conditions. For different poling conditions of temperature and voltage, we conducted detailed characterization of the surface depleted layers to reveal Aluminium and Boron coordination variations as a function of the initial alkalis and alkaline earth concentrations. To characterize the chemistry variation with thermal poling, we compared the binding energies of these glasses with a water layer before and after the poling. This is followed by a study of the glasses response to nano-indentation before and after the thermal poling. Overall, our Molecular Dynamics based study reveals that glass surface properties are tunable to critical mechanical and/or chemical properties from a combination of thermal poling conditions and choice of the initial glass composition.

10:20 AM

(GOMD-S3-150-2015) Distinguishability of Particles in Glass-Forming Systems

J. C. Mauro*[1]; M. M. Smedskjaer[2]; 1. Corning Incorporated, USA; 2. Aalborg University, Denmark

The distinguishability of particles has important implications for calculating the partition function in statistical mechanics. While there are standard formulations for systems of identical particles that are either fully distinguishable or fully indistinguishable, many realistic systems do not fall into either of these limiting cases. In particular, the glass transition involves a continuous transition from an ergodic liquid system of indistinguishable particles to a nonergodic glassy system where the particles become distinguishable. While the question of partial distinguishability of microstates has been treated previously in quantum information theory, this issue has not yet been addressed for a system of classical particles. We present a general formalism for quantifying particle distinguishability in classical systems. Example calculations for a simple glass-forming system demonstrate the continuous onset of distinguishability as temperature is lowered. We also examine the loss of distinguishability in the limit of long observation time, coinciding with the restoration of ergodicity. We discuss some of the general implications of our work, including the direct connection to topological constraint theory of glass. We also discuss qualitative features of distinguishability as they relate to the Second and Third Laws of thermodynamics.

10:40 AM

(GOMD-S3-151-2015) Structural simulations of oxy-fluoride glasses

H. Inoue*[1]; A. Masuno[1]; 1. The Univeristy of Tokyo, Japan

Oxy-fluoride glasses have attractive optical properties. The doped rare earth ions show the broad emission bands. It indicates that there are fluoride and oxide sites. Their properties will depend on the coordinated states of oxygen and fluorine ions. In this study, the glasses based on AlF_3 with $AlPO_4$ were prepared and the high-energy x-ray diffraction was measured at the BL04B2 beamline in the Spring-8 synchrotron radiation facility. The structural models were prepared by the classical molecular dynamics simulation. Born-Mayer type of pair potentials was used. The effective charges of the ions were used. The initial coordinates of ions were given by random. The temperature was reduced from 4000K to 293K for 200000 time steps. The experimental total correlation function was reproducible from the function obtained from the structural models. In the structural models, the average coordination numbers of P ions were from 4.01 to 3.95. In the coordination sphere of P ions, the ratios of oxide anions were more than 90 %. The ratio of oxygen in the anion was 23 % in the maximum. Therefore, the oxide anions have selectively coordinated with the P ions. The vibrational frequencies of PO_n polyhedra were evaluated. It was found that the isolated PO_4 tetrahedra in the structural models were obtained by the potential optimization.

11:00 AM

(GOMD-S3-152-2015) Large Scale Simulation of Structure and Properties of Slicate and Metallic Glass (Invited)

N. Li*[1]; X. Zhao[1]; 1. Wuhan University of Technology, China

Amorphous SiO2 (a-SiO2) and bulk metallic glasses (BMG) are both noncrystalline solids without long-range order (LRO), but have distinctively different structures, properties and applications. The structure of a-SiO2 is that of a continuous random network (CRN) with well-defined short range order (SRO) whereas BMG has additional medium range order (MRO) which is far less understood. In this talk, I describe the simulation of a large of amorphous SiO2 (a-SiO2) model with 432 SiO2 molecules and no broken bonds or over-/under-coordinated Si or O atoms, the densification mechanism of a-SiO2 glass; and a series of binary ZrCu BMG models containing 1024 atoms with compositions. These large periodic models were first relaxed by using VASP (Vienna Ab Initio Simulation Package) with high accuracy and their physical properties are calculated using the first first-principles OLCAO (orthogonalized linear combination of atomic orbitals) method. The electronic structure and bonding between these two different types of glasses are compared and contrasted. The significance and implications of these results will be discussed.

11:20 AM

(GOMD-S3-153-2015) Source of instability in amorphous semiconducting oxides (Invited)

S. Han*[1]; 1. Seoul National University, Republic of Korea

Ultra-definition, large-area displays with three-dimensional visual effects represent megatrend in the current/future display industry. On the hardware level, such a "dream" display requires faster pixel switching and higher driving current, which in turn necessitate thin-film transistors (TFTs) with high mobility of 30~50 cm^2/Vs. The traditional *a*-Si TFT performs far below than this requirement and amorphous semiconducting oxides (ASOs) such as In-Ga-Zn-O are poised to enable the high-mobility TFTs. However, the device instabilities under various stress conditions such as voltage, temperature, and light become the main hurdle against the massive commercialization of the AOS-based TFTs. Therefore, the microscopic understanding on the device instability is highly demanded at this moment. In this presentation, I will summarize our recent ab initio calculations on the source of instability in ASO. To explain various instability sources, we calculated the absorption spectrum of ASO, the interface between ASO and SiO2, and the oxygen vacancies. In addition, through the combined study with experiments, we investigated the device instability more directly and proposed how to improve the stability.

11:40 AM

(GOMD-S3-154-2015) State of the Surface of a Thin Sheet of Glass, and its Strength

O. Prokhorenko*[1]; 1. L.G.P. International, USA

The present work describes some initial results of investigation of the influence of the state of the surface of the glass on its mechanical strength. Thin sheet of glass having finite size (100 mm x 100 mm x 1 mm) has been chosen for this study. Physical properties critical from the point of view of formation of thermal stresses in the sheet in the course of its heat treatment (viscosity, CTE, and structural and stress relaxation parameters) were measured using precision methods available at this time. Mathematical modeling of the stress distributions in the sheet in the course of its cooling at different regimes has been performed by using the most accurate analytical, and numerical solutions available at present. A special model simulating behavior of the thin sheet of glass under different kinds of deformation (simple bending, twisting, and local impact) has been developed and used to estimate probability of formation of cracks at presence of initial small defects. Criteria of formation of cracks at the surface of flat or curved thin sheet of glass are discussed in the present paper.

Session 6: Non-Oxide and Metallic Glasses III

Room: Symphony Ballroom II
Session Chair: Ozgur Gulbiten, Corning Incorporated

9:20 AM

(GOMD-S3-155-2015) Structure and Properties of Sulfophosphate Glasses (Invited)

L. Wondraczek*[1]; 1. University of Jena, Germany

Ionic and superionic sulfophosphate glasses of the type $M^1{}_2O$-M^2O-SO_3-P_2O_5, sometimes comprising further anion species, exhibit surprising glass stability and a variety of interesting properties such as tailorable dissolution behaviour, transition and nobel metal ion solubility, tailorable photosensitivity and, generally, low-temperature melting and forming ability. This talk will review our recent understanding of their chemistry and structure, and will also discuss some correlations between structure and macroscopic properties.

9:50 AM

(GOMD-S3-156-2015) Investigation of Structure and Properties in the $GeSe_2$-As_2Se_3-PbSe System with Varying PbSe

C. Smith*[1]; K. Chamma[1]; D. McClane[1]; L. Sisken[1]; A. K. Buff[1]; A. Swisher[2]; A. Pogrebnyakov[2]; T. Mayer[2]; K. Richardson[1]; 1. University of Central Florida, USA; 2. Pennsylvania State University, USA

Chalcogenide glasses have generated significant interest due to their infrared (IR) transmission which allows for their use as lenses or fibers in IR optical systems. In this work we present the characterization of glasses in the $GeSe_2$-As_2Se_3-PbSe system. Techniques such as differential scanning calorimetry (DSC), microhardness testing, and Raman spectroscopy; in addition to optical and electron transmission measurements, were used to determine the effects of PbSe additions on the $GeSe_2$-As_2Se_3 composition. With increasing PbSe two crystallization peaks develop in the DSC spectra and, initially, there is a decrease in the glass transition temperature (T_g), with no change after 10 mol% PbSe. The optical band edge varies non-linearly with PbSe content and can be related to the DSC data and microstructure of the glasses. The changes in properties were also correlated with variations in the Raman spectroscopy data which show systematic changes in relative band intensities for different species, including a decrease in As-Se associated peaks, with the addition of PbSe. The role of PbSe in the glass structure will be assessed and described.

10:10 AM

(GOMD-S3-157-2015) Rare earth doped chalcogenide glasses for environmental sensing

R. Chahal*[1]; F. Starecki[1]; C. Boussard-Pledel[1]; J. Doualan[7]; L. Quetel[2]; K. Michel[3]; S. Marre[8]; S. Morais[8]; Y. Garrabos[8]; C. Prestipino[1]; A. Trapananti[4]; A. Moreac[5]; G. Tricot[6]; A. Braud[7]; P. Camy[7]; B. Bureau[1]; V. Nazabal[1]; 1. Institut des Sciences Chimiques de Rennes UMR CNRS 6226, France; 2. IDIL Fibres Optiques, France; 3. Bureau des Recherches Geologiques et Minieres (BRGM), France; 4. ESRF, France; 5. Institut de Physique de Rennes UMR CNRS 6251, France; 6. ENSC Lille Unite de Catalyse et Chimie du Solide UMR 8181, France; 7. Centre de Recherche sur les Ions, les Materiaux et la Photonique (CIMAP) UMR 6252 CEA-CNRS-ENSICaen, France; 8. Institut de Chimie de la Matiere Condensee de Bordeaux CNRS (ICMCB) UPR 9048, France

Sulfur and Selenium based glasses doped with rare earth (RE) are useful to develop optical sensor for detecting pollutants and monitoring CO_2 stored in underground. Chemical molecules (as CO_2) are presenting absorbing bands in the middle Infrared (mid-IR) and therefore, can be detected in this spectral range. Chalcogenide glasses doped with RE can be used as mid-IR source emitting in the 3 to 5 μm range. They are attractive materials due to their wide optical transparence in the IR region, high refractive indices and low phonon energy that limits non-radiative relaxations. Characterizations were performed to obtain absorption, emission, refractive index, T_g, density and matrix structure. Several compositions of the Ga-Ge-Sb-S(Se) system were investigated to change the band-gap absorption in order to improve the RE pumping efficiency . Dy^{3+}, Er^{3+}, Nd^{3+} and Pr^{3+} absorptions and emissions were observed for bulk and fiber. First, CO_2 gas was detected by an optical sensing prototype based on Dy^{3+} sulfide fiber dipped in a deep well with sensitivity required for final user. Second, Pr^{3+} doped glass fiber was successfully used to detect chemical pollutants by FEWS (Fiber Evanescent Wave Spectroscopy) method. Compare to the classical passive FEWS, which requires the use a black body source, the main benefit of this technology lies in the compactness of the final device and the brightness of the fluorescent mid-IR sources.

10:30 AM

(GOMD-S3-158-2015) Viscosity of $As_{40}Se_{60}$ glass during the fiber drawing process

J. Troles*[1]; G. yang[1]; B. Bureau[1]; C. Boussard[1]; P. Houizot[1]; C. Sangleboeuf[1]; T. Rouxel[1]; 1. University of Rennes 1, France

The viscosity of $As_{40}Se_{60}$ Glass within the hot zone region of the fiber drawing process was estimated using the actual temperature distribution and standard continuum mechanics equations for a linear viscous material. The obtained values for the shear viscosity lie between 10^{3} and 10^{6} Pa.s and are in good agreement with those extrapolated from bending and penetration tests at a lower temperature. In our condition, neck-down region is to be found almost independent on the drawing rate or on the fiber tension.

10:50 AM

(GOMD-S3-159-2015) Optical Property Extrema and Correlation in GeAsSe ternary glass forming system

B. Gleason*[1]; L. Sisken[2]; C. Smith[2]; R. Whitsitt[2]; A. Qiao[3]; N. Anheier[3]; K. Richardson[2]; 1. Clemson University, USA; 2. University of Central Florida, USA; 3. Pacific Northwest National Laboratory, USA

Seventeen infrared-transmitting GeAsSe chalcogenide glasses were fabricated to determine the role of chemistry and structure on various intrinsic optical properties. The refractive index and thermoptic coefficients of samples were measured using an infrared-modified Metricon prism coupler, located at Pacific Northwest National Laboratory. Thermoptic coefficient values were shown to range from approximately -30 ppm/C to +80 ppm/C, and refractive index was shown to vary between approximately 2.5000 and 2.8000. Additional results showed a positive correlation between the density, refractive index, and short wavelength cut-off, all of which displayed a non-linear trend with increasing network coordination. Thermoptic coefficients showed no direct correlation to other measured properties, but can be used to extrapolate ϕ, the materials' thermal polarizability coefficient. Two separate methods of calculating ϕ have been analyzed in the scope of this study. Overall this work demonstrated the ability to compositionally tune, or tailor, optical properties to suit optical design needs.

Session 7: Glass under Extreme Conditions III

Room: Symphony Ballroom I
Session Chair: Anne Tanguy, Université Lyon 1

9:20 AM

(GOMD-S3-160-2015) Unique Effects of Pressure and Thermal History: Implications for Glass Mechanics and Chemical Strengthening (Invited)

M. M. Smedskjaer*[1]; M. Bauchy[2]; M. N. Svenson[1]; J. C. Mauro[3]; L. M. Thirion[3]; S. J. Rzoska[4]; M. Bockowski[4]; 1. Aalborg University, Denmark; 2. University of California, Los Angeles, USA; 3. Corning Incorporated, USA; 4. Polish Academy of Sciences, Poland

The properties of glass are determined not only by temperature, pressure, and composition, but also by their complete thermal and pressure histories. Through both experiments and MD simulations, we reveal that glasses of identical composition produced through thermal annealing and through quenching from elevated pressure can result in samples with identical density and mean interatomic distances, yet different bond angle distributions, medium-range structures, and, thus, macroscopic properties. Specifically we show that changes in micromechanical properties (e.g., hardness) and an ion-exchange induced surface compressive stress are more pronounced when a density increase is obtained through thermal annealing rather than through pressure-quenching, since pressure-quenching has larger effect on medium-range order, while annealing has larger effect on short-range structures. On the other hand, the change in other properties such as alkali diffusivity and bulk modulus upon densification is independent of the type of treatment used to induce the density increase. Our work opens a new avenue towards industrially useful glasses that are identical in terms of composition and density, but with differences in some thermodynamic, mechanical, and rheological properties due to unique structural characteristics.

9:50 AM

(GOMD-S3-161-2015) Transport in thermally grown borosilicate glasses (Invited)

E. J. Opila*[2]; K. Shugart[1]; B. McFarland[2]; M. Wilson[2]; 1. Air Force Research Lab, USA; 2. University of Virginia, USA

Thermally grown borosilicate glasses are important for oxidation protection of ceramics in high temperature oxidizing environments. However, the transport of oxidants through the growing scale is highly sensitive to composition and the temperature dependence of transport is therefore expected to have a complex dependence on boria volatilization which in turn depends on the reactive gas environment. In this work, we explore the oxidation kinetics of ZrB_2-SiC and SiC/BN/SiC composites as a function of temperature and oxidant (dry O_2 and wet oxygen) through thermogravimetric analysis, compositional analysis, and microstructural characterization. In addition, model borosilicate bulk glasses and thin films on SiC substrates were synthesized using a sol gel technique to explore glass compositional effects of boria volatility and SiC oxidation. Results indicate the surface of both thermally grown and model borosilicate glasses are depleted in boria in both dry and wet environments resulting in a boron gradient through the thickness of the scale. Oxidation kinetics are interpreted in terms of the glass composition with a long term goal of developing thermochemical life prediction models for application of these ceramic systems in high temperature oxidizing environments.

10:20 AM

(GOMD-S3-162-2015) Density of Silicate Glass Melts and Glasses Using Aerolevitation

M. Affatigato*[1]; P. Pinchuk[1]; A. Kline[2]; M. Welninski[1]; G. Wehr[1]; S. Feller[1]; 1. Coe College, USA; 2. Iowa State University, USA

We report on our studies of the density of alkaline earth silicate glasses and melts using aerolevitation. We strat by discussing the range of compositions that can be formed into glass for several alkaline earth silicate families, and the reasons for the differences between modifiers. We will also report on our investigations of the density over a wide temperature range (up to 2000 Celsius). The size of the bead, and hence its density in both the liquid and solid states, was accurately measured as a function of temperature using a high speed camera and various imaging techniques. More recent preliminary work includes the use of sound waves to set the bead into different modes of oscillations, which permits us to determine the surface tension (during the oscillation) and viscosity (as the oscillation decays once the driving sound waves are removed) of the melt. This work was supported by the U.S. National Science Foundation under grants REU PHY 1004860, REU PHY 1358968, DMR CER 1407404, and DMR MRI 0922924.

10:40 AM

(GOMD-S3-163-2015) Raman spectroscopy of v-SiO_2 under rare gas compression

C. Weigel[1]; B. Hehlen[1]; M. Foret*[1]; M. Kint[1]; R. Vacher[1]; B. Ruffle[1]; 1. University of Montpellier, France

The normalized VV- and VH-polarized Raman spectra of SiO_2 glass pressurized in helium and in argon at pressure in the range 0 – 8 GPa by means of diamond anvil cell are presented. We detail the evolution of structural changes associated with the compressed state of the glass. In the case of compression under argon atmosphere, one observes a strong narrowing and a closing of the broad Si-O-Si angle distribution that is characteristic of the tetrahedral network glass. In contrast, with helium as pressurizing medium, the reduction of the intertetrahedral angle distribution is to a large extent hindered by the penetration of helium atoms in the silica network.

11:00 AM

(GOMD-S3-164-2015) Optical properties of permanently densified silica glass

A. Masuno*[1]; N. Nishiyama[2]; F. Sato[3]; T. Taniguchi[4]; H. Inoue[1]; 1. The University of Tokyo, Japan; 2. Deutsches Elektronen-Synchrotron, Germany; 3. Nippon Electric Glass Co., Ltd., Japan; 4. National Institute for Materials Science, Japan

Large-sized densified silica glasses were fabricated at a high pressure of 7.7 GPa. As the synthesis temperature was increased from room temperature to 1200°C, the densification increased to 23%. The refractive index at 587.56 nm, n_d, increased linearly to 1.55680, which is higher than that of crystalline silica (α-quartz). Furthermore, the Abbe number, ν_d, also increased and approached that of α-quartz. According to the Sellmeier equation, the increase in ν_d that accompanied densification was caused by a shift of the glasses' absorption band in the UV region to shorter wavelengths. The densified silica glasses with a refractive index and a wavelength dispersion comparable to those of α-quartz are promising materials for the design of advanced optics.

11:20 AM

(GOMD-S3-165-2015) Structural Relaxation of Isostatically Compressed Sodium-Borate Glass

M. N. Svenson*[3]; M. M. Smedskjær[3]; Y. Yue[3]; R. Youngman[1]; S. Rzoska[2]; M. Bockowski[2]; L. R. Jensen[3]; 1. Corning Incorporated, USA; 2. Polish Academy of Sciences, Poland; 3. Aalborg University, Denmark

The short- and intermediate-range structures and thus properties of glasses can be modified by subjecting them to sufficiently high pressure. However, the relaxation behavior of such compressed glasses upon subsequent heat-treatment at ambient pressure is poorly understood. Relaxation studies of compressed glasses could shed light on the relations between certain structural features and the macroscopic glass properties. In this work, we address this issue by performing ^{11}B and ^{23}Na NMR, Raman spectroscopy, and density measurements on a sodium-borate glass, which has first been isostatically compressed at 1 GPa at the glass transition temperature (T_g) and then annealed at ambient pressure at various times and temperatures around T_g. In general, the isostatically compressed glass gradually returns to its state prior to compression upon annealing at ambient pressure. As expected, the rate of relaxation increases with increasing annealing temperature. The structural analysis reveals strong correlations between density and both short- and intermediate-range structural features. We thus find that density and the pressure-induced change in boron coordination from BO_3 to BO_4 relax on a similar timescale, in contrast to recent findings on an analogous composition.

11:40 AM

(GOMD-S3-166-2015) Structure and Properties of Silica Glass Densified by Pressure-quenching

M. Guerette[1]; L. Huang*[1]; 1. RPI, USA

Pressure quenching from the non-rigid state near the glass transition temperature was used to effectively change the glass atomic packing and to make densified silica glass (up to 25% increase in density). The resulting structure and properties of as-quenched samples were investigated using XRD, Raman and Brillouin spectroscopy. In-situ Raman and Brillouin light scattering techniques were developed to study the structure, elastic and dynamic properties of silica glass under high temperature and high pressure conditions. High temperature measurements were carried out in an optical furnace up to 1500 °C, a diamond anvil cell was used to carry out high pressure experiments up to 25 GPa. Our studies show that pressure quenching imparts structural signatures to densified silica glass that cannot be accomplished through cold compression at room temperature. The unique structures of pressure-quenched silica glass are reflected in decreased anomalous response of elastic moduli to external stimuli of high temperature or high pressure, and therefore greater thermo-mechanical stability.

Symposium 4: Optical and Electronic Materials and Devices - Fundamentals and Applications

Session 4: Glass Ceramics

Room: Concerto A
Session Chair: Yiquan Wu, Alfred University

9:20 AM

(GOMD-S4-056-2015) Effects of Thermal Processing Parameters on Material Properties for Chalcogenide Glass Ceramics in the Ge-As-Pb-Se System

L. Sisken*[1]; C. Smith[1]; P. Wachtel[2]; K. Chama[1]; A. K. Buff[1]; K. Richardson[1]; 1. University of Central Florida, USA; 2. Irradiance Glass, USA

There is increasing interest in chalcogenide-based glass ceramics to create infrared materials that are easier to manufacture than single crystals and have material properties that are more desirable then their base chalcogenide glass. Detailed studies of the effect of the processing temperatures away from the peak nucleation and growth temperatures on the material properties are sparse. The properties of a glass ceramic are dependent on the nucleation and growth treatments performed, due to the different microstructures that are grown. A multi-component Ge-As-Se-Pb glass composition was nucleated and grown at different temperatures base on prior experimental data, and evaluated for resulting physical properties in its post-processed state. The properties were evaluated as a function of different heat treatment protocols and include index, thermal conductivity, hardness, and the absorption edge. The Raman spectra were also taken after the heat treatments in order to correlate property changes with configurational changes. A range of material properties was observed, which has been correlated to microstructure.

9:40 AM

(GOMD-S4-057-2015) Glass-ceramics based on the bulk formation of "anti-glass" spherulites in the TeO_2-Nb_2O_5-Bi_2O_3 system

M. Shimoda[2]; A. Bertrand[1]; J. Carreaud[1]; G. Delaizir[1]; J. Duclere*[1]; M. Colas[1]; J. Cornette[1]; T. Hayakawa[2]; O. Masson[1]; C. Genevois[3]; E. Véron[3]; M. Allix[3]; P. Thomas[1]; 1. Laboratoire SPCTS, France; 2. Nagoya Institute of Technology, Japan; 3. Conditions Extrêmes et Matériaux : Haute Température et Irradiation (CEMHTI), France

Glass-ceramics in the TeO_2-Nb_2O_5-Bi_2O_3 system were studied. The kinetics parameters and the Avrami exponent, as well as the nucleation and growth parameters, were determined. The glass-ceramics consist in crystalline spherulites present throughout the bulk. The crystal structure corresponds to a cubic phase, similar to β-$Bi_2Te_4O_{11}$, but containing Nb. Such structure is analogous to the "anti-glass" phases described by Trömel. The optical transparency of the bulk materials is progressively reduced with the increase in the density of spherulite/glass matrix interfaces. The photoluminescence (PL) properties of (1% wt) Er_2O_3-doped compositions, as a function of the devitrification time at T = 380°C, were investigated. A careful analysis of the evolution of the PL signal ($^4I_{13/2}$ - $^4I_{15/2}$ transition) allows the indirect detection of the first steps of the devitrification. The corresponding time determined from PL measurements match very well with the one directly derived from X-ray diffraction (XRD) data. Finally, the evolution of the integrated PL intensity and lifetime values as a function of the devitrification time is monitored. It is noticed that both quantities show very comparable trends, and that the increase/decrease in the PL intensity is systematically accompanied by a respective increase/decrease of the lifetime value.

10:00 AM

(GOMD-S4-058-2015) The effect of trivalent iron on the properties of fluorochlorozirconate glass ceramic

A. Evans*[1]; J. Hah[1]; R. Leonard[1]; C. Johnson[1]; J. A. Johnson[1]; 1. University of Tennessee Space Institute, USA

Fluorochlorozirconate (FCZ) glasses doped with europium (II) or (III) chloride and iron (III) chloride were prepared in order to ascertain the effect of trivalent iron on the properties of (FCZ) materials. The samples were subsequently heat treated to produce glass ceramics containing barium chloride nanocrystals in either the hexagonal or orthorhombic structure. Characterization methods include differential scanning calorimetry to determine crystallization temperatures for the heat treatment process, x-ray diffraction to give the crystalline phase of the nanocrystals, Mössbauer Spectroscopy to determine the valency of both europium and iron and phosphorimetry to tie together the optical and structural properties. The addition of trivalent iron had a marked effect on the crystallization of the glasses.

10:20 AM

(GOMD-S4-059-2015) Scratch resistance of glass-ceramics in the $MgO-Al_2O_3-SiO_2$ (MAS) system

B. Hota*[1]; O. Hochrein[2]; I. Burger[2]; I. Mitra[2]; M. Bockmeyer[2]; J. Deubener[1]; 1. Clausthal University of Technology, Germany; 2. SCHOTT AG, Germany

Glass-ceramics in the $MgO-Al_2O_3-SiO_2$ system (MAS-GC) are of increasing interest due to multiple precipitation of binary and ternary crystal phases of superior mechanical properties (high Young modulus, high hardness etc.). Nevertheless, MAS-GC are scratched in contact with sharp, even harder materials. Damage to the surface leads to an optical impairment of the GC component and to a reduction of its mechanical strength and fatigue limit. In contrast to glasses, where the governing factors to initiate and propagate scratches are the surface state (roughness and initial cracks) and the stress conditions (contact tensile stresses vs. engineered compressive stresses), for GC additionally microstructural gradients and residual stresses induced by the thermal expansion mismatch of crystals and glass matrix are significant. In order to address the latter effects we have varied the ceramization conditions of selected MAS green glasses. DWeibull plot of the probability for chipping vs. indentation load as adopted from Yoshida et alThe results show that in the case of iso crystalline MAS-GC (constant crystalline volume fraction) the resistance against scratching was highest for Mg-bearing GC whereas Al-rich GC decreases the scratch resistance.

10:40 AM

(GOMD-S4-060-2015) Fusion Formable Glass-Ceramics with High Strength

M. Dejneka*[1]; I. Dutta[1]; C. Smith[1]; 1. Corning Incorporated, USA

Strong, black materials are needed for electronic device backs and appliance facings. While glass ceramics have good strength and toughness, their liquidus viscosity is too low to enable economical forming of these devices by the fusion or slot draw methods. Thus we invented a new class of low crystallinity glass ceramics with 10-20nm crystallites in the $Fe_2O_3-TiO_2-MgO$ system. These materials were formed into transparent glasses and then heat treated to make black opaque glass-ceramics containing magnetite, pseudobrookite, and/or $\varepsilon-Fe_2O_3$. The $\varepsilon-Fe_2O_3$ phase exhibited extensive solid solution (ss) between Fe_2O_3 and $MgTiO_3$. The blackness and opacity of the $\varepsilon-Fe_2O_3$ glass-ceramics peaked at a ceram temperature of 750°C where the Fe^{2+} in the crystallites was maximized, resulting in peak Fe^{2+} - Ti^{4+} charge transfer absorption. The liquidus viscosity was increased to more than 100 kPa*s by optimizing the base glass composition and minimizing the amount of crystallinity thereby enabling fusion formability. These fusion formable glass-ceramics had strengths exceeding the best commercially available glasses after ion exchange. This work provides a new class of low crystallinity fusion formable glass ceramics with high strength.

11:00 AM

(GOMD-S4-061-2015) Tailoring Nanoscale Phase Separation in New Gallogermanate and Gallosilicate Oxide Glasses: Application to Highly Transparent Glass-ceramics (Invited)

M. Allix*[1]; S. Chenu[1]; E. Véron[1]; C. Genevois[1]; G. Matzen[1]; 1. Laboratoire CEMHTI - CNRS, France

New nanostructured gallogermanate- and gallosilicate-based glass materials exhibiting high transparency in the visible range have been fabricated by conventional melt-quenching. These materials can accommodate wide oxide compositions and present nanoscale phase separation. The size of the nanostructuring can be tailored depending on the nominal composition. A single heat treatment then allows selective crystallization of the phase separated glass, resulting in glass-ceramic materials exhibiting nanostructures and transparency similar to the parent glass. The wide possibilities of designing new nanostructured glass-ceramics with tunable optical properties will be illustrated in the case of a highly transparent $ZnGa_2O_4$ glass-ceramic exhibiting 50 wt% of nanocrystals with homogeneous and tunable sizes. High resolution scanning transmission electron microscopy analysis coupled with in situ high temperature X-ray diffraction and optical measurements led to a detailed description of the crystallization process. Remarkably, red long-lasting luminescence arising from the entire sample volume is observed in this Cr^{3+} doped material, opening the route to a wider range of performing applications for this famous zinc gallate persistent phosphor.

Symposium 5: Glass Technology and Cross-cutting Topics

Session 2: Transparent Protective Systems

Room: Concerto B

Session Chairs: Andrew Wereszczak, Oak Ridge National Laboratory; Parimal Patel, Army Research Laboratory

9:20 AM

(GOMD-S5-068-2015) Responses of Silicate Glasses to High Pressure

A. Wereszczak*[1]; T. Morrissey[2]; M. Ferber[1]; K. Bortle[2]; E. Rodgers[2]; G. Tsoi[3]; Y. Vohra[3]; 1. Oak Ridge National Laboratory, USA; 2. ORISE, USA; 3. University of Alabama @ Birmingham, USA

Several silicate glasses (float glasses and vitreous silica) were subjected to high pressure loading using spherical indentation, diamond anvil cell (DAC) testing, and laser shock impact. The investigated materials are either presently used in armor applications or are candidates for such. The three employed test methods were chosen because they can apply many GPa of pressure, are relatively quick and inexpensive to experimentally conduct, produce repeatable results, and induce a bulk material response. Small diameter diamond indenters were used to apply many GPa of Hertzian contact stress, and resulting indenter depth-of-penetration provided insights into apparent stress-strain response under concurrent shear and hydrostatic loadings. A DAC was used to apply a hydrostatic pressure and each material's Raman and x-ray diffraction spectra were interpreted as a function of pressure up to ~ 20 GPa. Laser shock impact testing applied many GPa in a few nanoseconds so this dynamic test method enabled a cursory examination of any rate effect at high pressures. The test methods and their produced stress states are described, and the mechanical and morphological responses of the materials caused by them are contrasted.

9:50 AM

(GOMD-S5-069-2015) Laser-shock spall testing of glass and glass-ceramics

M. J. Davis*[1]; C. Weinhold[1]; P. Vullo[1]; 1. SCHOTT North America, Inc., USA

The identification of a useful screening test for armor materials remains a subject of considerable interest. We report on high strain-rate experiments (> 10^6 sec^{-1}) using laser-shock techniques in which the energy of a 10-nsec laser pulse is converted at the sample surface into a sharp pressure wave which then propagates into the sample. Well-defined spall threshold conditions were quantified for a variety of glass and glass-ceramic materials. In general, glasses all exhibited higher spall thresholds than the glass-ceramics, although some of the glass-ceramics exhibited low levels of subsequent fracturing even when tested above threshold conditions. Finally, calculated spall stresses for the glasses are compared with quasi-static tensile breaking stresses for pristine glass fibers, perhaps the only other test method for which surface flaws play a negligible role in the fracture of glass.

10:20 AM

(GOMD-S5-070-2015) Equibiaxial Flexure Strength of Glass: Influence of Glass Plate Size and Equibiaxial Ring Ratio

J. Swab*[1]; P. Patel[1]; S. Kilczewski[1]; 1. U.S. Army Research Laboratory, USA

Glass plays an important role in many engineering applications including transparent armor. Determining the actual strength of a glass is problematic because typical glass strength numbers are presented in the literature as ranges. Minor changes in surface finish, composition, test method employed, and processing all influence the mechanical strength of glass. A standardized method needs to be utilized to ensure that strength data can be compared universally. The use of a standard methodology is vital when comparing glass compositions or multiple sample lots of the same composition in order to attribute any real strength variations to the glass itself. While the procedures established in ASTM C1499 provide a good framework for glass strength measurement, flexibility in the experimental parameters of the standard allow for substantial strength variations when testing glass materials. The ratio between the load and support ring diameters, as well as the specimen dimensions, are shown to lead to variations in both the measured strength, as well as the percentage of number of valid/invalid tests based on where fracture initiates. The goal of this study is to quantify these effects in order to establish optimized testing conditions for determining the strength of float glass.

10:40 AM

(GOMD-S5-071-2015) Investigation of failure mechanisms in glass under dynamic loading using high speed x-ray contrast imaging

N. Parab[1]; W. W. Chen*[1]; 1. Purdue University, USA

Glasses are critical materials for transparent armor applications because of high hardness, low weight, low cost and high transparency. In this study, failure/damage mechanisms under dynamic loading in different types of glasses are investigated using high speed x-ray phase contrast imaging (PCI) synchronized with a modified Kolsky bar setup. Borosilicate and soda-lime glasses were investigated under a dynamic indentation loading using a knife edge indenter driven at a velocity of 8-10 m/s. It was observed that an angular crack develops in front of the indenter in borosilicate glass similar to Hertzian cone cracks commonly observed in penetration experiments in brittle materials. Straight line cracking was observed to initiate from the indenter in soda-lime glass. To investigate the effects of indenter geometry on the damage mechanisms, a cylindrical indenter was driven into the glass with the same velocity as that of the knife edge indenter. Conical cracking was observed to initiate in front of the indenter in borosilicate glass and predominantly straight line cracking was observed in soda-lime glass. It can be concluded that there are significant differences in the damage mechanisms in different types of glasses which might be the reason behind the differences in ballistic performance.

11:00 AM

(GOMD-S5-072-2015) Internal Pores in Thick Silicate Glasses Revealed by High-Strain-Energy Fracture

A. Wereszczak*[1]; S. Waters[1]; L. D. Pye[2]; 1. Oak Ridge National Laboratory, USA; 2. Alfred University, USA

Sub-micron-sized pores are described in context to silicate glass plates having thicknesses greater than 6 mm and subjected to a large strain energy of fracture. These pores, ranging in size from ~ 300-1000 nm as estimated by fractography via scanning electron microscopy, are suspected to form during glass melting having not been eliminated prior to solidification. They are located on the surfaces and edges of a fraction of the smaller-sized fragments resulting from high-strain-energy fracture (initial imposed strain greater than 1%) and subsequent inter-particle comminution from the event. This pore-positioning on the fracture surfaces, with positioning sometimes at the front of crack bifurcation, suggests these pre-existing pores could have provided localized preferred paths of crack propagation or lower crack-propagation resistance. These pores do not appear to be randomly distributed but rather often have a porous seam or planar habit to their positioning. The size-range of these interior pores is several orders of magnitude smaller than surface-located flaw sizes that typically limit glass flexure strength, so high-strain-energy appears to be a prerequisite for these pores to be exposed in the fracture of these glasses. These sub-micron-pores in several silicate glasses and their potential relevance in a ballistic event are described.

Session 4: Waste Glass Chemistry

Room: Concerto C

Session Chair: Kevin Fox, Savannah River National Laboratory

9:20 AM

(GOMD-S5-073-2015) Sulfur Solubility in Hanford Waste Glass Melts

J. Vienna*[1]; D. Kim[1]; A. Kruger[2]; 1. PNNL, USA; 2. DOE-ORP, USA

The concentration of sulfur in Hanford waste glass melter feed will be maintained below the point where the salt accumulates on the melt surface. The allowable concentrations may range from near zero to over 2.05 wt% (of SO_3 on a calcined oxide basis) depending on the composition of the melter feed and processing conditions. If the amount of sulfur exceeds the melt tolerance level, a molten salt will accumulate which may upset melter operations and potentially shorten the useful life of the melter. At the Hanford site, relatively conservative limits have traditionally been placed on sulfur loading in melter feed, which in turn significantly increases the projected amount of waste glasses that will be produced. Crucible-scale sulfur solubility data and scaled melter sulfur tolerance data have been collected on simulated Hanford waste glasses over the last 15 years. These data were compiled and analyzed. An empirical model was developed to predict the solubility of SO_3 in simulated waste glass compositions. This model represents the data well, accounting for over 85% of the variation in data, and was well validated. The model was also found to accurately predict the maximum amount of sulfur in melter feed that did not form a salt layer in scaled melter tests of simulated Hanford waste glasses.

9:40 AM

(GOMD-S5-074-2015) Effects of Chloride on Sulfate Solubility in LAW Glass Melts

H. Gan*[1]; Z. Feng[1]; I. L. Pegg[1]; 1. the Catholic University of America, USA

Many low-activity waste (LAW) streams at Hanford contain significant amounts of sulfate, leading to the potential for the formation of deleterious molten salt phases during vitrification. Salt formation depends on many factors, including the underlying phase equilibria, the melter feed and glass compositions, and the dynamic processes occurring in the cold cap. In addition to sulfate, the presence of other salt-prone components in the waste (such as halides, chromate, phosphate), and interactions between them, further complicates the mitigation of molten salt formation. Understanding these effects can provide the basis for the design of improved LAW glass formulations that mitigate this risk while maximizing waste loadings. This work investigated the effect of chloride on sulfate solubility in LAW glass melts using a technique that maintained a stable molten sulfate/chloride salt phase in equilibrium with the glass melt. Sulfate solubility decreased with increasing chloride concentration and analysis of the coexisting phases suggests that this is due primary to the effect of chloride on the activity of sulfate in the molten salt phase. Sulfate solubility obeyed Henry's Law over wide concentration ranges and the Henry's constant was significantly smaller when vanadium was present in the melt. Various other glass additives were also tested for their effectiveness in increasing solubility.

10:00 AM

(GOMD-S5-075-2015) Current state of knowledge of yellow phase in HLW glasses

S. Schuller*[1]; E. Boué[1]; E. Régnier[1]; 1. CEA, France

In the field of high level waste vitrification, the main issues facing current nuclear R&D challenges are to accommodate new types of waste and higher waste loading while enhancing the glass quality and increasing the production capacity. This requires in-depth knowledge of the glassy materials physical and chemical properties. In this context, understanding yellow phase formation in High Level Waste (HLW) glasses is a fundamental step toward managing the microstructure and the quality of nuclear glass. Based on the literature and research carried out at the CEA concerning phase separation and chemical reactivity between glass frit and calcine, this contribution describes current state of knowledge concerning the yellow phase formation. Following a general introduction on French nuclear glass waste forms, this presentation focuses on a number of key issues related to yellow phase. Its chemical compositions, radiological variability, the impacts of the precursor physical properties and the process parameters will be discussed. Then, the mechanisms of yellow phase formation and dissolution during glass synthesis and the hypotheses taken into account will be shown. Finally, based on publications and patents, the different approaches used to avoid yellow phase formation and the limitation of molybdenum concentration in the nuclear glasses will be presented.

10:20 AM

(GOMD-S5-076-2015) Retention of Iodine in Hanford Waste Glasses

K. S. Matlack*[1]; I. L. Pegg[1]; 1. The Catholic University of America, USA

The long half-life, high environmental mobility, and biological activity of ^{129}I make it a constituent of concern in the treatment and disposal of nuclear wastes at the Hanford site. Iodine is also one of the more volatile radionuclides and its retention in glass under the high temperature conditions prevailing during vitrification can vary over a relatively wide range, depending on the melter feed and glass compositions, redox conditions, and melter operating parameters. High retention of iodine in the glass is desirable in order to minimize the fraction that is directed to secondary waste treatment and disposal in non-glass waste forms. In this work, a wide range of Hanford LAW and HLW simulants containing iodine were processed in joule-heated ceramic melters at four different scales spanning a scale-up of a factor of ~160. Tests were also conducted on systems that included off-gas treatment components that are prototypical of those in the Hanford Waste Treatment Plant. The effects of glass and waste composition, additives and additive forms, reductant type and amount, bubbling rate and bubbling gas composition, glass temperature, and melter size on iodine partitioning in the melter and prototypical off-gas system components were investigated. Iodine retention in the glass product spanned a wide range, from a few percent to over 60% and, as expected, increased significantly with recycle.

10:40 AM

(GOMD-S5-077-2015) Alkali Technetium Oxides as Model Compounds for ^{99}Tc Incorporation in Glass

J. L. Weaver*[1]; J. McCloy[1]; N. Wall[1]; C. Soderquist[2]; 1. Washington State University, USA; 2. Pacific Northwest National Labratory, USA

A priority goal of the United States Department of Energy is to dispose of nuclear wastes accumulated in underground tanks at the Hanford Nuclear Reservation in Richland, WA. Incorporation and stability of technetium (^{99}Tc) into vitrified waste forms is a concern to the waste glass community and DOE due to its long half-life (2.110^5 y), and its high mobility in the subsurface environment under oxidizing conditions. We provide a progress report on our efforts to obtain first-of-a-kind chemical structure determination of poorly understood, environmentally relevant, alkali technetium oxide pure compounds. Knowledge of the structure and spectral signature of these compounds, will aid in refining the understanding of ^{99}Tc incorporation into and release from oxide nuclear waste glasses. Compounds currently under investigation, which are all, all non-pertechnetate Tc^{7+}, include Na_3TcO_5, K_3TcO_5, Na_5TcO_6, K_5TcO_6, and their rhenium analogs. This work provides much needed data for assessing reactions of water with Tc in glass, and thus improving understanding of Tc environmental release which impacts performance assessment models for waste repositories.

11:00 AM

(GOMD-S5-078-2015) Crystallization kinetics of Na_2O-Al_2O_3-Fe_2O_3-SiO_2 glasses

Y. Shahrayar[1]; E. Han[1]; A. Maron[1]; J. Marcial[2]; J. Weaver[2]; J. McCloy[2]; A. Goel*[1]; 1. Rutgers - The State University of New Jersey, USA; 2. Washington State University, USA

As per the current strategy, the sodium and alumina-rich high level radioactive wastes (HLW) stored at Hanford site in Washington will be vitrified into chemically durable borosilicate glasses. However, in the presence of SiO_2 and B_2O_3, the melt rich in Na_2O, Al_2O_3 and Fe_2O_3 is prone to crystallization of nepheline and iron-containing spinel ($NiFe_2O_4$). While volume nucleation of $NiFe_2O_4$ crystals in the melt pool would be problematic as large insoluble crystals can settle to the floor of the glass melter and block the pour spout, the crystallization of nepheline in glass melt can result in severe deterioration of the chemical durability of the waste form. Therefore, it becomes mandatory to understand the nucleation and crystallization kinetics of these multicomponent glasses. However, their compositional complexity does not allow the creation of holistic datasets needed to design glasses with high waste loading and minimal crystallization tendency. Since HLW borosilicate glasses are similar in composition to basalt glass on a borate-free basis, and as no borate phases crystallize on the liquidus, the crystallization chemistry of waste glasses can be described by the known phase relations of the Na_2O-Al_2O_3-Fe_2O_3-SiO_2 quaternary system. Therefore, the present study is focused on understanding the influence of redox chemistry of iron on the crystallization kinetics of simplified iron-containing model nuclear waste glasses.

11:20 AM

(GOMD-S5-079-2015) Nepheline crystallization in boron-rich alumino-silicate glasses as investigated by multi-nuclear NMR, Raman, & Mössbauer spectroscopies

J. McCloy*[1]; N. Washton[3]; P. Gassman[2]; J. Marcial[1]; J. Weaver[1]; R. Kukkadapu[3]; 1. Washington State University, USA; 2. Pacific Northwest National Laboratory, USA; 3. Environmental Molecular Sciences Laboratory, USA

A spectroscopic study was conducted on six simulant nuclear waste glasses using multi-nuclear NMR, Raman, and Mössbauer spectroscopies exploring the role of Si, Al, B, Na, and Fe in the glass network with the goal of understanding melt structure precursors to deleterious nepheline crystal formation. NMR showed two sites each for Al, Si, and Na in the samples which crystallized significant amounts of nepheline, and B speciation changed, typically resulting in more B(IV) after crystallization. Raman spectroscopy suggested some of the glass structure is composed of metaborate chains or rings, thus significant numbers of non-bridging oxygen and a separation of the borate from the alumino-silicate network. Mössbauer, combined with Fe redox chemical measurements, showed Fe playing a minor role in these glasses, mostly as Fe^{3+}, but iron oxide spinel forms with nepheline in all cases. A model of the glass network and allocation of non-bridging oxygens (NBOs) was computed using experimental B(IV) fractions which predicted a large amount of NBO consistent with Raman spectra of metaborate features.

11:40 AM

(GOMD-S5-080-2015) Iron Phosphate Waste Forms for Simulated Fission Products Waste Streams

C. Kim*[1]; L. Ma[2]; R. K. Brow[2]; 1. MO-SCI Corporation, USA; 2. Missouri University of Science and Technology, USA

Most liquid high-level nuclear waste is currently being immobilized to a solid form as a borosilicate glass by vitrification. However, many nuclear wastes have complex and diverse chemical compositions that reduce their compatibility with borosilicate glass. The current baseline spent nuclear fuel reprocess generates secondary waste streams that generally include large amounts of MoO_3 and lanthanides that are poorly soluble in borosilicate glasses and thereby limit the waste loading. New waste forms as alternatives to borosilicate glass are being sought to increase the waste loading while retaining acceptable chemical durability and thus to decrease the total nuclear waste volume required for storage and disposal. Iron phosphate waste forms containing up to 60 wt% of the MoO_3-rich waste (Collins-CLT composition) were prepared. Physical properties and chemical durability of the iron phosphate waste forms are discussed.

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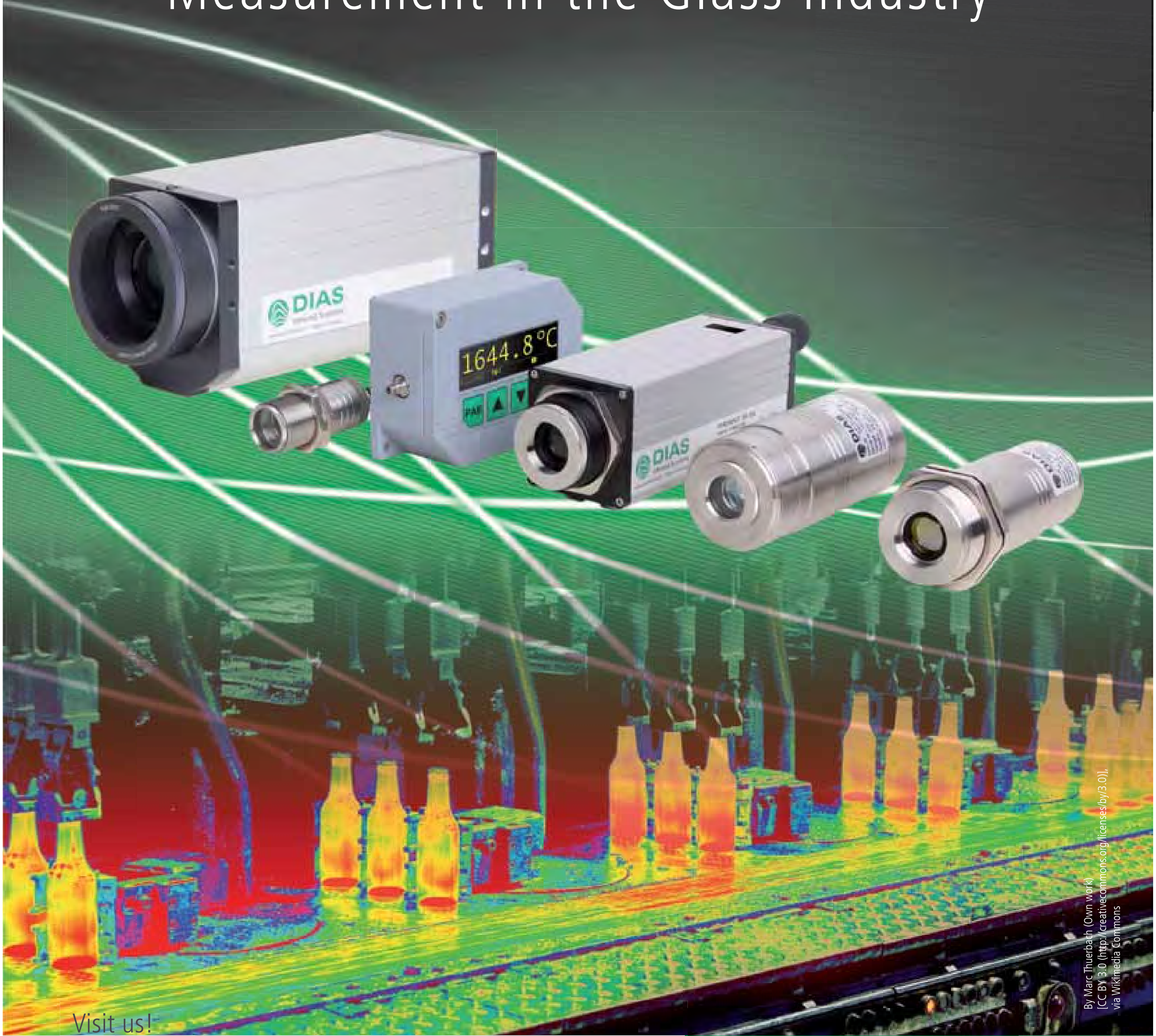

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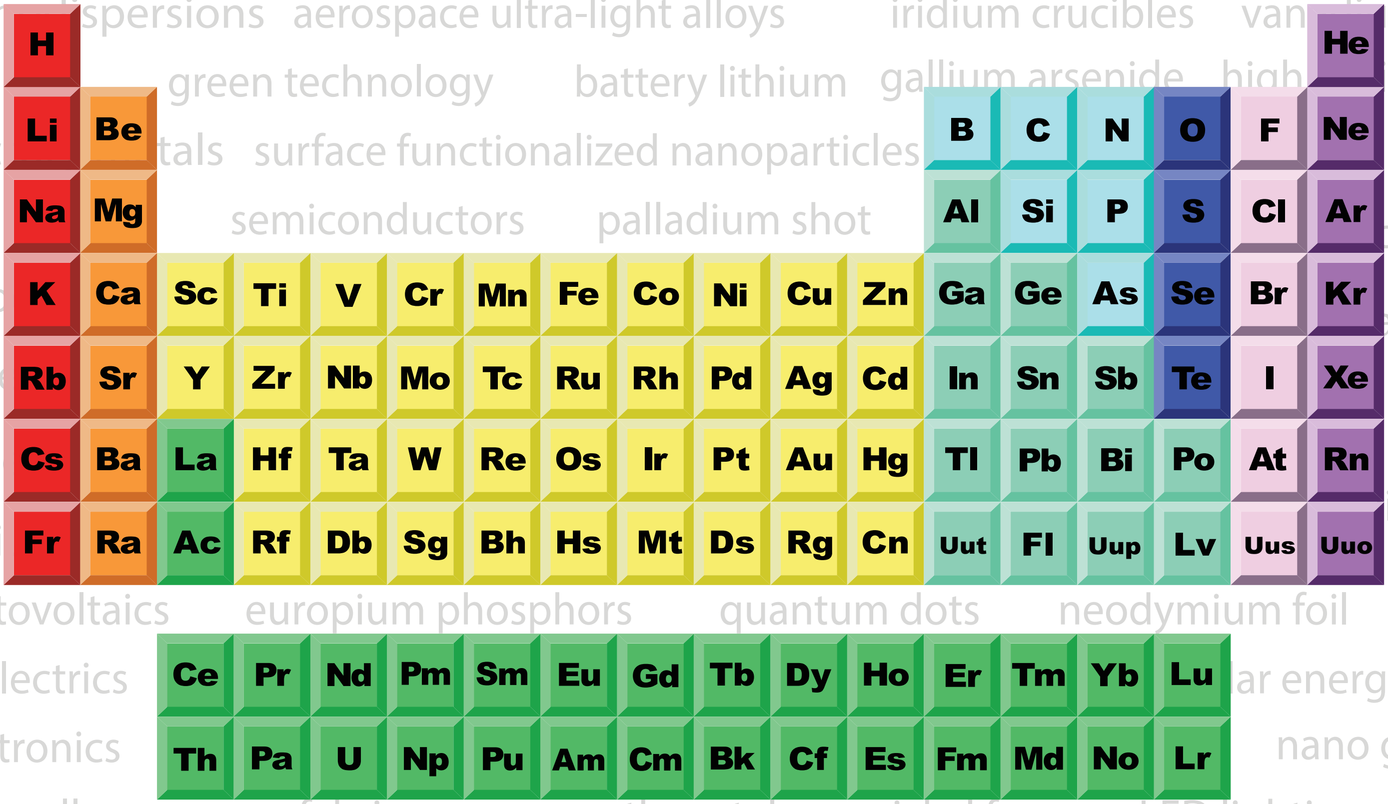

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