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# conference program

[ceramics.org/gomd2016](http://ceramics.org/gomd2016)

The Madison Concourse Hotel and Governor's Club | Madison, WI USA

# **2016 GLASS AND OPTICAL MATERIALS DIVISION ANNUAL MEETING**

May 22–26, 2016





ELSEVIER

# JOURNAL OF NON-CRYSTALLINE SOLIDS

PROUD SPONSOR OF THE GOMD 2016 POSTER SESSION



2014 Impact Factor\*

**1.766**

## 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 23**

**Time: 6.30 – 8.30 pm**

## Announcing the 2016 N.F. Mott Award

The Senior Scientist Award for Outstanding contributions to the science of Non-Crystalline Solids over many years.

**The winner will be announced during the conference banquet.**

FOR MORE INFORMATION

[www.elsevier.com/locate/jnoncrysol](http://www.elsevier.com/locate/jnoncrysol)

# welcome

## **Dear Colleagues and Friends,**

On behalf of The American Ceramic Society, welcome to the Glass & Optical Materials Division Meeting (GOMD 2016). We have over 360 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. GOMD2016 will provide a unique opportunity for glass scientists and technologists to interact.

GOMD2016 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 ***The International Journal of Applied Glass Science (IJAGS)***, ***Deltech Furnaces***, ***Saint-Gobain*** and the ***Journal of Non-Crystalline Solids***.

**The American Ceramic Society thanks you for participating in this year's meeting.**

## The 2016 Organizing Committee:



**Liping Huang**  
Rensselaer Polytechnic  
Institute



**John Kieffer**  
University of Michigan

# award speakers



## **Stookey Lecture of Discovery**

Monday, May 23, 2016 | 8 – 9 a.m.

**David L. Griscom**, impactGlass research international

Title: *The life and unexpected discoveries of an intrepid glass scientist*

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



## **George W. Morey Lecture**

Tuesday, May 24, 2016 | 8 – 9 a.m.

**Hellmut Eckert**, Institute of Physics in São Carlos, University of São Paulo, Brazil & Institute of Physical Chemistry, University of Münster, Germany

Title: *Spying with spins on messy materials: 50 years of glass structure elucidation by NMR spectroscopy*

Sponsored by **PPG Industries, Inc.**



## **The Norbert J. Kreidl Award for Young Scholars Lecture**

Tuesday, May 24, 2016 | Noon – 1 p.m.

**Lan Li**, Massachusetts Institute of Technology

Title: *Materials and devices for mechanically flexible integrated photonics*



## **Darshana and Arun Varshneya Frontiers of Glass Science Lecture**

Wednesday, May 25, 2016 | 8 – 9 a.m.

**Matteo Ciccotti**, Professeur de l'ESPCI, Laboratoire de Science et Ingénierie de la Matière Molle, France

Title: *Multiscale investigation of stress-corrosion crack propagation mechanisms in oxide glasses*



## **Darshana and Arun Varshneya Frontiers of Glass Technology Lecture**

Thursday, May 26, 2016 | 8 – 9 a.m.

**Matthew J. Dejneka**, Research fellow, Corning Glass Research Group

Title: *Chemically strengthened glasses and glass-ceramics*

# table of contents

Award Speakers .....	ii
Schedule at a Glance .....	iv
Student Events .....	v
Symposia/Session Matrix .....	vi-ix
Hotel Floor plan .....	x
Presenting Author List .....	1-3

## final program

Monday morning .....	4-5
Monday afternoon .....	5-9
Tuesday morning .....	9-11
Tuesday afternoon .....	11-14
Wednesday morning .....	14-16
Wednesday afternoon .....	16-18
Thursday morning .....	19-20
Thursday afternoon .....	20-21
Abstracts .....	22-89
Author index .....	90-94

## sponsors



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The American Ceramic Society is a nonprofit scientific organization that facilitates the exchange of knowledge meetings and publication of papers for future reference. The Society owns and retains full right to control its publications and its meetings. The Society has an obligation to protect its members and meetings from intrusion by others who may wish to use the meetings for their own private promotion purpose. Literature found not to be in agreement with the Society's goals, in competition with Society services or of an offensive nature will not be displayed anywhere in the vicinity of the meeting. Promotional literature of any kind may not be displayed without the Society's permission and unless the Society provides tables for this purpose. Literature not conforming to this policy or displayed in other than designated areas will be disposed. The Society will not permit unauthorized scheduling of activities during its meeting by any person or group when those activities are conducted at its meeting place in interference with its programs and scheduled activities. The Society does not object to appropriate activities by others during its meetings if it is consulted with regard to time, place, and suitability. Any person or group wishing to conduct any activity at the time and location of the Society meeting must obtain permission from the Executive Director or Director of Meetings, giving full details regarding desired time, place and nature of activity.

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# schedule at a glance

## SUNDAY, MAY 22, 2016

Registration	4:00 p.m. – 7:00 p.m.	Madison Foyer
Welcome reception	6:00 p.m. – 8:00 p.m.	Capitol Ballroom

## MONDAY, MAY 23, 2016

Registration	7:00 a.m. – 5:30 p.m.	
Stokey Lecture of Discovery – <b>David L. Griscom</b>	8:00 a.m. – 9:00 a.m.	Madison
*Concurrent Sessions	9:20 a.m. – 5:40 p.m.	
Lunch on own	12:00 p.m. – 1:20 p.m.	
GOMD General Business Meeting	5:45 p.m. – 6:30 p.m.	Madison
Poster Session & Student Poster Competition	6:30 p.m. – 8:30 p.m.	Senate & Assembly

## TUESDAY, MAY 24, 2016

Registration	7:30 a.m. – 5:30 p.m.	
George W. Morey Award Lecture – <b>Hellmut Eckert</b>	8:00 a.m. – 9:00 a.m.	Madison
*Concurrent Sessions	9:20 a.m. – 6:00 p.m.	
The Norbert J. Kreidl Award for Young Scholars Lecture – <b>Lan Li</b>	12:00 p.m. – 1:00 p.m.	Madison
Lunch on own	12:00 p.m. – 1:20 p.m.	
Conference Banquet	7:00 p.m. – 10:00 p.m.	Capitol Ballroom

## WEDNESDAY, MAY 25, 2016

Registration	7:30 a.m. – 5:00 p.m.	
Darshana and Arun Varshneya Frontiers of Glass Science Lecture – <b>Matteo Ciccotti</b>	8:00 a.m. – 9:00 a.m.	Madison
*Concurrent Sessions	9:20 a.m. – 5:40 p.m.	
<i>Practical Tips for Getting Your Research Published</i> , sponsored by <b>Saint-Gobain and ACerS Global Graduate Research Network</b>	12:00 p.m. – 1:15 p.m.	Madison
Lunch on own	12:00 p.m. – 1:20 p.m.	
*Concurrent Sessions	1:30 p.m. – 5:40 p.m.	
Career Discussion Round tables	5:45 p.m. – 6:45 p.m.	Capitol B

## THURSDAY, MAY 26, 2016

Registration	7:30 a.m. – 12:00 p.m.	
Darshana and Arun Varshneya Frontiers of Glass Technology Lecture – <b>Matthew J. Dejneka</b>	8:00 a.m. – 9:00 a.m.	Madison
*Concurrent Sessions	9:20 a.m. – 12:00 p.m.	
Lunch on own	12:00 p.m. – 1:20 p.m.	
*Concurrent Sessions	1:20 p.m. – 3:40 p.m.	

\*Concurrent sessions are in the Madison, Wisconsin, Capitol, University and Senate rooms.

# student events

Brought to you by



## Practical Tips for Getting Your Research Published

Wednesday, May 25, 12 – 1:15 p.m. | MADISON ROOM

and the **ACerS Global Graduate Researcher Network**

All student and young professional attendees are invited. Professor Mario Affatigato will provide advice for students on the wild world of scientific publishing. More specifically, he will discuss:

- Content suitable for publication
- Desire for cutting-edge work
- Reviews and topical issues
- Vexing problem of plagiarism, both naive and intentional
- Technical issues with manuscripts, like image resolution and English language editing
- Getting involved as a journal reviewer
- Writing clarity and the expected audience
- Some of the ethical principles behind research publishing
- Brief mention of the current environment in the scientific journal world, with an emphasis on trends like Open Access publishing and discussions on impact.

Expect a friendly, educational presentation with much time for questions.

Professor Mario Affatigato is the co-Editor of the *International Journal of Applied Glass Science*. He holds the Fran Allison and Francis Halpin Professorship in Physics at Coe College, where he has developed a research effort primarily investigating the relationship between the optical properties and structure of glassy materials. He is a Fellow of The American Ceramic Society and the UK Society of Glass Technology, and in 2015, he became a Research Corporation Cottrell Scholar.

Lunch will be provided on a first come, first served basis.

## Student, Post-doc, and Young Professional Career Discussion Roundtables

Wednesday, May 25, 5:45 – 6:45 p.m. | CAPITOL B

Students, post-docs, and young professionals are invited to an informal group discussion with 9 panelists representing industry, government, and academia. This is an opportunity to ask questions of professionals in a casual environment on a number of diverse topics (work-life balance, career opportunities, etc.). The career professionals will rotate every 15 minutes, so attendees will get a chance to have candid discussions with several professionals during this session. Light refreshments will be served.

### **PANELISTS:**

#### **Academia:**

**Juejun Hu**, Massachusetts Institute of Technology  
**Mathieu Bauchy**, University of California, Los Angeles  
**Liping Huang**, Rensselaer Polytechnic Institute

#### **National Lab:**

**Tayyab Suratwala**, Lawrence Livermore National Laboratory  
**Todd Alam**, Sandia National Laboratories  
**Joseph Ryan**, Pacific Northwest National Laboratory

#### **Industry:**

**Mathieu Hubert**, CelSian Glass & Solar, The Netherlands  
**John Mauro**, Corning Incorporated  
**Clara Rivero-Baleine**, Lockheed Martin Corporation

## GOMD Student Poster Contest Information

Sponsored by **CORNING**

The GOMD Student Poster Contest, sponsored by Corning Incorporated, will take place on Monday evening as part of the regular poster session from 6:30 - 8:30 p.m. in Senate A/B and Assembly—first floor of the hotel. This year's contest is organized by Mathieu Bauchy of UCLA.

- Set up posters from 3:20 – 5:00 p.m. Pins will be provided.
- Students are expected to remain with their poster for judging.
- All posters must be removed from the boards at 8:30 p.m.
- Winners announced at the conference dinner on Tuesday 7:00 – 10:00 p.m.

**Good luck to all students, and thanks to Corning for their generous sponsorship!**

# 2016 GLASS AND OPTICAL MATERIALS

## symposia schedule and organizers

### SYMPOSIUM 1: FUNDAMENTALS OF THE GLASSY STATE

SESSION 1: GLASS FORMATION AND RELAXATION I (Organized by: **John Mauro**, Corning Incorporated; **Ozgur Gulbitten**, Corning Incorporated; **Sabyasachi Sen**, UC Davis)

SESSION 1: GLASS FORMATION AND RELAXATION II

SESSION 1: GLASS FORMATION AND RELAXATION III

SESSION 2: FUNDAMENTALS (**Edgar D. Zanotto**, Federal University of São Carlos; **Mark J. Davis**, SCHOTT North America Inc.)

SESSION 2: GLASS-CERAMICS

SESSION 3: NMR (Organized by: **Paul Voyles**, University of Wisconsin–Madison; **Mario Affatigato**, Coe College; **Randall E. Youngman**, Corning Incorporated; **Dominique de Ligny**, Universität Erlangen-Nürnberg)

SESSION 3: SCATTERING TECHNIQUES

SESSION 3: NEW TECHNIQUES AND APPLICATIONS

SESSION 3: OPTICAL AND VIBRATIONAL MEASUREMENTS

SESSION 4: POTENTIAL DEVELOPMENT AND MD SIMULATIONS OF MULTICOMPONENT GLASSES (Organized by: **Jincheng Du**, University of North Texas; **Walter Kob**, Université Montpellier II; **Carlo Massobrio**, Institut de Physique et Chimie des Matériaux de Strasbourg)

SESSION 4: PREDICTING GLASS PROPERTIES FROM SIMULATIONS

SESSION 4: FIRST PRINCIPLES METHODS AND AB INITIO MD SIMULATIONS OF GLASSES

SESSION 4: SIMULATIONS OF CHALCOGENIDE AND METALLIC GLASSES

SESSION 5: MECHANICAL PROPERTIES OF GLASSES I (Organized by: **Lothar Wondraczek**, University of Jena; **Timothy Gross**, Corning Incorporated; **Satoshi Yoshida**, The University of Shiga Prefecture; **Tanguy Rouxel**, Université de Rennes)

SESSION 5: MECHANICAL PROPERTIES OF GLASSES II

SESSION 5: MECHANICAL PROPERTIES OF GLASSES III

SESSION 5: MECHANICAL PROPERTIES OF GLASSES IV

SESSION 5: MECHANICAL PROPERTIES OF GLASSES V

SESSION 6: CARBIDE AND NITRIDE GLASSES (Organized by: **Pierre Lucas**, University of Arizona; **Tanguy Rouxel**, Université de Rennes)

SESSION 6: METALLIC GLASSES

SESSION 6: CHALCOGENIDE GLASSES I

SESSION 6: CHALCOGENIDE GLASSES II

SESSION 7: SYNTHESIS, STRUCTURE AND PROPERTIES OF GLASS UNDER EXTREME CONDITIONS (Organized by: **Benoit Rufflé**, Université Montpellier II; **Morten Matstrup Smedskjær**, Aalborg University; **Yann Vaills**, University of Orléans)

SESSION 7: RESPONSE OF GLASS TO EXTREME CONDITIONS

SESSION 7: CHARACTERIZATION OF GLASS UNDER EXTREME CONDITIONS I

SESSION 7: MODELING OF GLASS UNDER EXTREME CONDITIONS

SESSION 7: CHARACTERIZATION OF GLASS UNDER EXTREME CONDITIONS II

## award speakers

Stokey Lecture of Discovery | **David L. Griscom** | Monday, May 23, 2016 | 8 – 9 a.m. | Madison

George W. Morey Lecture | **Hellmut Eckert** | Tuesday, May 24, 2016 | 8 – 9 a.m. | Madison

The Norbert J. Kreidl Award for Young Scholars Lecture | **Lan Li** | Tuesday, May 24, 2016 | Noon – 1 p.m. | Madison



# DIVISION ANNUAL MEETING

	Mon - AM	Mon - PM	Tues - AM	Tues - PM	Wed - AM	Wed - PM	Thurs - AM	Thurs - PM
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Darshana and Arun Varshneya Frontiers of Glass Science Lecture | **Matteo Ciccotti** |  
 Wednesday, May 25, 2016 | 8 – 9 a.m. | Madison

Darshana and Arun Varshneya Frontiers of Glass Technology Lecture | **Matthew J. Dejneka** |  
 Thursday, May 26, 2016 | 8 – 9 a.m. | Madison

# 2016 GLASS AND OPTICAL MATERIALS

## symposia schedule and organizers

### SYMPOSIUM 2: LARRY L. HENCH MEMORIAL SYMPOSIUM ON BIOACTIVE GLASSES

LARRY L. HENCH MEMORIAL SYMPOSIUM ON BIOACTIVE GLASSES I (Organized by: **Julian Jones**, Imperial College London; **Delia S. Brauer**, Friedrich Schiller University Jena; **Ashutosh Goel**, Rutgers, The State University of New Jersey)

LARRY L. HENCH MEMORIAL SYMPOSIUM ON BIOACTIVE GLASSES II: SOL-GEL GLASSES

LARRY L. HENCH MEMORIAL SYMPOSIUM ON BIOACTIVE GLASSES III

LARRY L. HENCH MEMORIAL SYMPOSIUM ON BIOACTIVE GLASSES IV: STRUCTURE

### SYMPOSIUM 3: OPTICAL AND ELECTRONIC MATERIALS AND DEVICES FUNDAMENTALS AND APPLICATIONS

SESSION 1: IONIC CONDUCTING MATERIALS (Organized by: **David A. Drabold**, Ohio University; **Parthapratim Biswas**, The University of Southern Mississippi; **Xiang-hua Zhang**, Université de Rennes I)

SESSION 1: ELECTRONIC CONDUCTING MATERIALS I

SESSION 1: ELECTRONIC CONDUCTING MATERIALS II

SESSION 2: OPTICAL FIBERS (Organized by: **Johann Troles**, Université de Rennes; **Daniel Milanese**, Politecnico di Torino)

SESSION 3: OPTICAL MATERIALS FOR COMPONENTS AND DEVICES I (Organized by: **Juejun Hu**, Massachusetts Institute of Technology; **Shibin Jiang**, Photonics Inc.)

SESSION 3: OPTICAL MATERIALS FOR COMPONENTS AND DEVICES II

SESSION 4: F<sub>s</sub> LASER INTERACTIONS WITH GLASS I (Organized by: **Jianrong Qiu**, South China University of Technology; **Himanshu Jain**, Lehigh University)

SESSION 4: F<sub>s</sub> LASER INTERACTIONS WITH GLASS II

SESSION 5: GLASS-CERAMICS AND OPTICAL CERAMICS I (Organized by: **Yiquan Wu**, Alfred University; **Kathleen Richardson**, University of Central Florida)

SESSION 5: GLASS-CERAMICS AND OPTICAL CERAMICS II

SESSION 5: GLASS-CERAMICS AND OPTICAL CERAMICS III

### SYMPOSIUM 4: GLASS TECHNOLOGY AND CROSS-CUTTING TOPICS

SESSION 1: GLASS SURFACES AND FUNCTIONAL COATINGS (Organized by: **Carlo Pantano**, The Pennsylvania State University; **Nathan P. Mellott**, Alfred University; **Nick Smith**, Corning Incorporated)

SESSION 2: LIQUID SYNTHESIS AND SOL-GEL-DERIVED MATERIALS I (Organized by: **John Kieffer**, University of Michigan; **Lisa C. Klein**, Rutgers University)

SESSION 2: LIQUID SYNTHESIS AND SOL-GEL-DERIVED MATERIALS II

SESSION 3: CHALLENGES IN MANUFACTURING I (Organized by: **Irene Peterson**, Corning Incorporated; **Mathieu Hubert**, CelSian Glass & Solar in Eindhoven)

SESSION 3: CHALLENGES IN MANUFACTURING II

SESSION 4: GLASS FORMULATION I (Organized by: **Stephane Gin**, CEA; **Joseph Ryan**, Pacific Northwest National Laboratory; **S. K. Sundaram**, Alfred University; **Ashutosh Goel**, Rutgers, The State University of New Jersey)

SESSION 4: GLASS FORMULATION II

SESSION 4: GLASS CORROSION: GENERAL ASPECTS

SESSION 4: GLASS CORROSION: MECHANISMS AND RATE I

SESSION 4: GLASS CORROSION: MECHANISMS AND RATE II

SESSION 4: GLASS CORROSION: ANALYTICAL TECHNIQUES

### SYMPOSIUM 5: FESTSCHRIFT FOR PROFESSOR DONALD R. UHLMANN

CRYSTALLIZATION (Organized by: **Lisa C. Klein**, Rutgers University; **Pierre Lucas**, University of Arizona; **Edgar D. Zanotto**, Federal University of São Carlos)

MODELS AND CONNECTIONS

GELS AND APPLICATIONS

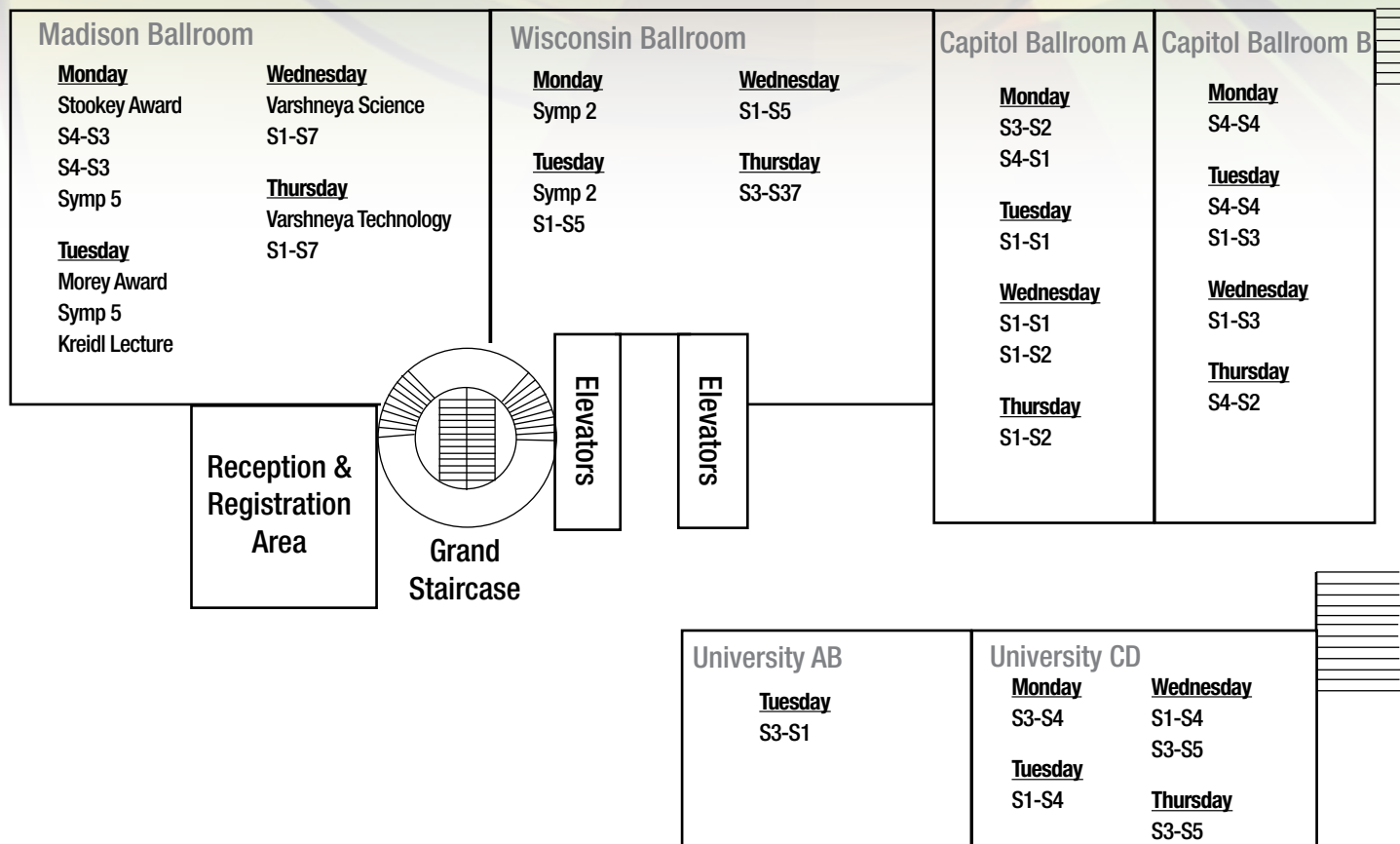
LEGACY

# DIVISION ANNUAL MEETING

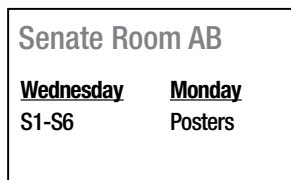
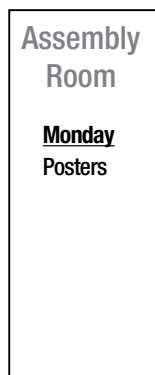
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# floor plan

## second floor



## first floor



### Key code –

#### S1: FUNDAMENTALS OF THE GLASSY STATE

- Session 1: Glass Formation and Structural Relaxation
- Session 2: Fundamentals and Applications of Glass-Crystallization
- Session 3: Structural Characterization of Glasses
- Session 4: Computational and Theoretical Studies of Glasses
- Session 5: Mechanical Properties of Glasses
- Session 6: Non-oxide and Metallic Glasses
- Session 7: Glass Under Extreme Conditions

#### S2: LARRY L. HENCH MEMORIAL SYMPOSIUM ON BIOACTIVE GLASSES

#### S3: OPTICAL AND ELECTRONIC MATERIALS AND DEVICES—FUNDAMENTALS AND APPLICATIONS

- Session 1: Amorphous Ionic and Electronic Conductors: Materials and Devices

#### Session 2: Optical Fibers

- Session 3: Optical Materials for Components and Devices
- Session 4: Laser Interactions with Glass
- Session 5: Glass-ceramics and Optical Ceramics

#### S4: GLASS TECHNOLOGY AND CROSS-CUTTING TOPICS

- Session 1: Glass Surfaces and Functional Coatings
- Session 2: Liquid Synthesis and Sol-gel-derived Materials
- Session 3: Challenges in Glass Manufacturing
- Session 4: Waste Immobilization—Waste Form Development: Processing and Performance

#### S5: FESTSCHRIFT FOR PROFESSOR DONALD R. UHLMANN

## Oral Presenters

Name	Date	Time	Room	Page Number	Name	Date	Time	Room	Page Number
<b>A</b>									
Aaldenberg, E.	24-May	3:00PM	Wisconsin	12	Doyle, W.F.	24-May	3:40PM	Madison	14
Adhikari, P.	25-May	10:40AM	University C/D	15	Drabold, D.	24-May	2:20PM	University A/B	13
Agnello, G.	23-May	4:10PM	Capitol A	6	Du, J.	24-May	9:20AM	University C/D	9
Aitken, B.	26-May	10:20AM	Capitol A	19	Duran, C.A.	23-May	1:40PM	Madison	7
Akola, J.	25-May	1:20PM	University C/D	17	Dutra Zanotto, E.	23-May	3:40PM	Madison	7
Alam, T.M.	24-May	3:40PM	Capitol B	11	Dutta, I.	26-May	11:20AM	Capitol A	19
Alderman, O.L.	25-May	10:10AM	Capitol B	14	<b>E</b>				
Ali, S.	25-May	10:20AM	Senate A/B	15	Ebert, W.	23-May	3:40PM	Capitol B	7
Almeida, R.M.	26-May	1:20PM	Capitol B	21	Ebert, W.	23-May	4:40PM	Capitol B	7
Anderson, M.A.	26-May	9:20AM	Capitol B	20	Eckert, H.	24-May	8:00AM	Madison	9
<b>B</b>					Eden, M.	24-May	9:50AM	Wisconsin	10
Bado, P.	23-May	2:50PM	University C/D	6	Ediger, M.D.	24-May	1:20PM	Capitol A	11
Baker, S.P.	24-May	4:00PM	Wisconsin	12	Ediger, M.D.	25-May	1:50PM	Madison	18
Baleine, C.R.	26-May	9:20AM	University C/D	20	Evans, A.	26-May	3:10PM	University C/D	21
Ballato, J.	23-May	9:20AM	Capitol A	4	<b>F</b>				
Baral, K.	25-May	11:30AM	University C/D	15	Fabes, B.	24-May	11:10AM	Madison	11
Barthel, E.	25-May	1:50PM	Wisconsin	17	Ferreira, J.M.	23-May	11:00AM	Wisconsin	4
Bauchy, M.	24-May	3:50PM	University C/D	12	Foret, M.	25-May	11:40AM	Madison	16
Bauchy, M.	26-May	10:40AM	Madison	19	Freudenberger, P.	24-May	10:20AM	Wisconsin	10
Beaucage, G.	26-May	10:50AM	Capitol B	20	Fu, Q.	26-May	9:50AM	Capitol A	19
Bellouard, Y.	23-May	9:50AM	University C/D	4	<b>G</b>				
Bhattarai, B.	24-May	2:40PM	University A/B	13	Gaddam, A.	26-May	12:00PM	Capitol A	19
Birnie, D.P.	24-May	9:20AM	Madison	11	Gaerke, D.A.	23-May	11:20AM	Madison	5
Bista, S.	26-May	11:10AM	Madison	19	Galoisy, L.	24-May	11:40AM	Capitol B	11
Biswas, P.	24-May	1:50PM	University A/B	13	Ganisetti, V.	24-May	2:40PM	University C/D	12
Boero, M.	25-May	9:20AM	University C/D	15	George, J.	23-May	10:40AM	Capitol B	5
Boioli, F.	25-May	2:10PM	Wisconsin	17	Giboire, I.	23-May	9:40AM	Capitol B	5
Bokas, G.	25-May	2:40PM	University C/D	17	Gin, S.	24-May	11:00AM	Capitol B	11
Bouzd, A.	24-May	4:10PM	University A/B	13	Goel, A.	25-May	2:40PM	Capitol A	16
Bouzd, A.	25-May	2:10PM	Senate A/B	17	Gong, Y.	23-May	3:50PM	Capitol A	6
Brauer, D.S.	23-May	4:10PM	Wisconsin	6	Gong, Y.	24-May	11:20AM	Capitol B	11
Burov, E.	25-May	11:00AM	Capitol A	14	Gouillart, E.	23-May	10:10AM	Madison	5
<b>C</b>					Gouillart, E.	26-May	9:50AM	Madison	19
Calas, G.	25-May	4:10PM	Capitol B	16	Griscom, D.L.	23-May	8:00AM	Madison	4
Calvert, P.	24-May	1:50PM	Madison	13	Gross, T.M.	24-May	4:40PM	Wisconsin	12
Cao, Y.	26-May	11:20AM	University C/D	20	Gueguen, Y.	25-May	2:50PM	Wisconsin	17
Cassar, D.R.	24-May	4:10PM	Capitol A	11	Gujral, A.	25-May	10:50AM	Capitol B	14
Cavillon, M.	23-May	10:20AM	Capitol A	4	Gulbitten, O.	24-May	10:20AM	Capitol A	9
Chapman, C.L.	23-May	3:30PM	Capitol A	6	Gupta, P.	24-May	9:50AM	Capitol A	9
Chass, G.	24-May	9:20AM	Wisconsin	10	Gupta, P.	25-May	1:20PM	Capitol A	16
Chen, G.	24-May	1:20PM	University A/B	13	<b>H</b>				
Chen, W.	24-May	10:10AM	University C/D	10	Han, Z.	26-May	1:50PM	Wisconsin	21
Chevreux, P.	23-May	1:40PM	Capitol B	7	Hannon, A.C.	25-May	10:30AM	Capitol B	14
Ching, W.	25-May	10:50AM	Senate A/B	15	Harrison, M.T.	23-May	10:00AM	Capitol B	5
Ciccotti, M.	25-May	8:00AM	Madison	14	Holbrook, C.	25-May	4:30PM	Capitol B	16
Conradt, R.	23-May	9:50AM	Madison	5	Hsu, J.	23-May	2:20PM	Capitol B	7
Copenhaver, K.E.	26-May	2:30PM	Capitol B	21	Hu, J.	26-May	9:50AM	University C/D	20
Corkhill, C.L.	23-May	9:20AM	Capitol B	5	Huang, L.	26-May	9:20AM	Madison	19
Cormier, L.	25-May	4:10PM	Madison	18	Huang, Q.	26-May	10:40AM	University C/D	20
Crawford, C.L.	23-May	4:00PM	Capitol B	7	Hubert, M.	23-May	10:40AM	Madison	5
Criscenti, L.	24-May	9:50AM	University C/D	9	Hubert, M.	23-May	2:20PM	Madison	7
Curtis, B.	24-May	11:00AM	University A/B	10	<b>I</b>				
<b>D</b>					Icenhower, J.P.	24-May	10:00AM	Capitol B	10
Damart, T.	24-May	2:20PM	University C/D	12	Inoue, H.	24-May	10:30AM	University C/D	10
Dasmahapatra, A.	24-May	5:00PM	University C/D	12	Ionescu, E.	25-May	9:20AM	Senate A/B	15
Davis, M.J.	25-May	4:40PM	Madison	18	Ispas, S.	25-May	11:00AM	University C/D	15
Day, D.E.	23-May	9:30AM	Wisconsin	4	<b>J</b>				
de Ligny, D.	25-May	4:50PM	Capitol B	17	Jaffe, M.	24-May	2:20PM	Madison	14
de Oliveira, M.	24-May	5:00PM	Capitol B	12	Jain, H.	23-May	4:30PM	Wisconsin	6
Dejneka, M.	26-May	8:00AM	Madison	19	Jantzen, C.M.	23-May	4:20PM	Capitol B	7
Dejneka, M.	26-May	9:50AM	Wisconsin	19	Jiang, S.	23-May	11:40AM	Capitol A	4
Deubener, J.	23-May	4:40PM	Madison	7	Jin, T.	23-May	11:40AM	Capitol B	5
Deubener, J.	24-May	2:20PM	Capitol A	11	Johnson, N.	24-May	4:20PM	Wisconsin	12
Dixon, D.	23-May	10:20AM	Capitol B	5	Jones, J.	23-May	10:00AM	Wisconsin	4
Dolekcekic, E.	23-May	2:50PM	Wisconsin	6					
Dong, G.	23-May	10:40AM	University C/D	5					
Dongol, R.	24-May	5:20PM	University C/D	12					
Dousti, M.	26-May	10:50AM	Wisconsin	20					

# Presenting Author List

## Oral Presenters

Name	Date	Time	Room	Page Number	Name	Date	Time	Room	Page Number
<b>K</b>									
Kaseman, D.C.	25-May	1:50PM	Senate A/B	17	Morin, E.I.	24-May	4:00PM	Capitol B	11
Keryvin, V.	25-May	1:20PM	Wisconsin	17	Muralidharan, K.	24-May	11:10AM	University C/D	10
Kieffer, J.	25-May	1:20PM	Madison	18	Muralidharan, K.	25-May	5:30PM	Capitol A	16
Kieffer, J.	25-May	3:40PM	Capitol A	16	<b>N</b>				
Kim, C.	23-May	2:00PM	Capitol B	7	Naruphontjirakul, P.	23-May	2:30PM	Wisconsin	6
Kim, D.	23-May	11:20AM	Capitol B	5	Neeway, J.	23-May	2:40PM	Capitol B	7
Kim, H.	25-May	4:40PM	University C/D	18	Neill, L.M.	24-May	10:40AM	Capitol B	10
Kim, J.	23-May	4:30PM	Capitol A	6	Neuefeind, J.	25-May	9:50AM	Capitol B	14
Kim, S.H.	23-May	1:20PM	Capitol A	6	Nishiyama, N.	25-May	9:20AM	Wisconsin	15
Kim, W.	26-May	1:20PM	University C/D	21	Norris, E.G.	23-May	1:50PM	Wisconsin	5
King, E.A.	24-May	2:40PM	Capitol A	11	Novak, S.	26-May	2:40PM	Wisconsin	21
Klein, L.C.	24-May	1:20PM	Madison	13	<b>O</b>				
Klein, L.C.	26-May	1:50PM	Capitol B	21	Oelgoetz, J.R.	26-May	3:00PM	Wisconsin	21
Klein, L.C.	26-May	10:10AM	Capitol B	20	Ohishi, Y.	23-May	9:50AM	Capitol A	4
Kob, W.	24-May	9:20AM	Capitol A	9	Ono, M.	25-May	4:40PM	Wisconsin	17
Kramer, D.	23-May	2:10PM	Capitol A	6	Ori, G.	24-May	10:40AM	University A/B	10
Krol, D.	23-May	9:20AM	University C/D	4	Ori, G.	25-May	2:10PM	University C/D	17
Kroll, P.	25-May	10:20AM	University C/D	15	<b>P</b>				
Kroll, P.	26-May	2:50PM	Capitol B	21	Pandey, A.	24-May	4:40PM	University A/B	13
<b>L</b>					Patel, A.	23-May	1:50PM	University C/D	6
LaComb, M.M.	24-May	4:20PM	Capitol B	11	Perepezko, J.H.	25-May	1:50PM	Capitol A	16
Lampin, E.	24-May	4:20PM	University C/D	12	Peterson, I.	23-May	1:20PM	Madison	7
Langevin, G.	25-May	5:20PM	Madison	18	Pföss, B.S.	24-May	11:10AM	Wisconsin	10
Lee, H.	25-May	3:40PM	University C/D	18	Philipps, K.	25-May	11:00AM	Wisconsin	15
Lee, S.	25-May	11:10AM	Madison	16	Pierce, E.M.	24-May	2:20PM	Capitol B	13
Lemmens, K.	23-May	3:00PM	Capitol B	7	Pierre, A.C.	24-May	2:50PM	Madison	14
Lepicard, A.	26-May	11:10AM	Wisconsin	20	Ponomarev, I.	25-May	11:50AM	University C/D	15
Lepry, W.C.	23-May	2:10PM	Wisconsin	5	Poologasundarampillai, G.	23-May	1:20PM	Wisconsin	5
Letz, M.	26-May	9:20AM	Capitol A	19	Powell, C.T.	25-May	5:10PM	Capitol A	16
Li, A.	23-May	1:50PM	Capitol A	6	Pradel, A.	24-May	9:20AM	University A/B	10
Li, L.	24-May	12:00PM	Madison	11	Pradel, A.	26-May	2:10PM	Wisconsin	21
Li, L.	26-May	10:30AM	Wisconsin	19	Prange, A.	23-May	9:20AM	Madison	5
Li, N.	25-May	9:50AM	University C/D	15	Prasai, K.	24-May	3:00PM	University A/B	13
Li, Y.	26-May	2:50PM	University C/D	21	Priven, A.	25-May	10:00AM	Capitol A	14
Linford, M.R.	23-May	2:30PM	Capitol A	6	<b>R</b>				
Linford, M.R.	23-May	2:50PM	Capitol A	6	Ranasinghe, K.S.	23-May	4:50PM	Wisconsin	6
Liu, Y.	26-May	11:00AM	University C/D	20	Reiser, J.	24-May	9:40AM	Capitol B	10
Locker, S.T.	23-May	10:20AM	University C/D	4	Rice, J.A.	24-May	9:20AM	Capitol B	10
Lonegan, J.M.	25-May	4:00PM	Senate A/B	18	Rimsza, J.M.	24-May	1:20PM	Capitol B	13
Lonnroth, N.	26-May	11:00AM	Capitol A	19	Rino, J.P.	24-May	10:50AM	University C/D	10
Lousteau, J.	23-May	11:20AM	Capitol A	4	Rocherullé, J.	24-May	10:20AM	University A/B	10
Lu, X.	24-May	2:40PM	Capitol B	13	Ronchetto, E.	24-May	2:20PM	Wisconsin	12
Lucas, P.	24-May	10:40AM	Capitol A	9	Rosales Sosa, G.A.	25-May	10:20AM	Wisconsin	15
Lucas, P.	26-May	1:20PM	Wisconsin	21	Roth, J.	25-May	5:00PM	Madison	18
Luksic, S.A.	23-May	11:00AM	Capitol B	5	Rouxel, T.	24-May	3:40PM	Wisconsin	12
Luo, J.	25-May	11:10AM	Capitol B	14	Rouxel, T.	25-May	11:20AM	Senate A/B	15
Luo, J.	25-May	3:40PM	Wisconsin	17	Ruffle, B.	26-May	1:50PM	Madison	20
<b>M</b>					Ryan, J.	25-May	1:20PM	Capitol B	16
Mabrouk, A.	26-May	2:30PM	Madison	20	Rygel, J.	23-May	11:00AM	Madison	5
Marple, M.A.	25-May	3:40PM	Senate A/B	18	<b>S</b>				
Martin, S.W.	24-May	9:50AM	University A/B	10	Saitoh, A.	26-May	11:30AM	Wisconsin	20
Martinez, V.	25-May	2:10PM	Capitol B	16	Savitsky, D.	23-May	11:10AM	University C/D	5
Martinez, V.	26-May	2:10PM	Madison	20	Schaut, R.	25-May	10:20AM	Madison	16
Massera, J.	23-May	3:40PM	Wisconsin	6	Scherer, G.W.	24-May	10:20AM	Madison	11
Masuno, A.	25-May	9:50AM	Wisconsin	15	Schmidt, V.	25-May	9:20AM	Capitol B	14
Mauro, J.C.	25-May	9:20AM	Capitol A	14	Schropp, R.E.	24-May	3:40PM	University A/B	13
McAnany, S.	23-May	11:30AM	University C/D	5	Schweizer, K.	24-May	1:50PM	Capitol A	11
McCloy, J.	24-May	4:20PM	Madison	14	Seaman, J.H.	24-May	2:40PM	Wisconsin	12
McFarland, B.	26-May	2:10PM	Capitol B	21	Sen, S.	25-May	10:40AM	Madison	16
McLaren, C.	24-May	11:20AM	Capitol A	9	Seward, T.P.	24-May	9:50AM	Madison	11
Micoulaut, M.	25-May	1:50PM	University C/D	17	Sglavo, V.M.	25-May	5:00PM	Wisconsin	17
Micoulaut, M.	25-May	4:10PM	Capitol A	16	Shen, Y.	25-May	2:20PM	Capitol A	16
Micoulaut, M.	25-May	9:50AM	Madison	15	Sheth, N.	25-May	1:50PM	Capitol B	16
Milanesi, D.	23-May	10:40AM	Capitol A	4	Shih, Y.	25-May	10:40AM	Capitol A	14
Miller, A.	25-May	4:10PM	University C/D	18	Shimotsuma, Y.	23-May	1:20PM	University C/D	6
Mishra, A.	23-May	11:30AM	Wisconsin	4	Shinozaki, K.	24-May	5:00PM	Wisconsin	12
Möncke, D.	24-May	10:40AM	Wisconsin	10					
Möncke, D.	25-May	3:40PM	Capitol B	16					



## Monday, May 23, 2016

### Stokey Lecture of Discovery

Room: Madison

**8:00 AM**

**(GOMD-AW-001-2016) The life and unexpected discoveries of an intrepid glass scientist (Invited)**

D. L. Griscorn<sup>\*</sup>; 1. impactGlass research international, Mexico

**9:00 AM**

**Break**

### Symposium 2: Larry L. Hench Memorial Symposium on Bioactive Glasses

#### Larry L. Hench Memorial Symposium on Bioactive Glasses I

Room: Wisconsin

Session Chairs: Julian Jones, Imperial College London; Ashutosh Goel, Rutgers University

**9:20 AM**

**Opening Remarks - Kathleen Richardson**

**9:30 AM**

**(GOMD-S2-001-2016) Tribute to Larry Hench: Educator, Scientist, Author (Invited)**

D. E. Day<sup>\*</sup>; 1. Missouri University of Science and Technology, USA

**10:00 AM**

**(GOMD-S2-002-2016) Larry Hench: from Bioglass to Boing Boing and back again (Invited)**

J. Jones<sup>\*</sup>; 1. Imperial College London, United Kingdom

**10:30 AM**

**(GOMD-S2-003-2016) Development of unique ceramic scaffolds for regeneration of large bone defects under load (Invited)**

H. Zreiqat<sup>\*</sup>; 1. University of Sydney, Australia

**11:00 AM**

**(GOMD-S2-004-2016) Additive manufacturing of highly bioactive and strong 3D porous alkali-free bioactive glass scaffolds for healthcare applications (Invited)**

J. M. Ferreira<sup>\*</sup>; A. Brito<sup>2</sup>; B. C. Silva<sup>1</sup>; A. C. Marques<sup>1</sup>; S. H. Olhero<sup>1</sup>; 1. University of Aveiro, Portugal; 2. Reg4life-Regeneration Technology, Portugal

**11:30 AM**

**(GOMD-S2-005-2016) Characterization of Ag, Cu and Fe doped phosphate bioactive glasses**

A. Mishra<sup>\*</sup>; J. Rocherullé<sup>2</sup>; J. Massera<sup>1</sup>; 1. Tampere University of Technology, Finland; 2. Université de Rennes I, France

**11:50 AM**

**Donald Uhlmann - "Larry Hench, the Man for All Seasons and Dearest Friend"**

### Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications

#### Session 2: Optical Fibers

Room: Capitol A

Session Chair: Daniel Milanese, Politecnico di Torino

**9:20 AM**

**(GOMD-S3-001-2016) Novel Effects from Old Glasses in Next Generation Optical Fibers (Invited)**

J. Ballato<sup>\*</sup>; P. Dragic<sup>2</sup>; 1. Clemson University, USA; 2. University of Illinois at Urbana-Champaign, USA

**9:50 AM**

**(GOMD-S3-002-2016) Recent status of lightwave generation and processing using soft glass specialty optical fibers (Invited)**

Y. Ohishi<sup>\*</sup>; T. Suzuki<sup>1</sup>; 1. Toyota Technological Institute, Japan

**10:20 AM**

**(GOMD-S3-003-2016) Brillouin-related properties of novel alkaline earth oxide silicate glass optical fibers**

M. Cavillon<sup>\*</sup>; J. Ballato<sup>1</sup>; P. Dragic<sup>2</sup>; C. Kucera<sup>1</sup>; T. Hawkins<sup>1</sup>; M. Jones<sup>1</sup>; 1. Clemson University, USA; 2. University of Illinois at Urbana-Champaign, USA

**10:40 AM**

**(GOMD-S3-004-2016) Bio-resorbable phosphate optical fibers for biophotonics**

D. Milanese<sup>\*</sup>; E. Ceci-Ginistrelli<sup>1</sup>; N. Boetti<sup>2</sup>; J. Lousteau<sup>3</sup>; A. Ambrosone<sup>1</sup>; G. Novajra<sup>1</sup>; C. Vitale-Brovarone<sup>1</sup>; D. Pugliese<sup>1</sup>; 1. Politecnico di Torino, Italy; 2. Istituto Superiore Mario Boella, Italy; 3. University of Southampton, United Kingdom

**11:00 AM**

**(GOMD-S3-005-2016) Elaboration of a chalcogenide microstructured optical fiber presenting high birefringence**

J. Troles<sup>\*</sup>; C. Caillaud<sup>1</sup>; C. Gilles<sup>2</sup>; L. Provino<sup>2</sup>; L. Brilland<sup>1</sup>; L. Jumpertz<sup>2</sup>; S. Ferre<sup>2</sup>; M. Carras<sup>2</sup>; M. Brun<sup>2</sup>; J. Adam<sup>1</sup>; 1. University of Rennes I, France; 2. Mirsense, France; 3. Perfos, France; 4. Selenoptics, France

**11:20 AM**

**(GOMD-S3-006-2016) Core/clad tellurite glass pairs for Mid-IR Supercontinuum Generation in high NA step index optical fibre (Invited)**

J. Lousteau<sup>\*</sup>; D. Pugliese<sup>2</sup>; N. Boetti<sup>2</sup>; P. Janicek<sup>3</sup>; E. Ceci-Ginistrelli<sup>2</sup>; F. Poletti<sup>1</sup>; D. Milanese<sup>2</sup>; 1. University of Southampton, United Kingdom; 2. Politecnico di Torino, Italy; 3. University of Pardubice, Czech Republic

**11:40 AM**

**(GOMD-S3-007-2016) Glass Fiber Lasers for Glass Applications (Invited)**

S. Jiang<sup>\*</sup>; 1. AdValue Photonics Inc, USA

#### Session 4: Fs Laser Interactions with Glass I

Room: University C/D

Session Chair: Jianrong Qiu, South China University of Technology

**9:20 AM**

**(GOMD-S3-008-2016) Dynamic processes of femtosecond laser induced phenomena in glass (Invited)**

J. Hernandez-Rueda<sup>1</sup>; D. Krol<sup>\*</sup>; 1. UC Davis, USA

**9:50 AM**

**(GOMD-S3-009-2016) Femtosecond laser-induced material modifications to control stress states in silica: A step toward metastable polymorphic phase generation (Invited)**

Y. Bellouard<sup>\*</sup>; 1. Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

**10:20 AM**

**(GOMD-S3-010-2016) Strengthening of Aluminoborosilicate and Soda-Lime Silicate Glasses Using Femtosecond Pulse Laser**

S. T. Locker<sup>\*</sup>; P. Tumurugoti<sup>1</sup>; S. K. Sundaram<sup>1</sup>; 1. Alfred University, USA



**10:40 AM****(GOMD-S3-011-2016) Femtosecond laser-induced element distribution and crystallization in glass (Invited)**G. Dong\*; J. Qiu<sup>1</sup>; 1. South China University of Technology, China**11:10 AM****(GOMD-S3-012-2016) Laser-induced oriented Sb<sub>2</sub>S<sub>3</sub> single crystal dots on the surface of Sb-S-I glasses using spatial light modulator**D. Savvitsky\*; V. Dierolf; H. Jain<sup>1</sup>; 1. Lehigh University, USA**11:30 AM****(GOMD-S3-013-2016) Formation of Ferroelectric LaBGeO<sub>5</sub> Single Crystal Architecture in Glass by Femtosecond Laser Irradiation**S. McAnany\*; K. Veenhuizen<sup>1</sup>; D. Nolan<sup>1</sup>; V. Dierolf; H. Jain<sup>1</sup>; 1. Lehigh University, USA; 2. Corning Incorporated, USA**Symposium 4: Glass Technology and Cross-Cutting Topics****Session 3: Challenges in Manufacturing I**

Room: Madison

Session Chairs: Elizabeth Sturdevant, Corning Incorporated; Irene Peterson, Corning Incorporated

**9:20 AM****(GOMD-S4-001-2016) A critical review of methods employed for studying the batch-to-melt conversion (Invited)**A. Prange\*; V. Niessen<sup>1</sup>; R. Conrad<sup>1</sup>; 1. RWTH Aachen University, Germany**9:50 AM****(GOMD-S4-002-2016) Identifying the rate determining step of the batch-to-melt conversion**

R. Conrad\*; 1. RWTH Aachen University, Germany

**10:10 AM****(GOMD-S4-003-2016) A particle-scale view of glass batch melting thanks to in situ microtomography (Invited)**E. Gouillart\*; W. Woelffel<sup>1</sup>; E. Burov<sup>1</sup>; M. Toplis<sup>1</sup>; M. Chopinet<sup>1</sup>; 1. Joint Unit CNRS/Saint-Gobain, France; 2. IRAP, France**10:40 AM****(GOMD-S4-004-2016) Batch reactions and melting-in of alkali-lean borosilicate glasses prepared with different borate raw materials**

M. Hubert\*; 1. CelSian Glass &amp; Solar, Netherlands

**11:00 AM****(GOMD-S4-005-2016) HTXRD investigation of batch reactions for phosphate raw materials in a multicomponent sodium aluminosilicate glass**J. Rygel\*; B. Wheaton<sup>1</sup>; K. Rossington<sup>1</sup>; 1. Corning Incorporated, USA**11:20 AM****(GOMD-S4-006-2016) Current Glass Melting Sensor Needs (Invited)**

D. A. Gaerke\*; 1. Owens-Illinois Inc., USA

**Session 4: Glass Formulation I**

Room: Capitol B

Session Chairs: Claire Corkhill, University of Sheffield; Isabelle Giboire, CEA

**9:20 AM****(GOMD-S4-007-2016) Development and characterisation of Mg-based glasses for uranium-containing Sellafield legacy wastes**C. L. Corkhill\*; S. T. Barlow<sup>1</sup>; A. J. Fisher<sup>1</sup>; M. C. Stennett<sup>1</sup>; N. C. Hyatt<sup>1</sup>; 1. University of Sheffield, United Kingdom**9:40 AM****(GOMD-S4-008-2016) Study of peraluminous glass formulations for fission products and minor actinides containment**I. Giboire\*; V. Montouillout<sup>1</sup>; V. Piovesan<sup>1</sup>; E. Gasnier<sup>1</sup>; N. Pellerin<sup>1</sup>; 1. CEA, France; 2. CEMHTI CNRS Orléans, France**10:00 AM****(GOMD-S4-009-2016) Chemical durability of UK vitrified high level waste using a Ca/Zn alkali borosilicate glass**M. T. Harrison\*; C. J. Steele<sup>1</sup>; 1. National Nuclear Laboratory, United Kingdom; 2. Sellafield Ltd, United Kingdom**10:20 AM****(GOMD-S4-010-2016) Rhenium Mass Balance in a Laboratory-Scale Melter**D. Dixon\*; M. J. Schweiger<sup>1</sup>; C. Fischer<sup>1</sup>; C. D. Lukins<sup>1</sup>; D. Kim<sup>1</sup>; P. Hrma<sup>1</sup>; 1. Pacific Northwest National Lab, USA**10:40 AM****(GOMD-S4-011-2016) Effects of Reducing Agents on Retention of Rhenium during Melting of Low-Activity Waste Glasses**J. George\*; D. Kim<sup>1</sup>; M. J. Schweiger<sup>1</sup>; A. A. Kruger<sup>2</sup>; 1. Pacific Northwest National Lab, USA; 2. DOE Office of River Protection, USA**11:00 AM****(GOMD-S4-012-2016) Proposed mechanisms for Tc volatility from waste glass feed simulants**

S. A. Luksic\*; 1. Pacific Northwest National Lab, USA

**11:20 AM****(GOMD-S4-013-2016) Volatile Species of Technetium and Rhenium Relevant to Vitrification of Hanford Low-Activity Wastes**D. Kim\*; A. A. Kruger<sup>2</sup>; 1. PNNL, USA; 2. DOE-ORP, USA**11:40 AM****(GOMD-S4-014-2016) Experimental Study of Sulfur Solubility in Low-Activity Waste Glass**T. Jin\*; D. Kim<sup>1</sup>; L. P. Darnell<sup>1</sup>; B. L. Weese<sup>1</sup>; N. L. Canfield<sup>1</sup>; M. Bliss<sup>1</sup>; J. R. Davies<sup>1</sup>; C. C. Bonham<sup>1</sup>; M. J. Schweiger<sup>1</sup>; A. A. Kruger<sup>1</sup>; 1. Pacific Northwest National Laboratory, USA; 2. US Department of Energy - Office of River Protection, USA**Symposium 2: Larry L. Hench Memorial Symposium on Bioactive Glasses****Larry L. Hench Memorial Symposium on Bioactive Glasses II: Sol-gel Glasses**

Room: Wisconsin

Session Chairs: Julian Jones, Imperial College London; Delia Brauer, Friedrich-Schiller-Universität

**1:20 PM****(GOMD-S2-006-2016) Bioactive glass reactions in physiological fluids and their competitive protein adsorption (Invited)**G. Poologasundarampillai\*; J. Jones<sup>1</sup>; 1. University of Manchester, United Kingdom; 2. Imperial College, United Kingdom**1:50 PM****(GOMD-S2-007-2016) 3-D Electrospun bioactive glasses for wound healing**E. G. Norris\*; Q. Ju<sup>2</sup>; G. Poologasundarampillai<sup>2</sup>; A. Obata<sup>3</sup>; J. Jones<sup>1</sup>; 1. Imperial College, United Kingdom; 2. University of Manchester, United Kingdom; 3. Nagoya Institute of Technology, Japan**2:10 PM****(GOMD-S2-008-2016) Processing Parameters Affect the Bioactivity of Sol-Gel Derived Borate Glasses**W. C. Lepry\*; S. N. Nazhat<sup>1</sup>; 1. McGill University, Canada

**2:30 PM****(GOMD-S2-009-2016) Development of strontium incorporating sol-gel derived bioactive glass nanoparticles for bone regeneration applications**

P. Naruphontjirakul\*; S. L. Greasley; S. Chen; L. Siwei; A. E. Porter; J. Jones; 1. Imperial College London, United Kingdom

**2:50 PM****(GOMD-S2-010-2016) Preparation of Lithium Disilicate Glass-Ceramics by the Sol-Gel Method**

H. Celik; L. Romero-Sanchez; A. Diaz Cuenca; E. Dolekcekic\*; 1. Anadolu University, Turkey; 2. Materials Science Institute of Seville, Spain

**3:10 PM****Break****Larry L. Hench Memorial Symposium on Bioactive Glasses III**

Room: Wisconsin

Session Chairs: Ashutosh Goel, Rutgers University; José Ferreira, University of Aveiro

**3:40 PM****(GOMD-S2-011-2016) Bioactive glasses for fiber drawing and particles sintering (Invited)**

J. Massera\*; 1. Tampere University of Technology, Finland

**4:10 PM****(GOMD-S2-012-2016) Influence of lithium and potassium substitution on the dissolution behavior of Bioglass 45S5**

R. Brückner; L. Hupa; D. S. Brauer\*; 1. Friedrich-Schiller-Universität, Germany; 2. Åbo Akademi University, Finland

**4:30 PM****(GOMD-S2-013-2016) Effect of phase separation on protein adsorption and cell attachment on 45S5 bioactive glass**

R. Golovchak; T. Kowal; T. Chokshi; J. Harms; H. Jain\*; M. Falk; 1. Lehigh University, USA; 2. Austin Peay State University, USA

**4:50 PM****(GOMD-S2-014-2016) Thermal Analysis of Bio Active Borosilicate Glass doped with Cerium Oxide**

K. S. Ranasinghe\*; D. E. Day; G. Humble; 1. Kennesaw State University, USA; 2. Missouri University of Science & Technology, USA

**Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications****Session 4: Fs Laser Interactions with Glass II**

Room: University C/D

Session Chair: Himanshu Jain, Lehigh University

**1:20 PM****(GOMD-S3-014-2016) Femtosecond laser nanoprocessing and its application (Invited)**

Y. Shimotsu\*; 1. Kyoto University, Japan

**1:50 PM****(GOMD-S3-015-2016) Advancing the Art of Ultrafast Laser Writing (Invited)**

P. G. Kazansky; M. Beresna; R. Drevinskas; A. Patel\*; A. Cerkauskaite; F. Zhang; S. Lotarev; A. Okhrimchuk; V. Sigaev; 1. University of Southampton, United Kingdom; 2. Advanced Laser Technologies Centre, Mendeleev University of Chemical Technology, Russian Federation

**2:20 PM****(GOMD-S3-016-2016) Modification of surface properties of glasses by ultrashort pulsed lasers (Invited)**

Q. Zhao\*; 1. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, China

**2:50 PM****(GOMD-S3-017-2016) Precision micromachining of fused silica glass using femtosecond lasers: Fabrication of flexure elements with integrated waveguides (Invited)**

P. Bado\*; M. Dugan; A. Said; 1. Translume, USA

**Symposium 4: Glass Technology and Cross-Cutting Topics****Session 1: Glass Surfaces and Functional Coatings**

Room: Capitol A

Session Chairs: Nathan P Mellott, Alfred University; Carlo Pantano, The Pennsylvania State University

**1:20 PM****(GOMD-S4-015-2016) Characterization of hydrous species at multicomponent glass surfaces using non-linear optical spectroscopy (Invited)**

S. H. Kim\*; 1. Pennsylvania State University, USA

**1:50 PM****(GOMD-S4-016-2016) Impacts of Aqueous Chemical Treatments and Aging on Glass Durability and Surface Appearance of Silicate Glasses**

A. Li\*; Y. Jin; X. Guo; S. Chen; K. Hughes; J. Hou; 1. Corning Incorporated, USA

**2:10 PM****(GOMD-S4-017-2016) Surface Chemistry of Calcium Aluminosilicate Glasses in Response to Aqueous Corrosion**

D. Kramer\*; J. Kopatz; C. G. Pantano; 1. Pennsylvania State University, USA

**2:30 PM****(GOMD-S4-018-2016) Angle-Resolved X-Ray Photoelectron Spectroscopy and Low-Energy Ion Scattering of Alkali-free Display Glasses**

C. V. Cushman; N. J. Smith; B. Sturgell; G. I. Major; B. M. Lunt; P. Bruener; J. Zake; T. Greh; M. R. Linford\*; 1. Brigham Young University, USA; 2. Corning Incorporated, USA; 3. ION-TOF, Germany

**2:50 PM****(GOMD-S4-019-2016) Chemometric Analysis of Time-of-flight Secondary Ion Mass Spectrometry Data from Display Glass Surfaces**

M. R. Linford\*; C. V. Cushman; B. Sturgell; G. I. Major; B. M. Lunt; P. Bruener; J. Zake; T. Greh; N. J. Smith; 1. Brigham Young University, USA; 2. ION-TOF, Germany; 3. Corning Incorporated, USA

**3:10 PM****Break****3:30 PM****(GOMD-S4-020-2016) Antimicrobial substrates made using an aqueous ion exchange process**

C. L. Chapman\*; 1. Corning Incorporated, USA

**3:50 PM****(GOMD-S4-021-2016) Copper Oxide Thin Films on Glass via Chemical Solution Deposition**

Y. Gong\*; P. Gao; S. T. Mixture; N. Mellott; 1. Alfred University, USA

**4:10 PM****(GOMD-S4-022-2016) Investigation of contact-induced charging kinetics on variably modified glass surfaces**

G. Agnello\*; J. Hamilton; R. Manley; E. Steltsova; W. LaCourse; A. Cormack; 1. Corning Incorporated, USA; 2. Alfred University, USA

**4:30 PM****(GOMD-S4-023-2016) Coating of Self-cleaning TiO<sub>2</sub>-SiO<sub>2</sub> Double Layers for the Photocatalytic Glass**

J. Kim\*; H. M. Yadav; B. Kim; 1. University of Seoul, Republic of Korea

**Session 3: Challenges in Manufacturing II**

Room: Madison

Session Chairs: Mathieu Hubert, CelSian Glass &amp; Solar; Andreas Prange, RWTH Aachen University

**1:20 PM****(GOMD-S4-024-2016) Reactions Between Glass and Zirconia Refractory**I. Peterson\*; M. DeLamielleure<sup>1</sup>; M. Mack<sup>1</sup>; D. Schnare<sup>1</sup>; 1. Corning Incorporated, USA**1:40 PM****(GOMD-S4-025-2016) Fine-Tuning of CTE in Ultra-Low Expansion Glass through Annealing (Invited)**

C. A. Duran\*; 1. Corning Incorporated, USA

**2:20 PM****(GOMD-S4-026-2016) Attracting New Talents: The Biggest Challenge in Glass Manufacturing?**

M. Hubert\*; 1. CelSian Glass &amp; Solar, Netherlands

**Session 4: Glass Formulation II**

Room: Capitol B

Session Chairs: Isabelle Giboire, CEA; Claire Corkhill, University of Sheffield

**1:20 PM****(GOMD-S4-027-2016) Spectroscopic Characterization of the Effects of Sulfate Addition on the Structure of Silicate Glasses – a Raman, NMR and Neutron Diffraction Study**S. Vaishnav\*; E. Barney<sup>2</sup>; A. C. Hannon<sup>3</sup>; P. A. Bingham<sup>1</sup>; 1. Sheffield Hallam University, United Kingdom; 2. University of Nottingham, United Kingdom; 3. Rutherford Appleton Laboratory, United Kingdom**1:40 PM****(GOMD-S4-028-2016) Interactions between an aluminosilicate glass melt and molten metals investigated by SEM analysis for a nuclear issue**P. Chevreux\*; A. Laplace<sup>1</sup>; E. Delouie<sup>2</sup>; L. Tissandier<sup>2</sup>; 1. CEA, France; 2. CNRS, France**2:00 PM****(GOMD-S4-029-2016) Development of Iron Phosphate Waste Forms for a High MoO<sub>3</sub> Collins-CLT Waste**C. Kim\*; J. Szabo<sup>1</sup>; A. Zervos<sup>1</sup>; J. Hsu<sup>2</sup>; J. Bai<sup>2</sup>; R. Brow<sup>2</sup>; 1. MO-SCI Corporation, USA; 2. Missouri University of Science and Technology, USA**2:20 PM****(GOMD-S4-030-2016) Chemical durability of iron phosphate waste forms containing 40 wt% of a high MoO<sub>3</sub> Collins-CLT waste**J. Hsu\*; J. Bai<sup>1</sup>; C. Kim<sup>2</sup>; R. Brow<sup>1</sup>; J. Szabo<sup>2</sup>; A. Zervos<sup>2</sup>; 1. Missouri University of Science and Technology, USA; 2. MO-SCI Corporation, USA**Session 4: Glass Corrosion: General Aspects**

Room: Capitol B

Session Chairs: Joseph Ryan, Pacific Northwest National Lab; Cory Trivelpiece, Pennsylvania State University

**2:40 PM****(GOMD-S4-031-2016) The Dissolution Rate of a Several High-Level and Low-Level Waste Glass Compositions**J. Neeway\*; M. Asmussen<sup>1</sup>; J. Ryan<sup>1</sup>; 1. Pacific Northwest National Lab, USA**3:00 PM****(GOMD-S4-032-2016) Evaluation of the behaviour of vitrified waste in the Belgian supercontainer disposal conditions**K. Lemmens\*; K. Ferrand<sup>1</sup>; S. Liu<sup>1</sup>; A. Elia<sup>1</sup>; 1. Belgian Nuclear Research Centre, Belgium**3:20 PM****Break****3:40 PM****(GOMD-S4-033-2016) Parameterizing a Glass Degradation Model**

W. Ebert\*; 1. Argonne National Lab, USA

**4:00 PM****(GOMD-S4-034-2016) Long term corrosion testing to assess durability of glass ceramics and glass waste forms**C. L. Crawford\*; C. M. Jantzen<sup>1</sup>; J. McCloy<sup>2</sup>; 1. Savannah River National Laboratory, USA; 2. Washington State University, USA**4:20 PM****(GOMD-S4-035-2016) Stage III Dissolution for High Level Waste (HLW) and Low Activity Waste (LAW) Glasses: Role of Leachate Hydroxide and Aqueous Aluminate**C. M. Jantzen\*; C. L. Crawford<sup>1</sup>; C. L. Trivelpiece<sup>1</sup>; 1. Savannah River National Laboratory, USA**4:40 PM****(GOMD-S4-036-2016) Implementing the ANL Stage 3 Glass Dissolution Model**W. Ebert\*; J. Jerden<sup>1</sup>; 1. Argonne National Lab, USA**Symposium 5: Festschrift for Professor Donald R. Uhlmann****Crystallization**

Room: Madison

Session Chair: Lisa Klein, Rutgers University

**3:40 PM****(GOMD-S5-001-2016) A random walk through Don Uhlmann's crystallization research (Invited)**

E. Dutra Zanotto\*; 1. Federal University of São Carlos, Brazil

**4:10 PM****(GOMD-S5-002-2016) A journey through time: Working with Don on time-dependent problems in nucleation, crystallization and glass formation (Invited)**

V. A. Shneidman\*; 1. New Jersey Institute of Technology, USA

**4:40 PM****(GOMD-S5-003-2016) Statistical approach to crystal nucleation in silicate glasses (Invited)**J. Deubener\*; S. Krüger<sup>1</sup>; 1. Clausthal University of Technology, Germany**5:10 PM****Donald Uhlmann - "Recent Advances in Antimicrobials"****Poster Session and Student Poster Competition**

Room: Senate A/B and Assembly

**6:30 PM****(GOMD-S1-P001-2016) Glass stability, crystal growth rate and microstructure after isothermal crystallization of glasses in the system Na<sub>2</sub>O-CaO-SiO<sub>2</sub>**

E. B. Ferreira\*; 1. EESC-USP, Brazil

**(GOMD-S1-P002-2016) Crack initiation in metallic glasses under nanoindentation**Y. Yang<sup>1</sup>; J. Luo<sup>2</sup>; L. Huang<sup>1</sup>; G. Hu<sup>2</sup>; K. Vargheese<sup>2</sup>; Y. Shi<sup>1</sup>; J. C. Mauro\*; 1. Rensselaer Polytechnic Institute, USA; 2. Corning Incorporated, USA**(GOMD-S1-P003-2016) Determination of the Network Dilation Coefficient in Ion-Exchanged Glass**S. Tietje\*; R. Schaut<sup>1</sup>; 1. Corning Incorporated, USA**(GOMD-S2-P004-2016) Effect of P<sub>2</sub>O<sub>5</sub>-SiO<sub>2</sub>-based bioglass powder preparation route on body formation by Yb<sup>3+</sup>-doped fiber laser**

J. Wang\*; 1. NSYSU, Taiwan

**(GOMD-S3-P005-2016) Chalcogenide Fibers and Fiber Bundles for Mid-infrared Applications**

Z. Yang<sup>\*</sup>; B. Zhang<sup>1</sup>; C. Zhai<sup>1</sup>; S. Qi<sup>1</sup>; H. Ren<sup>1</sup>; W. Guo<sup>1</sup>; Y. Yu<sup>2</sup>; B. Luther-Davies<sup>3</sup>; G. Tao<sup>3</sup>; D. Tang<sup>1</sup>; 1. Jiangsu Normal University, China; 2. The Australian National University, Australia; 3. University of Central Florida, USA

**(GOMD-S3-P006-2016) Optical Properties of Zinc Tellurite Glasses doped with Ni<sup>2+</sup> ions**

O. Zamiatin<sup>\*</sup>; E. Torokhova<sup>1</sup>; I. Fedotova<sup>1</sup>; A. Sibirkin<sup>1</sup>; 1. Lobachevsky State University of Nizhni Novgorod, Russian Federation

**(GOMD-S3-P007-2016) Specification of the glass-forming range of the TeO<sub>2</sub> - MoO<sub>3</sub> - Bi<sub>2</sub>O<sub>3</sub> system and the characterization of the glasses prepared**

O. Zamiatin<sup>\*</sup>; E. Torokhova<sup>1</sup>; I. Fedotova<sup>1</sup>; A. Sibirkin<sup>1</sup>; 1. Lobachevsky State University of Nizhni Novgorod, Russian Federation

**(GOMD-S3-P008-2016) Design, synthesis and characterization of innovative glasses with erbium-doped nanoparticles**

P. Lopez Iscoa<sup>1</sup>; L. Petit<sup>2</sup>; J. Massera<sup>3</sup>; D. Milanese<sup>4</sup>; G. Baldi<sup>5</sup>; M. Salvo<sup>6</sup>; M. Ferraris<sup>7</sup>; 1. Politecnico di Torino, Italy; 2. nLight, Finland; 3. Colorobbia S.p.A., Italy; 4. Tampere University of Technology, Finland

**(GOMD-S3-P009-2016) Direct Measurement of Photo-Elastic Processes in Chalcogenide Glasses**

P. Lucas<sup>\*</sup>; P. Deymier<sup>1</sup>; G. Coleman<sup>1</sup>; N. Boechler<sup>2</sup>; A. Khanolkar<sup>2</sup>; 1. University of Arizona, USA; 2. University of Washington, USA

**(GOMD-SP-001-2016) Characterisation of glass alteration layers: A combined microscopic and spectroscopic approach**

D. J. Backhouse<sup>1</sup>; C. L. Corkhill<sup>2</sup>; P. Zeng<sup>3</sup>; N. C. Hyatt<sup>1</sup>; R. J. Hand<sup>1</sup>; 1. University of Sheffield, United Kingdom

**(GOMD-SP-002-2016) Medium-Range Structure of Zr-Cu-Al Bulk Metallic Glasses from Structural Refinement Based on Fluctuation Electron Microscopy**

J. Maldonis<sup>\*</sup>; P. Zhang<sup>1</sup>; M. Besser<sup>2</sup>; M. Kramer<sup>2</sup>; P. Voyles<sup>1</sup>; 1. University of Madison, Wisconsin, USA; 2. Ames Laboratory, USA

**(GOMD-SP-003-2016) Optimization of Quantitative Analysis of Glass Surfaces with Electron Probe Microanalysis**

L. M. Neill<sup>\*</sup>; O. K. Neill<sup>1</sup>; J. Weaver<sup>1</sup>; J. Reiser<sup>1</sup>; N. Wall<sup>1</sup>; 1. Washington State University, USA

**(GOMD-SP-004-2016) Surface diffusion of molecular glasses and its material dependence**

W. Zhang<sup>\*</sup>; S. Ruan<sup>1</sup>; Y. Chen<sup>1</sup>; L. Yu<sup>1</sup>; 1. University of Wisconsin-Madison, USA

**(GOMD-SP-005-2016) Raman spectroscopic and high-pressure liquid chromatography study of the structures of Na<sub>2</sub>O-MoO<sub>3</sub>-Fe<sub>2</sub>O<sub>3</sub>-P<sub>2</sub>O<sub>5</sub> glasses**

J. Bai<sup>\*</sup>; J. Hsu<sup>1</sup>; R. Brown<sup>1</sup>; C. Kim<sup>2</sup>; J. Szabo<sup>2</sup>; A. Zervos<sup>2</sup>; 1. Missouri University of Science & Technology, USA; 2. MO-SCI Corporation, USA

**(GOMD-SP-006-2016) Dynamic Light Scattering in Mixed Na-Zn Metaphosphate Melts**

D. Vu<sup>\*</sup>; D. Sidebottom<sup>1</sup>; 1. Creighton University, USA

**(GOMD-SP-007-2016) Possible Existence of Two Amorphous Phases of D-Mannitol Related by a First-Order Transition**

M. Zhu<sup>\*</sup>; J. Wang<sup>1</sup>; J. H. Perepezko<sup>1</sup>; L. Yu<sup>1</sup>; 1. University of Wisconsin-Madison, USA

**(GOMD-SP-008-2016) Lithium Oxy-Thio Borate Glasses for Glassy Solid-State Electrolytes**

P. A. Enz<sup>1</sup>; M. R. Hoyt<sup>2</sup>; S. W. Martin<sup>1</sup>; 1. Iowa State University, USA

**(GOMD-SP-009-2016) Effect of transition metals addition on structural and mechanical properties of three-alkali zinc borate glass system**

S. Lakshminantha<sup>\*</sup>; N. Udayashankar<sup>1</sup>; H. Shashikala<sup>1</sup>; 1. National Institute of Technology Karnataka, Surathkal, India

**(GOMD-SP-010-2016) Fracture of molecular glasses under tension and fracture-induced crystallization**

Y. Chen<sup>\*</sup>; C. T. Powell<sup>1</sup>; L. Yu<sup>1</sup>; 1. University of Wisconsin, USA

**(GOMD-SP-011-2016) Structure - Property Relationships in Borosilicate and Aluminosilicate Glasses**

J. Y. Cheng<sup>\*</sup>; R. Youngman<sup>2</sup>; J. Matthewson<sup>1</sup>; A. Goel<sup>1</sup>; 1. Rutgers University, USA; 2. Corning Incorporated, USA

**(GOMD-SP-012-2016) Topological Control on Borosilicate Glass Dissolution Kinetics**

M. Wang<sup>\*</sup>; B. Wang<sup>1</sup>; J. C. Mauro<sup>2</sup>; M. Bauchy<sup>1</sup>; 1. UCLA, USA; 2. Corning Incorporated, USA

**(GOMD-SP-013-2016) Densification of ZnS-CaLa<sub>2</sub>S<sub>4</sub> infrared composite optical ceramics**

Y. Li<sup>\*</sup>; Y. Wu<sup>1</sup>; 1. Alfred University, USA

**(GOMD-SP-014-2016) Sintering and mechanical properties of mineral-glass composites for development of engineered stones**

G. Guimarães dos Santos<sup>\*</sup>; M. Camuri Crovace<sup>1</sup>; E. Dutra Zanotto<sup>1</sup>; 1. Federal University of Sao Carlos, Brazil

**(GOMD-SP-015-2016) Interpretation of space charge potential in ceramics with a presence of an electric field**

Y. Liu<sup>\*</sup>; Y. Wu<sup>1</sup>; 1. Alfred University, USA

**(GOMD-SP-016-2016) Mechanical properties of silver nanoparticle embedded BaO-CaF<sub>2</sub>-P<sub>2</sub>O<sub>5</sub> glasses**

M. Narayanan<sup>\*</sup>; H. Shashikala<sup>1</sup>; 1. National Institute of Technology Karnataka Surathkal, India

**(GOMD-SP-017-2016) Structural Study of Tellurite Glasses**

B. Hauke<sup>\*</sup>; A. Crego<sup>1</sup>; G. Tarantino<sup>1</sup>; M. Affatigato<sup>1</sup>; S. Feller<sup>1</sup>; E. Barney<sup>2</sup>; 1. Coe College, USA; 2. University of Nottingham, United Kingdom

**(GOMD-SP-018-2016) Metal-to-Insulator Transition in Conducting Bridge Memory Materials**

K. Prasai<sup>\*</sup>; B. Bhattarai<sup>1</sup>; G. Chen<sup>1</sup>; D. Drabold<sup>1</sup>; 1. Ohio University, USA

**(GOMD-SP-019-2016) Pores arising due to non-isothermal crystallization of diopside glass particles**

R. G. Fernandes<sup>\*</sup>; R. R. Tobar<sup>1</sup>; E. B. Ferreira<sup>1</sup>; 1. University of São Paulo, Brazil

**(GOMD-SP-020-2016) Surface diffusion and crystallization of molecular glasses**

S. Ruan<sup>\*</sup>; Y. Sun<sup>1</sup>; W. Zhang<sup>1</sup>; M. D. Ediger<sup>1</sup>; L. Yu<sup>1</sup>; 1. University of Wisconsin-Madison, USA

**(GOMD-SP-021-2016) Crystallization of iron-containing sodium aluminosilicate glasses**

M. Ahmadzadeh<sup>1</sup>; J. Marcial<sup>1</sup>; M. Saleh<sup>1</sup>; M. Rehman<sup>2</sup>; A. Goel<sup>2</sup>; J. McCloy<sup>1</sup>; 1. Washington State University, USA; 2. Rutgers University, USA

**(GOMD-SP-022-2016) Experimentally constrained materials modeling: Application to disorder and glassy materials**

A. Pandey<sup>\*</sup>; P. Biswas<sup>2</sup>; D. Drabold<sup>1</sup>; 1. Ohio Univeristy, USA; 2. The University of Southern Mississippi, USA

**(GOMD-SP-023-2016) Study of thermal stability and optical properties of phospho-silicate glasses**

K. Garg<sup>1</sup>; N. Kaur<sup>1</sup>; G. Kaur<sup>2</sup>; V. Kumar<sup>1</sup>; 1. SGGSWU, India; 2. Thapar University, India

**(GOMD-SP-024-2016) Sol-gel Derived Alumina-rich Binary Aluminosilicate Glasses**

K. E. Johnson<sup>\*</sup>; S. H. Risbud<sup>1</sup>; 1. "University of California, Davis", USA

**(GOMD-SP-025-2016) Formation of liquid-crystalline structures in glasses**

R. Teerakapibal<sup>\*</sup>; C. Huang<sup>1</sup>; A. Gujral<sup>1</sup>; M. D. Ediger<sup>1</sup>; L. Yu<sup>1</sup>; 1. University of Wisconsin-Madison, USA

**(GOMD-SP-026-2016) Ce<sup>3+</sup> Luminescence in UV Transparent Phosphate Glasses**

M. W. Kielty<sup>\*</sup>; M. Dettmann<sup>2</sup>; V. Herrig<sup>2</sup>; U. Akgun<sup>2</sup>; L. Jacobsohn<sup>1</sup>; 1. Clemson University, USA; 2. Coe College, USA

**(GOMD-SP-027-2016) Effect of iron content on the structure and disorder of iron-bearing sodium silicate glasses: Insights from high-resolution solid-state NMR study**

H. Kim<sup>\*</sup>; S. Lee<sup>1</sup>; 1. Seoul National University, Republic of Korea

**(GOMD-SP-028-2016) Novel Approach to Crystal Derived Optical Fibers**

M. A. Tuggle<sup>\*</sup>; J. Ballato<sup>1</sup>; 1. Clemson University, USA

**(GOMD-SP-029-2016) Recycling solid wastes into high strength glass foams**

Y. Gong<sup>\*</sup>; R. Dongol<sup>1</sup>; C. Yatongchai<sup>2</sup>; A. W. Wren<sup>1</sup>; S. K. Sundaram<sup>1</sup>; N. Mellott<sup>1</sup>; 1. Alfred University, USA; 2. Maejo University, Thailand

**(GOMD-SP-030-2016) Physical properties and Structure of Sodium Borogermanate Glasses as Part of the Mixed Glass Former Effect**

D. Hynek<sup>\*</sup>; D. Shadle<sup>1</sup>; G. Bohach<sup>1</sup>; S. Verkey<sup>1</sup>; S. Keizer<sup>1</sup>; J. Wang<sup>1</sup>; S. Feller<sup>1</sup>; M. Affatigato<sup>1</sup>; S. Kmiec<sup>2</sup>; K. Hakanson<sup>2</sup>; C. Francis<sup>2</sup>; S. W. Martin<sup>2</sup>; 1. Coe College, USA; 2. Iowa State University, USA

**(GOMD-SP-031-2016) Influence of transition metal oxide on the properties and dissolution behaviors of simplified high-level nuclear waste glasses**

X. Yu<sup>\*</sup>; J. Neeway<sup>2</sup>; J. Ryan<sup>2</sup>; J. Du<sup>1</sup>; 1. University of North Texas, USA; 2. Pacific Northwest National Lab, USA

**(GOMD-SP-032-2016) Effect of composition and heat treatment on the microstructure and properties of  $\text{Li}_{1-x}\text{Al}_x\text{Ge}_{2-x}(\text{PO}_4)_3$  NASICON structured glass-ceramics solid-state electrolytes**

P. Kuo<sup>\*</sup>; J. Du<sup>1</sup>; 1. University of North Texas, USA

**(GOMD-SP-033-2016) Probing Inhomogeneity of Glasses by Small-angle X-ray Scattering**

M. Sundararajan<sup>\*</sup>; H. Abu Jeib<sup>1</sup>; G. Chen<sup>1</sup>; 1. Ohio University, USA

**(GOMD-SP-034-2016) Effect of the Surface Topology on the Reactivity of Silica: Insights from Reactive Molecular Dynamics**

Y. Yu<sup>\*</sup>; B. Wang<sup>1</sup>; M. Wang<sup>1</sup>; M. Bauchy<sup>1</sup>; 1. University of California, Los Angeles, USA

**(GOMD-SP-035-2016) Study of the 2<sup>nd</sup> order nonlinear optical properties (SONL) induced in thermally poled alkali-doped chalcogenide glasses**

A. Lepicard<sup>\*</sup>; F. Adamietz<sup>1</sup>; V. Rodriguez<sup>1</sup>; K. Richardson<sup>2</sup>; M. Dussauze<sup>1</sup>; 1. University of Bordeaux, France; 2. University of Central Florida, USA

**(GOMD-SP-036-2016) Mesoscale Structure Engineering in Photonic Glass for Tunable Luminescence**

Y. Xu<sup>\*</sup>; S. Zhou<sup>1</sup>; J. Qiu<sup>1</sup>; 1. South China University of Technology, China

**(GOMD-SP-037-2016) Phosphate glass-clad  $\text{Se}_x\text{Te}_{1-x}$  semiconductor core optical fibers**

G. Tang<sup>\*</sup>; Q. Qian<sup>1</sup>; Z. Yang<sup>1</sup>; 1. State Key Laboratory of Luminescent Materials and Devices and Institute of Optical Communication Materials, South China University of Technology, China

**(GOMD-SP-038-2016) Phosphate single core and core-clad fiber: impact of fibers immersion in TRIS on light loss and mechanical properties**

A. Mishra<sup>\*</sup>; F. Smektala<sup>1</sup>; J. Massera<sup>1</sup>; 1. Tampere University of Technology, Finland; 2. Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB), France

**(GOMD-SP-039-2016) Growth and characterization of vacuum sintering Pr/Ce-doped YAG transparent ceramic for the excellent white LED**

Y. Tang<sup>\*</sup>; S. Zhou<sup>1</sup>; X. Yi<sup>1</sup>; D. Hao<sup>1</sup>; S. Zhang<sup>1</sup>; 1. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, China

**(GOMD-SP-040-2016) Low-temperature fluorescence of Pr-doped TAS glasses**

C. Thomas<sup>\*</sup>; Y. Shpotyuk<sup>2</sup>; R. Golovchak<sup>1</sup>; 1. Austin Peay State University, USA; 2. University of Rzeszow, Poland

**(GOMD-SP-041-2016) Structure and properties of complex Bi-containing chalcogenide glasses**

T. L. Hodge<sup>\*</sup>; R. Golovchak<sup>1</sup>; Y. Shpotyuk<sup>2</sup>; B. Bureau<sup>3</sup>; H. Jain<sup>4</sup>; 1. Austin Peay State University, USA; 2. Centre for Innovation and Transfer of Natural Sciences and Engineering Knowledge, Poland; 3. Université de Rennes 1, France; 4. Lehigh University, USA

**(GOMD-SP-042-2016) Thermal Analysis of Borosilicate Glass for its Biological Applications**

K. S. Ranasinghe<sup>1</sup>; G. Humble<sup>\*</sup>; D. E. Day<sup>2</sup>; 1. Kennesaw State University, USA; 2. Missouri University of Science & Technology, USA

**(GOMD-SP-043-2016) Tellurium Vanadate Glasses: Conductivity, Structure, Decay**

L. McDonald<sup>\*</sup>; S. Xian<sup>1</sup>; S. Feller<sup>1</sup>; C. Love<sup>2</sup>; B. Baker<sup>2</sup>; M. Affatigato<sup>1</sup>; 1. Coe College, USA; 2. William Jewell College, USA

**(GOMD-SP-044-2016) Modelling thermally deposited chalcogenide glass thin films using time-dependent density functional theory**

L. R. Nichols<sup>\*</sup>; J. R. Oelgoetz<sup>1</sup>; 1. Austin Peay State University, USA

**Tuesday, May 24, 2016****George W. Morey Award Lecture**

Room: Madison

**8:00 AM**

**(GOMD-AW-002-2016) Spying with Spins on Messy Materials: 50 Years of Glass Structure Elucidation by NMR Spectroscopy (Invited)**

H. Eckert<sup>\*</sup>; 1. University of Muenster, Germany

**9:00 AM**

Break

**Symposium 1: Fundamentals of the Glassy State****Session 1: Glass Formation and Relaxation I**

Room: Capitol A

Session Chair: John Mauro, Corning Incorporated

**9:20 AM**

**(GOMD-S1-001-2016) Excitations in glasses at low temperatures (Invited)**

W. Kob<sup>\*</sup>; 1. Laboratoire Charles Coulomb, France

**9:50 AM**

**(GOMD-S1-002-2016) Glass Transition: The Broken-Ergodicity View (Invited)**

P. Gupta<sup>\*</sup>; 1. Ohio State University, USA

**10:20 AM**

**(GOMD-S1-003-2016) Viscosity of Westminster Cathedral Glass**

O. Gulbitten<sup>\*</sup>; X. Guo<sup>1</sup>; J. C. Mauro<sup>1</sup>; 1. Corning Incorporated, USA

**10:40 AM**

**(GOMD-S1-004-2016) Structure and properties of  $\text{ZnCl}_2$  melts: indication of a strong-to-fragile transition**

P. Lucas<sup>\*</sup>; A. Edwards<sup>1</sup>; M. Venkateswara<sup>1</sup>; P. Deymier<sup>1</sup>; K. Muralidharan<sup>1</sup>; A. Al Sayoud<sup>1</sup>; 1. University of Arizona, USA

**11:00 AM**

**(GOMD-S1-005-2016) Characterizing and Predicting Stress and Structural Relaxation in Glass**

K. T. Strong<sup>\*</sup>; B. Elisberg<sup>1</sup>; R. Jamison<sup>1</sup>; K. Ewsuk<sup>1</sup>; 1. Sandia National Laboratories, USA

**11:20 AM**

**(GOMD-S1-006-2016) Depletion layer formation by electro-thermal poling of alkali silicate glasses**

C. McLaren<sup>\*</sup>; M. Balabajew<sup>2</sup>; B. Roling<sup>2</sup>; H. Jain<sup>1</sup>; 1. Lehigh University, USA; 2. University of Marburg, Germany

**Session 4: Potential Development and MD Simulations of Multicomponent Glasses**

Room: University C/D

Session Chairs: Walter Kob, Laboratoire Charles Coulomb; Jincheng Du, University of North Texas

**9:20 AM**

**(GOMD-S1-007-2016) Structures and properties of multicomponent oxide glasses with mixed glass formers from molecular dynamics simulations (Invited)**

J. Du<sup>\*</sup>; 1. University of North Texas, USA

**9:50 AM**

**(GOMD-S1-008-2016) Molecular Dynamics Simulations of Multicomponent Aluminosilicate Glass and Glass Surfaces**

L. Criscenti<sup>\*</sup>; T. Zeitler<sup>1</sup>; K. Ewsuk<sup>1</sup>; 1. Sandia National Laboratories, USA

10:10 AM

**(GOMD-S1-009-2016) Simulations of nepheline glasses: A study of relation between nanostructure and properties**W. Chen<sup>\*</sup>; N. Greaves<sup>1</sup>; 1. Aberystwyth University, United Kingdom

10:30 AM

**(GOMD-S1-010-2016) Structural simulations of Yb-doped aluminum fluoride glasses**H. Inoue<sup>\*</sup>; A. Masuno<sup>1</sup>; 1. The University of Tokyo, Japan

10:50 AM

**(GOMD-S1-011-2016) Barium Dissilicate: A molecular Dynamics study**J. P. Rino<sup>\*</sup>; 1. Universidade Federal de São Carlos, Brazil

11:10 AM

**(GOMD-S1-012-2016) An Environment Dependent Dynamic Charge Interatomic Potential for Modeling Nano and Bulk Silica Polymorphs**K. Muralidharan<sup>\*</sup>; K. Runge<sup>1</sup>; 1. University of Arizona, USA

11:30 AM

**(GOMD-S1-013-2016) Optimizing Molecular Dynamics Potentials for Multi-component Glasses**S. Sundararaman<sup>\*</sup>; S. Ispas<sup>2</sup>; W. Kob<sup>2</sup>; L. Huang<sup>1</sup>; 1. Rensselaer Polytechnic Institute, USA; 2. Université de Montpellier 2, France**Symposium 2: Larry L. Hench Memorial Symposium on Bioactive Glasses****Larry L. Hench Memorial Symposium on Bioactive Glasses IV: Structure**

Room: Wisconsin

Session Chairs: Julian Jones, Imperial College London; Jonathan Massera, Tampere University of Technology

9:20 AM

**(GOMD-S2-015-2016) First observation of the atomistic source of mechanical toughness in glass bio-cements during setting (Invited)**N. Greaves<sup>1</sup>; G. Chass<sup>2</sup>; Y. Yue<sup>3</sup>; 1. University of Cambridge, United Kingdom; 2. Queen Mary University of London, United Kingdom; 3. Aalborg University, Denmark

9:50 AM

**(GOMD-S2-016-2016) Composition-Structure Trends of Bioactive Phosphosilicate and Borophosphosilicate Glasses Probed by Solid-State NMR and MD Simulations (Invited)**R. Mathew<sup>1</sup>; Y. Yu<sup>1</sup>; B. Stevansson<sup>1</sup>; M. Eden<sup>\*</sup>; 1. Stockholm University, Sweden

10:20 AM

**(GOMD-S2-017-2016) The Structure and Properties of 20Na<sub>2</sub>O-30[(1-x)CaO-xSrO]-50P<sub>2</sub>O<sub>5</sub> Glasses for a Biomedical Application**P. Freudenberger<sup>\*</sup>; R. Brow<sup>1</sup>; A. Saitoh<sup>2</sup>; H. Takebe<sup>2</sup>; S. Nakane<sup>2</sup>; H. Ikeda<sup>3</sup>; 1. Missouri University of Science & Technology, USA; 2. Ehime University, Japan; 3. Nippon Electric Glass, Japan

10:40 AM

**(GOMD-S2-018-2016) Study of Bioglasses and Glass Ceramics by Infrared and Raman Spectroscopy (Invited)**D. Möncke<sup>\*</sup>; 1. Friedrich-Schiller University Jena, Germany

11:10 AM

**(GOMD-S2-019-2016) A thermodynamic discourse on the dissolution behavior of bioactive glasses**B. S. Pföss<sup>\*</sup>; R. Conradt<sup>1</sup>; 1. RWTH Aachen University, Germany

11:30 AM

**Edgar Dutra Zanotto - "Hench's key role in the development of the most bioactive glass-ceramic (BioSilicate)"**

11:50 AM

Parting Thoughts

**Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications****Session 1: Ionic Conducting Materials**

Room: University A/B

Session Chair: Xiang-hua Zhang, Université de Rennes I

9:20 AM

**(GOMD-S3-018-2016) Ion conducting oxide and sulfide glasses and development of all solid state batteries (Invited)**A. Pradel<sup>\*</sup>; M. Ribes<sup>1</sup>; 1. Université de Montpellier, France

9:50 AM

**(GOMD-S3-019-2016) Development and Characterization of Fast Ion Conducting Solid Electrolytes for All-Solid-State Sodium Batteries (Invited)**S. W. Martin<sup>\*</sup>; 1. Iowa State University, USA

10:20 AM

**(GOMD-S3-020-2016) Characterization of a new Na bulk ionic conductor prepared from a glass reactive sintering route**S. Chenu<sup>2</sup>; P. Bénard-Rocherullé<sup>1</sup>; R. Lebullenger<sup>1</sup>; J. Rocherullé<sup>\*</sup>; X. Zhang<sup>1</sup>; 1. University of Rennes, France; 2. University of Limoges, France

10:40 AM

**(GOMD-S3-021-2016) Transition metal oxides based glasses for solid-state batteries: Insights from a combined first-principles and classical molecular dynamics modeling approach**G. Ori<sup>\*</sup>; L. Sementa<sup>2</sup>; M. Boero<sup>1</sup>; C. Massobrio<sup>1</sup>; M. Montorsi<sup>1</sup>; 1. IPCMS, CNRS - University of Strasbourg, France; 2. University of Modena and Reggio Emilia, Italy

11:00 AM

**(GOMD-S3-022-2016) Structure and Physical Properties of the Glassy Solid State Electrolyte of the 0.64 Na<sub>2</sub>S+ 0.46 [xB<sub>3/2</sub>+ (1-x)GeS<sub>2</sub>] System**B. Curtis<sup>\*</sup>; S. W. Martin<sup>1</sup>; 1. Iowa State University, USA**Symposium 4: Glass Technology and Cross-Cutting Topics****Session 4: Glass Corrosion: Mechanisms and Rate I**

Room: Capitol B

Session Chairs: Eric Pierce, Oak Ridge National Lab; Stephane Gin, CEA

9:20 AM

**(GOMD-S4-037-2016) Corrosion Behavior of Mixed Simulated Radioactive Waste Glasses SON-68 and AFCI**J. A. Rice<sup>\*</sup>; 1. Pennsylvania State University, USA

9:40 AM

**(GOMD-S4-038-2016) Investigation of Alteration Gel Layers' Porosities using Positron Annihilation Spectroscopy**J. Reiser<sup>\*</sup>; J. McCloy<sup>1</sup>; M. Weber<sup>1</sup>; B. Parruzot<sup>1</sup>; L. M. Neill<sup>1</sup>; J. Ryan<sup>2</sup>; J. Neeway<sup>2</sup>; N. Wall<sup>1</sup>; 1. Washington State University, USA; 2. Pacific Northwest National Lab, USA

10:00 AM

**(GOMD-S4-039-2016) Dissolution of International Simple Glass (ISG) in Sodium Chloride Brine Solution**J. P. Icenhower<sup>\*</sup>; 1. Sandia National Laboratories, USA

10:20 AM

**(GOMD-S4-040-2016) Corrosion behavior of ISG fibers from pH 9.5 - 12.5**C. L. Trivelpiece<sup>\*</sup>; C. G. Pantano<sup>1</sup>; 1. Pennsylvania State University, USA

10:40 AM

**(GOMD-S4-041-2016) Effect of Magnetite on Nuclear Waste Glass Alteration Layers**L. M. Neill<sup>\*</sup>; S. Gin<sup>2</sup>; P. Jollivet<sup>2</sup>; B. Parruzot<sup>1</sup>; N. Wall<sup>1</sup>; 1. Washington State University, USA; 2. CEA, France

11:00 AM

**(GOMD-S4-042-2016) The role played by inter-diffusion in glass dissolution: The case of basaltic and nuclear glasses**S. Gin<sup>\*</sup>; T. Ducasse<sup>1</sup>; M. Collin<sup>1</sup>; 1. CEA, France

11:20 AM

**(GOMD-S4-043-2016) A Leap Towards the Quantification of Glass Dissolution Rate: An Atomic Force Microscopy Approach**Y. Gong<sup>\*</sup>; C. L. Trivelpiece<sup>2</sup>; C. G. Pantano<sup>2</sup>; N. Mellott<sup>1</sup>; 1. Alfred University, USA; 2. Pennsylvania State University, USA

11:40 AM

**(GOMD-S4-044-2016) Role of zirconium in nuclear waste glass and in the corresponding alteration gels**L. Galois<sup>\*</sup>; G. Calas<sup>1</sup>; P. Jollivet<sup>2</sup>; F. Angeli<sup>2</sup>; S. Gin<sup>2</sup>; 1. UPMC, France; 2. LCLT, CEA-Marcoule, France**Symposium 5: Festschrift for Professor Donald R. Uhlmann****Models and Connections**

Room: Madison

Session Chair: Lisa Klein, Rutgers University

9:20 AM

**(GOMD-S5-004-2016) Modeling of Glass-Ceramics with Anisotropic Crystallization (Invited)**D. P. Birnie<sup>\*</sup>; 1. Rutgers University, USA

9:50 AM

**(GOMD-S5-005-2016) Connections: From metallurgy, to glass science, to phase separation, to localization of light (Invited)**T. P. Seward<sup>\*</sup>; 1. Retired, USA

10:20 AM

**(GOMD-S5-006-2016) The Spherical Cow and Associated Technological Breakthroughs: A tribute to Don Uhlmann**G. W. Scherer<sup>\*</sup>; 1. Princeton, USA

10:40 AM

**(GOMD-S5-007-2016) Cigars and Tiny Bubbles (Invited)**G. Wicks<sup>\*</sup>; 1. Wicks Consulting Services, LLC, USA

11:10 AM

**(GOMD-S5-008-2016) Applications of the Uhlmann Conjecture in Non-Traditional Domains (Invited)**B. Fabes<sup>\*</sup>; 1. Civic Consulting Alliance, USA**Norbert J. Kreidl Award Lecture**

Room: Madison

12:00 PM

**(GOMD-AW-003-2016) Materials and devices for mechanically flexible integrated photonics (Invited)**L. Li<sup>\*</sup>; 1. Massachusetts Institute of Technology, USA**Symposium 1: Fundamentals of the Glassy State****Session 1: Glass Formation and Relaxation II**

Room: Capitol A

Session Chair: Sabyasachi Sen, UC Davis

1:20 PM

**(GOMD-S1-014-2016) Structural relaxation of organic and metallic glasses: A new mechanism for relaxation in glasses of high kinetic stability (Invited)**M. D. Ediger<sup>\*</sup>; 1. University of Wisconsin-Madison, USA

1:50 PM

**(GOMD-S1-015-2016) Microscopic Theory of Elasticity-Mediated Activated Relaxation in Glass-Forming Liquids (Invited)**K. Schweizer<sup>\*</sup>; 1. University of Illinois, USA

2:20 PM

**(GOMD-S1-016-2016) Viscosity of hydrous borate and silicate glasses**J. Deubener<sup>\*</sup>; H. Behrens<sup>2</sup>; R. Müller<sup>2</sup>; 1. Clausthal University of Technology, Germany; 2. Institute of Mineralogy, Leibniz University of Hannover, Germany; 3. Federal Institute for Materials Research and Testing (BAM), Berlin, Germany

2:40 PM

**(GOMD-S1-017-2016) Role of Structural Relaxation in the Network Dilution of Ion-Exchanged Glasses**E. A. King<sup>\*</sup>; D. C. Allan<sup>1</sup>; J. C. Mauro<sup>1</sup>; 1. Corning Incorporated, USA

3:00 PM

**(GOMD-S1-018-2016) Structural Relaxation Time of Supercooled Pt<sub>57.5</sub>Cu<sub>14.7</sub>Ni<sub>5.3</sub>P<sub>22.5</sub> Nanowires in the Supercooled Liquid State from Electron Correlation Microscopy**P. Zhang<sup>\*</sup>; L. He<sup>1</sup>; Z. Liu<sup>2</sup>; J. Schroers<sup>2</sup>; P. Voyles<sup>1</sup>; 1. University of Wisconsin-Madison, USA; 2. Yale University, USA

3:20 PM

**Break**

3:40 PM

**(GOMD-S1-019-2016) Enthalpy relaxation in melt-quenched metal-organic framework glasses (Invited)**Y. Yue<sup>\*</sup>; 1. Aalborg University, Denmark

4:10 PM

**(GOMD-S1-020-2016) Which equation best describes the equilibrium viscosity of glass-forming liquids?**D. R. Cassar<sup>\*</sup>; M. L. Nascimento<sup>1</sup>; A. M. Rodrigues<sup>3</sup>; T. D. Fragoso<sup>2</sup>; F. Louzada Neto<sup>2</sup>; E. Dutra Zanotto<sup>1</sup>; 1. Institute of Humanities, Arts & Sciences, Federal University of Bahia, Brazil; 2. Institute of Mathematical and Computational Sciences, University of São Paulo, Brazil; 3. Department of Materials Engineering, Federal University of São Carlos, Brazil

4:30 PM

**(GOMD-S1-021-2016) Connectivity Patterns in the Fragility of Network-forming Glasses**D. Sidebottom<sup>\*</sup>; 1. Creighton University, USA**Session 3: NMR**

Room: Capitol B

Session Chair: Randall Youngman, Corning Incorporated

3:40 PM

**(GOMD-S1-022-2016) Connecting NMR Spectroscopy Results and MD Simulations of Ba-Silicate Glasses**T. M. Alam<sup>\*</sup>; T. Zeitler<sup>1</sup>; K. Ewsuk<sup>1</sup>; B. A. Hammann<sup>2</sup>; 1. Sandia National Laboratories, USA; 2. Washington University in St. Louis, USA

4:00 PM

**(GOMD-S1-023-2016) Temperature effects on the distribution of non-bridging oxygens on Si and Al in aluminosilicate glass**E. I. Morin<sup>\*</sup>; J. Stebbins<sup>1</sup>; 1. Stanford University, USA

4:20 PM

**(GOMD-S1-024-2016) Oxygen Speciation in Calcium Aluminosilicate and Aluminoborosilicate Glasses as Quantified Through <sup>17</sup>O Double-Resonance NMR**M. M. LaComb<sup>\*</sup>; D. M. Rice<sup>1</sup>; J. Stebbins<sup>1</sup>; 1. Stanford University, USA

4:40 PM

**(GOMD-S1-025-2016) Measuring bond angle distribution in silicate glasses with 2D J PIETA NMR**D. Srivastava<sup>\*</sup>; P. Florian<sup>2</sup>; P. Grandinetti<sup>1</sup>; J. Baltisberger<sup>3</sup>; 1. Ohio State University, USA; 2. CEMHTI-CNRS UPR3079, France; 3. Berea College, USA

**5:00 PM****(GOMD-S1-026-2016) Network Structure and Rare-earth Ion Local Environments in Fluorophosphate Photonic Glasses Studied by Solid State NMR and EPR Spectroscopies**

M. de Oliveira<sup>\*1</sup>; T. Uesbeck<sup>2</sup>; T. Gonçalves<sup>1</sup>; C. Magon<sup>1</sup>; P. S. Pizani<sup>3</sup>; A. de Camargo<sup>1</sup>; H. Eckert<sup>1</sup>; 1. University of Sao Paulo, Brazil; 2. Westfälische Wilhelms-Universität Münster, Germany; 3. Federal University of Sao Carlos, Brazil

**Session 4: Predicting Glass Properties from Simulations**

Room: University C/D

Session Chairs: Carlo Massobrio, CNRS-IPCMS-UNR 7504; Jincheng Du, University of North Texas

**1:20 PM****(GOMD-S1-027-2016) Molecular dynamics simulations study on the relation between dynamical heterogeneity, structural relaxation, and self diffusion in viscous silica (Invited)**

M. Vogel<sup>\*1</sup>; P. Henritzi<sup>1</sup>; F. Klameth<sup>1</sup>; A. Bormuth<sup>1</sup>; J. Geske<sup>1</sup>; B. Drossel<sup>1</sup>; 1. Institute of Condensed Matter Physics, TU Darmstadt, Germany

**1:50 PM****(GOMD-S1-028-2016) Glass surface properties design with thermal poling: A Molecular Dynamics study (Invited)**

A. Tandia<sup>\*1</sup>; 1. Corning Incorporated, USA

**2:20 PM****(GOMD-S1-029-2016) Atomic-Scale Study of High-Frequency Energy Dissipation in Oxide Glasses**

T. Damart<sup>\*1</sup>; A. Tanguy<sup>2</sup>; D. Rodney<sup>1</sup>; 1. Institut Lumière Matière, Université Lyon 1, France; 2. LAMCOS, INSA de Lyon, France

**2:40 PM****(GOMD-S1-030-2016) Influence of Deformation Induced Topological Anisotropy on Mechanical Properties of Silica Glass: An Atomistic Study**

V. Ganisetti<sup>\*1</sup>; E. Bitzek<sup>1</sup>; 1. Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

**3:00 PM****(GOMD-S1-031-2016) Dispersion and pressure-dependence of photoelastic response in inorganic glass (Invited)**

J. Zwanziger<sup>\*1</sup>; 1. Dalhousie University, Canada

**3:30 PM****Break****3:50 PM****(GOMD-S1-032-2016) Stretched Exponential Relaxation of Glasses at Low Temperature (Invited)**

Y. Yu<sup>1</sup>; M. Wang<sup>1</sup>; D. Zhang<sup>1</sup>; B. Wang<sup>1</sup>; G. Sant<sup>1</sup>; M. Bauchy<sup>\*1</sup>; 1. University of California, Los Angeles, USA

**4:20 PM****(GOMD-S1-033-2016) Atomic-scale calculation of thermal properties via the "approach-to-equilibrium" methodology**

E. Lampin<sup>\*1</sup>; P. Palla<sup>1</sup>; F. Cleri<sup>1</sup>; G. Ori<sup>2</sup>; A. Bouzid<sup>2</sup>; C. Massobrio<sup>2</sup>; M. Boero<sup>2</sup>; 1. IEMN, France; 2. IPCMS, France

**4:40 PM****(GOMD-S1-034-2016) Multiscale cohesive zone model for simulation of brittle glass material**

S. Urata<sup>\*1</sup>; S. Li<sup>2</sup>; 1. Asahi Glass Co., Ltd., Japan; 2. University of California, Berkeley, USA

**5:00 PM****(GOMD-S1-035-2016) Network modeling and Simulation of Amorphous Silicon Boron Nitride (SiBN)**

A. Dasmahapatra<sup>\*1</sup>; Y. Ni<sup>2</sup>; T. Dumitrica<sup>2</sup>; P. Kroll<sup>1</sup>; 1. The University of Texas at Arlington, USA; 2. University of Minnesota, USA

**5:20 PM****(GOMD-S1-036-2016) Molecular Dynamics Simulation of Glasses for Photomultiplier Tubes in Neutrino Detection**

R. Dongol<sup>\*1</sup>; S. K. Sundaram<sup>1</sup>; A. Tandia<sup>1</sup>; 1. Alfred University, USA; 2. Corning Inc., USA

**Session 5: Mechanical Properties of Glasses I**

Room: Wisconsin

Session Chair: Tanguy Rouxel, Université de Rennes 1

**1:20 PM****(GOMD-S1-037-2016) Water-Enhanced Swelling of Silica Glass: Role of Applied Stress (Invited)**

S. Wiederhorn<sup>\*1</sup>; G. Rizzi<sup>2</sup>; M. Hoffmann<sup>2</sup>; T. Fett<sup>2</sup>; 1. National Institute of Science and Technology, USA; 2. Karlsruhe Institute of Technology, Germany

**1:50 PM****(GOMD-S1-038-2016) Glass Strength and Water (Invited)**

M. Tomozawa<sup>\*1</sup>; 1. Rensselaer Polytechnic Institute, USA

**2:20 PM****(GOMD-S1-039-2016) Effect of Water on Aging and Fatigue of Soda-Lime-Silicate Glass**

E. Ronchetto<sup>\*1</sup>; R. Brow<sup>1</sup>; 1. Missouri University of Science and Technology, USA

**2:40 PM****(GOMD-S1-040-2016) Origin of the Fatigue Limit in Oxide Glasses: Fracture Mechanics Modelling**

J. H. Seaman<sup>\*1</sup>; T. Blanchet<sup>1</sup>; M. Tomozawa<sup>1</sup>; 1. Rensselaer Polytechnic Institute, USA

**3:00 PM****(GOMD-S1-041-2016) The Size Effect of Surface Stress Relaxation**

E. Aaldenberg<sup>\*1</sup>; J. H. Seaman<sup>1</sup>; M. Tomozawa<sup>1</sup>; 1. Rensselaer Polytechnic Institute, USA

**3:20 PM****Break****Session 5: Mechanical Properties of Glasses II**

Room: Wisconsin

Session Chair: Minoru Tomozawa, Rensselaer Polytechnic Institute

**3:40 PM****(GOMD-S1-042-2016) Structural origin of the flaw sensitivity in glasses from different chemical systems: Interatomic bonding character and medium-range order**

T. Rouxel<sup>\*1</sup>; 1. University of Rennes 1, France

**4:00 PM****(GOMD-S1-043-2016) Mechanical Properties of Tectosilicate Calcium-Aluminosilicate, Magnesium-Aluminosilicate, and Calcium-Galliosilicate Glasses**

L. Lamberson<sup>1</sup>; R. Youngman<sup>2</sup>; S. P. Baker<sup>\*1</sup>; 1. Cornell University, USA; 2. Corning Incorporated, USA

**4:20 PM****(GOMD-S1-044-2016) Mechanical Properties of Denisified Tectosilicate Calcium-Aluminosilicate Glasses**

N. Johnson<sup>\*1</sup>; L. Lamberson<sup>2</sup>; M. M. Smedskjaer<sup>3</sup>; S. Baker<sup>1</sup>; 1. Cornell University, USA; 2. Corning Incorporated, USA; 3. Aalborg University, Denmark

**4:40 PM****(GOMD-S1-045-2016) Vickers Indentation of Ion-Exchanged Glasses at Quasi-Static and Dynamic Loading Rates**

T. M. Gross<sup>\*1</sup>; 1. Corning Incorporated, USA

**5:00 PM****(GOMD-S1-046-2016) Surface deformation and indentation-induced stress in various nanocrystallized glasses**

K. Shinozaki<sup>\*1</sup>; T. Honma<sup>1</sup>; T. Komatsu<sup>1</sup>; 1. Nagaoka University of Technology, Japan

**5:20 PM****(GOMD-S1-047-2016) Influence of mechanical properties on the dimple formation of non-alkaline glass substrate during the chemical thinning process**

H. Tokunaga<sup>\*1</sup>; K. Hayashi<sup>1</sup>; 1. Asahi Glass Co.,Ltd, Japan



### Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications

#### Session 1: Electronic Conducting Materials I

Room: University A/B

Session Chair: Ruud Schropp, Eindhoven University of Technology (TU/e)

**1:20 PM**

##### **(GOMD-S3-023-2016) Electron-conducting Filaments in Ion-conducting Ag-Ge-Se Glasses (Invited)**

G. Chen<sup>\*1</sup>; M. Sundararajan<sup>1</sup>; L. Zella<sup>1</sup>; H. Abu Jeib<sup>1</sup>; D. Drabold<sup>1</sup>; M. Kordesch<sup>1</sup>; D. Ingram<sup>1</sup>; 1. Ohio University, USA

**1:50 PM**

##### **(GOMD-S3-024-2016) Relation between hydrogen-bonding environment and high frequency Si-H stretching vibrations in hydrogenated amorphous silicon (Invited)**

P. Biswas<sup>\*1</sup>; D. Drabold<sup>2</sup>; 1. The University of Southern Mississippi, USA; 2. Ohio University, USA

**2:20 PM**

##### **(GOMD-S3-025-2016) Electron-phonon couplings for disordered systems**

D. Drabold<sup>\*1</sup>; K. Prasai<sup>1</sup>; 1. Ohio University, USA

**2:40 PM**

##### **(GOMD-S3-026-2016) Vibrations in amorphous silica**

B. Bhattarai<sup>\*1</sup>; D. Drabold<sup>1</sup>; 1. Ohio University, USA

**3:00 PM**

##### **(GOMD-S3-027-2016) Gap engineering using Hellmann-Feynman forces: method and applications**

K. Prasai<sup>\*1</sup>; P. Biswas<sup>2</sup>; D. Drabold<sup>1</sup>; 1. Ohio University, USA; 2. The University of Southern Mississippi, USA

**3:20 PM**

Break

#### Session 1: Electronic Conducting Materials II

Room: University A/B

Session Chair: Partha Biswas, The University of Southern Mississippi

**3:40 PM**

##### **(GOMD-S3-028-2016) Advanced electronic quality of narrow-gap amorphous silicon-germanium (Invited)**

R. E. Schropp<sup>\*1</sup>; Y. Kuang<sup>1</sup>; L. W. Veldhuizen<sup>1</sup>; 1. Eindhoven University of Technology (TU/e), Netherlands

**4:10 PM**

##### **(GOMD-S3-029-2016) The amorphous structure of prototypical phase change materials revisited: New first-principles molecular dynamics insights (Invited)**

A. Bouzid<sup>\*1</sup>; 1. Institut de physique et chimie des matériaux de Strasbourg, France

**4:40 PM**

##### **(GOMD-S3-030-2016) Force-enhanced Atomic Refinement (FEAR): A structural modeling technique for disordered and glassy materials**

A. Pandey<sup>\*1</sup>; P. Biswas<sup>2</sup>; D. Drabold<sup>1</sup>; 1. Ohio University, USA; 2. The University of Southern Mississippi, USA

### Symposium 4: Glass Technology and Cross-Cutting Topics

#### Session 4: Glass Corrosion: Mechanisms and Rate II

Room: Capitol B

Session Chairs: Eric Pierce, Oak Ridge National Lab; Stephane Gin, CEA

**1:20 PM**

##### **(GOMD-S4-045-2016) Interfacial behavior and dissolution gel structures of silicate glasses from ReaxFF and ab initio based computer simulations**

J. M. Rimsza<sup>\*1</sup>; J. Du<sup>1</sup>; 1. The University of North Texas, USA

**1:40 PM**

##### **(GOMD-S4-046-2016) Composition and Structural Trends in Static Corrosion of Calcium Aluminosilicate Glasses**

N. J. Smith<sup>\*1</sup>; R. Schaut<sup>1</sup>; J. Hamilton<sup>1</sup>; J. Klotz<sup>2</sup>; E. Bakowska<sup>3</sup>; A. Li<sup>1</sup>; K. Murphy<sup>1</sup>; 1. Corning Incorporated, USA

**2:00 PM**

##### **(GOMD-S4-047-2016) Topological Control on Silicates Dissolution Kinetics**

I. Pignatelli<sup>1</sup>; A. Kumar<sup>1</sup>; B. Wang<sup>\*1</sup>; M. Bauchy<sup>1</sup>; G. Sant<sup>1</sup>; 1. University of California, Los Angeles, USA

#### Session 4: Glass Corrosion: Analytical Techniques

Room: Capitol B

Session Chairs: Jonathan Icenhower, Sandia National Laboratories; S. Sundaram, Alfred University

**2:20 PM**

##### **(GOMD-S4-048-2016) Towards an Understanding of Surface Layer Formation, Growth, and Transformation at the Glass-Fluid Interface**

J. Hopf<sup>1</sup>; J. R. Eskelsen<sup>1</sup>; D. N. Leonard<sup>1</sup>; E. M. Pierce<sup>\*1</sup>; 1. Oak Ridge National Lab, USA

**2:40 PM**

##### **(GOMD-S4-049-2016) The influence of transition metal oxides induced absorption on LEAP detection efficiency and its glass alteration behaviors of ISG glasses**

X. Lu<sup>\*1</sup>; D. Schreiber<sup>2</sup>; J. Neeway<sup>2</sup>; J. Ryan<sup>2</sup>; J. Du<sup>1</sup>; 1. University of North Texas, USA; 2. Pacific Northwest National Lab, USA

**3:00 PM**

##### **(GOMD-S4-050-2016) Nanoscale Imaging of Li and B in Nuclear Waste Glass using APT, ToF-SIMS, and NanoSIMS**

Z. Zhu<sup>\*1</sup>; Z. Wang<sup>1</sup>; J. Liu<sup>1</sup>; J. Neeway<sup>1</sup>; D. Schreiber<sup>1</sup>; J. V. Crum<sup>1</sup>; J. Ryan<sup>1</sup>; F. Wang<sup>2</sup>; 1. Pacific Northwest National Laboratory, USA; 2. Institute of Chemistry, Chinese Academy of Sciences, China

### Symposium 5: Festschrift for Professor Donald R. Uhlmann

#### Gels and Applications

Room: Madison

Session Chair: Lisa Klein, Rutgers University

**1:20 PM**

##### **(GOMD-S5-009-2016) How I took Don's Advice and Signed up for Organic Chemistry (Invited)**

L. C. Klein<sup>\*1</sup>; 1. Rutgers University, USA

**1:50 PM**

##### **(GOMD-S5-010-2016) Strong gels and glass science (Invited)**

P. Calvert<sup>\*1</sup>; 1. NMT, USA

**2:20 PM****(GOMD-S5-011-2016) Fibers and Non-Wovens from Long Carbon Nanotubes: A Model for Extended Chain Polymers Process, Structure and Applications (Invited)**M. Jaffe\*<sup>1</sup>; 1. New Jersey Institute of Technology, USA**2:50 PM****(GOMD-S5-012-2016) From random glass networks to random silica gel networks and their use as host for biocatalytic applications (Invited)**A. C. Pierre\*<sup>1</sup>; 1. Retired, Université Claude Bernard Lyon 1, France**3:20 PM****Break****Legacy**

Room: Madison

Session Chair: Lisa Klein, Rutgers University

**3:40 PM****(GOMD-S5-013-2016) A Novel Cancer Therapy Utilizing Alternating Electric Fields Delivered via Lead Magnesium Niobate - Lead Titanate Transducers**W. F. Doyle\*<sup>1</sup>; 1. Novocure Ltd., USA**4:00 PM****(GOMD-S5-014-2016) Review of Anti-Reflection Sol-Gel Coatings in High Energy Lasers**T. I. Suratwala\*<sup>1</sup>; 1. Lawrence Livermore National Laboratory, USA**4:20 PM****(GOMD-S5-015-2016) Glass formation, crystallization, and Don (Invited)**J. McCloy\*<sup>1</sup>; 1. Washington State University, USA**Wednesday, May 25, 2016****Varshneya Frontiers of Glass Science Lecture**

Room: Madison

**8:00 AM****(GOMD-AW-004-2016) Multiscale investigation of stress-corrosion crack propagation mechanisms in oxide glasses (Invited)**M. Ciccotti\*<sup>1</sup>; 1. ESPCI, France**9:00 AM****Break****Symposium 1: Fundamentals of the Glassy State****Session 1: Glass Formation and Relaxation III**

Room: Capitol A

Session Chair: Ozgur Gulbiten, Corning Incorporated

**9:20 AM****(GOMD-S1-048-2016) Linking Equilibrium and Nonequilibrium Dynamics in Glass-Forming Systems**J. C. Mauro\*<sup>1</sup>; X. Guo<sup>1</sup>; M. M. Smedskjaer<sup>2</sup>; 1. Corning Incorporated, USA; 2. Aalborg University, Denmark**9:40 AM****(GOMD-S1-049-2016) Viscosity for low alkali binary silicate melts**J. Wu\*<sup>1</sup>; 1. Corning Incorporated, USA**10:00 AM****(GOMD-S1-050-2016) Near-Tg and sub-Tg structural relaxation in window glass: precise experiment vs. known models**A. Priven\*<sup>1</sup>; 1. Corning Korea, Republic of Korea**10:20 AM****(GOMD-S1-051-2016) Preparing organic glasses with high kinetic stability via physical vapor deposition: Role molecular structure**M. Tyllinski\*<sup>1</sup>; M. Beasley<sup>1</sup>; Y. Chua<sup>2</sup>; C. Schick<sup>2</sup>; M. D. Ediger<sup>1</sup>; 1. University of Wisconsin - Madison, USA; 2. University of Rostock, Germany**10:40 AM****(GOMD-S1-052-2016) Effect of network structure on the mixed cation phenomenon in lithium-calcium borosilicate glasses**Y. Shih\*<sup>1</sup>; J. Jean<sup>1</sup>; 1. National Tsing Hua University, Taiwan**11:00 AM****(GOMD-S1-053-2016) Silica network modification during multicomponent diffusion in the soda-lime glass**E. Burov\*<sup>1</sup>; E. Gouillart<sup>1</sup>; W. Woelffel<sup>1</sup>; M. Toplis<sup>2</sup>; 1. Saint-Gobain, France; 2. Observatoire Midi-Pyrénées, France**Session 3: Scattering Techniques**

Room: Capitol B

Session Chair: Paul Voyles, University of Wisconsin

**9:20 AM****(GOMD-S1-054-2016) Local density changes of deformed metallic glasses (Invited)**V. Schmidt\*<sup>1</sup>; H. Rösner<sup>1</sup>; M. Peterlechner<sup>1</sup>; P. Voyles<sup>2</sup>; G. Wilde<sup>1</sup>; 1. University of Münster, Germany; 2. University of Wisconsin, USA**9:50 AM****(GOMD-S1-055-2016) Isotope substitution neutron scattering of MgTiO<sub>3</sub> in the stable liquid supercooled liquid and crystalline state**J. Neuefeind\*<sup>1</sup>; C. J. Benmore<sup>2</sup>; R. Weber<sup>3</sup>; O. L. Alderman<sup>3</sup>; L. Skinner<sup>3</sup>; 1. Oak Ridge National Lab, USA; 2. Argonne National Lab, USA; 3. Materials Development, USA**10:10 AM****(GOMD-S1-056-2016) Local structural changes on melting and glass formation in alkali-free titanates**O. L. Alderman\*<sup>1</sup>; C. J. Benmore<sup>2</sup>; S. Heald<sup>2</sup>; M. Wilding<sup>4</sup>; S. Sendelbach<sup>1</sup>; A. Tamaloni<sup>1</sup>; J. B. Parise<sup>3</sup>; R. Weber<sup>3</sup>; 1. Materials Development Inc., USA; 2. Argonne National Lab, USA; 3. Stony Brook University, USA; 4. University of Bath, United Kingdom**10:30 AM****(GOMD-S1-057-2016) Structure of lithium germanate glasses by neutron diffraction with isotopic substitution**A. C. Hannon\*<sup>1</sup>; 1. ISIS Facility, United Kingdom**10:50 AM****(GOMD-S1-058-2016) Combining X-ray Scattering and Optical Techniques to Characterize the Structure of Organic Glasses formed by Physical Vapor Deposition**A. Gujral\*<sup>1</sup>; J. Jiang<sup>1</sup>; J. Gomez<sup>1</sup>; D. M. Walters<sup>1</sup>; C. Huang<sup>1</sup>; K. A. O'Hara<sup>2</sup>; M. F. Toney<sup>3</sup>; L. Yu<sup>1</sup>; M. L. Chabiny<sup>2</sup>; M. D. Ediger<sup>1</sup>; 1. University of Wisconsin, USA; 2. University of California, Santa Barbara, USA; 3. Stanford Synchrotron Radiation Lightsource, USA**11:10 AM****(GOMD-S1-059-2016) Subsurface structure of soda lime float glass and thermodynamics of water-glass interactions studied with vibrational sum frequency generation (SFG) spectroscopy**J. Luo\*<sup>1</sup>; J. Banerjee<sup>1</sup>; C. G. Pantano<sup>1</sup>; S. H. Kim<sup>1</sup>; 1. Pennsylvania State University, USA

## Session 4: First Principles Methods and ab initio MD Simulations of Glasses

Room: University C/D

Session Chairs: Jincheng Du, University of North Texas; Carlo Massobrio, CNRS-IPCMS-UNR 7504

**9:20 AM**

### (GOMD-S1-060-2016) Second Generation Car-Parrinello-type Molecular Dynamics: Advantages and Disadvantages (Invited)

M. Boero\*; 1. University of Strasbourg and CNRS, France

**9:50 AM**

### (GOMD-S1-061-2016) Large Scale Simulation of Structure and Properties of Metal-Organic Frameworks Hybrid Glasses: ZIF-4 (Invited)

N. Li\*; 1. Wuhan University of Technology, China

**10:20 AM**

### (GOMD-S1-062-2016) Structure Modeling and Thermochemical Properties of Tantalum-Silica Glasses

I. Ponomarev<sup>1</sup>; A. Dasmahapatra<sup>2</sup>; P. Kroll<sup>1</sup>; 1. UT Arlington, USA

**10:40 AM**

### (GOMD-S1-063-2016) Computational Studies of the Glass Phase in Hydrogrossular Mineral Series

P. Adhikari\*; C. C. Dharmawardhana<sup>1</sup>; W. Ching<sup>1</sup>; 1. University of Missouri, Kansas City, USA

**11:00 AM**

### (GOMD-S1-064-2016) First Principles study of silicate glasses: interplay between structural and vibrational properties (Invited)

S. Ispas\*; D. A. Kilymis<sup>1</sup>; J. Delaye<sup>2</sup>; B. Hehlen<sup>1</sup>; 1. University of Montpellier, France; 2. CEA Marcoule, France

**11:30 AM**

### (GOMD-S1-065-2016) Electronic structures, interatomic bonding and physical properties of $\text{Si}_x\text{Ge}_{1-x}\text{O}_2$ glass ( $x = 0$ to 1)

K. Baral\*; P. Adhikari<sup>1</sup>; W. Ching<sup>1</sup>; 1. University of Missouri, Kansas City, USA

**11:50 AM**

### (GOMD-S1-066-2016) Structure Modeling and DFT Calculations of Hafnia Soda Silicate Glasses

I. Ponomarev\*; A. Dasmahapatra<sup>1</sup>; J. P. Nimmo<sup>1</sup>; P. Kroll<sup>1</sup>; 1. University of Texas, Arlington, USA

## Session 5: Mechanical Properties of Glasses III

Room: Wisconsin

Session Chair: Satoshi Yoshida, The University of Shiga Prefecture

**9:20 AM**

### (GOMD-S1-067-2016) Fracture-induced amorphization of polycrystalline $\text{SiO}_2$ stishovite: nanoscale transformation toughening in the hardest oxide (Invited)

N. Nishiyama\*; F. Wakai<sup>1</sup>; 1. Deutsches Elektronen-Synchrotron, Germany; 2. Tokyo Institute of Technology, Japan

**9:50 AM**

### (GOMD-S1-068-2016) Mechanical properties of hard oxide glasses prepared by a levitation technique (Invited)

A. Masuno\*; 1. The University of Tokyo, Japan

**10:20 AM**

### (GOMD-S1-069-2016) Surface indentation topometry and fracture behavior of $\text{Al}_2\text{O}_3$ - $\text{SiO}_2$ glasses with high cracking initiation load

G. A. Rosales Sosa\*; A. Masuno<sup>1</sup>; Y. Higo<sup>2</sup>; T. Ishikawa<sup>3</sup>; H. Inoue<sup>1</sup>; 1. The University of Tokyo, Japan; 2. Japan Synchrotron Radiation Research Institute, Japan; 3. Japan Aerospace Exploration Agency, Japan

**10:40 AM**

### (GOMD-S1-070-2016) New route to ultra-stiff glass material composition

Y. Yu\*; Z. Maw<sup>1</sup>; B. Wang<sup>1</sup>; M. Wang<sup>1</sup>; M. Bauchy<sup>1</sup>; 1. University of California, Los Angeles, USA

**11:00 AM**

### (GOMD-S1-071-2016) Calculating elastic moduli from composition

K. Philipps\*; R. Conrad<sup>1</sup>; 1. RWTH Aachen University, Institute of Mineral Engineering, Germany

**11:20 AM**

### (GOMD-S1-072-2016) Tribochemical Wear of Phosphate Laser Glass

J. Yu\*; 1. Southwest University of Science and Technology, China

**11:40 AM**

### (GOMD-S1-073-2016) In-situ observation of crack growth in LCD glass substrate during wheel scribing

N. Tomei\*; K. Murakami<sup>1</sup>; T. Fukunishi<sup>1</sup>; S. Yoshida<sup>2</sup>; J. Matsuoka<sup>2</sup>; 1. Mitsuboshi Diamond Industrial Co., Ltd, Japan; 2. The University of Shiga Prefecture, Japan

## Session 6: Carbide and Nitride Glasses

Room: Senate A/B

Session Chair: Tanguy Rouxel, Université de Rennes 1

**9:20 AM**

### (GOMD-S1-074-2016) High-Temperature Creep Behavior of $\text{SiO}_2$ Glasses and Glass Ceramics (Invited)

C. Stabler<sup>1</sup>; M. Narisawa<sup>2</sup>; M. Heilmaier<sup>3</sup>; H. Kleebe<sup>1</sup>; R. Riedel<sup>1</sup>; E. Ionescu\*; 1. Technical University Darmstadt, Germany; 2. Osaka Prefecture University, Japan; 3. Karlsruhe Institute of Technology, Germany

**9:50 AM**

### (GOMD-S1-075-2016) Silicon Oxycarbide Glasses: Synthesis, Structure and Properties (Invited)

G. Soraru\*; 1. University of Trento, Italy

**10:20 AM**

### (GOMD-S1-076-2016) Nitrogen rich oxynitride glasses – Difficulties and Opportunities (Invited)

S. Ali\*; 1. Linnæus University, Sweden

## Session 6: Metallic Glasses

Room: Senate A/B

Session Chair: Emanuel Ionescu, Technical University Darmstadt

**10:50 AM**

### (GOMD-S1-077-2016) An Alternative View on the Fundamental Structural Units in Bulk Metallic Glasses (Invited)

W. Ching\*; 1. University of Missouri-Kansas City, USA

**11:20 AM**

### (GOMD-S1-078-2016) Elastic properties and atomic bonding character in inorganic glasses: Metallic, oxide, and non-oxide

T. Rouxel\*; 1. University of Rennes 1, France

## Session 7: Synthesis, Structure and Properties of Glass under Extreme Conditions

Room: Madison

Session Chair: Mathieu Bauchy, University of California, Los Angeles

**9:20 AM**

### (GOMD-S1-079-2016) Structural changes in glass-forming silicates at high pressures, temperatures and extremes of composition: What's known and what's to be learned (Invited)

J. Stebbins\*; 1. Stanford University, USA

**9:50 AM**

### (GOMD-S1-080-2016) Anomalous dynamics during glass transition linked with rigidity properties (Invited)

M. Micoulaut\*; M. Bauchy<sup>1</sup>; 1. UPMC, France; 2. UCLA, USA

10:20 AM

**(GOMD-S1-081-2016) Chemical durability of 'forbidden' glasses: Separating the effects of glass structure and chemistry**

R. Schaut\*; S. Tietje; 1. Corning Incorporated, USA

10:40 AM

**(GOMD-S1-082-2016) Structure-Property Transformations in Oxide and Non-Oxide Glasses and Supercooled Liquids Subjected to Extreme Conditions (Invited)**

S. Sen\*; 1. UC Davis, USA

11:10 AM

**(GOMD-S1-083-2016) Glasses under compression and surface confinement (Invited)**

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

11:40 AM

**(GOMD-S1-084-2016) Raman spectroscopy of  $v$ -SiO<sub>2</sub> under rare gas compression**

C. Weigel; B. Hehlen; A. Polian; B. Rufflé; R. Vacher; M. Foret\*; 1. University of Montpellier, France; 2. University Paris 6, France

**Session 2: Fundamentals**

Room: Capitol A

Session Chair: Edgar Dutra Zanotto, Federal University of Sao Carlos

1:20 PM

**(GOMD-S1-085-2016) Role of structural relaxation in crystal nucleation kinetics (Invited)**

P. Gupta\*; D. R. Cassar; E. Dutra Zanotto; 1. Ohio State University, USA; 2. Federal University of Sao Carlos, Brazil

1:50 PM

**(GOMD-S1-086-2016) Synthesis of Nanostructures during Devitrification of Metallic Glass Alloys (Invited)**

J. H. Perepezko\*; Y. Shen; 1. University of Wisconsin, USA

2:20 PM

**(GOMD-S1-087-2016) The Investigation of the Nucleation Delay Time in Al-based Metallic Glasses by the High Rate Calorimetry**

Y. Shen\*; J. H. Perepezko; 1. University of Wisconsin-Madison, USA

2:40 PM

**(GOMD-S1-088-2016) Crystallization of nepheline (Na<sub>2</sub>O-Al<sub>2</sub>O<sub>3</sub>·2SiO<sub>2</sub>) based glasses – Impact of cation mixing**

A. Deshkar; J. Marcial; S. Southern; L. Kobera; D. Bryce; J. McCloy; A. Goel\*; 1. Rutgers University, USA; 2. University of Ottawa, Canada; 3. Washington State University, USA

3:00 PM

**(GOMD-S1-089-2016) Characterization of CMAS and CMAS-TiO<sub>2</sub> crystallization behavior from the melt for EBC applications**

R. Webster\*; E. Opila; 1. University of Virginia, USA

3:20 PM

Break

3:40 PM

**(GOMD-S1-090-2016) Nucleation Mechanisms Revealed by Molecular Dynamics Simulations (Invited)**

H. Fang; Y. Zhang; R. Newman; J. Kieffer\*; 1. University Of Michigan, USA

4:10 PM

**(GOMD-S1-091-2016) Crystallization of liquids and glasses: learning from molecular simulations (Invited)**

M. Micoulaut\*; 1. UPMC, France

4:40 PM

**(GOMD-S1-092-2016) Crystallization of molecular glasses: A central role for surface mobility (Invited)**

L. Yu\*; C. Powell; Y. Chen; W. Zhang; M. D. Ediger; 1. University of Wisconsin, USA

5:10 PM

**(GOMD-S1-093-2016) Fast Crystal Growth in Organic Glasses: A Possible Role for Fracture and Surface Mobility**

C. T. Powell\*; Y. Chen; M. D. Ediger; L. Yu; 1. University of Wisconsin-Madison, USA

5:30 PM

**(GOMD-S1-094-2016) Computational modeling of synthesis of amorphous serpentine from olivine: Implications for planetary water delivery and formation of hydrous minerals in the solar nebula**

A. Asaduzzaman; K. Muralidharan\*; J. Ganguly; 1. University of Arizona, USA

**Session 3: New Techniques and Applications**

Room: Capitol B

Session Chair: Dominique de Ligny, University Erlangen-Nürnberg

1:20 PM

**(GOMD-S1-095-2016) Atom-probe tomography in the glass sciences (Invited)**

J. Ryan\*; D. Schreiber; 1. Pacific Northwest National Lab, USA

1:50 PM

**(GOMD-S1-096-2016) Usable Strength of Glass - Surface Science Perspective**

N. Sheth; J. Luo; C. G. Pantano; S. H. Kim; 1. Pennsylvania State University, USA

2:10 PM

**(GOMD-S1-097-2016) Structural characterization of mirror coating for gravitational waves detection**

V. Martinez\*; C. Elodie; G. Massimo; M. Christine; V. Dolique; A. Mermet; G. Cagnoli; 1. ILM, France; 2. LMA, France

2:30 PM

**(GOMD-S1-098-2016) Densification Mechanisms in Vitreous Ge<sub>x</sub>Se<sub>1-x</sub>**

C. Yildirim\*; M. Micoulaut; J. Raty; 1. University Paris 6, France; 2. Université de Liège, Belgium

2:50 PM

**(GOMD-S1-099-2016) Tunable Molecular Orientation in Vapor-Deposited Molecular Glasses**

D. M. Walters\*; S. S. Dalal; N. D. Johnson; M. D. Ediger; 1. University of Wisconsin-Madison, USA

3:10 PM

Break

**Session 3: Optical and Vibrational Measurements**

Room: Capitol B

Session Chair: Mario Affatigato, Coe College

3:40 PM

**(GOMD-S1-100-2016) Structural Studies by Vibrational Spectroscopy of Glasses Based on Less-conventional Glass Formers: from Sulfates to Tungstates (Invited)**

D. Möncke\*; E. I. Kamitsos; 1. Friedrich-Schiller University Jena, Germany; 2. National Hellenic Research Foundation, Greece

4:10 PM

**(GOMD-S1-101-2016) Structural control of optical properties linked to transition elements in borate glasses**

G. Calas\*; N. Capobianco; L. Cormier; L. Galois; M. Hunault; G. Lelong; 1. University P&amp;M Curie, Paris, France

4:30 PM

**(GOMD-S1-102-2016) Boson Mode, Topological Phases, Immiscibility Window, and Glass Structure in Ba-Borate glasses**

C. Holbrook\*; R. Chbeir; A. Czaja; P. Boolchand; 1. Air Force Research Lab, USA; 2. University of Cincinnati, USA

4:50 PM

**(GOMD-S1-103-2016) Structural modification of titanosilicate glasses with change of fictive temperature**D. Wenzel<sup>1</sup>; A. Veber<sup>1</sup>; M. Cicconi<sup>1</sup>; D. de Ligny<sup>1</sup>; 1. University Erlangen-Nürnberg, Germany**Session 4: Simulations of Chalcogenide and Metallic Glasses**

Room: University C/D

Session Chairs: Carlo Massobrio, CNRS-IPCMS-UNR 7504; Walter Kob, Laboratoire Charles Coulomb

1:20 PM

**(GOMD-S1-104-2016) Density functional/molecular dynamics simulations of functional chalcogenide materials (Invited)**J. Akola<sup>1</sup>; 1. Tampere University of Technology, Finland

1:50 PM

**(GOMD-S1-105-2016) Role of Van der Waals interactions in determining the structure of liquid tellurides**M. Micoulaut<sup>1</sup>; H. Flores-Ruiz<sup>1</sup>; A. Piarristeguy<sup>2</sup>; V. Coulet<sup>3</sup>; M. Johnson<sup>3</sup>; G. Cuello<sup>3</sup>; A. Pradel<sup>3</sup>; C. Bichara<sup>3</sup>; 1. UPMC, France; 2. Université Montpellier II, France; 3. Institut Laue Langevin, France; 4. Université Aix-Marseille, France

2:10 PM

**(GOMD-S1-106-2016) Atomic scale modeling of glassy chalcogenide surfaces: insights into their adsorption and gas separation properties (Invited)**G. Ori<sup>1</sup>; B. Coasne<sup>2</sup>; M. Boero<sup>1</sup>; C. Massobrio<sup>1</sup>; 1. IPCMS / CNRS - University of Strasbourg, France; 2. Laboratoire Interdisciplinaire de Physique, France

2:40 PM

**(GOMD-S1-107-2016) Properties of Vapor Deposited CuZrAl Glasses from Molecular Dynamics Simulations**G. Bokas<sup>1</sup>; I. Szlufarska<sup>1</sup>; 1. University of Wisconsin-Madison, USA

3:00 PM

**(GOMD-S1-108-2016) On the role of Sm in solidification process of Al-Sm metallic glasses**L. Zhao<sup>1</sup>; G. Bokas<sup>1</sup>; I. Szlufarska<sup>1</sup>; 1. University of Wisconsin - Madison, USA**Session 5: Mechanical Properties of Glasses IV**

Room: Wisconsin

Session Chair: Timothy Gross, Corning Incorporated

1:20 PM

**(GOMD-S1-109-2016) Deformation mechanisms in silica glass under hydrostatic conditions and underneath an indentation imprint (Invited)**V. Keryvin<sup>1</sup>; J. Guin<sup>2</sup>; J. Sangleboeuf<sup>3</sup>; L. Charleux<sup>3</sup>; 1. University of South Brittany, France; 2. University of Rennes 1, France; 3. University of Savoie Mont-Blanc, France

1:50 PM

**(GOMD-S1-110-2016) Perfectly plastic flow in silica glass**G. Kermouche<sup>2</sup>; G. Guillonnet<sup>3</sup>; J. Michler<sup>4</sup>; J. Teisseire<sup>5</sup>; E. Barthel<sup>1</sup>; 1. CNRS/ESPCI, France; 2. EMSE, France; 3. ECL, France; 4. Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland; 5. SVI, France

2:10 PM

**(GOMD-S1-111-2016) Mapping between atomistic simulations and Eshelby inclusions in the shear deformation of amorphous Silicon**F. Boioli<sup>1</sup>; T. Albaret<sup>1</sup>; D. Rodney<sup>1</sup>; 1. ILM, University of Lyon 1, France

2:30 PM

**(GOMD-S1-112-2016) Nano-Ductility in Silicate Glasses is Driven by Topological Heterogeneity**B. Wang<sup>1</sup>; Y. Yu<sup>1</sup>; M. Wang<sup>1</sup>; J. C. Mauro<sup>1</sup>; M. Bauchy<sup>1</sup>; 1. University of California, Los Angeles, USA; 2. Corning Incorporated, USA

2:50 PM

**(GOMD-S1-113-2016) Mechanoluminescence in a transparent glass composite (Invited)**Y. Gueguen<sup>1</sup>; M. Dubernet<sup>1</sup>; F. Célerié<sup>1</sup>; P. Houizot<sup>1</sup>; J. Sangleboeuf<sup>1</sup>; T. Rouxel<sup>1</sup>; 1. Institut de Physique de Rennes UMR UR1-CNRS 6251, France

3:20 PM

Break

**Session 5: Mechanical Properties of Glasses V**

Room: Wisconsin

Session Chair: Yann Gueguen, Institut de Physique de Rennes UMR UR1-CNRS 6251

3:40 PM

**(GOMD-S1-114-2016) Crack nucleation criterion and its application to impact indentation in oxide glasses**J. Luo<sup>1</sup>; K. Vargheese<sup>1</sup>; A. Tandia<sup>1</sup>; G. Hu<sup>1</sup>; J. C. Mauro<sup>1</sup>; 1. Corning Incorporated, USA

4:00 PM

**(GOMD-S1-115-2016) Compositional Dependence of Indentation-Induced Residual Stresses of Sodium Aluminosilicate Glasses**K. Yoshida<sup>1</sup>; S. Yoshida<sup>1</sup>; A. Yamada<sup>1</sup>; J. Matsuoka<sup>1</sup>; A. Errapart<sup>1</sup>; V. Pukhkaya<sup>1</sup>; J. Teisseire<sup>2</sup>; E. Barthel<sup>3</sup>; C. R. Kurkjian<sup>4</sup>; 1. The University of Shiga Prefecture, Japan; 2. Surface du Verre et Interfaces - CNRS / Saint-Gobain, France; 3. Science and Engineering of Soft Matter, UPMC / CNRS / ESPCI PPMU UMR 7615, France; 4. Rutgers University, USA; 5. Trenz Electronic GmbH, Germany

4:20 PM

**(GOMD-S1-116-2016) Mechanism and prediction of removal rate and surface roughness creation during optical polishing of glasses**T. I. Suratwala<sup>1</sup>; W. A. Steele<sup>1</sup>; M. D. Feit<sup>1</sup>; L. L. Wong<sup>1</sup>; N. Shen<sup>1</sup>; R. J. Dylla-Spears<sup>1</sup>; P. E. Miller<sup>1</sup>; R. P. Desjardins<sup>1</sup>; S. Elhadji<sup>1</sup>; 1. Lawrence Livermore National Laboratory, USA

4:40 PM

**(GOMD-S1-117-2016) Void Structure and Mechanical Properties of Corona-Discharged Glasses**M. Ono<sup>1</sup>; K. Uraji<sup>1</sup>; T. Sekine<sup>1</sup>; T. Suzuki<sup>1</sup>; K. Ito<sup>1</sup>; M. Miyai<sup>2</sup>; M. Fujinami<sup>3</sup>; S. Ito<sup>1</sup>; 1. Asahi Glass Company, Japan; 2. National Institute of Advanced Industrial Science and Technology (AIST), Japan; 3. Chiba University, Japan

5:00 PM

**(GOMD-S1-118-2016) Effect of salt impurities on the chemical strengthening of float glass by ion-exchange**V. M. Sglavo<sup>1</sup>; H. Hassani<sup>1</sup>; 1. University of Trento, Italy

5:20 PM

**(GOMD-S1-119-2016) Sequential Electric Field Assisted Ion Exchange: Engineered Stress Profile Glasses**A. Talimian<sup>1</sup>; V. M. Sglavo<sup>1</sup>; 1. Università degli Studi di Trento, Italy**Session 6: Chalcogenide Glasses I**

Room: Senate A/B

Session Chair: Pierre Lucas, Univ of Arizona

1:20 PM

**(GOMD-S1-120-2016) Ga-Sb-S Chalcogenide Glasses and Their Applications in the Mid-infrared (Invited)**Z. Yang<sup>1</sup>; A. Yang<sup>1</sup>; M. Zhang<sup>1</sup>; J. Qiu<sup>1</sup>; L. Li<sup>1</sup>; Y. Wang<sup>1</sup>; B. Zhang<sup>1</sup>; D. Tang<sup>1</sup>; 1. Jiangsu Normal University, China

1:50 PM

**(GOMD-S1-121-2016) Statistics of Selenium Chain Length Distribution in Ge<sub>x</sub>Se<sub>100-x</sub> glassy alloys: Unique Insights from NMR spectroscopy**D. C. Kaseman<sup>1</sup>; S. Sen<sup>1</sup>; 1. University of California Davis, USA

2:10 PM

**(GOMD-S1-122-2016) Relying on localized orbitals to understand structural features in chalcogenide glasses**A. Bouzid<sup>1</sup>; G. Ori<sup>1</sup>; M. Boero<sup>1</sup>; 1. Institut de physique et chimie des matériaux de Strasbourg, France

2:30 PM

**(GOMD-S1-123-2016) Synthesis and Characterization of Cs<sup>+</sup> Ion Conducting Gallo-Germanium Selenide Glasses**A. Whale\*; S. W. Martin<sup>1</sup>; 1. Iowa State University, USA

2:50 PM

**(GOMD-S1-124-2016) The Mixed Glass Former Effect in Glassy Solid State Electrolytes: The Physical Properties of the 0.5Na<sub>2</sub>S + 0.5[xSiS<sub>2</sub> + (1-x) PS<sub>5/2</sub>] glass system**D. Watson\*; S. W. Martin<sup>1</sup>; 1. Iowa State University, USA

3:10 PM

Break

**Session 6: Chalcogenide Glasses II**

Room: Senate A/B

Session Chair: Pierre Lucas, Univ of Arizona

3:40 PM

**(GOMD-S1-125-2016) Structure of binary Si-Se alloys: Results from one- and two-dimensional <sup>29</sup>Si and <sup>77</sup>Se NMR spectroscopy**M. A. Marple\*; I. Hung<sup>2</sup>; Z. Gan<sup>2</sup>; S. Sen<sup>1</sup>; 1. University of California Davis, USA; 2. National High Magnetic Field Laboratory, USA

4:00 PM

**(GOMD-S1-126-2016) Thermophysical Properties of As<sub>x</sub>Se<sub>1-x</sub> Glasses from x=0.2 to 0.5**J. M. Lonergan\*; C. Smith<sup>1</sup>; D. McClane<sup>1</sup>; K. Richardson<sup>1</sup>; 1. University of Central Florida, USA**Session 7: Response of Glass to Extreme Conditions**

Room: Madison

Session Chair: Randall Youngman, Corning Incorporated

1:20 PM

**(GOMD-S1-127-2016) Elastic Deformations and Structural Metrics in Chain-Like Amorphous Polymers (Invited)**A. Bielawski<sup>1</sup>; E. Woeltdgen<sup>1</sup>; J. Kieffer\*; 1. University Of Michigan, USA

1:50 PM

**(GOMD-S1-128-2016) Control of stability and molecular orientation in organic glasses (Invited)**

M. D. Ediger\*; 1. University of Wisconsin-Madison, USA

2:20 PM

**(GOMD-S1-129-2016) Annealing Effects in Sodium Silicate Glass around glass transition temperature and heterogeneous dynamics**Y. P. Vaills\*; M. Naji<sup>2</sup>; 1. CEMHTI - CNRS, France; 2. Institute for Transuranium Elements, Germany

2:40 PM

**(GOMD-S1-130-2016) Anomalies in Aging Behaviors of Supercooled Sodium Silicate Liquid under Pressure**D. Zhang<sup>1</sup>; B. Wang\*; M. Bauchy<sup>1</sup>; 1. University of California, Los Angeles, USA

3:00 PM

**(GOMD-S1-131-2016) Thermophysical Properties of Aerolevitated Glasses**I. Sorenson\*; B. Bailey<sup>1</sup>; M. Welninski<sup>1</sup>; S. Feller<sup>1</sup>; M. Affatigato<sup>1</sup>; 1. Coe College, USA

3:20 PM

Break

**Session 7: Characterization of Glass under Extreme Conditions I**

Room: Madison

Session Chair: Yann Vaills, CNRS-CEMHTI

3:40 PM

**(GOMD-S1-132-2016) Raman scattering in extreme conditions of high temperature and irradiation (Invited)**P. Simon\*; E. Fotsio Gueutue<sup>1</sup>; A. Canizares<sup>1</sup>; M. Ammar<sup>1</sup>; F. Duval<sup>1</sup>; Y. P. Vaills<sup>1</sup>; N. Raimboux<sup>1</sup>; M. Dutreilh-Colas<sup>2</sup>; R. Mohun<sup>3</sup>; L. Desgranges<sup>3</sup>; C. Jegou<sup>4</sup>; 1. CNRS-CEMHTI, France; 2. CNRS—Univ. Limoges-SPCTS, France; 3. CEA/DEN/DEC, France; 4. CEA/DEN/DTCDC, France

4:10 PM

**(GOMD-S1-133-2016) Temperature driven structural changes between oxide glasses and melts (Invited)**L. Cormier\*; G. Lelong<sup>1</sup>; L. Hennet<sup>2</sup>; 1. UPMC - CNRS, France; 2. CNRS, UPR 3049, France

4:40 PM

**(GOMD-S1-134-2016) Laser shock-induced spall and the intrinsic strength of glass**

M. J. Davis\*; 1. SCHOTT North America, Inc., USA

5:00 PM

**(GOMD-S1-135-2016) High Temperature Chalcogenide Glasses for Infrared Fiber Sensing in Advanced Small Modular Reactors**J. Roth\*; S. W. Martin<sup>1</sup>; J. Ballato<sup>2</sup>; A. Qiao<sup>2</sup>; 1. Iowa State University, USA; 2. Pacific Northwest National Lab, USA; 3. Clemson University, USA

5:20 PM

**(GOMD-S1-136-2016) Assessment of graveling impact phenomenon on helicopter glass windshields**G. Langevin\*; J. Sangleboeuf<sup>1</sup>; A. Perret<sup>1</sup>; 1. University of Rennes 1, France; 2. Airbus Helicopters, France**Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications****Session 5: Glass-Ceramics and Optical Ceramics I**

Room: University C/D

Session Chair: HeeDong Lee, UES, Inc.

3:40 PM

**(GOMD-S3-031-2016) Challenges Towards Transparent Oxide Ceramics (Invited)**

H. Lee\*; 1. UES, Inc., USA

4:10 PM

**(GOMD-S3-032-2016) Toughening of Transparent Magnesium Aluminate Spinel by Dissolution/Precipitation of Alumina (Invited)**A. Miller\*; W. Miao<sup>2</sup>; I. Reimanis<sup>1</sup>; 1. Colorado School of Mines, USA; 2. Corning, Incorporated, USA

4:40 PM

**(GOMD-S3-033-2016) Effect of Surface Roughness of Polycrystalline Ceramic Fiber on Scattering Loss**H. Kim\*; N. Usechak<sup>2</sup>; A. M. Urbas<sup>2</sup>; K. N. Shugart<sup>1</sup>; D. P. Brown<sup>1</sup>; B. Griffin<sup>1</sup>; R. S. Hay<sup>2</sup>; 1. AFRL & UES, USA; 2. Air Force Research Lab, USA

5:00 PM

**(GOMD-S3-034-2016) Study on Sintering of Calcium Fluoride Transparent Optical Materials**V. Veerapandiyani<sup>1</sup>; Y. Li<sup>1</sup>; Y. Wu\*; 1. Alfred University, USA

## Thursday, May 26, 2016

### Varshneya Frontiers of Glass Technology Lecture

Room: Madison

8:00 AM

#### (GOMD-AW-005-2016) Chemically Strengthened Glasses and Glass-Ceramics (Invited)

M. Dejneka\*; 1. Corning Incorporated, USA

9:00 AM

Break

### Symposium 1: Fundamentals of the Glassy State

#### Session 2: Glass-Ceramics

Room: Capitol A

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

9:20 AM

#### (GOMD-S1-137-2016) Glass ceramics as high temperature stable oxide thermoelectric materials (Invited)

M. Letz\*; J. Lingner<sup>1</sup>; 1. SCHOTT AG, Germany

9:50 AM

#### (GOMD-S1-138-2016) Strong and Tough Glass-ceramics for Emerging Markets (Invited)

Q. Fu\*; G. Beall<sup>1</sup>; C. Smith<sup>1</sup>; R. Youngman<sup>1</sup>; B. Wheaton<sup>1</sup>; O. Gulbitten<sup>1</sup>; 1. Corning Incorporated, USA

10:20 AM

#### (GOMD-S1-139-2016) Microstructural Evolution of Conductive WTi Phosphate Glass-Ceramics

B. Aitken\*; L. Moore<sup>1</sup>; I. Dutta<sup>1</sup>; 1. Corning Incorporated, USA

10:40 AM

#### (GOMD-S1-140-2016) Synthesis of afterglow glass-ceramics with SrAl<sub>2</sub>O<sub>4</sub> from SrO-Al<sub>2</sub>O<sub>3</sub> supercooling melt

K. Shinozaki\*; M. Kotaka<sup>1</sup>; T. Honma<sup>1</sup>; M. Affatigato<sup>2</sup>; T. Komatsu<sup>1</sup>; 1. Nagaoka University of Technology, Japan; 2. Coe College, USA

11:00 AM

#### (GOMD-S1-141-2016) Formation of Li<sub>1+x</sub>M<sub>x</sub>Ge<sub>y</sub>Ti<sub>2-x-y</sub>(PO<sub>4</sub>)<sub>3</sub> glasses with NZP stoichiometry and Li-ion conductivity of corresponding glass-ceramics

N. Lonnroth\*; B. Aitken<sup>1</sup>; 1. Corning Incorporated, USA

11:20 AM

#### (GOMD-S1-142-2016) In-situ Characterization of Conductive WTi Phosphate Glass-Ceramics

I. Dutta\*; B. Wheaton<sup>1</sup>; L. Moore<sup>1</sup>; B. Aitken<sup>1</sup>; G. Moore<sup>1</sup>; 1. Corning Incorporated, USA

11:40 AM

#### (GOMD-S1-143-2016) Silver Doped Lithium Disilicate Glass and Glass-Ceramics: Optical and Electrical Properties

S. Singh\*; S. Kundu<sup>1</sup>; P. Mattos<sup>1</sup>; A. Rodrigues<sup>1</sup>; E. Dutra Zanotto<sup>1</sup>; 1. Federal University of Sao Carlos, Brazil

12:00 PM

#### (GOMD-S1-144-2016) Influence of Al<sub>2</sub>O<sub>3</sub> and B<sub>2</sub>O<sub>3</sub> on sintering and crystallization of lithium silicate glass system

A. Gaddam\*; J. M. Ferreira<sup>1</sup>; 1. University of Aveiro, Portugal

### Session 7: Modeling of Glass under Extreme Conditions

Room: Madison

Session Chair: Benoit Ruffle, Montpellier University

9:20 AM

#### (GOMD-S1-145-2016) Densified Silica Glass Remembers Its Compression Pathway (Invited)

L. Huang\*; 1. Rensselaer Polytechnic Institute, USA

9:50 AM

#### (GOMD-S1-146-2016) Time-resolved in situ tomographic imaging of phase transformations in silicates (Invited)

E. Gouillart\*; E. Boller<sup>3</sup>; E. Burov<sup>1</sup>; W. Woelffel<sup>1</sup>; D. Bouttes<sup>1</sup>; D. Vandembroucq<sup>2</sup>; M. Toplis<sup>1</sup>; 1. Joint Unit CNRS/Saint-Gobain, France; 2. PMMH, ESPCI, France; 3. ESRF, France; 4. IRAP, France

10:20 AM

#### (GOMD-S1-147-2016) Constitutive Modeling of Glass Using Molecular Dynamics

V. Subramanian\*; S. Goyal<sup>1</sup>; 1. Corning Incorporated, USA

10:40 AM

#### (GOMD-S1-148-2016) Radiation-Induced Amorphization of Quartz: Insights from Rigidity Theory (Invited)

B. Wang<sup>1</sup>; Y. Yu<sup>1</sup>; M. Wang<sup>1</sup>; M. Bauchy\*; 1. University of California, Los Angeles, USA

11:10 AM

#### (GOMD-S1-149-2016) Pressure induced structural changes in Ca and Mg aluminosilicate glasses (MO/AL<sub>2</sub>O<sub>3</sub>≤1) recovered from 1-3 GPa: <sup>27</sup>Al MAS NMR studies

S. Bista\*; J. Stebbins<sup>1</sup>; 1. Stanford University, USA

11:30 AM

#### (GOMD-S1-150-2016) Influence of Network Topology on Ion-Exchange Strengthening of Glasses

M. Wang\*; Y. Yu<sup>1</sup>; B. Wang<sup>1</sup>; J. C. Mauro<sup>2</sup>; M. Bauchy<sup>1</sup>; 1. UCLA, USA; 2. Corning Incorporated, USA

### Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications

#### Session 3: Optical Materials for Components and Devices I

Room: Wisconsin

Session Chair: Pierre Lucas, Univ of Arizona

9:20 AM

#### (GOMD-S3-035-2016) Hydrothermal Synthesis and Characterization of 2D Nanomaterials for Optical Applications (Invited)

S. Whipkey<sup>1</sup>; Y. Liu<sup>1</sup>; Y. Wu\*; 1. Alfred University, USA

9:50 AM

#### (GOMD-S3-036-2016) High Anneal Point Rare Earth Aluminosilicates for Display Applications

M. Dejneka\*; C. L. Chapman<sup>1</sup>; 1. Corning Incorporated, USA

10:10 AM

#### (GOMD-S3-037-2016) Development of Germano-Gallate Glasses and Optical Fibers for Near- and Mid-Infrared Applications

T. Skopak\*; Y. Ledemi<sup>2</sup>; S. Morency<sup>2</sup>; M. Dussauze<sup>1</sup>; T. Cardinal<sup>1</sup>; E. Fargin<sup>1</sup>; Y. Messaddeq<sup>1</sup>; 1. Université de Bordeaux, France; 2. Université Laval, Canada

10:30 AM

#### (GOMD-S3-038-2016) Sol-Gel TiO<sub>2</sub> glass thin films for flexible cyto-compatible photonics

L. Li\*; P. Zhang<sup>2</sup>; H. Lin<sup>3</sup>; S. Geiger<sup>1</sup>; A. Zerdoum<sup>1</sup>; Y. Liu<sup>1</sup>; N. Xiao<sup>1</sup>; O. Ogbuu<sup>1</sup>; Q. Du<sup>3</sup>; X. Jia<sup>1</sup>; J. Hu<sup>3</sup>; 1. University of Delaware, USA; 2. Tianjin University, China; 3. Massachusetts Institute of Technology, USA

10:50 AM

**(GOMD-S3-039-2016) Role of metallic nanoparticles on the optical properties and luminescence intensities of rare earth doped tungsten phosphate glasses**M. Dousti\*; G. Poirier<sup>2</sup>; A. de Camargo<sup>1</sup>; 1. Universidade de São Paulo, Brazil, Brazil; 2. Instituto de Ciências e Tecnologia, Universidade Federal de Alfenas, Brazil

11:10 AM

**(GOMD-S3-040-2016) Micro-poling of a borosilicate glass employing laser-induced samarium absorption**A. Lepicard\*; T. Cardinal<sup>1</sup>; F. Adamietz<sup>2</sup>; V. Rodriguez<sup>3</sup>; K. Richardson<sup>3</sup>; M. Dussauze<sup>1</sup>; 1. University of Bordeaux, France; 2. ICMCB-CNRS, France; 3. University of Central Florida, USA

11:30 AM

**(GOMD-S3-041-2016) Substitution effect of ZnO on structure and properties in ZnO-SnO-P<sub>2</sub>O<sub>5</sub> glasses**A. Saitoh\*; Y. Hashida<sup>1</sup>; G. Tricot<sup>2</sup>; P. Freudenberger<sup>3</sup>; L. Ma<sup>3</sup>; R. Brow<sup>3</sup>; H. Takebe<sup>1</sup>; 1. Ehime University, Japan; 2. Université de Lille 1, France; 3. Missouri University of Science and Technology, USA**Session 5: Glass-Ceramics and Optical Ceramics II**

Room: University C/D

Session Chair: Yiquan Wu, Alfred University

9:20 AM

**(GOMD-S3-042-2016) Advanced Optical Materials for Next Generation EO/IR Sensors (Invited)**C. R. Baleine\*; A. Kirk<sup>1</sup>; S. Aiken<sup>1</sup>; C. Bungay<sup>1</sup>; S. Tuenge<sup>1</sup>; K. Richardson<sup>2</sup>; C. Smith<sup>2</sup>; L. Sisken<sup>2</sup>; T. Mayer<sup>2</sup>; A. Swisher<sup>2</sup>; M. Kang<sup>2</sup>; A. Pogrebnyakov<sup>2</sup>; C. G. Pantano<sup>3</sup>; 1. Lockheed Martin, USA; 2. University of Central Florida, USA; 3. Pennsylvania State University, USA

9:50 AM

**(GOMD-S3-043-2016) Thin film doped garnet materials and devices for monolithic on-chip optical isolation (Invited)**X. Sun<sup>2</sup>; Q. Du<sup>1</sup>; T. Goto<sup>3</sup>; M. Onbasli<sup>1</sup>; J. Hu\*<sup>1</sup>; C. Ross<sup>1</sup>; 1. Massachusetts Institute of Technology, USA; 2. Harbin Institute of Technology, China; 3. Toyohashi University of Technology, Japan

10:20 AM

**(GOMD-S3-044-2016) The Effects of Composition on the Refractive Index Change for GeSe<sub>2</sub>-As<sub>2</sub>Se<sub>3</sub>-PbSe Glass Ceramics**L. Sisken\*; C. Smith<sup>1</sup>; A. Buff<sup>1</sup>; B. Gleason<sup>2</sup>; K. Richardson<sup>1</sup>; 1. University of Central Florida, USA; 2. Clemson University, USA

10:40 AM

**(GOMD-S3-045-2016) Preparation of MgAl<sub>2</sub>O<sub>4</sub> Transparent Ceramic Mixed with phosphor by spark plasma sintering following by HIP sintering**Q. Huang\*; Q. Deng<sup>1</sup>; B. Han<sup>1</sup>; 1. Ningbo Institute of Material Technology and Engineering, Chinese Academy of Sciences, China

11:00 AM

**(GOMD-S3-046-2016) Conversion of ceramics into single crystals: grain boundary kinetics, impurity effects and space charge enhancement**Y. Liu\*; Y. Wu<sup>1</sup>; 1. Alfred University, USA

11:20 AM

**(GOMD-S3-047-2016) Spectral and laser properties of Yb:LuAG transparent ceramics fabricated by tape-casting method**Y. Cao\*; C. Ma<sup>1</sup>; 1. Renmin University of China, China**Symposium 4: Glass Technology and Cross-Cutting Topics****Session 2: Liquid Synthesis and Sol-gel-derived Materials I**

Room: Capitol B

Session Chair: John Kieffer, University Of Michigan

9:20 AM

**(GOMD-S4-051-2016) Building a Better Environment by Doing Things Porely (Invited)**

M. A. Anderson\*; 1. UW Madison (Retired Prof.), USA

9:50 AM

**(GOMD-S4-052-2016) Tuning the Bandgap of Nanoporous Glasses**M. Sundararajan\*; G. Chen<sup>1</sup>; 1. Ohio University, USA

10:10 AM

**(GOMD-S4-053-2016) Effect of Metal Nanoparticles on Melting Gels**L. C. Klein\*; S. Kallontzi<sup>1</sup>; L. Fabris<sup>1</sup>; A. Jitianu<sup>2</sup>; 1. Rutgers University, USA; 2. Lehman College, CUNY, USA

10:30 AM

**(GOMD-S4-054-2016) Solid-state electrolytes based on organically modified sol-gel derived silica networks**W. Wang\*; J. Kieffer<sup>1</sup>; 1. University of Michigan, USA

10:50 AM

**(GOMD-S4-055-2016) Branching and Fractal Structure in Ceramic Aggregates (Invited)**

G. Beaucage\*; 1. University of Cincinnati, USA

**Symposium 1: Fundamentals of the Glassy State****Session 7: Characterization of Glass under Extreme Conditions II**

Room: Madison

Session Chair: Patrick Simon, CNRS-CEMHTI

1:20 PM

**(GOMD-S1-151-2016) NMR Studies of Permanent Compression in Oxide Glasses (Invited)**R. Youngman\*; M. N. Svenson<sup>2</sup>; J. C. Mauro<sup>1</sup>; M. M. Smedskjaer<sup>2</sup>; 1. Corning Incorporated, USA; 2. Aalborg University, Denmark

1:50 PM

**(GOMD-S1-152-2016) Static vs dynamic compressibility of vitreous silica under pressure**C. Weigel<sup>1</sup>; B. Coasne<sup>2</sup>; A. Polian<sup>2</sup>; M. Foret<sup>1</sup>; R. Vacher<sup>1</sup>; B. Ruffle\*; 1. Montpellier University, France; 2. Université P. et M. Curie, France; 3. Joseph Fourier University, France

2:10 PM

**(GOMD-S1-153-2016) In-situ high pressure study of amorphous Ta<sub>2</sub>O<sub>5</sub> by Raman and Brillouin spectroscopies**V. Martinez\*; C. Elodie<sup>1</sup>; G. Massimo<sup>2</sup>; M. Christine<sup>1</sup>; V. Dolique<sup>2</sup>; G. Cagnoli<sup>2</sup>; A. Mermet<sup>1</sup>; 1. ILM, France; 2. LMA, France

2:30 PM

**(GOMD-S1-154-2016) Characterization of boron-aluminum substitution in lanthanum boroaluminosilicate glasses by Brillouin and NMR spectroscopy**A. Mabrouk\*; N. Pellerin<sup>1</sup>; Y. P. Vaills<sup>1</sup>; 1. University d'orleans, France



### **Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications**

#### **Session 3: Optical Materials for Components and Devices II**

Room: Wisconsin

Session Chair: Juejun Hu, Massachusetts Institute of Technology

**1:20 PM**

##### **(GOMD-S3-048-2016) Chalcogenide Glass-Based Sensors for Molecular Detection (Invited)**

P. Lucas\*; G. Coleman<sup>1</sup>; S. Jiang<sup>2</sup>; B. Bureau<sup>3</sup>; 1. University of Arizona, USA; 2. Advalue Photonics, USA; 3. University of Rennes, France

**1:50 PM**

##### **(GOMD-S3-049-2016) Mid-Infrared Methane Gas Sensing using Chalcogenide Glass on Silicon Platform**

Z. Han\*; P. Lin<sup>1</sup>; L. C. Kimerling<sup>1</sup>; A. Agarwal<sup>1</sup>; D. T. Tan<sup>2</sup>; 1. MIT, USA; 2. Singapore University of Technology and Design, Singapore; 3. Texas A&M University, USA

**2:10 PM**

##### **(GOMD-S3-050-2016) Development of micro-components for infrared integrated optics applications based upon Ge-Se-Te films (Invited)**

C. Vigreux<sup>1</sup>; A. Pradel\*; 1. universit  de Montpellier, France

**2:40 PM**

##### **(GOMD-S3-051-2016) Electro spraying of chalcogenide glass films to direct print gradient refractive index coating**

S. Novak\*; C. Li<sup>1</sup>; P. Lin<sup>2</sup>; C. Lumdee<sup>1</sup>; W. Deng<sup>3</sup>; P. G. Kik<sup>1</sup>; J. Hu<sup>2</sup>; A. Agarwal<sup>2</sup>; K. Richardson<sup>1</sup>; 1. University of Central Florida, USA; 2. Massachusetts Institute of Technology, USA; 3. Texas A&M University, USA; 4. Virginia Tech, USA

**3:00 PM**

##### **(GOMD-S3-052-2016) Influence of light flux and photon energy on photostructural evolution in thermally deposited As-S thin films**

J. R. Oelgoetz\*; J. Allen<sup>1</sup>; C. Thomas<sup>1</sup>; L. R. Nichols<sup>1</sup>; J. Buzek<sup>2</sup>; M. Vlcek<sup>2</sup>; R. Golovchak<sup>1</sup>; H. Jain<sup>3</sup>; A. Kovalskiy<sup>1</sup>; 1. Austin Peay State University, USA; 2. University of Pardubice, Czech Republic; 3. Lehigh University, USA

#### **Session 5: Glass-Ceramics and Optical Ceramics III**

Room: University C/D

Session Chair: Woohong (Rick) Kim, Naval Research Laboratory

**1:20 PM**

##### **(GOMD-S3-053-2016) Transparent Ceramics for Laser Materials (Invited)**

W. Kim\*; C. Baker<sup>1</sup>; G. Villalobos<sup>1</sup>; J. Frantz<sup>1</sup>; B. Shaw<sup>1</sup>; S. Bowman<sup>1</sup>; L. Busse<sup>1</sup>; S. Bayya<sup>1</sup>; M. Hunt<sup>1</sup>; B. Sadowski<sup>1</sup>; I. Aggarwal<sup>1</sup>; J. Sanghera<sup>1</sup>; 1. Naval Research Laboratory, USA; 2. Sotera Defense Solutions, USA

**1:50 PM**

##### **(GOMD-S3-054-2016) Fabrication of Re:YAG transparent ceramics for laser application (Invited)**

X. Chen<sup>1</sup>; T. Lu<sup>2</sup>; Y. Wu\*; J. Qi<sup>2</sup>; 1. Alfred University, USA; 2. Sichuan University, China

**2:20 PM**

##### **(GOMD-S3-055-2016) Fabrication of high-quality magneto-optical TAG transparent ceramics (Invited)**

S. Zhou\*; Y. Tang<sup>1</sup>; X. Yi<sup>1</sup>; D. Hao<sup>1</sup>; S. Zhang<sup>1</sup>; 1. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, China

**2:50 PM**

##### **(GOMD-S3-056-2016) Synthesis and Characterization of Calcium Lanthanum Sulfide using a Wet Chemistry Route**

Y. Li\*; Y. Wu<sup>1</sup>; 1. Alfred University, USA

**3:10 PM**

##### **(GOMD-S3-057-2016) Computed radiography at keV and MeV energies using glass-ceramic imaging plates**

R. L. Leonard<sup>1</sup>; A. Evans\*; A. Moses<sup>2</sup>; L. Arrowood<sup>2</sup>; A. Lubinsky<sup>3</sup>; J. Johnson<sup>1</sup>; 1. University of Tennessee Space Institute, USA; 2. Consolidated Nuclear Security, LLC, USA; 3. SUNY Stony Brook, USA

### **Symposium 4: Glass Technology and Cross-Cutting Topics**

#### **Session 2: Liquid Synthesis and Sol-gel-derived Materials II**

Room: Capitol B

Session Chair: Gregory Beaucage, University of Cincinnati

**1:20 PM**

##### **(GOMD-S4-056-2016) Sol-gel derived Yb:YAG ceramics for high-power thin disk lasers (Invited)**

R. M. Almeida\*; 1. Instituto Superior T cnico, ULisbon, Portugal

**1:50 PM**

##### **(GOMD-S4-057-2016) Collidal Silica Coatings for Textile Protection**

A. Chin<sup>1</sup>; N. Raiturcar<sup>1</sup>; L. C. Klein\*; 1. Rutgers University, USA

**2:10 PM**

##### **(GOMD-S4-058-2016) Boria Effects on High Temperature Silicon Carbide Oxidation: Comparison of Sol-Gel Derived and Thermally Grown Borosilicate Glass Films**

B. McFarland\*; E. Opila<sup>1</sup>; 1. University of Virginia, USA

**2:30 PM**

##### **(GOMD-S4-059-2016) Sol-Gel Synthesis and Characterization of Annealed Pyrolytic Graphite/Sodium Borosilicate Glass Composites**

K. E. Copenhaver\*; J. Nadler<sup>2</sup>; 1. Georgia Institute of Technology, USA; 2. Georgia Tech Research Institute, USA

**2:50 PM**

##### **(GOMD-S4-060-2016) Free Carbon embedded in Silicon Oxycarbide Glass: an Analysis of Experimental and Computational <sup>29</sup>Si NMR Data**

J. P. Nimmo<sup>1</sup>; P. Kroll\*; 1. The University of Texas at Arlington, USA

Monday, May 23, 2016

### Stookey Lecture of Discovery

Room: Madison

8:00 AM

#### (GOMD-AW-001-2016) The life and unexpected discoveries of an intrepid glass scientist (Invited)

D. L. Griscom<sup>\*1</sup>; 1. impactGlass research international, Mexico

Dave Griscom has been a glass physicist specializing in Electron Spin Resonance (ESR) since his 1996 Ph.D. He has advanced the state of the art in his 114 publications as first author. First came borate glasses, then lunar materials as Principle Investigator in the NASA Lunar Sample Program at the Naval Research Laboratory. His next foray treated Metal-Oxide-Semiconductor (MOS) issues, adding his ESR discoveries to those studying MOS by other methods. His greatest ESR discovery is what he termed “self-trapped holes” (STHs), created by irradiating pure silica glass at cryogenic temperatures. STHs have since been correlated with fictive temperature. His “homemade” optical spectrometer enabled simultaneous recording of the spectra of four different pure-silica-core fibers in factor-of-two intervals during continuous  $\gamma$ -irradiation from 10 seconds to 6 months, thereby discovering that the enormous attenuation peak near 1 hour later decreased monotonically ...going ever lower upon re-irradiation, thus “radiation hardening” them. Next he developed first- and second-order fractal kinetics in order to understand — and successively extrapolate! — the peculiar radiation-induced-attenuation growth curves of Ge-doped-silica-core fibers extensively recorded by others but never before understood. Dave also delved into impact geology, identifying significant deposits of quartz silt and ejecta from the Chesapeake Bay crater.

### Symposium 2: Larry L. Hench Memorial Symposium on Bioactive Glasses

#### Larry L. Hench Memorial Symposium on Bioactive Glasses I

Room: Wisconsin

Session Chairs: Julian Jones, Imperial College London; Ashutosh Goel, Rutgers University

9:30 AM

#### (GOMD-S2-001-2016) Tribute to Larry Hench: Educator, Scientist, Author (Invited)

D. E. Day<sup>\*1</sup>; 1. Missouri University of Science and Technology, USA

This brief tribute to Larry Hench traces (1) his illustrious professional career as an inspirational professor/educator at several prestigious universities, (2) his immensely important scientific discovery that certain glass compositions have the unique ability to bond to human bone and which led to what is now known through-out the world as Bioglass, and (3) his talent as a successful author of books for children (Boing-Boing the Bionic Cat). Over the past 45 years, thousands upon thousands of persons have benefited from Larry’s discovery that bioactive glasses can be used to repair damaged or diseased bones. His scientific contributions will continue to benefit mankind for years to come. What a success story, but it isn’t over. New medical applications for bioactive glasses continue to be found almost daily and their acceptance as a medical device continues to grow. Larry’s willingness to share his knowledge was well known and has inspired and attracted many young persons to the fields of Bioglass and Biomaterials. That is only one of the many enduring legacies that Larry leaves with us.

10:00 AM

#### (GOMD-S2-002-2016) Larry Hench: from Bioglass to Boing Boing and back again (Invited)

J. Jones<sup>\*1</sup>; 1. Imperial College London, United Kingdom

Larry Hench is best known for discovering Bioglass. In vivo studies showed 45S5 Bioglass bonds to bone faster, and encourages more bone growth, than other bioactive ceramics. In 1996, Larry arrived at Imperial College with the goal of finding out why his glass worked so well. He formed the Tissue Engineering and Regenerative Medicine Centre with Professor Dame Julia Polak to investigate the question. With PhD student Ioannis Xynos, and colleagues, they found that dissolution products stimulate bone cells at the genetic level, approved by the FDA as “osteostimulation”. This discovery has changed the mind-set again. Glasses can be used to deliver active ions for therapeutic benefit. As a student in Larry’s group in London, my role was to make 3D scaffolds out of the glasses, which led us to develop the sol-gel foaming process, producing the first bioactive glass scaffolds with open cell porosity similar to porous bone. Larry’s passion for science and his creativity led him to write fabulous children’s books: a series of adventures of Boing Boing the Bionic Cat. The concept of ions doing the work led to the development of toothpaste with Bioglass as the active ingredient. It is a privilege to try to continue his legacy at Imperial. Larry was more than a great supervisor and visionary. He was founder of fields, inspirer of people, a wonderful mentor, a gentle man and a great friend. His passing is a great loss to us all.

10:30 AM

#### (GOMD-S2-003-2016) Development of unique ceramic scaffolds for regeneration of large bone defects under load (Invited)

H. Zreiqat<sup>\*1</sup>; 1. University of Sydney, Australia

A challenge in bone tissue engineering is to treat large bone defects under load. A wide variety of 3D scaffolds of different structures and material properties has been reported in the literature for bone regeneration; however, these have struggled to meet the requirements for adequate pore geometry and bioactivity combined with the mechanical strength necessary for bone regeneration under load. We have developed the bioactive Sr-HT-Gahnite ceramic with combined requirements for bone regeneration under load. We used a 3D printing technology to fabricate glass-ceramic scaffolds with distinct pore geometries, which simultaneously display the properties of high mechanical strength and bone-like architecture. A particularly promising combination was Sr-HT Gahnite scaffolds with a hexagonal pore structure, which provided compressive strength of 110 MPa (comparable to cortical bone) at high porosity (70%) and interconnectivity (100%). Importantly, at similar porosity, the compressive strength recorded for our Sr-HT Gahnite scaffold with hexagonal geometry was higher than the values reported for polymeric and composite scaffolds by 150-fold, as well as ceramic and bioactive glass scaffolds (in clinical use or under development) by 5-fold. Such scaffolds opens avenues for treatment of load bearing bone defects in various clinical applications including orthopaedics, dental and maxillofacial.

11:00 AM

#### (GOMD-S2-004-2016) Additive manufacturing of highly bioactive and strong 3D porous alkali-free bioactive glass scaffolds for healthcare applications (Invited)

J. M. Ferreira<sup>\*1</sup>; A. Brito<sup>2</sup>; B. C. Silva<sup>1</sup>; A. C. Marques<sup>1</sup>; S. H. Olhero<sup>1</sup>;

1. University of Aveiro, Portugal; 2. Reg4life-Regeneration Technology, Portugal

An alkali-free bioactive glass composition, FastOs<sup>®</sup>BG (38.49% SiO<sub>2</sub> - 36.07% CaO - 19.24% MgO - 5.61% P<sub>2</sub>O<sub>5</sub> - 0.59% CaF<sub>2</sub>) belonging to the diopside (CaMgSi<sub>2</sub>O<sub>6</sub>)–fluorapatite (Ca<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>F)–tricalcium phosphate (Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>) system possesses a number of distinctive features, being promising for demanding applications in healthcare and tissue engineering. It exhibits fast in vitro biomineralization

and bonding ability to living tissues in vivo, and osteogenic properties that foster early cellular differentiation and proliferation. The purpose of the present study is to investigate the processing ability of this bioactive glass in aqueous media and obtaining high concentrated (up to 50 vol.% solids loading) inks for additive manufacturing. The effects of the type and amounts of the processing additives on the rheological properties of the fluid suspensions and on their transformation into extrudable pastes with enough stiffness for the cylindrical filaments to maintain the shape after extrusion, green and sintered properties were investigated. The excellent processing and sintering ability resulted in strong mechanical after sintering, essential for 3D porous scaffolds intended for bone regeneration and tissue engineering applications.

**11:30 AM**

**(GOMD-S2-005-2016) Characterization of Ag, Cu and Fe doped phosphate bioactive glasses**

A. Mishra\*<sup>1</sup>; J. Rocherullé<sup>2</sup>; J. Massera<sup>1</sup>; 1. Tampere University of Technology, Finland; 2. Université de Rennes I, France

Phosphate based glasses within the composition 50P2O5-20CaO-20SrO-10Na2O have been found to react in biological media and form a dicalcium phosphate di-hydrate (DCPD) layer at their surface upon immersion. However, the high phosphate content is responsible for the fast initial dissolution rate. As a consequence, human gingival fibroblasts cultured at their surface were found to have difficulties in attaching and proliferating during the first 3 days of culture. For longer immersion time the cells were found to proliferate at a rate similar to the typical silicate bioactive glass S53P4. In order to reduce the dissolution rate and confer additional properties to the glass, the base glass was doped with Ag, Cu or Fe. The newly obtained glasses were characterized in light of their thermal, structural and dissolution properties. DTA was used to measure the glass transition, onset of crystallization and crystallization peak temperatures, in order to assess if these glasses have potential for hot forming (scaffold sintering, fiber drawing). The in vitro bioactivity was studied by immersing the glass powders (particle size 125 - 200 µm) in TRIS buffer solution for various immersion time. Changes in glass structure, liquid chemical composition and the formation of a Ca-P layer were investigated using FTIR, ion chromatography and SEM-EDX, respectively.

**Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications**

**Session 2: Optical Fibers**

Room: Capitol A

Session Chair: Daniel Milanese, Politecnico di Torino

**9:20 AM**

**(GOMD-S3-001-2016) Novel Effects from Old Glasses in Next Generation Optical Fibers (Invited)**

J. Ballato\*<sup>1</sup>; P. Dragic<sup>2</sup>; 1. Clemson University, USA; 2. University of Illinois at Urbana-Champaign, USA

The global ubiquity and near-instantaneous nature of information today is owed to the remarkable successes of glass optical fibers. As new applications have emerged where optical fibers are again the enabling technology, practitioners have largely leveraged the manufacturing methods employed in telecommunications. While such processes are mature and highly scaled, they permit only a limited range of glass compositions that do not necessarily meet the performance demands of these new applications. This talk will highlight advances in silica-based optical fibers fabricated using the molten core approach which vastly expands the range of glass compositions that can be achieved. Particular attention will be paid to novel optical fibers that are either crystal-derived yet all-glass or gain their

performance from core/clad interactions in order to exhibit intrinsically low Brillouin and Raman gain, zero thermal dependence on Brillouin frequency, and enhanced upconversion.

**9:50 AM**

**(GOMD-S3-002-2016) Recent status of lightwave generation and processing using soft glass specialty optical fibers (Invited)**

Y. Ohishi\*<sup>1</sup>; T. Suzuki<sup>1</sup>; 1. Toyota Technological Institute, Japan

Highly nonlinear optical fibers have attracted much attention in recent years because they paved the way for the development of compact nonlinear devices for applications such as supercontinuum (SC) generation, wavelength conversion, pulse compression, parametric amplification, etc. Among nonlinear applications of highly nonlinear fibers, SC generation is attractive one. Studies on SC in optical fibers have been very active in recent years, because it has excellent properties, such as wide spectral bandwidth, high coherence, high brightness and potential compactness. For improving the applications of SC, continuous efforts to extend the SC spectral range to the mid-infrared (MIR) region have been made in the past several years. Fiber optical parametric amplification (FOPA) is another important application of the degenerate four wave mixing (DFWM). However, the potential of FOPA for soft glass highly nonlinear fibers have not yet been studied in details. We have fabricated microstructured optical fibers (MOF) made of tellurite and chalcogenide glass to control chromatic dispersion and shown that highly nonlinear soft glass MOFs are promising as mid-infrared SC generation and FOPA media. We report the present status and prospect of soft glass specialty optical fiber research.

**10:20 AM**

**(GOMD-S3-003-2016) Brillouin-related properties of novel alkaline earth oxide silicate glass optical fibers**

M. Cavillon\*<sup>1</sup>; J. Ballato<sup>2</sup>; P. Dragic<sup>2</sup>; C. Kucera<sup>1</sup>; T. Hawkins<sup>1</sup>; M. Jones<sup>1</sup>; 1. Clemson University, USA; 2. University of Illinois at Urbana-Champaign, USA

Stimulated Brillouin scattering (SBS) is a limitation in optical fiber telecommunication and high energy laser systems. In this work, material solutions to intrinsically low Brillouin gain optical fibers are developed. Specifically, alkaline earth oxides (AEO), such as BaO, SrO, CaO and MgO appear to be ideal dopants into silicate glasses due to their large negative Pockels' coefficient. However, in order to drastically lower Brillouin gain, the AEO has to be incorporated into the glass at relatively high concentrations (10 to 50 mol%), which is difficult due to tendencies in these glasses to phase separate. Accordingly, the molten core approach is employed as an effective method for realizing optical fibers from a very wide compositional range that could not otherwise be achieved using conventional processes. This work will provide a fundamental understanding of how the Group II oxides influence the properties of a silica-based optical fiber. Various physical and Brillouin-related properties of the AEO, such as the acoustic velocity, refractive index, mass density, thermo-optic and thermo-acoustic as well as strain-optic and strain-acoustic coefficients will be presented.

**10:40 AM**

**(GOMD-S3-004-2016) Bio-resorbable phosphate optical fibers for biophotonics**

D. Milanese\*<sup>1</sup>; E. Ceci-Ginistrelli<sup>1</sup>; N. Boetti<sup>2</sup>; J. Lousteau<sup>3</sup>; A. Ambrosone<sup>1</sup>; G. Novajra<sup>1</sup>; C. Vitale-Brovarone<sup>1</sup>; D. Pugliese<sup>1</sup>; 1. Politecnico di Torino, Italy; 2. Istituto Superiore Mario Boella, Italy; 3. University of Southampton, United Kingdom

Optical fibers are widely employed in biology and medicine because they allow minimally invasive procedures for diagnosis and therapy. In recent times, an emerging need of bioresorbable fibers has led to the exploration of several types of materials, mostly polymers and silk. This study aims to design and fabricate inorganic glass optical fibers able to combine optical functionalities and biocompatibility,

\*Denotes Presenter

together with bioresorbability. The core and cladding glasses were designed and fabricated by melt quenching. Glass thermal and optical characterizations were carried out in order to select the suitable core-cladding pair for the fabrication of the optical fibers. A dissolution test on single-material fibers was carried out to establish the solubility of the material in aqueous media. Core glasses were cast into rods, while the cladding glasses were obtained as tubes using the rotational casting technique. Optical fibers were drawn using a drawing tower developed in-house. All glasses showed typical  $T_g$  and CTE values of 440 °C and 12 °C<sup>-1</sup>, respectively. A core-cladding glass pair was selected and multi-mode and single-mode optical fibers were fabricated. The so-obtained fibers showed an attenuation loss of 6 and 2 dB/m at the wavelength of 1300 nm. Optical microscope and near field images were taken from the prepared fibers, showing good quality core/cladding interface and successful waveguiding property at 1300 nm.

**11:00 AM**

**(GOMD-S3-005-2016) Elaboration of a chalcogenide microstructured optical fiber presenting high birefringence**

J. Troles<sup>\*1</sup>; C. Caillaud<sup>1</sup>; C. Gilles<sup>2</sup>; L. Provino<sup>3</sup>; L. Brilland<sup>4</sup>; L. Jumpertz<sup>2</sup>; S. Ferre<sup>2</sup>; M. Carras<sup>2</sup>; M. Brun<sup>2</sup>; J. Adam<sup>1</sup>; 1. University of Rennes I, France; 2. Mirsense, France; 3. Perfos, France; 4. Selenoptics, France

Compared to oxide based glasses, vitreous materials composed of chalcogen elements (S, Se, Te) show large transparency windows in the infrared. Indeed, chalcogenide glasses can be transparent from the visible up to 12-15 μm, depending on their compositions. In addition, chalcogenide glasses contain large polarisable atoms and external lone electron pairs which induce exceptional non-linear properties. Consequently, the non-linear properties can be 100 or 1000 times as high as the non-linearity of silica. An original way to obtain single-mode fibers is to design microstructured optical fibers (MOFs). These fibers present unique optical properties thanks to the high degree of freedom in the design of their geometrical structure. In this context, a single-mode chalcogenide microstructured optical fiber (MOF) which presents high birefringence has been achieved in order to be connected to a Distributed Feedback Quantum Cascade Laser (DFB-QCL).

**11:20 AM**

**(GOMD-S3-006-2016) Core/clad tellurite glass pairs for Mid-IR Supercontinuum Generation in high NA step index optical fibre (Invited)**

J. Lousteau<sup>\*1</sup>; D. Pugliese<sup>2</sup>; N. Boetti<sup>2</sup>; P. Janicek<sup>3</sup>; E. Ceci-Ginistrelli<sup>2</sup>; F. Poletti<sup>1</sup>; D. Milanese<sup>1</sup>; 1. University of Southampton, United Kingdom; 2. Politecnico di Torino, Italy; 3. University of Pardubice, Czech Republic

We discuss the development of high numerical aperture (NA) step index optical tellurite glass fiber for developing Mid-IR SC source. While the high nonlinearity of tellurite glass allows compact and efficient Mid-R SC generation, the all-solid step index structure offers a level of integration not achievable with microstructured optical fiber. A core tellurite glass composition was developed to offer high nonlinearity, transparency up to 5 μm and superior thermo-mechanical properties. A serie of cladding glass compositions were designed to provide high NA fibre, up to 0.7 and a zero dispersion wavelength near 2 μm. Refractive index was assessed using prism coupling technique for VIS/NIR wavelengths and using variable angle spectroscopic ellipsometer in the Mid-IR region up to 5 μm. Refractive index values of 2.070 and 1.750 were measured at the wavelength of 2μm for the core and cladding glasses, respectively. Core and cladding glasses, namely SC1 and SC2, showed  $T_g$  values of 375 and 380 °C, respectively. A fiber preform was fabricated by the rod-in-tube technique. Fiber drawing trials suggest thermo-mechanical compatibility of SC1 and SC2 glasses. The tellurite glass compositions developed in this study indicate that the fabrication of an all solid high NA optical fiber from tellurite glass is achievable.

**11:40 AM**

**(GOMD-S3-007-2016) Glass Fiber Lasers for Glass Applications (Invited)**

S. Jiang<sup>\*1</sup>; 1. AdValue Photonics Inc, USA

The remarkable advances in fiber laser technology in recent years have rapidly changed the game of lasers in the marketplace. Due to their superior performances, in terms of high average power, high beam quality, high efficiency, and low ownership cost for maintenance and operation, fiber lasers have been replacing conventional solid-state lasers in most applications. This trend seems to continue in the foreseeable future. So far, fiber lasers have been widely used in a variety of industrial and military applications, such as material processing (marking, drilling, cutting, engraving, welding, micro-fabricating), medical/biomedical processing, free-space optical communications, fiber optical sensing, precise frequency metrology, 3D lidar, and high-energy laser weapons. Most efforts in fiber laser development focus on rare-earth doped silica fiber. We are actively design new glass compositions, fabricate new fibers, and design new fiber lasers to take advantages of multi-component glasses. Our current progresses including fibers with extremely high gain per unit length, single frequency fiber lasers with kilohertz linewidth, 2 micron Q-switched fiber laser, as well as 2 micron mode-locked fiber lasers will be presented. During this talk I will focus on lasers for glass applications.

**Session 4: Fs Laser Interactions with Glass I**

Room: University C/D

Session Chair: Jianrong Qiu, South China University of Technology

**9:20 AM**

**(GOMD-S3-008-2016) Dynamic processes of femtosecond laser induced phenomena in glass (Invited)**

J. Hernandez-Rueda<sup>1</sup>; D. Krol<sup>\*1</sup>; 1. UC Davis, USA

Femtosecond (fs)-laser processing of glass has been shown as a reliable method for producing 3-D waveguide structures that can be used to fabricate photonic devices. To harness the full potential of this technique we need a theoretical model to predict how the size and geometry of the structured volume depend on laser processing parameters (e.g. pulse energy, pulse duration) as well as materials composition. Such a model needs to adequately take into account the physical mechanisms associated with fs-laser processing including 1) absorption of the laser pulse, leading to free-carrier generation and 2) energy transfer of the electronic energy to the lattice and subsequent structural changes of the material. Modeling the interaction of a fs-laser pulse with a glass is a complex problem, since the optical properties of the interaction volume dynamically and spatially change within the time duration of a single laser pulse. To experimentally validate a model that describes such a scenario, it is necessary to monitor the laser-modified material with fs time resolution. In this talk, I will give an overview of our recent work, in which fs time-resolved experiments are coupled with numerical modeling of laser-matter interaction.

**9:50 AM**

**(GOMD-S3-009-2016) Femtosecond laser-induced material modifications to control stress states in silica: A step toward metastable polymorphic phase generation (Invited)**

Y. Bellouard<sup>\*1</sup>; 1. Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Driven by non-linear absorption effects, femtosecond laser exposure of fused silica in the non-ablative regime can induce a variety of localized structural changes in the bulk of the material. Depending on exposure conditions, these laser affected zones can be of different types: from densified volumes, to self-organized nanogratings and to micro-bubbles trapped in a molten volume. Each of these structural modifications finds interesting applications in particular in

micromechanics, fluidics and optics. Here, we review these morphological changes and their conditions of formation. In particular, we examine how these structural modifications can be a source for controlled anisotropic stress states in the material, for which we illustrate potential applications in micromechanics and optics as well as for the localized generation of metastable polymorphic phases.

**10:20 AM**

**(GOMD-S3-010-2016) Strengthening of Aluminoborosilicate and Soda-Lime Silicate Glasses Using Femtosecond Pulse Laser**

S. T. Locker<sup>\*1</sup>; P. Tumurugoti<sup>1</sup>; S. K. Sundaram<sup>1</sup>; I. Alfred University, USA

Strengthening a glass surface relies on the ability to replace small radial network modifiers with those of larger atomic radii, resulting in residual stress at or near the glass surface. This surface strengthening process is known as ion-exchange process. Similar to the ion-exchange effect, heating the surface of a glass instantaneously can cause ions to rapidly migrate and relax in a system with high stress fields at the surface. Femtosecond laser treatment of aluminoborosilicate (ABS) and soda-lime silicate (SLS) glass can strengthen the surface by rastering a high-intensity beam along the glass surface. The high-energy laser needs to be focused on the glass surface to prevent scattering or transmission of the beam. Polarized optical microscopy was used to observe the formation of surface stress as a result of superficial energy absorption. Wavelength-dispersive x-ray spectroscopy (WDS) analysis of both treated and untreated surfaces was used to measure the variation in elemental concentration as a function of depth. Mobile-ion concentration is expected to increase with respect to surface proximity. X-ray photoelectron spectroscopy (XPS) data supports the existence of a mobile-ion enriched surface compared to the bulk composition. Micron-surface indentation data shows that ABS and SLS glass surfaces can be strengthened using femtosecond laser treatment.

**10:40 AM**

**(GOMD-S3-011-2016) Femtosecond laser-induced element distribution and crystallization in glass (Invited)**

G. Dong<sup>\*1</sup>; J. Qiu<sup>1</sup>; 1. South China University of Technology, China

Due to the ultra-short pulse duration and extremely high energy intensity, femtosecond (fs) laser is expected to modulate the element distribution and crystallization in three dimensions inside transparent materials. After the irradiation of glasses by fs laser, the network formers (such as Si<sup>4+</sup>, B<sup>3+</sup>, etc.) enriched at the focal point, while the network modifiers (such as Na<sup>+</sup>, Ca<sup>2+</sup>, etc.) enriched in a ring-shaped region around the focal point. Subsequently, the spatial precipitation of nanocrystals in glasses can also be induced by fs laser irradiation. Different types of functional nanocrystals have been precipitation in glasses, such as nonlinear optical LiNbO<sub>3</sub>, Ba<sub>2</sub>TiSi<sub>2</sub>O<sub>8</sub> and BaAlBO<sub>3</sub>F<sub>2</sub> nanocrystals, luminescent host CaF<sub>2</sub>, Ga<sub>2</sub>O<sub>3</sub> and LaF<sub>3</sub> nanocrystals, metal Ag, Au and Pb nanoparticles, PbS, CdS and CdS<sub>x</sub>Se<sub>1-x</sub> quantum dots (QDs), etc. In the present talk, we will discuss the element distribution and crystallization in glasses induced by fs laser irradiation.

**11:10 AM**

**(GOMD-S3-012-2016) Laser-induced oriented Sb<sub>2</sub>S<sub>3</sub> single crystal dots on the surface of Sb-S-I glasses using spatial light modulator**

D. Savytskyy<sup>\*1</sup>; V. Dierolf<sup>1</sup>; H. Jain<sup>1</sup>; I. Lehigh University, USA

Laser induced crystallization can be exploited uniquely to grow oriented single crystals on surface of glasses. To elucidate the mechanism of the oriented crystal nucleation, we used a spatial light modulator (SLM), which allows to create arbitrary shape and intensity distributed laser beams on the sample surface. The intensity of the laser was chosen such that the temperature in the crystal growth region was kept below the melting temperature of the glass. The morphology, crystallinity and composition of crystallized dots were determined using Electron Backscatter Diffraction (EBSD), Raman scattering (RS) and Energy Dispersive X-ray Spectroscopy (EDS).

The results of EBSD mapping indicate that the crystal grows in dot with <001> crystallographic direction close to glass surface for beam with maximal light intensity at center of laser beam. Using laser beam with different spatial oriented elliptic shape we induce the nucleation and growth of Sb<sub>2</sub>S<sub>3</sub> single crystal with the fastest growth direction <001> parallel to the major axis of ellipse and the surface of glass matrix. Using glasses with different content of iodine we show that oriented Sb<sub>2</sub>S<sub>3</sub> single crystals were facilitated by SbI<sub>3</sub> evaporation on surface of glasses in Sb-S-I system. The laser induced chemical gradient preferentially "stimulate" the formation of oriented crystals.

**11:30 AM**

**(GOMD-S3-013-2016) Formation of Ferroelectric LaBGeO<sub>5</sub> Single Crystal Architecture in Glass by Femtosecond Laser Irradiation**

S. McAnany<sup>\*1</sup>; K. Veenhuizen<sup>1</sup>; D. Nolan<sup>2</sup>; V. Dierolf<sup>1</sup>; H. Jain<sup>1</sup>; 1. Lehigh University, USA; 2. Corning Incorporated, USA

Modification of glass by femtosecond laser irradiation provides a promising method for creating photonic integrated circuits (PICs) for use in optical communications. Recently, our team demonstrated for the first time the ability to create functional single crystal waveguides in a glass using the example of congruently crystallizing LaBGeO<sub>5</sub> composition for creating optically active PICs. In practice, however, the nucleation of unwanted secondary crystals in the vicinity of the single crystal is an issue that is yet to be addressed. One possible method of controlling nucleation would be to tailor the glass composition away from the stoichiometry of the desired crystal phase. In such a glass with excess of glass forming component relative to the desired crystal, the excess solute should be expelled into a region surrounding the crystal growth front, thereby inhibiting unwanted nucleation in that region. We have investigated this concept systematically. Using scanning electron microscopy, electron backscattered diffraction, Raman spectroscopy and differential scanning calorimetry, we have determined the feasibility of creating ferroelectric single crystal architectures in non-stoichiometric glass compositions in the xLa<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub>-2GeO<sub>2</sub> system with x = 0.8 - 1.2.

## Symposium 4: Glass Technology and Cross-Cutting Topics

### **Session 3: Challenges in Manufacturing I**

Room: Madison

Session Chairs: Elizabeth Sturdevant, Corning Incorporated; Irene Peterson, Corning Incorporated

**9:20 AM**

**(GOMD-S4-001-2016) A critical review of methods employed for studying the batch-to-melt conversion (Invited)**

A. Prange<sup>\*1</sup>; V. Niessen<sup>1</sup>; R. Conrad<sup>1</sup>; 1. RWTH Aachen University, Germany

For the investigation of reactions related to the batch-to-melt conversion process of industrial batches, a wide arsenal of methods has been described in literature, reaching from experiments at the mg scale to fully fledged industrial campaigns at the 10 - 100 t scale. In the present contribution, the methods are classified with respect to their ability to grasp the influence of grain size effects of raw materials, their feature of externally exposing of thermal history versus letting the thermal history evolve independently, their ability to grasp the competition between local chemical turnover and transport of heat and matter, their ability to feature the symmetry of the geometry given in a glass melting furnace. Based of the above compilation, a strategy for a reliable up-scaling of laboratory experiments to the expected behavior in industry is presented.

9:50 AM

**(GOMD-S4-002-2016) Identifying the rate determining step of the batch-to-melt conversion**

R. Conradt<sup>\*1</sup>; 1. RWTH Aachen University, Germany

The conversion of a raw materials batch into a continuous molten phase is the first high-T process of industrial glass melting. This process typically lasts 40 to 60 minutes and draws a power of about 600 kW per t of melted glass. The quality of its completion influences all consecutive steps of melting. There is a continued quest to make this process more efficient, so as to allow for higher pull rates or a lower overall energy consumption. Many efforts are directed towards enhancing heat transfer between combustion space and batch. As much as such measures may yield good results in individual cases, the approach rests on the prejudice that heat transfer is indeed the rate-determining step. This has never actually been verified. The intrinsic chemical turnover rate or the rate of within-batch heat transport might control the overall conversion rate as well. In a first part, the typical ranges of heat transfer, within-batch heat transport, and chemical turnover rates are compiled in their temperature dependence, and contrasted. Cases are presented where the chemical turnover rate poses a principal constraint. Finally, it is demonstrated how the nature of the rate determining step, may be read from the pull dependence of the heat balance of industrial furnaces.

10:10 AM

**(GOMD-S4-003-2016) A particle-scale view of glass batch melting thanks to in situ microtomography (Invited)**

E. Guillard<sup>\*1</sup>; W. Woelffel<sup>1</sup>; E. Burov<sup>1</sup>; M. Toplis<sup>2</sup>; M. Chopinet<sup>1</sup>; 1. Joint Unit CNRS/Saint-Gobain, France; 2. IRAP, France

Soda-lime window glass melting is an energy-intensive process, where granular raw materials react at high temperature to form silicate minerals, which then turn into melts. The efficiency of silica conversion depends crucially on the geometry of solid- and liquid-state reactions during decarbonation reactions, that occur in a few seconds in the case of liquid carbonates. We have used ultrafast in situ synchrotron microtomography to image in 3D the transformation of soda-lime glass batch at temperatures from 800 to 1100°C. With this technique, 3-D images of materials can be acquired in a few seconds, at micronic resolution. I will show how ultrafast tomographic imaging of glass batch reactions resulted in new insights about the geometry of reactions, and the origin of crystalline defects that are hard to dissolve in the industrial process. Importantly, time-resolved imaging reveals the presence of phases that are only present for a short time, such as mixed carbonates, but have important consequences for the later physical and chemical evolution of the system.

10:40 AM

**(GOMD-S4-004-2016) Batch reactions and melting-in of alkali-lean borosilicate glasses prepared with different borate raw materials**

M. Hubert<sup>\*1</sup>; 1. CelSian Glass & Solar, Netherlands

Borosilicate glasses are of utmost importance in a large number of commercial applications, and are among the most largely produced types of glass. For industrially produced borosilicate glasses, different borate raw materials can be chosen by the manufacturers (e.g. borax, boric acid, colemanite...). The selection of the borate raw material introduced in the batch will notably depend on the type of borosilicate produced, as well as on economic considerations. The choice of the borate raw materials can have an impact on the melting process itself, e.g. on the melting kinetics or on the energy demand to melt the batch. In this study, the influence of hydrated vs. anhydrous borate raw material (boric acid vs. boron oxide) on the melting behavior of alkali-lean borosilicate glasses is presented. Notably, a divergence in the low-temperature batch reaction kinetics for batches using different borate raw materials is highlighted.

11:00 AM

**(GOMD-S4-005-2016) HTXRD investigation of batch reactions for phosphate raw materials in a multicomponent sodium aluminosilicate glass**

J. Rygel<sup>\*1</sup>; B. Wheaton<sup>1</sup>; K. Rossington<sup>1</sup>; 1. Corning Incorporated, USA

High Temperature X-ray Diffraction (HTXRD) is an established technique that has been used extensively to study phase transitions and thermal expansion in crystalline materials. However, this technique also shows promise for investigating batch reactions during the glass melting process. Batch reactions for phosphate additions to multicomponent sodium aluminosilicate glasses using different raw materials were examined during heating to 1200 °C in 100 °C steps. For all of the phosphate raw materials investigated, sodium orthophosphate was formed at elevated temperatures due to reaction with sodium carbonate, though the pathway varied with starting material. Disodium phosphate and sodium trimetaphosphate first formed sodium pyrophosphate before sodium orthophosphate. Sodium hexametaphosphate was nanocrystalline and x-ray amorphous as-received, becoming crystalline by the 300 °C step. Additionally, monoammonium phosphate was observed to react at room temperature with sodium carbonate to produce diammonium phosphate and disodium phosphate. Finally, aluminum metaphosphate was inferred to form aluminum phosphate before sodium orthophosphate due to the increase in intensity of quartz diffraction peaks, the isostructural analog to aluminum phosphate.

11:20 AM

**(GOMD-S4-006-2016) Current Glass Melting Sensor Needs (Invited)**

D. A. Gaerke<sup>\*1</sup>; 1. Owens-Illinois Inc., USA

There are numerous commercial off the shelf sensors and measurement systems in use on modern glass melters. Most of these have been in use for years, although there are some newer technologies that have only been available for a few years. All of these are typically characterized by needing to operate in a harsh service environment with minimal maintenance. This paper will briefly cover potential improvements to existing sensors that could help with sustainability of the glass industry, but will also focus on potential new sensors that could improve melter operation, glass quality, and industry competitiveness.

### Session 4: Glass Formulation I

Room: Capitol B

Session Chairs: Claire Corkhill, University of Sheffield; Isabelle Giboire, CEA

9:20 AM

**(GOMD-S4-007-2016) Development and characterisation of Mg-based glasses for uranium-containing Sellafield legacy wastes**

C. L. Corkhill<sup>\*1</sup>; S. T. Barlow<sup>1</sup>; A. J. Fisher<sup>1</sup>; M. C. Stennett<sup>1</sup>; N. C. Hyatt<sup>1</sup>; 1. University of Sheffield, United Kingdom

Magnox sludge, the result of magnesium fuel alloy cladding corrosion in outdoor storage ponds, presents a significant challenge to the decommissioning of legacy ponds at the UK Sellafield nuclear site. The sludge comprises magnesium hydroxide with uranium, ranging from intact uranium metal pieces, to UO<sub>2</sub> and degraded UO<sub>3</sub>-like materials. We detail the development of a suite of glass formulations for the immobilisation of Magnox sludge via vitrification in magnesium borosilicate and magnesium aluminosilicate matrices, also immobilising uranium in the extreme bounding conditions of the waste envelope. Both metal and hydroxide were used as the source of magnesium in the base glass compositions. A range of suitable processing conditions were developed. The glasses were subsequently chemically characterised and their durability assessed. Compositions immobilising low waste loadings of uranium oxide formed a homogeneous glass matrix, while high waste loadings of

uranium metal were found to incorporate uranium both in the glass matrix and in crystallites of  $\text{UO}_2$ . Uranium speciation in the glass matrix and crystallites was confirmed using  $\mu$ -XANES. The chemical durability of the resulting glasses, determined using the PCT-B method, were found to surpass the "acceptance criteria" for geological disposal.

**9:40 AM**

**(GOMD-S4-008-2016) Study of peraluminous glass formulations for fission products and minor actinides containment**

I. Giboire<sup>\*1</sup>; V. Montouillout<sup>2</sup>; V. Piovesan<sup>1</sup>; E. Gasnier<sup>1</sup>; N. Pellerin<sup>2</sup>; 1. CEA, France; 2. CEMHTI CNRS Orléans, France

Part of the Research and Development program concerning waste containment glass aims to assess new glass formulations with good properties in terms of thermal stability, chemical durability, high waste content and process ability. This study focuses on new peraluminous glasses with high rare earth content, in which aluminum ions  $\text{Al}^{3+}$  are in excess regarding modifier elements such as  $\text{Na}^+$  or  $\text{Ca}^{2+}$ . The aim is to assess the potentiality of these glasses as waste conditioning matrices, especially by studying the rare earth incorporation in the network, as well as its crystallisation tendency and its structural role. Increasing aluminum content in such proportion seems to be very efficient to avoid crystallization of rare earth-rich apatite phase such as  $\text{Ca}_2\text{RE}_8(\text{SiO}_4)_6\text{O}_2$  or  $\text{NaRE}_9(\text{SiO}_4)_6\text{O}_2$ , that are well known to crystallize in other peralkaline systems, containing higher amount of modifier ions. Using microstructural (XRD, SEM, TEM, EPMA) and structural (NMR) characterization methods, the high thermal stability of these peraluminous glasses has been confirmed, thanks to the fact that rare earth elements enhance the aluminium incorporation in the network as well as aluminium ions enhance rare earth incorporation.

**10:00 AM**

**(GOMD-S4-009-2016) Chemical durability of UK vitrified high level waste using a Ca/Zn alkali borosilicate glass**

M. T. Harrison<sup>\*1</sup>; C. J. Steele<sup>2</sup>; 1. National Nuclear Laboratory, United Kingdom; 2. Sellafield Ltd, United Kingdom

In the UK, the Waste Vitrification Plant (WVP) at Sellafield converts the highly active liquid (HAL) waste from the reprocessing of spent nuclear fuel into a glass wastefrom suitable for long term storage and disposal. After the completion of reprocessing operations, the HAL storage tanks will be emptied and washed out to remove any accumulated solids. These solids are expected to contain high concentrations of molybdenum, which will limit the waste loading due to the low solubility this element in the current alkali borosilicate base glass composition used in WVP. Hence, a new glass formulation containing Al, Ca and Zn has been developed specifically for immobilisation of waste streams containing high concentrations of Mo. This Ca/Zn glass allows for significantly higher waste loadings by the formation of  $\text{CaMoO}_4$  crystals when the Mo content exceeds its solubility limit in the glass. The Ca/Zn vitrified product quality has to be validated for the full range of potential feeds. In particular, the chemical durability is an important product quality parameter for the long-term storage and final disposal of vitrified HLW. The durability of a range of Ca/Zn product glasses has been characterised using standard protocols for short- and long-term dissolution behaviour. The study reported here assesses these results, and compares them with those obtained for current vitrified product.

**10:20 AM**

**(GOMD-S4-010-2016) Rhenium Mass Balance in a Laboratory-Scale Melter**

D. Dixon<sup>\*1</sup>; M. J. Schweiger<sup>1</sup>; C. Fischer<sup>1</sup>; C. D. Lukins<sup>1</sup>; D. Kim<sup>1</sup>; P. Hrm<sup>1</sup>; 1. Pacific Northwest National Lab, USA

The path for immobilizing low-activity waste (LAW) for long-term storage is to mix these concentrated salt solutions with additive

chemicals and minerals and then vitrify the LAW slurry feed in an electric melter. One of the radionuclides present in LAW is technetium-99 ( $^{99}\text{Tc}$ ), a long-lived dose contributor. Rhenium (Re) is commonly used as a nonradioactive surrogate for  $^{99}\text{Tc}$  volatility behavior in glass. The presence of a cold cap, the layer of reacting feed on top of the molten glass pool, has been shown to affect the volatility of  $^{99}\text{Tc}$  and Re during vitrification. To study the effects of feed composition or feed components on  $^{99}\text{Tc}$  retention, an off-gas system was designed for capturing  $^{99}\text{Tc}$  during cold-cap melting of a LAW feed in a laboratory-scale melter (LSM). This system provides the capability to observe the evolution and coverage of the cold cap during feed charging. At the quasi-steady state time period where the cold cap maintains a consistent size and coverage, the amount of volatilized  $^{99}\text{Tc}$  in the off-gas can be used to determine the  $^{99}\text{Tc}$  retention in the glass. This paper presents the results of tests performed to evaluate the mass balance of Re in the LSM before this system is applied to LAW glass feeds spiked with  $^{99}\text{Tc}$  or containing actual tank waste.

**10:40 AM**

**(GOMD-S4-011-2016) Effects of Reducing Agents on Retention of Rhenium during Melting of Low-Activity Waste Glasses**

J. George<sup>\*1</sup>; D. Kim<sup>1</sup>; M. J. Schweiger<sup>1</sup>; A. A. Kruger<sup>2</sup>; 1. Pacific Northwest National Lab, USA; 2. DOE Office of River Protection, USA

A major concern in the vitrification of low-activity waste (LAW) at the U.S. Department of Energy's Hanford Site in Washington State is volatile loss of radioactive  $^{99}\text{Tc}$  to off-gas. We investigated the effect of redox on incorporation of Re (a non-radioactive surrogate for  $^{99}\text{Tc}$ ) into the glass melt during heating. Two simulated LAW solutions, AN-102 and AZ-102, were prepared and glass forming and modifying components were added to make the nominal glass feeds. The reduced glass feeds were prepared with Fe(II) oxalate replacing hematite as a glass modifying component and sucrose (AN-102 only). The slurry feeds were dried at 105 °C and heat treated to 400-1100 °C at 5 K/min then air-quenched to room temperature. X-ray diffraction (XRD) analyses were performed on the dried feeds and heat-treated samples and differential thermal analysis/thermogravimetric analysis (DTA/TGA) were performed on dried feeds to characterize the progress of feed-to-glass conversion. The dried feeds and heat-treated samples were leached with deionized water for 1 h at room temperature and a complete chemical analysis was performed on the resulting solutions and residual solids. The effect of reducing agents on the feed-to-glass conversion reactions and partitioning of Re into molten salt and glass-forming melts are evaluated to understand the role of reducing condition on retention of Re in glass.

**11:00 AM**

**(GOMD-S4-012-2016) Proposed mechanisms for Tc volatility from waste glass feed simulants**

S. A. Luksic<sup>\*1</sup>; 1. Pacific Northwest National Lab, USA

Technetium (Tc) and rhenium (Re) behavior in glass melts is explored under various conditions as a means for elucidating the differences between the two elements and qualifying the use of Re as a Tc surrogate. A low-activity waste (LAW) glass simulant feed spiked with  $\text{NaReO}_4$  and  $\text{KTcO}_4$  is heated to a series of temperatures from 100°C to 1000°C. The same LAW feed prepared without sulfate is run under identical conditions, and the behaviors of Tc and Re in both are compared. Tc retention increases from 43% to 65% in the case of the zero sulfate feed. The partitioning of Tc into the gas phase, molten salt and soluble phase, and glass matrix is examined by leach tests at each target temperature. Mechanisms of Tc and Re migration and volatilization are proposed based on their behavior in these waste glass simulants.

11:20 AM

### **(GOMD-S4-013-2016) Volatile Species of Technetium and Rhenium Relevant to Vitrification of Hanford Low-Activity Wastes**

D. Kim<sup>\*1</sup>; A. A. Kruger<sup>2</sup>; 1. PNNL, USA; 2. DOE-ORP, USA

Technetium-99 is one of the most difficult radionuclides to manage for the treatment of liquid low-activity waste (LAW) stored in underground tanks at the U.S. Department of Energy's Hanford site. The immobilization of LAW by vitrification is significantly challenged by extreme volatility of Tc and thus low retention in glass. Extensive crucible studies are being performed to understand the behavior of Tc-99 and Re (a surrogate for Tc-99) during melting of glass feeds (waste plus mineral and chemical additives) and to ultimately develop the methods to increase the Tc retention in the final glass product. One of the key elements important for understanding the mechanism of Tc loss is identifying the volatile species of Tc during high-temperature processing of slurry feeds in the melter. This paper reviews the literature information available on the volatile species of Tc and Re identified from previous studies including thermal analyses of Tc/Re-bearing phases, crucible melting tests of simulated waste glass feeds, and melter processing of actual and simulated waste glass feeds. The findings will be discussed in connection with the recent crucible test results on the partitioning of Re into different phases during melting of simulated LAW glass feeds in an effort to understand the major factors that affect Tc retention in glass.

11:40 AM

### **(GOMD-S4-014-2016) Experimental Study of Sulfur Solubility in Low-Activity Waste Glass**

T. Jin<sup>\*1</sup>; D. Kim<sup>1</sup>; L. P. Darnell<sup>1</sup>; B. L. Weese<sup>1</sup>; N. L. Canfield<sup>1</sup>; M. Bliss<sup>1</sup>; J. R. Davies<sup>1</sup>; C. C. Bonham<sup>1</sup>; M. J. Schweiger<sup>1</sup>; A. A. Kruger<sup>2</sup>; 1. Pacific Northwest National Laboratory, USA; 2. US Department of Energy - Office of River Protection, USA

During vitrification of high sulfur wastes in a Joule-heated melter, segregation and accumulation of sulfate salts causes processing problems such as corrosion of melter materials and increased volatile loss of radioactive components. Experiments were conducted to determine the sulfur solubility in Hanford low-activity waste (LAW) glasses. Sulfur-saturated glass samples were prepared by two different methods: bubbling method and salt-saturation method. The bubbling method involved bubbling the glass melt at 1150°C in a Pt crucible with a SO<sub>2</sub> containing gas mix. The salt-saturation method was performed by mixing a crushed glass with an excess amount of Na<sub>2</sub>SO<sub>4</sub> (target SO<sub>3</sub> of 4 wt% in glass, much higher than the solubility) and then melting it at 1150°C for one hour. After the glass melt and the segregated molten salt were air quenched, the glass-salt mixture was crushed, homogenized, and re-melted. The melt, quench, and crush process was repeated multiple times until the sulfur concentration in the glass plateaued. Inductively coupled plasma atomic emission spectroscopy and ion chromatography were used for chemical analyses of the samples. The results from both methods showed that LAW glasses were well saturated by sulfur in an air atmosphere. The bubbling method caused significant sodium loss from the glass, while the salt-saturation method had very minor losses of glass components.

## **Symposium 2: Larry L. Hench Memorial Symposium on Bioactive Glasses**

### **Larry L. Hench Memorial Symposium on Bioactive Glasses II: Sol-gel Glasses**

Room: Wisconsin

Session Chairs: Julian Jones, Imperial College London; Delia Brauer, Friedrich-Schiller-Universität

1:20 PM

### **(GOMD-S2-006-2016) Bioactive glass reactions in physiological fluids and their competitive protein adsorption (Invited)**

G. Poologasundarampillai<sup>\*1</sup>; J. Jones<sup>2</sup>; 1. University of Manchester, United Kingdom; 2. Imperial College, United Kingdom

Reactions of sol-gel derived bioactive glasses in physiological fluids are complex owing to their mesoporous structure and large specific surface area. As well as adsorption of large amounts of protein from the fluid, rapid ion exchange also takes place. This leads to a fluid environment in the vicinity of the bioactive glass that is different to the physiological conditions thereby influencing the cellular activity. In this talk, time resolved studies of competitive protein adsorption and reactions of sol-gel derived bioactive glass 70S30C (70mol% SiO<sub>2</sub> and 30 mol% CaO) in several different physiological fluids is presented. Bioactive glasses are known for their ability to rapidly form a hydroxyl carbonate apatite (HCA) layer on their surfaces which leads to bone bonding. Our study shows that the formation of HCA heavily depends on the composition of the physiological fluid and that the adsorption of physiological proteins is dependent on the phases that had nucleated on the surface of the bioactive glass.

1:50 PM

### **(GOMD-S2-007-2016) 3-D Electrospun bioactive glasses for wound healing**

E. G. Norris<sup>\*1</sup>; Q. Ju<sup>3</sup>; G. Poologasundarampillai<sup>2</sup>; A. Obata<sup>3</sup>; J. Jones<sup>1</sup>; 1. Imperial College, United Kingdom; 2. University of Manchester, United Kingdom; 3. Nagoya Institute of Technology, Japan

A challenge in wound healing is to produce a material that promotes cellular activity such as angiogenesis which can be used alongside current wound care procedures. Sol-gel derived bioactive glass compositions are flexible and allow biologically active cations to be added, offering valuable properties for wound healing. Herein a protocol for electrospinning a 3-D fibrous bioactive glass 70S30C (70 mol. % SiO<sub>2</sub> 30 mol. % CaO) has been developed with good reproducibility. This novel 3-D structure, ideal for packing into large defects, is very different architecturally from the typical 2-D structure traditionally produced by electrospinning. Factors such as sol-gel composition, relative humidity and solution viscosity were investigated. Results show that a combination of many factors contribute towards the production of the 3-D structure. Ag ions were additionally added for antibacterial properties, and by controlling these electrospinning parameters, it was possible to create 3-D structures with this composition. This suggests that other ions such as copper, cobalt and strontium could be incorporated into this network while maintaining the 3-D structure. This extends the possible applications of this material to bone in addition to skin for wound healing leading to materials with great potential for use in tissue regeneration.

2:10 PM

### **(GOMD-S2-008-2016) Processing Parameters Affect the Bioactivity of Sol-Gel Derived Borate Glasses**

W. C. Lepry<sup>\*1</sup>; S. N. Nazhat<sup>1</sup>; 1. McGill University, Canada

The sol-gel method is a flexible, low temperature, solution based process that can generate glasses with controlled morphologies. This approach is advantageous for biomedical applications since it



produces glasses with higher surface areas and porosities, allowing for more rapid conversion to bone-like mineral (hydroxy-carbonated apatite, HCA). Recently, it was demonstrated that sol-gel derived borate glasses (SGBGs) underwent surface conversion to HCA in as little as 30 minutes when submerged in simulated body fluid (SBF). However, aside from composition, it is not known how the processing parameters of the SGBGs modify their bioactivity. To this end, we altered the sol-gel processing parameters examined including precursor materials, ageing duration and temperature, as well as calcination rate and temperature of a borate substituted "45S5" glass ( $(46.1)\text{B}_2\text{O}_3-(26.9)\text{CaO}-(24.4)\text{Na}_2\text{O}-(2.6)\text{P}_2\text{O}_5$  in mol%). The result of these modifications were examined by characterizing the final structure, morphology, and textural properties, as well as the in vitro bioactivity. While all glasses converted to HCA, calcination temperature had the greatest effect on the rate of conversion. The results indicated that by controlling the sol-gel processing parameters, SGBGs can be modified for a wide range of tissue engineering applications.

### 2:30 PM

#### (GOMD-S2-009-2016) Development of strontium incorporating sol-gel derived bioactive glass nanoparticles for bone regeneration applications

P. Naruphontjirakul<sup>1</sup>; S. L. Greasley<sup>1</sup>; S. Chen<sup>1</sup>; L. Siwei<sup>1</sup>; A. E. Porter<sup>1</sup>; J. Jones<sup>1</sup>; 1. Imperial College London, United Kingdom

In this study, new dense sol-gel derived bioactive glass nanoparticles containing strontium (Sr) using a modified Stöber process were developed to enhance their osteogenic capability. Strontium oxide was used as a substitute for calcium oxide on a mol% basis (25 - 100%) in a  $\text{SiO}_2$ -CaO binary system (90 mol%  $\text{SiO}_2$ , 10 mol% CaO). Monodispersed Sr containing bioactive glass nanoparticles (Sr-BGNPs) had an amorphous spherical form with  $90 \pm 10$  nm in diameter. Sr-BGNPs were non-toxic to osteoblast-like cells (MC3T3-E1). Dissolution products of 75% Sr-BGNPs at 200 and 250  $\mu\text{g}\cdot\text{ml}^{-1}$  significantly increased cell proliferation ( $p < 0.05$ ). 75% Sr-BGNPs and their dissolution ions stimulated ALP activity and calcium deposition in the extracellular matrix of MC3T3-E1 cells following three weeks of culture in comparison to those cultured in basal and osteoinductive conditions. Markers associated with osteogenic differentiation including Col1a1, Osteopontin and Osteocalcin were also expressed. Sr-BGNPs had no toxic effect on murine bone marrow macrophages (M0). Following 24-h incubation of M0 with Sr-BGNPs, uptaken particles had internalised in the vesicles and released Sr and Ca from silica networks during degradation process. Sr and Ca were remained in the partially degraded particles. Sr-BGNPs with the great osteogenic ability have promising potential for bone regeneration.

### 2:50 PM

#### (GOMD-S2-010-2016) Preparation of Lithium Disilicate Glass-Ceramics by the Sol-Gel Method

H. Celik<sup>1</sup>; L. Romero-Sanchez<sup>2</sup>; A. Diaz Cuenca<sup>2</sup>; E. Dolekcecik<sup>1</sup>; 1. Anadolu University, Turkey; 2. Materials Science Institute of Seville, Spain

Lithium disilicate glass-ceramic materials are a type of glass-ceramic materials which have major composition in the  $\text{Li}_2\text{O}-2\text{SiO}_2$  system. Recent studies on compositional modifications of the lithium disilicate precursor glasses have yielded translucent glass-ceramics with high strength and excellent chemical durability. These type of materials are preferred for dental applications of veneers, crowns, bridges and implants. In recent years, the glasses prepared using a sol-gel route are found to have advantages over conventional glass meltings method in terms of better homogeneity, higher level of purity, lower stoichiometric losses and less contamination from crucibles. In the present study, a crystalline lithium disilicate ( $\text{Li}_2\text{Si}_2\text{O}_5$ ) phase was prepared from tetraethylorthosilicate (TEOS) and lithium nitrate ( $\text{LiNO}_3$ ) with addition of triethyl phosphate (TEP) and  $\text{Ca}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$  mixture with the help of the described sol-gel process. Lithium disilicate glass-ceramics materials were prepared having a

varying content of  $\text{Li}_2\text{O}$  (5, 10, 15 and 33.3 mol %). Results of the XRD analysis obtained from the samples revealed that formation of necessary lithium metasilicate and lithium disilicate could not be achieved for the 5, 10 and 15 mol %  $\text{Li}_2\text{O}$  containing samples. On the contrary, the XRD results of the 33 %  $\text{Li}_2\text{O}$  containing sample showed clearly the formation of lithium metasilicate and lithium disilicate phases.

### Larry L. Hench Memorial Symposium on Bioactive Glasses III

Room: Wisconsin

Session Chairs: Ashutosh Goel, Rutgers University; José Ferreira, University of Aveiro

### 3:40 PM

#### (GOMD-S2-011-2016) Bioactive glasses for fiber drawing and particles sintering (Invited)

J. Massera<sup>1</sup>; 1. Tampere University of Technology, Finland

Silicate bioactive glasses are well known for their ability to form hydroxyapatite and promote cell adhesion, proliferation and differentiation. However, the crystallization of these glasses inhibits proper hot forming at temperatures below crystallization limiting their applications as scaffolds or fibers. To reduce the tendency of the glass toward crystallization, boron can be added to the silica glass. However excess boron release may lead to negative effect on the differentiation of human stem cells. Phosphate bioactive glasses were found to be good candidates to replace silicate-based glass as they can be engineered with tailored thermal properties that enable hot forming into scaffolds or fibers. In this presentation, the different glass systems used as bioactive glasses will be reviewed. The crystallization mechanism of some (silicate and phosphate) bioactive glasses and its impact on particles sintering, fiber drawing and in vitro bioactivity will be discussed. Then we will discuss the successful manufacturing and characterization of 3D scaffolds and core/core-clad fibers. The impact of the glass composition on the cell proliferation, growth and differentiation will be discussed as well as the effect of the scaffolds and fibers immersion, in buffer solution, on their mechanical properties.

### 4:10 PM

#### (GOMD-S2-012-2016) Influence of lithium and potassium substitution on the dissolution behavior of Bioglass 45S5

R. Brückner<sup>1</sup>; L. Hupa<sup>2</sup>; D. S. Brauer<sup>1</sup>; 1. Friedrich-Schiller-Universität, Germany; 2. Åbo Akademi University, Finland

Partially substituting lithium or potassium for sodium in bioactive glasses can help to widen their processing window and facilitate sintering. Here, we investigated how replacing 0, 25, 50, 75 or 100% of sodium with lithium or potassium in melt-derived 45S5 ( $46.1\text{SiO}_2 - 2.6\text{P}_2\text{O}_5 - 26.9\text{CaO} - 24.4\text{Na}_2\text{O}$ ; mol%) affected ion release and dissolution. Static (6 hours to 3 days) and dynamic (continuous-flow; up to 2500 s) dissolution experiments were performed on glass powders in Tris buffer at pH 7.4, followed by ICP-OES analysis. Ion release was delayed with Li for Na substitution but accelerated with K for Na substitution. Although the mixed alkali effect affects ion release from more chemically stable silicate glasses, showing reduced ion release for mixed alkali compositions, here no such trend was observed. Density measurements and molar volume calculations showed that by replacing  $\text{Na}^+$  with the larger  $\text{K}^+$  ions, the molar volume increased, suggesting a less compact silicate network. For Li-substituted glasses, the opposite was true: the molar volume decreased with Li for Na substitution, resulting in a more compact network. This suggests that in bioactive glasses of low network connectivity, ion release is affected by the packing of the silicate network, which either facilitates (K) or inhibits (Li) diffusion of water molecules into the glass network and subsequent ion release.

4:30 PM

**(GOMD-S2-013-2016) Effect of phase separation on protein adsorption and cell attachment on 45S5 bioactive glass**

R. Golovchak<sup>2</sup>; T. Kowal<sup>1</sup>; T. Chokshi<sup>1</sup>; J. Harms<sup>2</sup>; H. Jain<sup>\*1</sup>; M. Falk<sup>1</sup>;  
1. Lehigh University, USA; 2. Austin Peay State University, USA

Recently we discovered strong impact of processing conditions on the nano/microstructure of 45S5 bioglass and consequently on cell response. Therefore, we have sought to correlate the effect of phase separation in this glass on the adsorption of bovine serum albumin (BSA) protein and the attachment of MC3T3-E1 pre-osteoblasts. In particular, BSA adsorption and cell attachment to the polished surfaces of spinodally phase separated and droplet-like phase separated 45S5 bioglass are compared. The cells demonstrated a significantly higher preference for the spinodal morphology compared to the droplet-like morphology. Similarly BSA proteins attached more efficiently to the surface of spinodally phase separated glass according to the quantitative chemical analysis by X-ray photoelectron spectroscopy. The conformational state of the attached BSA proteins, as obtained from Raman spectroscopy, indicated a better biocompatibility of spinodally phase separated glass. Thus, it appears from these results that cell attachment to 45S5 bioglass is mediated by a protein layer.

4:50 PM

**(GOMD-S2-014-2016) Thermal Analysis of Bio Active Borosilicate Glass doped with Cerium Oxide**

K. S. Ranasinghe<sup>\*1</sup>; D. E. Day<sup>2</sup>; G. Humble<sup>1</sup>; 1. Kennesaw State University, USA; 2. Missouri University of Science & Technology, USA

A bio active borosilicate glass doped with cerium oxide (BxSiCe) is investigated for biological applications. Cerium is known to be anti-inflammatory, anti-oxidant, a possible drug delivery mechanism for treating cancer and a therapeutic medicine for neurodegenerative diseases. Cerium exhibits coexistence of Ce<sup>3+</sup> and Ce<sup>4+</sup> states and the Ce<sup>3+</sup>/Ce<sup>4+</sup> ratio influences the microenvironment which plays an important role in determining the biological activity. A study of thermal analysis was conducted on this borosilicate glass doped with different wt% of cerium oxide, using SDT Q 600 thermal analyzer. A glass sample of 30mg, 400-500 μm particle size of different types of glass was heated to 1200C, to obtain glass transition, crystallization and melting temperatures. The glass samples were then heated to 900C at several heating rates between 2C/min to 100C/min and cooled to room temperature with the same rate. Results were compared with the glass samples made with different wt % of cerium.

### **Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications**

#### **Session 4: Fs Laser Interactions with Glass II**

Room: University C/D

Session Chair: Himanshu Jain, Lehigh University

1:20 PM

**(GOMD-S3-014-2016) Femtosecond laser nanoprocesing and its application (Invited)**

Y. Shimotsu<sup>\*1</sup>; 1. Kyoto University, Japan

Periodic nanostructures inside various materials ranging from glass to semiconductor have been induced by a focused beam of a femtosecond pulses. Such self-organized nanostructures are composed of defect formation and strained structure, depending on the material. We empirically classify the observed phenomenon into two types based on the bandgap structure and propose the mechanism for nanostructuring. Apart from the basic understanding, we have also proposed the possible optical and electrical application.

1:50 PM

**(GOMD-S3-015-2016) Advancing the Art of Ultrafast Laser Writing (Invited)**

P. G. Kazansky<sup>1</sup>; M. Beresna<sup>1</sup>; R. Drevinskas<sup>1</sup>; A. Patel<sup>\*1</sup>; A. Cerkauskaite<sup>1</sup>; F. Zhang<sup>1</sup>; S. Lotarev<sup>2</sup>; A. Okhrimchuk<sup>2</sup>; V. Sigaev<sup>2</sup>; 1. University of Southampton, United Kingdom; 2. Advanced Laser Technologies Centre, Mendeleev University of Chemical Technology, Russian Federation

Interaction of intense ultrashort light pulses with glass reveals new properties and phenomena, which challenge common beliefs in optics. Demonstrations of 3D nanograting formation and related self-assembled form birefringence uncover new science and applications including flat optics elements exploiting the Pancharatnam-Berry phase. The S-waveplate (Southampton-Super-Structured-waveplate) is one of the examples of such elements, which can be used for creating axially symmetric polarization state and optical vortexes. The applications of S-waveplates range from material processing to microscopy and optical trapping. Two independent parameters describing self-assembled form birefringence in quartz glass, the slow axis orientation and the strength of retardance, are also explored for the optical encoding of information in addition to three spatial coordinates. The data optically encoded into 5D is successfully retrieved by quantitative birefringence measurements. The storage allows unprecedented parameters including hundreds of terabytes per disc data capacity and thermal stability up to 1000°. The demonstrated recording of the first digital documents, including the eternal copy of King James Bible, which will survive the human race, is the vital step towards an eternal archive. These and more recent demonstrations of ultrafast laser calligraphy and anisotropic photosensitivity in glasses are reviewed.

2:20 PM

**(GOMD-S3-016-2016) Modification of surface properties of glasses by ultrashort pulsed lasers (Invited)**

Q. Zhao<sup>\*1</sup>; 1. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, China

Surface micro-/nanomodification of glasses has great demands in integrated photonic, microfluidic, and MEMS devices. Ultrashort pulsed laser processing has offered new prospects to miniaturize and integrate highly functional structures directly on glasses. In this talk, we review the recent progress in laser induced micro-/nanomodification on the surfaces of various glasses and their potential applications. Three aspects of laser induced surface modification of glasses will be introduced. Firstly, the history of laser induced surface modification of glasses is reviewed. The state-of-the-art applications and the mechanisms are discussed. Secondly, the efforts for achieving better micro-/nanomodification are introduced. At last, the future trends of laser induced surface modification of glasses will be given.

2:50 PM

**(GOMD-S3-017-2016) Precision micromachining of fused silica glass using femtosecond lasers: Fabrication of flexure elements with integrated waveguides (Invited)**

P. Bado<sup>\*1</sup>; M. Dugan<sup>1</sup>; A. Said<sup>1</sup>; 1. Translume, USA

Engineers that specialize in precision applications often use flexing elements to avoid some of the short-comings associated with other dynamic components. Traditionally, flexures are made from metals. Until recently, one could not procure one made out of fused silica glass, although many metrology practitioners have long recognized that fused silica glass, with a near-zero coefficient of thermal expansion, and its near-perfect elastic behavior, would provide exceptional characteristic suited for flexures that have to meet demanding requirements. Unfortunately traditional fabrication processes could not generate reliably flexures made out of glass. However, over the last decade, the development of fabrication process based on the use of femtosecond laser pulses has opened the door to the fabrication of dependable robust fused silica glass flexures. In addition, unlike any

other materials commonly used to fabricate high-quality flexures, fused silica is also transparent. This can be exploited to combine mechanical and optical functionalities in a metrology-grade component. To illustrate this uncommon juxtaposition, we have fabricated fused silica flexures with integrated optical waveguides. We will discuss the fabrication of a notch flexure made out of fused silica glass with an imbedded sub-surface Mach-Zehnder waveguide-based interferometer.

## **Symposium 4: Glass Technology and Cross-Cutting Topics**

### **Session 1: Glass Surfaces and Functional Coatings**

Room: Capitol A

Session Chairs: Nathan P Mellott, Alfred University; Carlo Pantano, The Pennsylvania State University

#### **1:20 PM**

#### **(GOMD-S4-015-2016) Characterization of hydrous species at multicomponent glass surfaces using non-linear optical spectroscopy (Invited)**

S. H. Kim<sup>\*1</sup>; 1. Pennsylvania State University, USA

Water adsorption and reaction on glass surfaces play important roles in chemical and mechanical durability of glasses. Compared to metals or crystalline oxide materials, the surface chemistry of multicomponent glasses in humid ambient is much less understood. This is in part because the adsorbed water can often be dissociated or diffused into the glass, especially in the case of alkali-containing silicate glasses; in addition, glass itself can have some hydrous species in the subsurface or bulk. The glass composition, thermal history, surface treatment, and environment condition can also affect the water adsorption and reaction behavior. We employed vibrational SFG spectroscopy, and other spectroscopy techniques that provide complementary information, to investigate water adsorption and reaction at the multicomponent silicate glasses containing leachable alkali ions. These studies revealed a unique role of the alkali ion leaching and exchange on the activity of water at glass surfaces, which could be correlated with surface mechanical and mechano-chemical properties of glass surfaces.

#### **1:50 PM**

#### **(GOMD-S4-016-2016) Impacts of Aqueous Chemical Treatments and Aging on Glass Durability and Surface Appearance of Silicate Glasses**

A. Li<sup>\*1</sup>; Y. Jin<sup>1</sup>; X. Guo<sup>1</sup>; S. Chen<sup>1</sup>; K. Hughes<sup>1</sup>; J. Hou<sup>1</sup>; 1. Corning Incorporated, USA

As part of the development of technical glasses for industrial applications, glass surfaces could be chemically strengthened and polished, and then undergo various aqueous chemical treatments for either cleaning purpose or stripping coatings from glass surfaces. After the treatments, glasses are required to remain good optical transparency for practical applications. In an effort of better understanding the relationship of aqueous chemical treatments and aging effects on glass surface appearance as a function of pristine glass surfaces, here we prepared polished and fusion-drawn glasses and exposed them to a wide variety of acidic and basic media. We discuss the impacts of aging and polishing on glass chemical durability of the silica glasses and connect the chemical durability data to the optical properties (particularly on glass transparency, color drift and haze) of treated surfaces.

#### **2:10 PM**

#### **(GOMD-S4-017-2016) Surface Chemistry of Calcium Aluminosilicate Glasses in Response to Aqueous Corrosion**

D. Kramer<sup>\*1</sup>; J. Kopatz<sup>1</sup>; C. G. Pantano<sup>1</sup>; 1. Pennsylvania State University, USA

The purpose of this work is to characterize the surface chemistry of calcium aluminosilicate glass surfaces in aqueous solutions across the pH range. A systematic series of glass compositions were studied e.g. constant silica content, variable non-bridging oxygen content, and a 1:1 CaO/Al<sub>2</sub>O<sub>3</sub> series. Glass surfaces studied include melt and polished surfaces which were then exposed to solutions of variable pH in both static and dynamic flow conditions, as well as to humidity. XPS surface compositional analysis, variable-angle XPS, infrared spectroscopy and solution analysis were used to obtain information about surface composition, in-depth leaching, hydration, and dissolution. In the absence of in-depth leaching of cations in strong acid and water, as observed for sodium aluminosilicate glasses under these conditions, the nature and extent of water reaction at and in the glass surface has been the focus of this study.

#### **2:30 PM**

#### **(GOMD-S4-018-2016) Angle-Resolved X-Ray Photoelectron Spectroscopy and Low-Energy Ion Scattering of Alkali-free Display Glasses**

C. V. Cushman<sup>1</sup>; N. J. Smith<sup>2</sup>; B. Sturgell<sup>1</sup>; G. I. Major<sup>1</sup>; B. M. Lunt<sup>1</sup>; P. Bruener<sup>3</sup>; J. Zakel<sup>3</sup>; T. Grehl<sup>3</sup>; M. R. Linford<sup>\*1</sup>; 1. Brigham Young University, USA; 2. Corning Incorporated, USA; 3. ION-TOF, Germany

Display glasses are extensively used as substrates for consumer electronics, where their surface composition(s) influences the manufacturing of the displays and their resulting performance. These compositions can be altered by various wet-chemical or gas-phase treatments. We have applied angle-resolved X-ray photoelectron spectroscopy (AR-XPS) and low-energy ion scattering (LEIS) to evaluate the surface of a model display glass, Corning Eagle XG, at different information depths. AR-XPS probes the outer ca. 2-10 nm of materials, and by taking data at multiple angles, information about compositional gradients is obtained. LEIS uses a beam of low-energy noble gas ions to probe the outermost atomic layer of materials. Because of its extreme surface sensitivity, there is often a direct correlation between elemental composition from LEIS and many surface phenomena, including wetting and adhesion. Samples analyzed here included the as-formed surface, a fracture surface, and surfaces exposed to HF, HCl, and tetramethylammonium hydroxide (TMAH). AR-XPS shows a gradient in the concentration of network modifiers in the as-formed surface relative to the fracture surface, as well as leaching of network modifiers during aqueous treatments. LEIS shows significant variations in the concentrations of network modifiers at the outermost surface as a function of surface preparation.

#### **2:50 PM**

#### **(GOMD-S4-019-2016) Chemometric Analysis of Time-of-flight Secondary Ion Mass Spectrometry Data from Display Glass Surfaces**

M. R. Linford<sup>\*1</sup>; C. V. Cushman<sup>1</sup>; B. Sturgell<sup>1</sup>; G. I. Major<sup>1</sup>; B. M. Lunt<sup>1</sup>; P. Bruener<sup>2</sup>; J. Zakel<sup>2</sup>; T. Grehl<sup>2</sup>; N. J. Smith<sup>3</sup>; 1. Brigham Young University, USA; 2. ION-TOF, Germany; 3. Corning Incorporated, USA

The surface composition of display glasses strongly influences the manufacturing process for making electronic displays and the performance of finished devices. This composition can be altered by exposure to wet-chemical or gas-phase treatments. We have probed the composition of the outer ca. 2 nm of a model display glass, Eagle XG, using time-of-flight secondary ion mass spectrometry (ToF-SIMS). Samples analyzed include the as-formed surface, a fracture surface, and surfaces exposed to aqueous chemistries, including HF, HCl, and tetramethylammonium hydroxide (TMAH). Both ToF-SIMS static spectra and depth profiles were obtained.

\*Denotes Presenter

The data were analyzed with chemometric techniques that included principle components analysis (PCA), multivariate curve resolution (MCR), and cluster analysis. This analysis, including radar plots of the ToF-SIMS intensities of the cationic glass components, showed that the elemental composition of the as-formed surface varied substantially from that of the fracture surface, and that the chemical treatments significantly altered the surface composition. Brief HF and HCl treatment leached network modifying components from the glass, creating similar surface compositions despite significantly different extents of network dissolution. Depth profiles showed a gradient in composition in the near-surface region of the material under different conditions.

**3:30 PM**

### **(GOMD-S4-020-2016) Antimicrobial substrates made using an aqueous ion exchange process**

C. L. Chapman<sup>\*1</sup>; 1. Corning Incorporated, USA

The silver ion, Ag<sup>1+</sup>, is a well-known antimicrobial agent that can be incorporated into a glass surface through ion exchange. With the use of an aqueous ion exchange the desired properties of the glass are not adversely affected. This process can be used to produce antimicrobial glass for touch-sensitive display screen, non-touch-sensitive surfaces or as an additive in a material.

**3:50 PM**

### **(GOMD-S4-021-2016) Copper Oxide Thin Films on Glass via Chemical Solution Deposition**

Y. Gong<sup>\*1</sup>; P. Gao<sup>1</sup>; S. T. Misture<sup>1</sup>; N. Mellott<sup>1</sup>; 1. Alfred University, USA

Copper oxide nanomaterials can be used in a variety of electronics including sensors, actuators, supercapacitors and energy storage systems. Rapidly growing demand in consumer electronics require the ability to produce cost effective nanostructured thin films for flexible products including electronic paper, wearable displays, and smart devices. However, nanomaterial in particulate form, as prepared via wet chemistry, is not conducive to the processing of thin films or devices. In this study, a series of copper oxide nanostructured thin films were deposited on activated glass surfaces via chemical solution deposition. The structural and morphological properties of the resultant thin films were studied as a function processing variables; in particular surfactant identity. Thin film morphology was compared to morphology of particulates prepared by traditional wet chemistry approaches. In addition, the gas sensing properties of the copper oxide thin films were evaluated.

**4:10 PM**

### **(GOMD-S4-022-2016) Investigation of contact-induced charging kinetics on variably modified glass surfaces**

G. Agnello<sup>\*1</sup>; J. Hamilton<sup>1</sup>; R. Manley<sup>1</sup>; E. Stelsova<sup>1</sup>; W. LaCourse<sup>2</sup>; A. Cormack<sup>2</sup>; 1. Corning Incorporated, USA; 2. Alfred University, USA

The accumulation and dissipation of electrical charge on glass surfaces is of considerable academic and industrial interest. The purpose of the present article, is to report on the differences in charging kinetics of several flat alumina-borosilicate (low alkali content) glass surfaces via a rolling sphere test (RST) that have been physically and/or chemically modified by different approaches and exposed to variable environmental conditions (i.e. relative humidity). Methods used for surface modification include chemical etching (HF based chemistries of variable molarity) and plasma processing/thin film deposition (CH<sub>4</sub> via Reactive Ion Etch (RIE) and/or Atmospheric Pressure Plasma Chemical Vapor Deposition (APPCVD)). Trends in glass surface charge rates, along with corresponding surface resistivity, energy and zeta potential measurements indicate that glass surface, and perhaps bulk, chemistry (specifically a surface' reactivity/affinity with/to water) play critical roles in charge dynamics. Based on the results, we propose an ion-based transfer model facilitated by surface-water molecular interactions

as the primary mechanism responsible for contact electrification in glass-metal contact systems.

**4:30 PM**

### **(GOMD-S4-023-2016) Coating of Self-cleaning TiO<sub>2</sub>-SiO<sub>2</sub> Double Layers for the Photocatalytic Glass**

J. Kim<sup>\*1</sup>; H. M. Yadav<sup>1</sup>; B. Kim<sup>1</sup>; 1. University of Seoul, Republic of Korea

The self cleaning properties of the TiO<sub>2</sub>-SiO<sub>2</sub> double layer films prepared by sol-gel method was investigated. Thin films were prepared by spin-coating onto glass and then thermally treated at different temperatures. The cross-sectional structure of the films was observed by a SEM analysis. The upper TiO<sub>2</sub> layer has a thickness of ca. 75 nm with a base SiO<sub>2</sub> layer of ca. 215 nm. The surface roughness of the films was characterized by AFM. The root mean square surface roughness of the thin films was below 2 nm; which should enhance their optical transparency. The photo-induced super-hydrophilicity of the films were evaluated by water contact angle measurement in air. The prepared thin films showed very good hydrophilicity. The stable Si-OH groups and the photocatalytic TiO<sub>2</sub> layer maintains the hydrophilicity of the double layer films by decomposing organic contaminants on the film surface. Optical measurements reveals a high transparency of the prepared thin films. The photocatalytic activity of the films were studied by the photocatalytic degradation of methylene blue under UV light irradiations. The TiO<sub>2</sub>-SiO<sub>2</sub> double layer thin films are plausibly applicable for developing self cleaning materials in various applications such as windows, solar panels, and tiles.

## **Session 3: Challenges in Manufacturing II**

Room: Madison

Session Chairs: Mathieu Hubert, CelSian Glass & Solar; Andreas Prange, RWTH Aachen University

**1:20 PM**

### **(GOMD-S4-024-2016) Reactions Between Glass and Zirconia Refractory**

I. Peterson<sup>\*1</sup>; M. DeLamielleure<sup>1</sup>; M. Mack<sup>1</sup>; D. Schnare<sup>1</sup>; 1. Corning Incorporated, USA

Zirconia refractory used in melting tanks can dissolve into the molten glass, and create a zirconia-rich stream in the glass. In colder regions of the melting system, crystallization of zirconia and zircon can occur. Laboratory testing was used to determine solubility limits of zirconia in a borosilicate glass, and precipitate a variety of different crystal morphologies.

**1:40 PM**

### **(GOMD-S4-025-2016) Fine-Tuning of CTE in Ultra-Low Expansion Glass through Annealing (Invited)**

C. A. Duran<sup>\*1</sup>; 1. Corning Incorporated, USA

Ultra-Low Expansion, ULE<sup>®</sup> Glass is a titania-doped silica glass produced for high-end applications requiring extreme shape stability over time and when exposed to changes in temperature. The material has a temperature-dependent coefficient of thermal expansion,  $\alpha(T)$ , which crosses zero at a temperature close to 300 K, and acquires values in the scale of  $1 \times 10^{-9} \text{ K}^{-1}$  for excursions of several K around the zero-crossing temperature,  $T_{ZC}$ .  $T_{ZC}$  is controlled by small changes in the level of doping of the glass, and methods are in place that seek to ensure consistency within each run and over time as well. Application of ULE<sup>®</sup> Glass as the substrate material for masks and key components for Extreme UV semiconductor manufacturing tools poses new challenges to the glass producer. These tools require  $T_{ZC}$  within a range narrower than existing methods can routinely achieve. Moreover, different components may require different  $T_{ZC}$  values, multiplying the challenges around efficient glass production. We have sought to overcome these difficulties through a post-production annealing process, which predictably modifies the

$\alpha(T)$  curve and enables fine control of  $T_{zc}$  while allowing the glass furnaces to run a consistent process. We discuss how annealing can also improve the shape of  $\alpha(T)$  to obtain a lower value of the “CTE slope”,  $\partial\alpha(T)/\partial T$ , in order to enable the parts to remain undistorted when subject to heavier thermal loads.

2:20 PM

**(GOMD-S4-026-2016) Attracting New Talents: The Biggest Challenge in Glass Manufacturing?**

M. Hubert\*<sup>1</sup>; 1. CelSian Glass & Solar, Netherlands

Benefiting from its versatility and the vast array of properties and shapes it can present, glass is one of the most ubiquitous materials around us in our everyday life, and is found in countless applications. Over the past century, the glass industry lived a revolution, the discontinuous, labor-intensive glassmaking by glass blowers being progressively replaced by continuous and automated processes, run in increasingly performant furnaces, allowing for production of several hundreds of tons of glass per day for most of the furnaces. Despite the importance of its production, the glass industry expresses more and more difficulty in finding and attracting new talents, point of crucial importance for an industry in constant need for sustainability and innovation. Unfortunately, while education on glass science is overall enjoying a stimulating growth, education on glass technology is globally slowing down. To reverse this trend, several programs have been put in place recently. In this presentation, the challenge that broadcasting glass technology and attracting new talents represents is discussed. The efforts made by the different programs, recent and more established, are highlighted.

**Session 4: Glass Formulation II**

Room: Capitol B

Session Chairs: Isabelle Giboire, CEA; Claire Corkhill, University of Sheffield

1:20 PM

**(GOMD-S4-027-2016) Spectroscopic Characterization of the Effects of Sulfate Addition on the Structure of Silicate Glasses – a Raman, NMR and Neutron Diffraction Study**

S. Vaishnav\*<sup>1</sup>; E. Barney<sup>2</sup>; A. C. Hannon<sup>3</sup>; P. A. Bingham<sup>1</sup>; 1. Sheffield Hallam University, United Kingdom; 2. University of Nottingham, United Kingdom; 3. Rutherford Appleton Laboratory, United Kingdom

The high content of sulfate anions ( $\text{SO}_4^{2-}$ ) present in some High and Intermediate Level radioactive Wastes (HLW / ILW) that require vitrification can limit the waste loading of the glass wastefrom and pose environmental issues due to water soluble secondary phase formation. Our aim is to understand the mechanisms underlying the incorporation of sulfate ions in radioactive waste glasses and thus to develop enhanced glass formulations providing greater sulfate capacities. As one step towards developing this understanding we have studied structural changes in simple binary and ternary silicate glass compositions upon addition of sulfate ions. The incorporation and speciation of  $\text{SO}_4^{2-}$  in  $\text{R}_x\text{O-SiO}_2$  and  $\text{R}_x\text{O-MO-SiO}_2$  glasses where  $\text{R} = \text{Li, Na}$  and  $\text{M} = \text{Ca, Ba}$  has been investigated. Initial results and conclusions based on Raman spectroscopy,  $^{29}\text{Si}$  MAS-NMR and Neutron Diffraction will be presented.

1:40 PM

**(GOMD-S4-028-2016) Interactions between an aluminosilicate glass melt and molten metals investigated by SEM analysis for a nuclear issue**

P. Chevreux\*<sup>1</sup>; A. Laplace<sup>1</sup>; E. Deloule<sup>2</sup>; L. Tissandier<sup>2</sup>; 1. CEA, France; 2. CNRS, France

A new conditioning matrix is currently being developed to immobilize nuclear intermediate level waste by a vitrification process. High actinides concentrations (uranium and plutonium) are expected and the final waste package contains both a vitreous phase and a metallic

phase coming from the waste. During the high temperature elaboration process, glass and metal phases are melted together which imposes a strongly reducing environment to the glass melt. This might modify actinides' oxidation state and thus affect their solubility in the glass, as for uranium. Moreover, redox reactions induced by the metal may have a substantial impact on the glass composition and microstructure. Some metals, such as aluminum, are able to reduce some glass elements up to their metallic form. Therefore the question of glass-metal interactions mechanisms, glass descriptions and actinides localization is raised. This paper presents the glass-metal interactions study for  $\text{CaO-Al}_2\text{O}_3\text{-SiO}_2$  and  $\text{Na}_2\text{O-CaO-Al}_2\text{O}_3\text{-SiO}_2$  glasses and stainless steel-Cu-Al metals. Neodymium was added as uranium and plutonium surrogate into the glass network. Glass was put in contact with metals at 1400°C and a kinetic study was followed. A thermodynamic approach using phase diagrams led us to describe the involved mechanisms; in particular redox reactions and crystallized phases formation and dissolution.

2:00 PM

**(GOMD-S4-029-2016) Development of Iron Phosphate Waste Forms for a High  $\text{MoO}_3$  Collins-CLT Waste**

C. Kim\*<sup>1</sup>; J. Szabo<sup>1</sup>; A. Zervos<sup>1</sup>; J. Hsu<sup>2</sup>; J. Bai<sup>2</sup>; R. Brow<sup>2</sup>; 1. MO-SCI Corporation, USA; 2. Missouri University of Science and Technology, USA

Iron phosphate (FeP) waste forms with high solubility for  $\text{MoO}_3$ ,  $\text{Cs}_2\text{O}$ , and lanthanide oxides are proposed as alternatives to borosilicate glasses to encapsulate secondary wastes from the uranium extraction process for spent fuel rods. Loadings of the Collins-CLT waste simulant as high as 40 wt% were achieved in as-cast FeP waste forms with acceptable chemical durability. Glass formation, crystallization tendency, and chemical composition were characterized using a variety of analytical techniques, including X-ray fluorescence (XRF), scanning electron microscopy with energy dispersive spectroscopy (SEM-EDS), X-ray diffraction (XRD), high-performance liquid chromatography (HPLC), and micro-Raman spectroscopy. Physical properties and chemical durability of the FeP waste forms are also discussed.

2:20 PM

**(GOMD-S4-030-2016) Chemical durability of iron phosphate waste forms containing 40 wt% of a high  $\text{MoO}_3$  Collins-CLT waste**

J. Hsu\*<sup>1</sup>; J. Bai<sup>1</sup>; C. Kim<sup>2</sup>; R. Brow<sup>1</sup>; J. Szabo<sup>2</sup>; A. Zervos<sup>2</sup>; 1. Missouri University of Science and Technology, USA; 2. MO-SCI Corporation, USA

The secondary waste stream produced by a uranium extraction process includes high concentrations of  $\text{MoO}_3$ ,  $\text{ZrO}_2$ , lanthanide oxides and noble metals that have low solubilities in borosilicate glasses, but greater solubilities in iron phosphate glasses. The chemical durability of the iron phosphate waste forms containing up to 40 wt% of a high  $\text{MoO}_3$  Collins-CLT waste simulant was determined at 90°C using the product consistency test (PCT) and the more aggressive vapor hydration test (VHT) at 200°C. From the elemental release information collected in the PCT tests, and the corrosion rate and corrosion product information from the VHT tests, the long-term degradation mechanism for these iron phosphate waste forms will be described.

**Session 4: Glass Corrosion: General Aspects**

Room: Capitol B

Session Chairs: Joseph Ryan, Pacific Northwest National Lab; Cory Trivelpiece, Pennsylvania State University

2:40 PM

**(GOMD-S4-031-2016) The Dissolution Rate of a Several High-Level and Low-Level Waste Glass Compositions**

J. Neeway\*<sup>1</sup>; M. Asmussen<sup>1</sup>; J. Ryan<sup>1</sup>; 1. Pacific Northwest National Lab, USA

The initial dissolution rate of high- and low-level waste glasses in dilute conditions depends principally on temperature, pH, and glass

\*Denotes Presenter

composition. The effect of pH and temperature on the rate of glass dissolution can be quantified and implemented into an affinity-based rate law. However, it is not possible to know a priori the value of the pH and temperature parameters from a given glass composition. Therefore, for every new glass composition, tests must be conducted to quantify these parameters. These parameters are obtained either from single-pass flow-through tests or from static tests with very low surface-to-volume ratios. Additionally, for a functioning affinity-based rate law, the pseudoequilibrium constant for a given glass composition must be determined. The pseudoequilibrium constant for a given glass is of utmost importance because it is the concentration of solution orthosilicic acid at which the glass corrodes at the residual rate. In this presentation, we have consolidated the existing body of literature of rate law parameters for a select number of glass compositions and we present values for some new glass compositions. Our discussion will focus on the importance of test conditions used to collect these parameters and to identify possible dissolution trends based on the composition of the given glass.

**3:00 PM**

### **(GOMD-S4-032-2016) Evaluation of the behaviour of vitrified waste in the Belgian supercontainer disposal conditions**

K. Lemmens<sup>\*1</sup>; K. Ferrand<sup>1</sup>; S. Liu<sup>1</sup>; A. Elia<sup>1</sup>; 1. Belgian Nuclear Research Centre, Belgium

The Belgian reference design for geological disposal of vitrified High-Level Waste foresees the use of supercontainers with an Ordinary Portland cement based concrete buffer. The stability of the vitrified waste in this highly alkaline environment is being studied at the Belgian Nuclear Research Centre (SCK-CEN). A summary of results obtained so far is presented. The research program comprises tests with reference glasses in cement waters simulating the expected evolution of the concrete pore water, and simple KOH solutions. Tests were performed with and without hardened cement paste, in static and dynamic mode. Validation tests were performed in more realistic mock-up cells. The interpretation was supported by surface analyses and geochemical modeling. The resulting set of dissolution rates varies over 4 orders of magnitude and can be explained semi-quantitatively by known glass alteration mechanisms. Under in situ disposal conditions, the dissolution rate is expected to be initially high due to the high pH and pozzolanic reaction with portlandite, but to decrease with time, due to a conversion of the portlandite into C-S-H phases and an accompanying pH decrease. To reach low dissolution rates, the pH close to the pristine glass surface should decrease to  $\leq 11.5$  (at 30°C) by the sequence of glass-concrete interactions. Whether this is possible, remains to be demonstrated.

**3:40 PM**

### **(GOMD-S4-033-2016) Parameterizing a Glass Degradation Model**

W. Ebert<sup>\*1</sup>; 1. Argonne National Lab, USA

A simple model that captures key aspects and dependencies of glass degradation kinetics has been developed to provide radionuclide source term values for reactive-transport-based performance models. Those include the initial rapid dissolution in dilute solutions (Stage 1), the very slow dissolution in solutions with high dissolved silica contents (Stage 2 residual rate), and the increased dissolution observed to occur for some glass coincidentally with the precipitation of zeolitic secondary phase (Stage 3). The model utilizes analytical functions representing the dependence of the dissolution rates of relevant glasses on key environmental variables including temperature, pH, and certain solutes. Tests are in progress to determine the key variables affecting the dissolution rates in the three reaction stages. The model is compatible with methods to represent waste form degradation in repository system performance simulations. The modeling approach, tests being conducted to determine the analytical forms of the environmental dependences, and envisioned implementation of the glass degradation model in performance calculations will be described.

**4:00 PM**

### **(GOMD-S4-034-2016) Long term corrosion testing to assess durability of glass ceramics and glass waste forms**

C. L. Crawford<sup>\*1</sup>; C. M. Jantzen<sup>1</sup>; J. McCloy<sup>2</sup>; 1. Savannah River National Laboratory, USA; 2. Washington State University, USA

The use of long term corrosion tests and accelerated durability test conditions involving high surface area to volume (SA/V) ratios can be utilized to investigate waste-form performance beyond the initial stages of corrosion. Powdered, static leach tests are currently being conducted at the Savannah River National Laboratory on glass ceramics and glasses to investigate their long term performance. Ongoing leach tests conducted for over 2 years (SA/V \* t ~ 1.5E+06 day/m) are in progress for glass ceramics designed for incorporation of large volumes of fission products separated from nuclear fuel by aqueous processing. Accelerated leach tests involving high SA/V conditions for the Environmental Assessment (EA) glass and other Waste Compliance Plan (WCP) high-level waste surrogate glasses linked to Savannah River Site vitrification have also been performed up to 6 months with SA/V \* t ~ 1E+07 day/m. An additional corrosion study on a simplified (Na,Al/B,Si) glass fabricated at the Washington State University is in progress to provide long term corrosion data that can be compared to published forward dissolution rate data obtained from single-pass flow through (SPFT) testing. Leachate data and secondary surface phases will be presented as well as modeling results as they relate to the ALTGLASS database.

**4:20 PM**

### **(GOMD-S4-035-2016) Stage III Dissolution for High Level Waste (HLW) and Low Activity Waste (LAW) Glasses: Role of Leachate Hydroxide and Aqueous Aluminate**

C. M. Jantzen<sup>\*1</sup>; C. L. Crawford<sup>1</sup>; C. L. Trivelpiece<sup>1</sup>; 1. Savannah River National Laboratory, USA

The durability of high level nuclear waste (HLW) glasses must be predicted on geological time scales. Waste glass surfaces form hydrogels when in contact with water for varying test durations. As the glass hydrogels age some exhibit an undesirable resumption of dissolution at long times while others exhibit near steady state dissolution. Resumption of dissolution is associated with the formation of zeolitic phases while non-resumption of dissolution is associated with the formation of clay minerals. Hydrogels with a stoichiometry close to 2Al:Si (imogolite) have been shown to be associated with waste glasses that resume dissolution. Hydrogels with a stoichiometry of Al:1.3-2Si have been shown to be associated with waste glasses that exhibit near steady state dissolution at long times. The solubility of the gel depends on the alkalinity of the leachate. The gel ensures the supersaturation of the system with respect to silica and is considered the primary building unit needed to form a zeolite framework. However,  $\text{AlO}_2^-$  is considered the origin of the zeolite framework charge and alkali cations are considered the counterions for the framework charge. Most importantly, the  $\text{OH}^-$  is considered the mineralizer.

**4:40 PM**

### **(GOMD-S4-036-2016) Implementing the ANL Stage 3 Glass Dissolution Model**

W. Ebert<sup>\*1</sup>; J. Jerden<sup>1</sup>; 1. Argonne National Lab, USA

A conceptual model for the increased glass dissolution rate observed in many laboratory tests and referred to as "Stage 3" has been developed recently. The ANL Stage 3 model is being implemented using Geochemists Workbench and applied to the ALTGLASS data base of long-term glass dissolution results from modified product consistency tests (PCT). Test results in that data base show nearly constant low dissolution rates for all glasses initially, but the dissolution rates of some glasses suddenly increase to higher constant rates, whereas the dissolution rates of other glasses remain low. The Stage 3 model attributes the sudden and continued increase in dissolution rate to the coupling of glass dissolution kinetics with the nucleation and

growth kinetics of particular secondary phases, respectively. Glass dissolution and secondary phase nucleation and growth kinetics are all modelled to depend on the solution composition, but the three processes have different dependencies on the solution composition. The objective of the GW study is to identify solution constituents that affect the kinetics of each process and derive the analytical forms of the reaction affinity terms that trigger and maintain the Stage 3 dissolution rates that were measured in tests included in the ALTGLASS data base. These analytical forms are needed to calculate the long-term degradation behavior of waste glasses in disposal systems.

## **Symposium 5: Festschrift for Professor Donald R. Uhlmann**

### **Crystallization**

Room: Madison

Session Chair: Lisa Klein, Rutgers University

#### **3:40 PM**

#### **(GOMD-S5-001-2016) A random walk through Don Uhlmann's crystallization research (Invited)**

E. Dutra Zanotto<sup>\*1</sup>; 1. Federal University of São Carlos, Brazil

Understanding the conditions that favor vitrification (over crystallization) has been a long-standing scientific endeavor, which also has a very relevant bearing on glass technology. As a matter of fact, "crystallization" is the keyword most frequently used in scientific articles published over the past 200 years of glass science. Prof. Uhlmann's contributions to this field in the seventies and eighties were numerous and seminal. In this talk, I will review some of his most relevant papers on crystal nucleation, crystal growth and kinetics of glass formation, and contextualize them within the state-of-the-art on these subjects. I will also discuss some remarkable old and new findings on why certain glasses "never" crystallize, the Kauzmann paradox, and on our joint work on superconducting glass-ceramics.

#### **4:10 PM**

#### **(GOMD-S5-002-2016) A journey through time: Working with Don on time-dependent problems in nucleation, crystallization and glass formation (Invited)**

V. A. Shneidman<sup>\*1</sup>; 1. New Jersey Institute of Technology, USA

Topics include. Quenching of a Brownian oscillator – the minimal model for the quench- and heating rate dependence of specific heat during glass transition. Transient nucleation: retardation of viscosity. Reconstructing the low-temperature growth rates from two-step annealing experiments. Nucleation and crystallization during rapid quench and heating: suppression of nucleation by non-steady-state effects, violation of adiabatic scaling and increase of the Avrami exponent. Implications for DTA. Some recent updates.

#### **4:40 PM**

#### **(GOMD-S5-003-2016) Statistical approach to crystal nucleation in silicate glasses (Invited)**

J. Deubener<sup>\*1</sup>; S. Krüger<sup>1</sup>; 1. Clausthal University of Technology, Germany

In order to study a stochastic phenomenon such as nucleation in silicate glasses it is necessary to collect data from a large set of nucleation events. Isothermal and isochronal (constant cooling rate) experiments are performed with the same small volume of a supercooled liquid under exactly the same conditions by repeating a thermal cycle for many times (> 300). This allows to measure induction times of crystal nucleation with statistical relevance at relative low degrees of supercooling. Results in glass ceramic model systems show an Poisson distribution of induction times in both types of experiments even when heterogeneous nucleation is occurring at the same favourable site. Nucleation histograms were

found to be free of memory effects confirming the stochastic nature of the nucleation process. Induction time statistics are essential for deriving continuous cooling-transformation (CCT) and isothermal time-temperature transformation (TTT) curves but they can be seen as a supplement to Uhlmann's kinetic treatment of glass formation, too.

### **Poster Session and Student Poster Competition**

Room: Senate A/B and Assembly

#### **(GOMD-S1-P001-2016) Glass stability, crystal growth rate and microstructure after isothermal crystallization of glasses in the system Na<sub>2</sub>O-CaO-SiO<sub>2</sub>**

E. B. Ferreira<sup>\*1</sup>; 1. EESC-USP, Brazil

It is a common sense that the higher the concentration of calcium and sodium in compositions of the system Na<sub>2</sub>O-CaO-SiO<sub>2</sub>, the more their glass forming ability deteriorates. However, there is still lack of information on the crystal growth rate and glass stability of glass forming compositions in this important system. Recently, we measured the glass stability and isothermal crystal growth of compositions in the phase compatibility triangle: CaO.SiO<sub>2</sub>-Na<sub>2</sub>O.2CaO.3SiO<sub>2</sub>-Na<sub>2</sub>O.3CaO.6SiO<sub>2</sub>, or CS-N<sub>1</sub>C<sub>2</sub>S<sub>3</sub>-N<sub>1</sub>C<sub>3</sub>S<sub>6</sub>, for compositions N<sub>1-x</sub>C<sub>2</sub>S<sub>3+x</sub>, where x = 0, 0.17, 0.33 and 0.5. Now, we extend the study for a set of compositions encompassing the whole sub-system CS-N<sub>1</sub>C<sub>2</sub>S<sub>3</sub>-N<sub>1</sub>C<sub>3</sub>S<sub>6</sub>. The glass forming ability was estimated from glass stability (GS) parameters calculated from the characteristic temperatures: glass transition, crystallization onset and liquidus obtained by differential scanning calorimetry (DSC). The microstructure of crystallized samples was characterized by optical and scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS). The crystal growth rate was obtained from the thickness of crystallized layers on the surface of samples isothermally treated at different temperatures and time periods. We present results aiming at understanding the transformation kinetics, nature and morphology of crystals in the microstructure.

#### **(GOMD-S1-P002-2016) Crack initiation in metallic glasses under nanoindentation**

Y. Yang<sup>1</sup>; J. Luo<sup>2</sup>; L. Huang<sup>1</sup>; G. Hu<sup>2</sup>; K. Vargheese<sup>2</sup>; Y. Shi<sup>1</sup>; J. C. Mauro<sup>\*2</sup>; 1. Rensselaer Polytechnic Institute, USA; 2. Corning Incorporated, USA

Simulated nanoindentation tests on a modified Lennard-Jones metallic glass reveal the initiation of crack occurs from the shear band area through cavitation process. The critical load at which crack initiates varies with the indenter geometry. A critical indentation size can be defined to account for the indenter geometry effect on the crack initiation load. Thermomechanical conditions of the shear-band area where crack initiates were determined to show that the crack initiation for different indenter geometry can be explained using cavitation stress. It is found that the cavitation is dictated by the normal stress component perpendicular with the shear band and the cavitation stress is reduced significantly by shear.

#### **(GOMD-S1-P003-2016) Determination of the Network Dilation Coefficient in Ion-Exchanged Glass**

S. Tietje<sup>\*1</sup>; R. Schaut<sup>1</sup>; 1. Corning Incorporated, USA

The network dilation coefficient quantifies the dimensional strain that occurs with chemistry changes. Traditionally this coefficient is determined by measuring molar volume differences of melt-derived glasses of sequential chemistry. This approach generally produces values that are about 3 times greater than those determined through stress profile measurements after ion-exchange. Here we demonstrate a new approach to its determination through characterization of molar volume, composition, and use of a novel ion-exchange process. The results will be discussed with respect to various historical approaches and changes in glass structure.

\*Denotes Presenter

### (GOMD-S2-P004-2016) Effect of $P_2O_5$ - $SiO_2$ -based bioglass powder preparation route on body formation by $Yb^{3+}$ -doped fiber laser

J. Wang<sup>\*1</sup>; 1. NSYSU, Taiwan

As known, bioglass can provide many favor bio-active properties which could be very attractive for tissue engineering. These include highly tunability in glass toward various requirements of surface reactivity, in vivo resorption, bonding to hard and soft tissue, and tissue-bioglass interaction. In this study, we would like to investigate the effect of  $P_2O_5$ - $SiO_2$ -based bioglass compositions and their preparation routes on the bioglass body formation by  $Yb^{3+}$ -doped fiber laser. Glass compositions to be studied include  $18Na_2O-25MgO-4P_2O_5-53SiO_2$ ,  $6Na_2O-12K_2O-25MgO-4P_2O_5-53SiO_2$ ,  $18Na_2O-5MgO-20CaO-4P_2O_5-53SiO_2$ , and  $6Na_2O-12K_2O-5MgO-20CaO-4P_2O_5-53SiO_2$  (all in wt %). Because a clearer fundamental understanding the correlation among composition, preparation route, and final body formation could be important to further developing better processing control and performance of bioglass body for various bone healing applications (bone grafting, implantation, etc.). In the report, the dependence of structural properties (shape, porosity, and strength) of final body of the  $P_2O_5$ - $SiO_2$ -based bioglasses on initial glass powder size, proportions of hydroxypropyl-cellulose-based thickener, ammonium polyacrylate (dispersant), and water-ethanol solution, and pH would be reported. Then their correlations aiming to better bioglass body formation will be discussed.

### (GOMD-S3-P005-2016) Chalcogenide Fibers and Fiber Bundles for Mid-infrared Applications

Z. Yang<sup>\*1</sup>; B. Zhang<sup>1</sup>; C. Zhai<sup>1</sup>; S. Qi<sup>1</sup>; H. Ren<sup>1</sup>; W. Guo<sup>1</sup>; Y. Yu<sup>2</sup>; B. Luther-Davies<sup>3</sup>; G. Tao<sup>3</sup>; D. Tang<sup>1</sup>; 1. Jiangsu Normal University, China; 2. The Australian National University, Australia; 3. University of Central Florida, USA

Step-index chalcogenide glass fibers for mid-infrared supercontinuum generation were designed and fabricated. By pumping an optimized fiber at its anomalous dispersion region using a femto-second laser, a SC spanning from 2 to  $12\mu m$  and with an average power of about 20mW was achieved. High-resolution chalcogenide fiber bundles for infrared imaging were designed and fabricated. The fiber bundles consisted of more than 20,000 single fibers with a diameter of less than  $20\mu m$ , had an active area of more than 50%, showed a resolution of more than 20 lp/mm and presented a crosstalk of less than 2.5%. Fine thermal images of hot objects were delivered through the fiber bundles.

### (GOMD-S3-P006-2016) Optical Properties of Zinc Tellurite Glasses doped with $Ni^{2+}$ ions

O. Zamiatin<sup>\*1</sup>; E. Torokhova<sup>1</sup>; I. Fedotova<sup>1</sup>; A. Sibirkin<sup>1</sup>; 1. Lobachevsky State University of Nizhni Novgorod, Russian Federation

Tellurite glasses possess some of specific properties which make them an attractive material for optical applications. But the impurity atoms of transition metals provides a high level of optical losses in tellurite glasses. The purpose of this research was to prepare zincate-tellurite glasses doped with  $Ni^{2+}$  ion to study their optical properties. The presence of nickel ions in the glasses provides the intensive absorption bands with maxima at 430, 800 and 1310 nm in the transmission spectra. The specific absorption rate of  $Ni^{2+}$  ions was calculated from the spectra of glass samples containing variable quantities of the dopant. The  $Ni^{2+}$  minimum content in the glass to ensure the preset level of optical losses was estimated. The nickel ions were found to be the strongly absorbing impurities and their content was to be controlled carefully. The  $Ni^{2+}$  ions content contributes much to the value of energy gap. The reported study was funded by RFBR according to the research project 16-03-00785 a.

### (GOMD-S3-P007-2016) Specification of the glass-forming range of the $TeO_2$ - $MoO_3$ - $Bi_2O_3$ system and the characterization of the glasses prepared

O. Zamiatin<sup>\*1</sup>; E. Torokhova<sup>1</sup>; I. Fedotova<sup>1</sup>; A. Sibirkin<sup>1</sup>; 1. Lobachevsky State University of Nizhni Novgorod, Russian Federation

The particular properties of tellurite glasses determine the possibility of their use as a material for manufacturing of optical fibers and amplifiers. The addition of bismuth or molybdenum oxide to tellurite glasses increase the stability of these glasses to crystallization and modifies their optical and thermal properties. The purpose of this work was to find out the boundaries of the glass-forming range in the triple system  $TeO_2$  -  $MoO_3$  -  $Bi_2O_3$  and to study of the properties of the glasses. The possibility of conversion the tellurium (IV), molybdenum(VI), and bismuth(III) oxides mixture into stable glasses was proved. The nature of the successive crystalline phases which form in the course of heating of the initial oxide mixture up to the preparation of a glass-forming melt was elucidated. The glasses of the triple system described was prepared to study of their optical transmittance over the entire transparency range. The values of the energy gap width elicited from optical measurements showed their dependence on the composition of the glass. It was noticed that the increase in the content of molybdenum trioxide in the system shifts the glass short wave boundary cutoff to longer wavelengths. The thermal properties of glasses were studied by DSC method. The reported study was funded by RFBR according to the research project No. 16-33-00187 mol\_a.

### (GOMD-S3-P008-2016) Design, synthesis and characterization of innovative glasses with erbium-doped nanoparticles

P. Lopez Iscoa<sup>1</sup>; L. Petit<sup>2</sup>; J. Massera<sup>4</sup>; D. Milanese<sup>\*1</sup>; G. Baldi<sup>3</sup>; M. Salvo<sup>1</sup>; M. Ferraris<sup>1</sup>; 1. Politecnico di Torino, Italy; 2. nLight, Finland; 3. Colorobbia S.p.A., Italy; 4. Tampere University of Technology, Finland

In the development of optical devices based on Rare Earth (RE) ions, the local environment around the RE is of paramount importance for determining the optical properties. Recently, nanoparticles approaches to manufacture doped optical fibres have been shown to improve doping efficiency. Using nanoparticles, it is also possible to control the rare-earth optical response independently of the core glass matrix composition. This new doping technology opens a supplementary degree of freedom in the design of novel active optical fibres, which could be used as sensors for monitoring muscles or ligaments movements. We report on the synthesis of novel active glasses based on the incorporation of erbium-doped nanoparticles. Different techniques of fabrication of micro and nanoparticles were explored and compared using soft chemistry.  $Al_2O_3$ ,  $TiO_2$  were selected as crystalline hosts for the erbium ions. Phosphate glasses were selected as host materials and were fabricated by melt-quenching techniques. The doping of the micro and nanoparticles was carried out. Preliminary results concerning structural, optical and spectroscopic properties are reported. The project leading to this result has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 642557.

### (GOMD-S3-P009-2016) Direct Measurement of Photo-Elastic Processes in Chalcogenide Glasses

P. Lucas<sup>\*1</sup>; P. Deymier<sup>1</sup>; G. Coleman<sup>1</sup>; N. Boechler<sup>2</sup>; A. Khanolkar<sup>2</sup>; 1. University of Arizona, USA; 2. University of Washington, USA

Light-induced control of phonon transport in materials is key to the realization of novel phenomena such as loss-less transport of acoustic waves or opto-acoustic devices such as tunable phononic filters. Here we present the first direct measurements of photo-elastic processes in Ge-Se glasses using a transient grating method to directly measure the speed of acoustic waves propagating through the glass during irradiation. Large changes in elastic constant are observed upon irradiation and these changes are shown to increase exponentially with intensity of irradiating light. The compositional dependence of this process is also investigated through the Ge-Se



system and a direct correlation is observed between the covalent network coordination and the magnitude of change in elastic constant. No effect is observed at the rigidity percolation threshold. These observations are consistent with the composition and intensity dependence of other photo-structural effects such as photo-fluidity, photodarkening or photo-expansion.

**(GOMD-SP-001-2016) Characterisation of glass alteration layers: A combined microscopic and spectroscopic approach**

D. J. Backhouse<sup>1</sup>; C. L. Corkhill<sup>\*1</sup>; P. Zeng<sup>1</sup>; N. C. Hyatt<sup>1</sup>; R. J. Hand<sup>1</sup>;  
1. University of Sheffield, United Kingdom

The long-term behaviour of glass, important in both nuclear waste and archaeological applications, is governed by the alteration of the surface by aqueous solutions, such as groundwater. An alteration layer, comprising elements from both the glass and the solution, is understood to play an important role in long-term glass alteration, although the exact details of this role and the mechanisms of formation are heavily debated. Despite the great number of glass dissolution experiments reported in the literature, analysis of the alteration layer is not often reported. The hydrated gel layer is fragile and susceptible to damage when prepared for microscopy; the largely amorphous nature of the layer provides challenges in composition identification; and when crystalline materials are formed, their size is often below the resolution for conventional diffraction techniques. We present alteration layer analysis of natural and nuclear waste simulant glasses formed during dissolution in alkali media. Characterisation of a basaltic glass, the International Simple Glass and the UK simulant high level waste glass, MW25, was performed using <sup>11</sup>B, <sup>29</sup>Si and <sup>27</sup>Al NMR. Analysis of crystalline phases in the alteration layer was performed using TEM in conjunction with selective area electron diffraction. We also present a novel analysis of the alteration layer using synchrotron-based  $\mu$ -XRD.

**(GOMD-SP-002-2016) Medium-Range Structure of Zr-Cu-Al Bulk Metallic Glasses from Structural Refinement Based on Fluctuation Electron Microscopy**

J. Maldonis<sup>\*1</sup>; P. Zhang<sup>1</sup>; M. Besser<sup>2</sup>; M. Kramer<sup>2</sup>; P. Voyles<sup>1</sup>; 1. University of Madison, Wisconsin, USA; 2. Ames Laboratory, USA

Bulk metallic glasses (BMGs) show a variety of outstanding properties including high yield strength, high elastic limit, and excellent nanoprocessability. However, applications of BMGs are limited by the high critical cooling rates required to avoid crystallization and create a glass. We aim to identify important links between structure and glass-forming ability by combining experimental data from fluctuation electron microscopy (FEM) with simulated system energies from an empirical interatomic potential in a hybrid reverse Monte Carlo (HRMC) structural refinement. Within HRMC, FEM data constrain the medium-range order of the structure, and the potential constrains the short-range and chemical order. The result is an atomistic model with realistic structure at multiple length scales. We have studied the structures of two Zr-Cu-Al BMGs, both of which show two competing forms of nanoscale structure, one icosahedral, and the other more crystal-like. In  $Zr_{50}Cu_{35}Al_{15}$ , the poorer glass former, the crystal-like structure is more stable under annealing below the glass transition temperature than in  $Zr_{50}Cu_{45}Al_5$ , the better glass former. From these correlations in structural trends during annealing, we find that destabilizing crystal-like structures may be more important to high glass forming ability than enhancing non-crystalline structures.

**(GOMD-SP-003-2016) Optimization of Quantitative Analysis of Glass Surfaces with Electron Probe Microanalysis**

L. M. Neill<sup>\*1</sup>; O. K. Neill<sup>1</sup>; J. Weaver<sup>1</sup>; J. Reiser<sup>1</sup>; N. Wall<sup>1</sup>; 1. Washington State University, USA

Silicate glasses are considered an acceptable host for high level nuclear waste, but continued research into the rates and mechanisms associated with the alteration of these waste forms is necessary to understand their long-term viability as waste storage media. Studies

of such glasses involving both solid and solution analysis are used to understand the alteration behavior of glasses under aqueous conditions. Previous work (Weaver et al., 2015) showed the quantitative determination of the composition of both altered and unaltered glass surfaces by electron probe microanalysis and wavelength dispersive X-ray spectroscopy (WDS) with a simple six-oxide glass form known as International Simple Glass. While this study was able to accurately determine the composition of heavier elements in borosilicate glasses (i.e. silicon, aluminum, and calcium) it is more difficult to quantify boron due to boron's low fluorescent yield, the low energy of its  $K\alpha$  line, the strong absorbance of the B  $K\alpha$  by the sample matrix, and issues of peak shift and shape effects on measure B via WDS, which limit the sensitivity of WDS measurements of boron (McGee and Anovitz, 1996). Variables such as the type of diffracting crystal used to measure boron, background corrections, and electron beam conditions are all considered to optimize a procedure to determine the boron concentration within the total glass composition.

**(GOMD-SP-004-2016) Surface diffusion of molecular glasses and its material dependence**

W. Zhang<sup>\*1</sup>; S. Ruan<sup>1</sup>; Y. Chen<sup>1</sup>; L. Yu<sup>1</sup>; 1. University of Wisconsin-Madison, USA

Molecular glasses are useful for drug delivery, organic electronics, and food formulations. In all these applications, the amorphous materials must resist crystallization. Motivated by recent observations of fast surface crystallization, we have systematically studied the surface diffusion of molecular glasses and its impact on physical stability. Surface-grating decay was used to measure surface diffusion coefficients of molecular glasses. Wavelength dependence of decay rate was used to identify the conditions under which surface diffusion is the mechanism for surface evolution (low temperatures and short wavelengths). Surface diffusion coefficients have been measured for organic glasses composed of molecules of different sizes and abilities to form hydrogen bonds. The results show that surface diffusion of molecular glasses can be 5 – 8 orders of magnitude faster than bulk diffusion. We also find that surface diffusion slows down with the increase of molecular size and hydrogen bonding, whereas bulk diffusion has a weaker material dependence. The molecular size effect is attributed to a sharp mobility gradient beneath the surface and deeper penetration of larger molecules. These results are relevant for predicting the rates of surface crystallization and the ability to form stable glasses by vapor deposition.

**(GOMD-SP-005-2016) Raman spectroscopic and high-pressure liquid chromatography study of the structures of Na<sub>2</sub>O-MoO<sub>3</sub>-Fe<sub>2</sub>O<sub>3</sub>-P<sub>2</sub>O<sub>5</sub> glasses**

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Chemically durable iron phosphate glasses have displayed great potential for accommodating nuclear waste streams, including those with significant concentrations of species like MoO<sub>3</sub> that have low solubilities in borosilicate melts. To better understand how the incorporation of waste components affect structure and properties, four series of Na<sub>2</sub>O-MoO<sub>3</sub>-Fe<sub>2</sub>O<sub>3</sub>-P<sub>2</sub>O<sub>5</sub> glasses were prepared with constant concentrations of Na<sub>2</sub>O (0-22.5 mole%) and with MoO<sub>3</sub> replacing Fe<sub>2</sub>O<sub>3</sub> in three sub-series with constant nominal O/P ratios of 3.1, 3.25 and 3.4. Raman spectroscopy indicates that the type of molybdate species incorporated into the glass depends on the Na<sub>2</sub>O content and that smaller phosphate anions are present in glasses with greater O/P ratios; the latter observation was confirmed by the high-pressure liquid chromatography results. Compositional trends in glass properties, including glass transition temperature and chemical durability, will be explained using this structural information.

### (GOMD-SP-006-2016) Dynamic Light Scattering in Mixed Na-Zn Metaphosphate Melts

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Dynamic light scattering has been conducted on a series of mixed metaphosphate glass melts of the form  $[\text{Zn}(\text{PO}_3)_2]_y[\text{NaPO}_3]_{1-y}$  near the glass transition point. Scattering provides a representation of the liquid's dynamic structure factor from which the relaxation time and KWW stretching exponent can be evaluated as a function of temperature. The fragility of each glass composition has been determined and is compared with values recently reported in the literature as well as with predictions of a coarse-grained connectivity model. We observe that the fragility of the  $\text{NaPO}_3$  is systematically decreased by the introduction of 4-coordinated Zn units that increase the average bridging oxygen bond density. This decrease with increasing connectivity is consistent with model predictions.

### (GOMD-SP-007-2016) Possible Existence of Two Amorphous Phases of D-Mannitol Related by a First-Order Transition

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We report that the common polyalcohol D-mannitol may have two amorphous phases related by a first-order transition. Slightly above  $T_g$  (284 K), the supercooled liquid (SCL) of D-mannitol transforms to a low-energy, apparently amorphous phase ("Phase X"). The enthalpy of Phase X is roughly halfway between those of the known amorphous and crystalline phases. The amorphous nature of Phase X is suggested by its absence of birefringence, transparency, broad X-ray diffraction, and broad Raman and NIR spectra. Phase X has larger molecular spacing, higher molecular order and stronger hydrogen bonds (HBs) than the SCL. On fast heating, Phase X transforms back to the SCL near  $T_g + 50$  K. Upon temperature cycling, it shows a glass-transition-like change of heat capacity. Near IR reveals that SCL-to-Phase-X transition is a two-state, nucleation-growth process with breaking of intra- and formation of inter-molecular HBs. The presence of D-sorbitol enables the observation of a first-order liquid-liquid transition from the SCL to Phase X. The SCL-to-Phase X transition has intriguing similarities with polyamorphic transitions reported for triphenyl phosphite and water. This is the first report of possible polyamorphism for a substance of pharmaceutical relevance. As amorphous solids are explored for many applications, polyamorphism could offer a tool to engineer the properties of materials.

### (GOMD-SP-008-2016) Lithium Oxy-Thio Borate Glasses for Glassy Solid-State Electrolytes

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Ion-conductive  $0.7\text{Li}_2\text{S} + (1-x)\text{B}_2\text{S}_3 + x\text{B}_2\text{O}_3$  glasses have been prepared for testing as solid-state lithium battery electrolytes. Samples were either annealed in a 140-160 °C brass mold or quenched at room temperature. For annealing, samples were cooled to 30 °C at 1 °C/min. Infrared spectroscopy confirmed higher molar ratios of  $\text{Li}_2\text{S}$  and  $\text{B}_2\text{S}_3$  in the annealed glass compared to  $\text{B}_2\text{O}_3$ . Pour method, mold design, and melt temperature were adjusted to produce strong, void-free disk samples. Differential scanning calorimetry revealed onset  $T_g$ 's and  $T_c$ 's of ~170 °C, and ~230 °C, respectively. Increasing mole fraction of  $\text{B}_2\text{O}_3$  dramatically reduced sample transparency. Yet, powder x-ray diffraction showed amorphous structure past onset of opaque appearance. Improved sample strength also accompanied increasing mole fraction of  $\text{B}_2\text{O}_3$ . Pours of  $x \geq 0.09$  required higher melt temperature, due to greater viscosity.

### (GOMD-SP-009-2016) Effect of transition metals addition on structural and mechanical properties of three-alkali zinc borate glass system

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Studies on structural and mechanical properties of three-alkali zinc borate glass system with nominal composition  $5\text{Li}_2\text{O}-5\text{K}_2\text{O}-20\text{Na}_2\text{O}-60\text{B}_2\text{O}_3-9.9\text{ZnO}-0.1\text{M}$  (M= Cr, Mn, Fe, Co and Ni) are reported. The samples were prepared using standard melt quenching technique. X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Density measurement, Fourier transform infrared (FTIR) spectroscopy and Vickers indentation studies were performed to investigate the effect of transition metal on three alkali zinc borate glass system. XRD measurements confirmed the amorphous nature of prepared glasses, SEM images have not shown any precipitates and aggregates which indicated the homogeneity of glasses. Variation of density may be attributed to the respective ionic radii of transition ions. FTIR studies confirmed the presence of both  $[\text{BO}_3]$  and  $[\text{BO}_4]$  units, indicating the present glass networks to be made up of these two units placed in different structural groups. The variation of peak positions of B-O-B bending and stretching of  $[\text{BO}_3]$  and  $[\text{BO}_4]$  units of each glass sample explain the role of modifier alkali elements and transition ions. The micro-hardness and fracture toughness of the samples were measured using Vickers micro indentation technique.

### (GOMD-SP-010-2016) Fracture of molecular glasses under tension and fracture-induced crystallization

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Molecular glasses are formed and fractured by cooling a liquid on a less thermally expansive substrate. In-plane tension is created by the mismatch of thermal expansion coefficients and accumulates to cause catastrophic network fracture. This simple experiment allowed the first measurement of fracture toughness and the heat of fracture of molecular glasses. For the systems studied (o-terphenyl, indomethacin, and sucrose benzoate), the fracture condition is well described by recent theories and a material-specific energy release rate (fracture toughness)  $G_c$ . Small-molecule glasses are highly brittle, with  $G_c \approx 1 \text{ J/m}^2$ , and can be made significantly tougher with the addition of polymers. The heat of fracture was found to be anomalously large relative to the value expected for the fracture energy release rate and the surface area created. The large release of heat is caused by the reduction of heat capacity for a glass film constrained on a rigid substrate. Rapid crystal growth was observed along fracture surfaces.

### (GOMD-SP-011-2016) Structure - Property Relationships in Borosilicate and Aluminosilicate Glasses

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Silicate glasses are by far the most important materials for the US glass industry and various other non-industrial technological applications. In particular, alkali/alkaline-earth borosilicate and aluminosilicate glasses form the basis for some of the most advanced technological applications including display glasses, glasses for nuclear waste immobilization, and ultra-strong glasses. Since the macroscopic properties of a glass are a direct result of its underlying structure, it is crucial to understand the structure - property relationships of glasses in order to engineer them for advanced technological applications. With this perspective, our work focuses on understanding the influence of glass structure on thermal, physical and mechanical properties of melt-quenched ternary alkali borosilicate and aluminosilicate glasses, including their selected silica-rich binary end members. The as-obtained results from these studies will be presented at the symposium.

**(GOMD-SP-012-2016) Topological Control on Borosilicate Glass Dissolution Kinetics**

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Driven by the need of corrosion-resistant glasses, e.g., for nuclear waste immobilization, improving the intrinsic chemical durability of glasses in aqueous environment is of fundamental and practical interest. However, the relation between composition, structure, and durability remains poorly understood. In this study, we investigate the chemical durability of sodium calcium borosilicate glasses by coupling dissolution rates, measured by vertical scanning interferometry (VSI), with topological constraint theory, which captures the essential features of the atomic topology that govern the dissolution behavior, while filtering out less relevant structural details. Based on our newly developed empirical potential for modified borosilicate glasses, the chemical topological constraints of glasses are evaluated using molecular dynamics simulations. The observed linkage between topological constraints and dissolution rates provides a realistic model to predict glass compositions with improved intrinsic chemical durability.

**(GOMD-SP-013-2016) Densification of ZnS-CaLa<sub>2</sub>S<sub>4</sub> infrared composite optical ceramics**

Y. Li<sup>\*1</sup>; Y. Wu<sup>1</sup>; 1. Alfred University, USA

Zinc sulfide (ZnS) and calcium lanthanum sulfide (CaLa<sub>2</sub>S<sub>4</sub>) are both suitable for the applications as infrared optical materials because of their good optical transmittances in the infrared range. In the present study, ZnS-CaLa<sub>2</sub>S<sub>4</sub> infrared composite optical ceramics have been fabricated through a pressure-assisted sintering (hot pressing and field-assisted sintering) of the mixed ZnS-CaLa<sub>2</sub>S<sub>4</sub> powders. The effects of densification conditions and ZnS/CaLa<sub>2</sub>S<sub>4</sub> composition ratios on the ZnS sphalerite-wurtzite phase transition were investigated by phase composition analysis through X-ray diffraction. The investigation has also sought to uncover the densification mechanism by analyzing the microstructural features and densities of the as-sintered ZnS-CaLa<sub>2</sub>S<sub>4</sub> composite ceramics in order to further study the influences of different ZnS/CaLa<sub>2</sub>S<sub>4</sub> compositions on microstructural evolution during the sintering. Furthermore, the optical and mechanical properties were characterized to achieve a better understanding on the correlation between compositions, phases, microstructure and properties of the ZnS-CaLa<sub>2</sub>S<sub>4</sub> composite ceramics.

**(GOMD-SP-014-2016) Sintering and mechanical properties of mineral-glass composites for development of engineered stones**

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Engineered stones are composite materials made of crushed minerals combined with a resin binder. They have been increasingly used in decoration and interior design due to easy handling, aesthetic appeal and a smaller degree of environmental impact in comparison to natural stones, such as granite and marble. However, the use of polymer resins brings some disadvantages such as degradation by UV exposure, permanent damage when submitted to high temperatures and low scratch resistance. In this work we aim to develop engineered stones composed of different minerals by replacing the polymer by an inorganic glass matrix. Minerals with distinct thermal expansion coefficients were selected and their sintering behavior when mixed with different quantities of glass, the level of residual stress and the resulting flexural strength were investigated. Compositions were weighted, homogenized and manually pressed in a stainless steel mold at 25 MPa in the form of cylindrical pellets that were analyzed by heating stage optical dilatometry. The sintering behavior for the samples was similar: the onset temperature lies between 820-850°C and the linear shrinkage reaches 15% at 1075°C. The density and porosity were determined by Archimedes principle and image analysis, respectively, and the best results are p

= 2.26 g/cm<sup>3</sup> with 5% porosity. The best result for flexural strength was 64 MPa.

**(GOMD-SP-015-2016) Interpretation of space charge potential in ceramics with a presence of an electric field**

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The space charge and other related dielectric properties hold a long discussion for ceramic materials. However, there has been little work done on the optical ceramics. Because the solid-state processing, densification and grain boundary behaviors are some key research indexes with respect to dielectric properties for optical ceramics, it is necessary to investigate the contribution of space charge to optical-grade ceramics or single- and poly-crystal conjunction towards a fully converted single crystal. In this regard, an external electric field was applied on Sr<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>F materials with different crystal conjunctions and green body geometries during sintering and heat-treatment processing. The space charge potential was interpreted by two approaches. In the first approach, a space charge potential associated with reduced capillary force was estimated from isothermal grain growth. In the second approach, the samples were examined by AC impedance spectra and the space charge potential was obtained directly from grain and grain boundary resistivity. Furthermore, the cation diffusion, solute drag and grain orientation misfit were considered in an attempt to correlate the calculated space charge potential with that obtained experimentally.

**(GOMD-SP-016-2016) Mechanical properties of silver nanoparticle embedded BaO-CaF<sub>2</sub>-P<sub>2</sub>O<sub>5</sub> glasses**

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Silver-doped glasses of composition 30BaO-20CaF<sub>2</sub>-50P<sub>2</sub>O<sub>5</sub>-4Ag<sub>2</sub>O-4SnO were prepared by conventional melt-quenching method. Silver doped glasses were heat treated for a fixed duration of 10 h at temperatures 500 °C, 525 °C and 550 °C to embed silver nanoparticles of different sizes into the glass matrix. Nanoindentation and microindentation techniques were used to investigate mechanical properties of prepared samples. Young's modulus, Vickers hardness and fracture toughness increased while brittleness decreased with increase in heat treatment temperature, which can be ascribed to the increase in size of nanoparticles embedded in the glass matrix with temperature. Median-radial cracks generated around the indentations on the surface of samples were further analysed using scanning electron microscopy (SEM) to confirm the reduction in brittleness of glasses. Transmission electron microscopy (TEM) analysis of samples confirmed the formation of well dispersed and non-agglomerated spherical silver nanoparticles inside the matrix. The observed mechanical properties could be explained based on the size of silver nanoparticles in the glass matrix.

**(GOMD-SP-017-2016) Structural Study of Tellurite Glasses**

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Tellurite glasses show the potential for use in mid-infrared optical applications, but their structure has not been intensively studied. While they do not conduct light better than chalcogenides, which are currently the best glasses for infrared optics, they are much easier to produce. Alkaline earth tellurite glasses, including single component, rapidly cooled TeO<sub>2</sub> are reported and studied here. Specifically barium, strontium, calcium, and magnesium tellurites were evaluated. The results include Tg measurements, Raman spectra and resulting structural models are discussed. Acknowledgement: The NSF is thanked for support under grant number DMR-1407407.

**(GOMD-SP-018-2016) Metal-to-Insulator Transition in Conducting Bridge Memory Materials**

K. Prasai<sup>\*1</sup>; B. Bhattacharai<sup>1</sup>; G. Chen<sup>1</sup>; D. Drabold<sup>1</sup>; 1. Ohio University, USA

Silver-doped chalcogenide glasses are used in conducting bridge random access memory (CBRAM) materials. The conductivity

\*Denotes Presenter

of these materials can change by a factor of  $10^6$  on a nanosecond time scale under an external bias. This remarkable transition from metallic phase to insulating phase is a complex process involving both ionic as well as electronic conductivities and depends on many details of the network. In this work, we investigate both types of conductivities as a function of silver concentration and discuss the characteristics of the network close to this transition. We discuss the role of phase separation, silver trapping, voids etc on the conductivity of these materials. And, finally we present the results of employing a novel method of gap engineering to explore the most-conducting and most-insulating configurations of these materials. All calculations are carried out with plane-wave LDA.

### **(GOMD-SP-019-2016) Pores arising due to non-isothermal crystallization of diopside glass particles**

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Glass particles with the diopside stoichiometric composition present only surface crystallization. On sufficiently large particles, i.e., with a size much larger than that of crystals growing on their surface, the crystals grow until they impinge with each other, forming a continuous layer which afterwards continues to grow into the interior of the particles. When the crystals have a density much higher than the glass, the growing layer gives rise to tensile stresses in the glass, which is finally relieved by the formation of a pore in the interior of the particles. Pores arising due to isothermal crystallization of diopside glass particles have been studied theoretically and experimentally in the literature. In the present work, we evaluate the arising of pores in diopside glass particles with different sizes due to non-isothermal crystallization. Diopside glass particles with different sizes from 7 to 650  $\mu\text{m}$  were compacted and heat treated for crystallization at 10 C/min up to different maximum temperatures, set according to DSC crystallization peaks, and then quenched in air. The microstructure evolution due to crystallization and pore formation was evaluated by microscopy. A comprehensive study is presented and discussed.

### **(GOMD-SP-020-2016) Surface diffusion and crystallization of molecular glasses**

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Surface diffusion has been studied for molecular glasses tris-naphthylbenzene (TNB) and PMMA oligomers ( $\sim 1$  kg/mole) by surface grating decay. Surface diffusion on TNB is vastly faster than bulk diffusion, by a factor of 107 at  $T_g$ , while the process is very slow on PMMA. TNB and other small-molecule glasses show fast crystal growth on the free surface. We find a general relation between the coefficient of surface diffusion and the velocity of crystal growth on the free surface. This relation holds for 4 molecular glasses (o-terphenyl, indomethacin, nifedipine, and TNB) and amorphous silicon. The relation indicates that fast surface crystallization is supported by high surface mobility.

### **(GOMD-SP-021-2016) Crystallization of iron-containing sodium aluminosilicate glasses**

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From both geological and technological viewpoints, Fe is a significant transition metal which affects the crystallization behavior of silicate melts. In this study, the effects of Fe addition and heat-treatment on crystallization of sodium-aluminosilicate glasses were investigated using X-ray diffraction (XRD) and Vibrating-sample magnetometry (VSM) methods. Melt-quench methods were used to prepare nepheline-( $\text{NaAlSiO}_4$ ) based glasses with the compositions of  $\text{NaAl}_{1-x}\text{Fe}_x\text{SiO}_4$ , as well as a few other stoichiometric higher Si sodium-iron-silicates ( $\text{NaFeSi}_2\text{O}_6$  and  $\text{Na}_3\text{FeSi}_4\text{O}_{12}$ ). Heat treatments were performed at select temperatures (700-1000°C) and in some cases different atmospheres (air, nitrogen). Results show

that for high values of Fe ( $x > 0.2$ ), quenched glasses contain some Fe-containing crystals. Increasing the heat treatment temperature and addition of Fe promote the crystallization of the nepheline phase for low values of Fe and suppress it for high values of Fe. XRD suggested traces of magnetite crystallization for heat treated low-Fe samples, specifically for those in reducing atmosphere, as the main phase responsible for magnetism. However, magnetic measurements indicate existence of more than a single magnetic phase and/or behavior. Therefore, applying VSM as a complementary method, we conclude that magnetite may not be the only Fe-containing phase in the present glass-ceramics, and hematite is suspected.

### **(GOMD-SP-022-2016) Experimentally constrained materials modeling: Application to disorder and glassy materials**

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An ideal approach to computational modeling of complex amorphous materials should incorporate state-of-the-art total energy and force methods and the judicious application of a priori information—experimental data pertaining to the material. When these schemes are suitably merged, the resulting structural models should reflect our full state of knowledge about the material. This has led to the development of hybrid approaches that successfully couple a total-energy functional (quantum mechanical or otherwise) with a priori information. We apply these methods to amorphous silicon (a-Si), amorphous carbon (a-C) and amorphous silica (a-SiO<sub>2</sub>). We employ structural information from neutron or x-ray diffraction experiments, and electronic information from photoemission spectroscopy. Here, we present preliminary examples of these techniques.

### **(GOMD-SP-023-2016) Study of thermal stability and optical properties of phospho-silicate glasses**

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60SiO-(30-x) ZnO-xCaO-10P<sub>2</sub>O<sub>5</sub> (x = 8, 6, 4, 2) glasses with varying compositions of Calcium Oxide and Zinc Oxide are synthesized using Sol-gel technique. Sol-gel is a chemical solution process used to make ceramic and glass materials in the form of thin films, fibers, or powders. Thermal stability and optical properties of Phospho-Silicate glasses have been analyzed using Fourier Transformation Infrared Spectroscopy (FTIR), Differential Thermal Analysis (DTA) and UV- visible spectroscopy characterization technique. The dual role of divalent ion ZnO in modifying the optical band gap energy and increase in the chemical durability of this present glasses with the fixed Phosphosilicate content and significant increase in ZnO have been studied. The optical properties of zinc Phosphosilicate glasses is studied in the range of visible and ultraviolet spectrum. Therefore, Differential Thermal Analysis with changing glass transition temperature indicates towards structural rearrangement of network and stability of studied glasses with the addition of ZnO.

### **(GOMD-SP-024-2016) Sol-gel Derived Alumina-rich Binary Aluminosilicate Glasses**

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Alumina-rich aluminosilicate glasses hold great promise as highly efficient optical fibers. Glasses and glass-ceramics with high alumina compositions are also candidates for high-temperature applications due to potential high mechanical and chemical stability. However, due to the onset of rapid crystallization during melt cooling possibly preceded by the thermodynamically predicted liquid-liquid immiscibility region at the alumina-rich end of this binary phase diagram, conventional methods of glass melting and quenching are not adequate to produce amorphous materials with alumina contents higher than approximately 60mol%. A bottom-up approach provides a pathway to access these metastable amorphous states in the temperature range where glass-in-glass immiscibility is predicted. Low-temperature sol-gel synthesis is an effective method

for studying glassy materials at the alumina-rich region of the binary alumina-silica system as it allows for the production of high-purity materials while circumventing potential regions of liquid-liquid immiscibility often encountered during melt-quenching. In this work, we used sol-gel synthesis to make alumina-rich glassy materials with compositions ranging from 60 to 90mol% alumina. The glass powders were then characterized in order to better understand the microstructure of such materials and the effects of high temperature heat treatments on the evolution of the microstructure.

**(GOMD-SP-025-2016) Formation of liquid-crystalline structures in glasses**

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Some liquids transform to liquid crystals upon cooling. Such transformations are typically so fast that it is difficult to avoid them. Itraconazole, an anti-fungal drug, offers an interesting counterexample. Upon slow cooling, itraconazole undergoes an isotropic/nematic transition, a nematic/smectic transition, and finally the glass transition ( $T_g = 329$  K). At sufficiently fast cooling rate ( $>100$  K/min), however, the system enters the glassy state without developing the smectic order. This property allows us to study the formation of liquid crystals in a glass and compare the behavior with the formation of normal crystals. Differential Scanning Calorimetry and X-ray Diffraction were used to follow the development of the smectic phase of itraconazole and its orientation. We find very different behaviors depending on the temperature of annealing. Above  $T_g$ , the smectic order emerges gradually on a timescale that approximately tracks the structural relaxation time. The presence of a free surface tends to organize the smectic layers parallel to it. Below  $T_g$ , however, glass aging is observed, but there is no evidence for the smectic order to develop. These results are relevant for understanding the stability of molecular glasses against crystallization and suggest that the formation of liquid crystals can differ from the formation of normal crystals.

**(GOMD-SP-026-2016) Ce<sup>3+</sup> Luminescence in UV Transparent Phosphate Glasses**

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The ability to be produced with considerably lower cost, large areas, and tailored size and shape is increasing the interest in the development of glass scintillators as an alternative to single crystals. Ce-doped phosphate glasses were investigated focusing on the effect of different modifiers on their optical properties and luminescence. Two series of glasses were prepared aiming at the detection of gamma-rays taking advantage of high Z elements Ba and Pb: 50 or 60 mol%  $PO_4 + 5, 15$  or 25 mol%  $SiO_2 + 9$  or 19 mol% BaO or PbO + 15 mol%  $Al_2O_3 + 1$  mol%  $CeO_2$  such to add up to 100 mol%. Structural characteristics determined by Raman spectroscopy were coupled with results from photoluminescence and UV-visible transmission measurements, while the index of refraction was estimated using the Gladstone-Dale relation using experimentally obtained density values. The optical and luminescence behavior were found to depend on the chemical composition, with the transmission cutoff wavelength being  $\sim 317$  nm for the Ba series and within 316-332 nm for the Pb series. Luminescence of the Ba series was centered within 340-355 nm and for the Pb series within 355-375 nm besides being considerably broader and asymmetric. Further, the luminescence results were analyzed within the framework of the optical basicity toward developing predictive capability for the search of suitable luminescent glasses.

**(GOMD-SP-027-2016) Effect of iron content on the structure and disorder of iron-bearing sodium silicate glasses: Insights from high-resolution solid-state NMR study**

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Understanding the structure and disorder of iron-bearing glasses remains a difficult problem in geochemistry and glass science. Here, we present high-resolution  $^{29}Si$  and  $^{17}O$  solid-state NMR spectra of iron-bearing sodium silicate glasses with varying iron content (up to 22.9 wt%  $Fe_2O_3$ ). For both nuclides, a decrease in the NMR signal intensity with increasing iron content is prevalent due to paramagnetic effect. The observed trend of the  $^{29}Si$  NMR intensity with varying iron content suggests that the effective paramagnetic radius (within which paramagnetic interactions result in signal loss) can be larger than  $\sim 1$  nm. Despite the intrinsic difficulties that result from paramagnetic effect, the NMR results yield structural details regarding the Q speciation, spatial distribution of iron, and the extent of polymerization in the iron-bearing glasses. The  $^{29}Si$  and  $^{17}O$  NMR results indicate that the degree of polymerization apparently increases by replacing  $Na_2O$  with  $Fe_2O_3$  and that  $Fe^{3+}$  is predominantly a network-former. The  $^{17}O$  NMR results suggest a moderate degree of preferential partitioning of iron and local oxygen clusters while maintaining nanoscale homogeneity in the glasses. While further efforts are certainly necessary, the present results hold strong promise for studying iron-bearing glasses using solid-state NMR.

**(GOMD-SP-028-2016) Novel Approach to Crystal Derived Optical Fibers**

M. A. Tuggle<sup>\*1</sup>; J. Ballato<sup>1</sup>; 1. Clemson University, USA

Recent years have seen significant growth in the demands for higher performing optical fibers necessitating new materials and fabrication processes. Materials previously thought to be impossible to incorporate into a core for a fiber are now possible using the molten core method. In this method a precursor core material is sleeved inside a glass cladding tube. The core is molten at the draw temperature of the cladding. As the fiber cools, the molten core quenches and glass compositions not permissible due to immiscibilities or instabilities are possible. In an effort to reduce diffusion of the cladding material into the core melt, thereby shifting its composition upon drawing a preform to a fiber, high purity aluminum foil in various thicknesses were used in an attempt to better oxide migration into the core of a yttrium aluminum garnet (YAG) derived core. Energy dispersive x-ray spectroscopy was performed to analyze the compositions of the fibers. Results relating to the amount of diffusion of the silica into the core, as well as fiber performance will be discussed.

**(GOMD-SP-029-2016) Recycling solid wastes into high strength glass foams**

Y. Gong<sup>\*1</sup>; R. Dongol<sup>1</sup>; C. Yatongchai<sup>2</sup>; A. W. Wren<sup>1</sup>; S. K. Sundaram<sup>1</sup>; N. Mellott<sup>1</sup>; 1. Alfred University, USA; 2. Maejo University, Thailand

Solid wastes are primarily disposed into landfills, and only small proportions of them are recycled. Recycling the solid wastes increases the cost-efficiency of desired recycle-end product and minimizes the potential environment impact on the landfill sites. In this study, the concept of recycled materials was adopted to fabricate novel glass foams: green body composed of pulverized waste amber glass and porcine bone is sintered at 850 °C for 600 seconds. Prepared glass foams were thermally, structurally and mechanically characterized to investigate the processing-property relationship. High flexural strength values between  $16.71 \pm 1.73$  and  $29.69 \pm 3.23$  MPa were reported for glass foams prepared in this study. In particular, the glass foams show potential to be used in a variety of advanced structural and energy material systems, given their unique properties including heat retardation, sound adsorption and shock-wave adsorption.

## (GOMD-SP-030-2016) Physical properties and Structure of Sodium Borogermanate Glasses as Part of the Mixed Glass Former Effect

D. Hynek<sup>1</sup>; D. Shadle<sup>1</sup>; G. Bohach<sup>1</sup>; S. Verkey<sup>1</sup>; S. Keizer<sup>1</sup>; J. Wang<sup>1</sup>; S. Feller<sup>1</sup>; M. Affatigato<sup>1</sup>; S. Kmiec<sup>2</sup>; K. Hakanson<sup>2</sup>; C. Francis<sup>2</sup>; S. W. Martin<sup>2</sup>; 1. Coe College, USA; 2. Iowa State University, USA

Glass electrolytes are crucial for creating alkaline-Ion batteries and fuel cells that are cheaper, more stable, and have increased Ion conducting capabilities. We have been examining the Mixed Glass Former Effect (MGFE), which is defined as the non-linear, non-additive trend in physical properties of systems with more than one glass former as a function of modifier content. Sodium borosilicate glasses are relatively well studied due to their presence in industry. In light of this and because Christiansen et al. have recently completed a n MGFE study of these borosilicates, analogue sodium borogermanate glasses were chosen for study due to their favorable glass forming characteristics and since this system has been relatively understudied. Density, glass transition temperatures ( $T_g$ ), Raman spectra, and the fraction of four-coordinated boron from NMR measurements were obtained for the sodium borogermanate system. Analysis of data collected suggests that there is a positive MGFE in regards to  $T_g$  and four-coordinated boron concentrations, and negative in terms of density. Acknowledgements The National Science Foundation is thanked for support under grant DMR 1407404

## (GOMD-SP-031-2016) Influence of transition metal oxide on the properties and dissolution behaviors of simplified high-level nuclear waste glasses

X. Lu<sup>1</sup>; J. Neeway<sup>2</sup>; J. Ryan<sup>2</sup>; J. Du<sup>1</sup>; 1. University of North Texas, USA; 2. Pacific Northwest National Lab, USA

Transition metal oxides are commonly present in nuclear waste and they can alter the structure, property and especially dissolution behaviors of the glasses to immobilize these wastes. In this paper, we investigated vanadium and cobalt oxide induced changings on physical properties and dissolution behaviors of International Simple Glass (ISG), a model nuclear waste glass system. Static chemical durability tests were performed at 90 °C with a PH value of 7 and a surface-area-to-solution-volume of 200 m<sup>-1</sup> for 112 days, on three samples: ISG, 0.5 mol% Co<sub>2</sub>O<sub>3</sub> doped ISG and 2.0 mol% V<sub>2</sub>O<sub>5</sub> doped ISG. ICP-MS was used to analyze the dissolved ion solutions and it was found that both doping with vanadium and cobalt oxide reduce the leaching rate. The normalizes mass loss of Na and B decreases as comparing with undoped ISG, while there is no significant influence on Ca. Differential Scanning Calorimetry (DSC) curves showed that V doping could reduce the transition temperature ( $T_g$ ) of ISG and the effect became significant with increasing dopant amount, while Co doping slightly increased the  $T_g$  of ISG. In addition, solid characterization indicated that X-ray diffraction (XRD) and Raman spectrometer couldn't identify secondary phases in our experiment due to the large amount of amorphous phases.

## (GOMD-SP-032-2016) Effect of composition and heat treatment on the microstructure and properties of $\text{Li}_{1-x}\text{Al}_x\text{Ge}_{2-x}(\text{PO}_4)_3$ NASICON structured glass-ceramics solid-state electrolytes

P. Kuo<sup>1</sup>; J. Du<sup>1</sup>; 1. University of North Texas, USA

All solid state lithium ions batteries represent a new generation of energy storage systems that provide higher safety, energy density and thermal stability as compared to conventional lithium ion batteries. NASICON structured glass-ceramics is a promising solid electrolyte.  $\text{Li}_{1-x}\text{Al}_x\text{Ge}_{2-x}(\text{PO}_4)_3$  samples were prepared in different ratios of Phosphate and Germanium and different heat treatment schemes to investigate the effect of composition and treatment schemes on phase composition. Differential scanning calorimetry (DSC) was used to obtain characteristic temperatures and activation energies for crystallization by using modified Kissinger equation. X-ray diffraction (XRD) and scanning electron microscope (SEM) were used to characterize phase composition and microstructures of the samples after heat treatment. All the samples crystallizes the

high lithium ion conductive phase  $\text{LiGe}_2(\text{PO}_4)_3$ , and the highest phase purity was observed in P/Ge range of 2.3 to 2.4, instead of the commonly used composition with P/Ge ration of 2.0.

## (GOMD-SP-033-2016) Probing Inhomogeneity of Glasses by Small-angle X-ray Scattering

M. Sundararajan<sup>1</sup>; H. Abu Jeib<sup>1</sup>; G. Chen<sup>1</sup>; 1. Ohio University, USA

Small-angle X-ray Scattering (SAXS) is an effective technique for studying heterogeneous glasses, especially those with nanostructures. In this poster, we show a few examples of application of SAXS to the study of heterogeneous glasses such as two-phase glasses, glass ceramics, nanoporous glasses and ion-diffusion-induced heterogeneous glasses. A tabletop SAXS system was employed and structural information such as shape and size distribution of the inhomogeneous features is obtained. The results are used to explain interesting phenomena in glass and glass-related materials.

## (GOMD-SP-034-2016) Effect of the Surface Topology on the Reactivity of Silica: Insights from Reactive Molecular Dynamics

Y. Yu<sup>1</sup>; B. Wang<sup>1</sup>; M. Wang<sup>1</sup>; M. Bauchy<sup>1</sup>; 1. University of California, Los Angeles, USA

Glassy silica is the base material for various silicate glasses of geological and technological interest. As it is often exposed to humid conditions, which can, e.g., induce stress corrosion, understanding the mechanism and extent of its surface reactivity is of primary importance. Here, based on reactive molecular dynamics simulations relying on the ReaxFF potential, we bring new insights on the hydration mechanism of silica. We find that the predicted surface density of hydroxyl groups is in good agreement with experimental data. In addition, we investigate the effect of annealing (from 700 to 1600 K) on the surface topology and reactivity. Annealing is found to decrease the number of surface defects (non-bridging oxygen and under-coordinated silicon atoms), thereby increasing the connectivity and stability of the exposed surface. This induces a decrease of the number of possible adsorption sites which, ultimately, reduces the reactivity of the surface. This study suggests new routes to understand and tune the surface reactivity of disordered silicate materials.

## (GOMD-SP-035-2016) Study of the 2<sup>nd</sup> order nonlinear optical properties (SONL) induced in thermally poled alkali-doped chalcogenide glasses

A. Lepicard<sup>1</sup>; F. Adamietz<sup>1</sup>; V. Rodriguez<sup>1</sup>; K. Richardson<sup>2</sup>; M. Dussauze<sup>1</sup>; 1. University of Bordeaux, France; 2. University of Central Florida, USA

Integrated photonics, optoelectronics and photonics are technological domains where candidate materials demand specific control of optical properties. Chalcogenide glasses (ChGs) are widely considered for these applications due to their large transparency window in the infrared. In this talk, we discuss use of a thermal poling process to tune the optical properties of these glasses. Thermal poling induces a strong static electric field in the glass which allows for Second Harmonic Generation (SHG) through a process known as Electric Field Induced Second Harmonic (EFISH). As the main issue in thermally poled ChGs is the rapid decay of the SHG, we focused on the stability and origin of this SHG. ChGs lack the cationic conductivity necessary for an effective poling, the strategy in this effort has been to dope glasses from the ternary Ge-Sb-S with Na<sub>2</sub>S. Stable glasses were obtained and characterized using Raman and IR spectroscopy. After poling, the nonlinear response was measured using the Maker fringes technique. Several contributions to the signal were observed. A first contribution was linked to the expected EFISH process. In addition, a contribution in the plane of the surface, usually absent has been found. These contributions are highly Na-dependent. This exploratory study gives us a possibility to better control the process of thermal poling in ChGs.

**(GOMD-SP-036-2016) Mesoscale Structure Engineering in Photonic Glass for Tunable Luminescence**Y. Yu\*<sup>1</sup>; S. Zhou<sup>1</sup>; J. Qiu<sup>1</sup>; 1. South China University of Technology, China

Novel light sources emitting in the near-infrared spectral range are especially attractive, due to their important application in the biological and optical telecommunication. The existing methods for the fabrication of these special material candidates mainly involve the management of active centers, including exploitation of novel dopants, combination of multiple dopants and modulation of their energy transfer. Although numerous efforts have been made, the development of advanced materials with satisfactory bandwidth and flat feature remains an arduous task. Here, we describe an effective strategy for management of photon emission by manipulation of mesoscale heterogeneity in optically active materials. We present experimental observation and mechanistic investigation of emission control through phase tailoring in unique multi-phase glasses. We demonstrate that the mesoscale engineering approach results in dramatic inhomogeneous spectral broadening, and for the first time show success in simultaneously extending emission bandwidth and flattening spectral shape. Our results highlight that the findings connect the understanding and manipulation at the mesoscale realm to functional behavior at the macroscale, and the approach to managing the dopants based on mesoscale engineering may provide new opportunity for construction of robust fiber light source.

**(GOMD-SP-037-2016) Phosphate glass-clad  $\text{Se}_x\text{Te}_{1-x}$  semiconductor core optical fibers**G. Tang\*<sup>1</sup>; Q. Qian<sup>1</sup>; Z. Yang<sup>1</sup>; 1. State Key Laboratory of Luminescent Materials and Devices and Institute of Optical Communication Materials, South China University of Technology, China

In recent years, glass-clad semiconductor core optical fibers have attracted great attention for their potential utility as novel waveguides for applications in nonlinear optics, mid-infrared power delivery, sensing, biomedicine, optical switch, and photodetecting devices. Phosphate glass-clad optical fibers comprising  $\text{Se}_x\text{Te}_{1-x}$  ( $x=0, 0.8, 1$ ) semiconductor core were fabricated by using conventional fiber fabrication techniques. Both of the Se core ( $x=1$ ) and  $\text{Se}_{0.8}\text{Te}_{0.2}$  ( $x=0.8$ ) core of as-drawn fibers were found to be amorphous, while the Te core ( $x=0$ ) of as-drawn fibers was confirmed to be crystalline. Phase-pure Se crystals and  $\text{Se}_{0.8}\text{Te}_{0.2}$  crystals can be precipitated in their core region by a postdrawing annealing process. A two-cm-long crystalline  $\text{Se}_{0.8}\text{Te}_{0.2}$  semiconductor core optical fiber, electrically contacted to external circuitry through the fiber end facets, exhibits two-orders-of-magnitude change in conductivity between dark and illuminated. The great discrepancy in light and dark conductivity suggests that such crystalline  $\text{Se}_{0.8}\text{Te}_{0.2}$  semiconductor core optical fibers have promising applications in optical switch and photoconductivity of optical fiber array. This work verifies that by fine-tuning the initial core composition of Se and Te powder and using the reactive molten core method, it can tune the photoconductivity of optical fibers which containing crystalline Se-Te alloy semiconductor core.

**(GOMD-SP-038-2016) Phosphate single core and core-clad fiber: impact of fibers immersion in TRIS on light loss and mechanical properties**A. Mishra\*<sup>1</sup>; F. Smektala<sup>2</sup>; J. Massera<sup>1</sup>; 1. Tampere University of Technology, Finland; 2. Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB), France

Phosphate based glasses (PBG) have been found to be good alternative to typical silicate bioactive glasses in medical applications. PBG were found to have thermal properties more suitable for fiber drawing than typical silicate bioactive glasses. Indeed, commercial silicate bioactive glasses were found to crystallize rapidly at temperatures at which they should be drawn into fiber from preform. PBG fibers could be used as bioactive reinforcing fiber in composite or biodegradable optical sensor. Here, glasses within the  $(1-x)(0.5\text{P}_2\text{O}_5+0.2\text{CaO}+0.2\text{SrO}+0.1\text{Na}_2\text{O}) + x(\text{CeO}_2)$  ( $x$  from 0 to 0.05 mol%) composition were studied in terms of their thermal and optical properties. Single core and core-clad (clad  $x=0$  and

core  $x=0.01$ ) fibers were drawn into fibers with 125  $\mu\text{m}$  diameter. Change in the thermal properties post drawing were evidenced by DTA. Fibers were then immersed in TRIS buffer solution and the changes in light loss as a function of immersion time were assessed using a broadband light source and a CCD spectrometer (from 200 to 1000 nm). In the case of the core-clad fiber the clad was etched away to reveal the core prior to the measurement. The mechanical properties (tensile strength and elastic modulus) of the fibers were estimated using an Instron mechanical tester. The impact of glass dissolution/reaction on the mechanical properties was assessed.

**(GOMD-SP-039-2016) Growth and characterization of vacuum sintering Pr/Ce-doped YAG transparent ceramic for the excellent white LED**Y. Tang\*<sup>1</sup>; S. Zhou<sup>1</sup>; X. Yi<sup>1</sup>; D. Hao<sup>1</sup>; S. Zhang<sup>1</sup>; 1. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, China

Abstract: Pr/Ce-doped YAG transparent ceramics are synthesized by the vacuum sintering method, and their crystal structure and morphology, luminescence properties, and the energy transfer between  $\text{Ce}^{3+}$  and  $\text{Pr}^{3+}$  are discussed. The characteristic emission peaks of  $\text{Pr}^{3+}$  ions at 608 nm and 638 nm are observed, and it can be attributed to the complicated energy-transfer. Therefore, white light-emitting diodes (LEDs) with improved color-rendering properties obtained by using modified  $\text{Pr}^{3+}$ -doped Ce:YAG phosphors. Furthermore, with the increase of  $\text{Pr}^{3+}$  doping concentration, the CRI (Color Render Index) increases and the emission intensity of  $\text{Ce}^{3+}$  ions decrease. The distribution densities and homogeneity of Pr and Ce ions in transparent ceramic also have been identified, and these influenced the result of luminous efficacy and CRI. The composite phase ceramic with  $\text{Al}_2\text{O}_3$  as the second phase distributed in Pr/Ce-doped matrix has been designed for improving the luminous efficacy.

**(GOMD-SP-040-2016) Low-temperature fluorescence of Pr-doped TAS glasses**C. Thomas\*<sup>1</sup>; Y. Shpotyuk<sup>2</sup>; R. Golovchak<sup>1</sup>; 1. Austin Peay State University, USA; 2. University of Rzeszow, Poland

Rare earth doped chalcogenide glasses are being extensively studied recently because of their potential applications in chemical monitoring and spectroscopy, detecting complex biological substances and lasers, optical amplifiers and broad band sources in the mid-infrared spectral range. In this regard, glasses of Te-As-Se (TAS) family have been proposed as perspective host matrix for rare earth, combining high infrared transparency, good fiber drawing capability and substantial glass stability. In this work we have investigated structural features and low-temperature (liquid nitrogen) fluorescence of TAS glasses doped with Pr. To improve solubility and spatial distribution of Pr in host glass matrix, small concentration of gallium was added to the initial glass compositions. The emission spectra were recorded in 1000-1700 nm range of wavelengths, using Horiba Fluorolog-3 spectrometer. The samples were immersed into liquid nitrogen and excited with light from 300-950 nm spectral range. At this cryogenic temperature distinct emission lines at 1.35  $\mu\text{m}$ , 1.42  $\mu\text{m}$  and  $\sim 1.52 \mu\text{m}$  can be resolved, which, presumably, correspond to electronic down-transitions to  $^3\text{H}_5$  level of  $\text{Pr}^{3+}$  ions. These fluorescent signals, however, vanish at room temperatures.

**(GOMD-SP-041-2016) Structure and properties of complex Bi-containing chalcogenide glasses**T. L. Hodge\*<sup>1</sup>; R. Golovchak<sup>1</sup>; Y. Shpotyuk<sup>2</sup>; B. Bureau<sup>3</sup>; H. Jain<sup>4</sup>; 1. Austin Peay State University, USA; 2. Centre for Innovation and Transfer of Natural Sciences and Engineering Knowledge, Poland; 3. Université de Rennes 1, France; 4. Lehigh University, USA

Bismuth is considered as a unique dopant in chalcogenide glasses, which can either modify or enhance their intrinsic physical properties. In particular, Bi can cause conduction type reversal from p- to n-type, or transform the glass into a topological insulator upon crystallization. Additionally, Bi-containing chalcogenide glasses are

\*Denotes Presenter

considered as the most promising bulk materials for thermoelectric applications. The high tendency of Bi to induce crystallization can be exploited to optimize the structure of Bi-containing glasses with nanocrystalline inclusions or compositional inhomogeneities, which then dramatically suppress the lattice thermal conductivity needed to achieve high thermoelectric figure of merit. In this work, we have investigated the structural modification of mixed Ge(As,Sb)-based selenides, tellurides and sulphides with additions of Bi, using X-ray photoelectron spectroscopy (XPS), Raman scattering and extended X-ray absorption fine structure (EXAFS) spectroscopy. The results show that Bi enters the glass network in the form of pyramidal units, most probably forming dispersed partially ordered nanophases. These nanodomains of trivalent Bi may be a reason for the conductivity percolation and type reversal in these glasses as well as their thermoelectric behavior. At higher concentrations, Bi triggers crystallization even during the quenching of melt.

### **(GOMD-SP-042-2016) Thermal Analysis of Borosilicate Glass for its Biological Applications**

K. S. Ranasinghe<sup>1</sup>; G. Humble<sup>1</sup>; D. E. Day<sup>2</sup>; 1. Kennesaw State University, USA; 2. Missouri University of Science & Technology, USA

Borosilicate glass doped with varying wt% of cerium oxide is investigated for biological applications. Thermal studies of each formulation were conducted using an SDT Q600 differential scanning calorimeter. 30mg samples of 350-425  $\mu\text{m}$  particle size of each type of glass were heated to 1200C in order to obtain the glass transition, crystallization, and melting temperatures. Samples were then heated to 900C at several heating rates, ranging from 2C/min to 100C/min, then compared against each other as well as against an undoped borosilicate glass.

### **(GOMD-SP-043-2016) Tellurium Vanadate Glasses: Conductivity, Structure, Decay**

L. McDonald<sup>1</sup>; S. Xian<sup>1</sup>; S. Feller<sup>1</sup>; C. Love<sup>2</sup>; B. Baker<sup>2</sup>; M. Affatigato<sup>1</sup>; 1. Coe College, USA; 2. William Jewell College, USA

The focus of this research is the binary tellurium vanadate glasses. These glasses are compositionally described by  $x\text{TeO}_2 - (1-x)\text{V}_2\text{O}_5$ . We report on the temperature-dependent conductivity, calculated from resistance measured by a modified furnace and electrometer setup. Alternating currents of 100 V also produced a decay curve that was then analyzed on the computer. Alongside these electrical measurements, the structure was studied through use of FTIR followed by multi-peak fitting. As chemical titration proved ineffective for determining the ratio of  $\text{V}^{4+}$  to  $\text{V}^{5+}$  in these tellurium-containing glasses, EPR was used to obtain the abundances of these different ionic species. The understanding of structure and  $\text{V}^{4+}/\text{V}^{5+}$  levels gives insight into why the glasses display the conductivity they do. This research was supported by Argonne National Laboratory under contract 3F-32104, the National Science Foundation under grant DMR-RUI 1407404, and Coe College.

### **(GOMD-SP-044-2016) Modelling thermally deposited chalcogenide glass thin films using time-dependent density functional theory**

L. R. Nichols<sup>1</sup>; J. R. Oelgoetz<sup>1</sup>; 1. Austin Peay State University, USA

It is well-known that thermally deposited chalcogenide glass thin films (ChGF) exhibit several photo-induced effects caused by modification of electronic and/or atomic structure under irradiation. The mechanism of the accompanied photostructural transformations is quite complex and not completely understood. It likely includes bond switching and defect formation processes both on the surface and the inside of ChGF. This work reports on the results of time-dependent density functional theory modeling which aims to illuminate the atomistic mechanisms behind these transformations. A handful of structures were first optimized using density functional theory. These structures were then re-optimized using time-dependent density functional theory with respect to the first electronic excited state. This optimal geometry was then used to seed a ground

state optimization. Raman spectra of structures that show bond switching or defect formation were then modeled for comparison to experimental spectra.

## Tuesday, May 24, 2016

### **George W. Morey Award Lecture**

Room: Madison

**8:00 AM**

#### **(GOMD-AW-002-2016) Spying with Spins on Messy Materials: 50 Years of Glass Structure Elucidation by NMR Spectroscopy (Invited)**

H. Eckert<sup>1</sup>; 1. University of Muenster, Germany

Glasses remain a focus of attraction to fundamental researchers and materials engineers alike. The desire of controlling physical property combinations by compositional design inspires the search for fundamental structural concepts describing the short and medium-range order of the glassy state. From its early beginnings about 50 years ago, solid state nuclear magnetic resonance (NMR) spectroscopy has been making significant contributions towards this objective. Being element-selective, inherently quantitative as well as selective to the local environment, NMR in many ways presents an ideal experimental tool of structural investigation of glasses. Over the years, substantial NMR methods development, along with advances in the theoretical understanding of NMR parameters have produced an inventory of powerful complementary techniques offering new concepts of medium-range order to glass scientists and useful structure/property correlations to materials engineers. The lecture will sketch this trajectory from the early beginnings to the present state of the art, with a focus on applications to ionically conductive and photonic glasses.

## **Symposium 1: Fundamentals of the Glassy State**

### **Session 1: Glass Formation and Relaxation I**

Room: Capitol A

Session Chair: John Mauro, Corning Incorporated

**9:20 AM**

#### **(GOMD-S1-001-2016) Excitations in glasses at low temperatures (Invited)**

W. Kob<sup>1</sup>; 1. Laboratoire Charles Coulomb, France

At low temperatures glasses show a variety of properties that are very different from the ones found in crystals, such as the temperature dependence of the specific heat or the thermal conductivity. Since many years these anomalies have been rationalized by means of the so-called two-level systems in which a local group of particles can undergo a tunneling motion between two different states. Although this explanation is appealing and is able to give a correct phenomenological description of the experimental data, it has the flaw that so far nobody has been able to identify what these relaxing entities really are. In this talk I will discuss the experimental facts and the ideas that have been put forward regarding the nature of the relaxing entities. Subsequently I will argue that from a quantitative point of view these ideas are not able to explain the experimental findings and that hence one has to reconsider our view on what is really relaxing. Using large scale computer simulations we have recently been able to identify a new kind of two level system that seem to have the right features to explain the properties of glasses at low temperatures. In this talk I will discuss these results and speculate on the implication that they have on the local structure of glasses.



9:50 AM

**(GOMD-S1-002-2016) Glass Transition: The Broken-Ergodicity View (Invited)**P. Gupta<sup>\*1</sup>; 1. Ohio State University, USA

While there is little debate about glass transition being an ergodicity-breaking transition in which the ergodic (equilibrium) liquid state is transformed into a broken-ergodic glassy state strictly because of finite observation time, there is persistent resistance to adopt some of the basic consequences of broken-ergodicity in formulating the thermodynamics of glasses. This is principally because the physics of broken-ergodicity challenges the traditional notion of continuation of configurational entropy through the glass transition – a notion that has unfortunately become firmly rooted in the canons of glass science as a result of treating glass transition as a spontaneous non-equilibrium process. In this talk, I will review arguments as to why the process of breaking ergodicity is not a conventional spontaneous process and that the loss of configurational entropy during glass transition does not require an extension of the equilibrium definition of entropy to time dependent nonequilibrium situations.

10:20 AM

**(GOMD-S1-003-2016) Viscosity of Westminster Cathedral Glass**O. Gulbitten<sup>\*1</sup>; X. Guo<sup>1</sup>; J. C. Mauro<sup>1</sup>; 1. Corning Incorporated, USA

It had been a long lasting myth that medieval cathedral glasses were thicker at the bottom due to the flow at room temperature, until this myth was busted by Zanotto and Gupta's studies. They showed that relaxation times of cathedral glasses at room temperature are too long to observe a significant amount of flow in human times. Recent relaxation studies of silicate glasses (at room temperature) indicated small but observable volumetric changes in a few years. A rigorously developed non-equilibrium viscosity model (MAP) and new capabilities of viscosity measurements over a wide range of viscosities in the equilibrium and non-equilibrium ranges allow us to estimate the relaxation times of glasses well below their glass transition temperature. These results and developments motivated us to revisit the old question of relaxation times of cathedral glasses. In this study we focus on a glass composition that was used in the windows of Westminster Cathedral. An accurate calculation of the non-equilibrium viscosity was performed by utilization of a modified beam bending viscometer and application of the MAP model. Relaxation times derived from the non-equilibrium viscosity estimations elucidated the viscosity of cathedral glasses at room temperature.

10:40 AM

**(GOMD-S1-004-2016) Structure and properties of ZnCl<sub>2</sub> melts: indication of a strong-to-fragile transition**P. Lucas<sup>\*1</sup>; A. Edwards<sup>1</sup>; M. Venkateswara<sup>1</sup>; P. Deymier<sup>1</sup>; K. Muralidharan<sup>1</sup>; A. Al Sayoud<sup>1</sup>; 1. University of Arizona, USA

High temperature Raman spectroscopy was conducted on ultra-dry molten ZnCl<sub>2</sub> to characterize the temperature dependence of the melt structure. A complex mixture of edge and corner sharing tetrahedra is observed which is corroborated with ab-initio molecular dynamic models as well as previously reported neutron diffraction data. The effect of the conversion from corner-to-edge sharing tetrahedra and its consequence on dynamic properties such as viscosity is interpreted in terms of topological constraints counting. The low temperature viscosity is then estimated by calorimetric method from the activation energy for enthalpy relaxation which yields the fragility index "m". A severe mismatch between low and high temperature viscosity is observed which suggest the presence of a strong-to-fragile transition.

11:00 AM

**(GOMD-S1-005-2016) Characterizing and Predicting Stress and Structural Relaxation in Glass**K. T. Strong<sup>\*1</sup>; B. Elisberg<sup>1</sup>; R. Jamison<sup>1</sup>; K. Ewsuk<sup>1</sup>; 1. Sandia National Laboratories, USA

Residual stress in bimaterial components such as glass-to-metal seals can significantly impact component performance and reliability. Predicting residual stress requires an accurate determination of strain. In addition to large strain from differences in thermo-physical response, smaller strain from structural and/or stress relaxation can also be important. To better quantify and understand the effects of stress and structural relaxation in glass, experiments and modeling have been completed on Schott 8061 glass. The nonlinear viscoelastic simplified potential energy clock (SPEC) model, originally developed at Sandia National laboratories for organic thermosets, was employed to predict glass strain in this study. The model was calibrated and tested using data from dynamic (i.e., dynamic and thermal mechanical analysis) and static (i.e., creep) experiments. In comparison to the measured strain from the structural relaxation associated with thermal excursions about the glass transition temperature (T<sub>g</sub>=460C), and from stress relaxation due to creep, the physically-based SPEC viscoelasticity model predicts strain with engineering accuracy. Examples will be presented and discussed. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, of the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000

11:20 AM

**(GOMD-S1-006-2016) Depletion layer formation by electro-thermal poling of alkali silicate glasses**C. McLaren<sup>\*1</sup>; M. Balabajew<sup>2</sup>; B. Roling<sup>2</sup>; H. Jain<sup>1</sup>; 1. Lehigh University, USA; 2. University of Marburg, Germany

Electro-thermal poling is a processing technique used to induce second-order nonlinear optical susceptibility of glasses by use of DC electric fields. The technique can also be used to enhance biological, physical and chemical properties of glass. Tailoring of these properties critically depends on the formation of a depletion layer due to charge transport toward opposing DC electrodes. Despite numerous studies, mechanisms responsible for depletion layer formation and charge compensation remain only partially understood. We have investigated possible depletion layer formation mechanisms by use of electrical and chemical characterization techniques. Impedance spectroscopy, in situ poling current measurements and ToF-SIMS were done on several glass compositions in order to determine the role of alkali ion migration in depletion layer formation. Two binary alkali (lithium and sodium) disilicate glasses along with two mixed alkali lithium-sodium disilicate glasses were prepared by standard melt quench method for this study. Two relaxation time scales of electro-thermal poling current have been identified. The first time scale appears to be related to alkali ion migration followed by a slower process of either irreversible electrolysis or gaseous oxygen evolution near the anode. Implications of electro-thermal poling for recently discovered electrical field-induced softening of glass are discussed.

### Session 4: Potential Development and MD Simulations of Multicomponent Glasses

Room: University C/D

Session Chairs: Walter Kob, Laboratoire Charles Coulomb; Jincheng Du, University of North Texas

9:20 AM

#### (GOMD-S1-007-2016) Structures and properties of multicomponent oxide glasses with mixed glass formers from molecular dynamics simulations (Invited)

J. Du<sup>\*1</sup>; 1. University of North Texas, USA

Computer simulations of multicomponent glasses, especially those with mixed glass formers, have been a challenge due to the availability and validity of empirical potentials and structure complexity of these glasses. In this talk, I will summarize our recent work on potential development and applications of these potentials in the study of multicomponent glasses, including aluminosilicate, borosilicate and boroaluminosilicate glasses, using classical molecular dynamics simulations. Analyses of the bulk and surface structure features of these glasses from MD simulations and comparison with experimental data, insight on the short and medium range structures of these glasses, and discussion of the structure effect on mechanical property and chemical durability of these glasses will be given.

9:50 AM

#### (GOMD-S1-008-2016) Molecular Dynamics Simulations of Multicomponent Aluminosilicate Glass and Glass Surfaces

L. Criscenti<sup>\*1</sup>; T. Zeitler<sup>1</sup>; K. Ewsuk<sup>1</sup>; 1. Sandia National Laboratories, USA

Molecular simulation of multicomponent glass may provide a predictive capability to determine correlations in glass structures and properties as a function of composition. Molecular dynamics (MD) simulations have been used to investigate if molecular-scale structure and composition can be correlated to macroscopic glass properties to help design glasses for glass-to-metal seals. Simulations have been performed for three-component BaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> and CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> glasses; and for glasses with up to eight components with contributions as low as 1 mol%, that are nearly as complex as those used in actual glass-to-metal seals. Bulk structural properties (bond and angle distributions) and other macroscopic properties of interest (i.e., CTE, T<sub>g</sub>, and density) have been calculated for these glasses. In addition, simulations have been performed to investigate the migration of network modifiers to glass surfaces in vacuum. We will discuss simulation methods, calculated correlations (with uncertainties) between glass composition, bulk, and surface properties. In addition, we will present preliminary calculations on glass-to-metal seal interfaces. Our modeling efforts are strongly tied to ongoing experimental research including EXAFS and NMR that can be used to validate our simulation results. Comparisons will be made between modeling and experimental results where possible.

10:10 AM

#### (GOMD-S1-009-2016) Simulations of nepheline glasses: A study of relation between nanostructure and properties

W. Chen<sup>\*1</sup>; N. Greaves<sup>1</sup>; 1. Aberystwyth University, United Kingdom

The distribution of mobile metallic ions, which fundamentally affects the properties of glasses, has been simulated in this study to understand the roles mobile ions played. In particular, we are interested in the micro-segregation of ions which form into percolation channels. Molecular dynamics simulations of alumina-silicate nepheline have been performed to obtain the molten structure. Different alkali ratios have been taken to verify the effect of ionic field strength on segregation. Radial Distribution functions, REDOR second moments, Vibrational Densities of States and molecular structure snapshots reveal how alkali ions distributed non-randomly, formed channels in between the framework. When K<sup>+</sup> replaces Na<sup>+</sup>, it provides less distortion to system due to its lower field strength thus

resulting in a higher viscosity. Moreover, a dramatically increasing of both melt viscosity and boson peak intensity in quenched glass, due to the effect of K<sup>+</sup> percolation, can be observed. To replicate the thermal properties, simulations with varied alumina-silicate, including nepheline, containing different ratio of Al/Si, have been performed. Mean square displacements were calculated at 2000K to derive the diffusion constant. Compared to Einstein-Stokes equation, the viscosity results derived from Eyring relation show a better replication of a fitted Adam-Gibbs model with measured values.

10:30 AM

#### (GOMD-S1-010-2016) Structural simulations of Yb-doped aluminum fluoride glasses

H. Inoue<sup>\*1</sup>; A. Masuno<sup>1</sup>; 1. The University of Tokyo, Japan

White luminescent Yb-doped glasses of fluoride and/or chloride excited with near-UV light have been prepared. These glasses are expected to be a candidate for white LED. The YbF<sub>3</sub>-doped glass based on AlF<sub>3</sub> was melted under a reductive atmosphere. In the obtained glass Yb<sup>2+</sup> and Yb<sup>3+</sup> were present. The ratio of Yb<sup>2+</sup> ions and the structure around the ions will give a significant influence on the luminescence properties. In this study, the glasses based on AlF<sub>3</sub> with YbF<sub>3</sub> were prepared and the high-energy x-ray diffraction was measured 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 and was kept at 293K for 20000 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 Al and Yb ions were 6 and 8, respectively. About 20% of F ions did not coordinate with Al ions. It seems that the network of this glass consist of AlF<sub>6</sub> octahedra and YbF<sub>8</sub> polyhedra. Furthermore, the electronic state of Yb ions in the glass will be discussed.

10:50 AM

#### (GOMD-S1-011-2016) Barium Dissilicate: A molecular Dynamics study

J. P. Rino<sup>\*1</sup>; 1. Universidade Federal de São Carlos, Brazil

An effective two-body interaction potential is proposed in order to describe the amorphous phase of the barium dissilicate mineral. The two-body potential takes into account steric repulsion, Coulomb interactions due to charge transfer, charge-induced dipole attractions due the electronic polarizability of ions and van der Waals attraction. The proposed potential is used to study structural and dynamical properties of amorphous BaSi<sub>2</sub>O<sub>5</sub>. Results for pair correlation function, static structure factor, bond angle distributions, statistic of rings and phonon density of states are presented. Results are in good agreement with neutron and Raman experiments.

11:10 AM

#### (GOMD-S1-012-2016) An Environment Dependent Dynamic Charge Interatomic Potential for Modeling Nano and Bulk Silica Polymorphs

K. Muralidharan<sup>\*1</sup>; K. Runge<sup>1</sup>; 1. University of Arizona, USA

The environment dependent dynamic charge (EDD-Q) paradigm represents a new framework for developing and parameterizing interatomic potentials. EDD-Q is constructed using first-principles data obtained on a hierarchical set of atomic clusters. This enables EDD-Q to model molecules, nanostructures and bulk counterparts within a single framework. EDD-Q has a functional form formally based on density functional theory, and is couched in a fundamentally appealing method of accounting for atomic charge and electron density fluctuations as a function of the atoms' chemical environment, thereby naturally capturing the underlying chemistry of electrons. To illustrate the EDD-Q potential

development, we focus on silica ( $\text{SiO}_2$ ) and assess its capabilities, by examining its ability to describe silica nanoclusters as well as bulk silica polymorphs (crystalline and amorphous) with respect to density functional theory (DFT) calculations. The ability to emulate DFT calculations signifies the success of the EDD-Q framework and provides a new first-principles based hierarchical approach to developing predictive interatomic potentials for a wide variety of complex glass formers.

**11:30 AM**

**(GOMD-S1-013-2016) Optimizing Molecular Dynamics Potentials for Multi-component Glasses**

S. Sundaraman\*<sup>1</sup>; S. Ispas<sup>2</sup>; W. Kob<sup>2</sup>; L. Huang<sup>1</sup>; 1. Rensselaer Polytechnic Institute, USA; 2. Université de Montpellier 2, France

A major stumbling block in modelling multi-component oxide glasses is the lack of satisfactory potentials that can reasonably describe a wide range of properties of these glasses. In this work, a new optimization scheme for parameterizing potentials for molecular dynamics (MD) simulations of multi-component glasses was developed. The main motivation was to improve predictions of static properties like elastic moduli and dynamic properties like vibrational density of states (VDOS) that MD simulations have generally not been able to estimate correctly, while still using a simple functional form for computational efficiency. Our approach was to fit the potentials to results from accurate first principles calculations to predict both the static and dynamic properties correctly, by explicitly incorporating the radial distribution function (RDF) and the VDOS into the cost function of the fitting scheme. This new optimization scheme has successfully improved the potentials for silica glass. It will be extended to binary alkali silicate glasses, and then multi-component oxide glasses. These newly developed potentials will be used to study the elastic response of multi-component oxide glasses to external stimuli such as high temperatures, high pressures and high strains, and their deformation modes under different loading conditions.

**Symposium 2: Larry L. Hench Memorial Symposium on Bioactive Glasses**

**Larry L. Hench Memorial Symposium on Bioactive Glasses IV: Structure**

Room: Wisconsin

Session Chairs: Julian Jones, Imperial College London; Jonathan Massera, Tampere University of Technology

**9:20 AM**

**(GOMD-S2-015-2016) First observation of the atomistic source of mechanical toughness in glass bio-cements during setting (Invited)**

N. Greaves<sup>1</sup>; G. Chass<sup>2</sup>; Y. Yue<sup>3</sup>; 1. University of Cambridge, United Kingdom; 2. Queen Mary University of London, United Kingdom; 3. Aalborg University, Denmark

Bio-cements, notably glass-ionomer cements, have been in widespread use for over 40 years in dentistry and medicine. Progress in improving their mechanical properties, however, lags behind the toughness needed for permanent implants. A significant impediment to improvement has been the need to use conventional mechanical failure methods, which are necessarily retrospective. Through the novel use of neutron Compton scattering, and also terahertz spectroscopy and DSC (Nature Communications 6 8631 pp 1-10 (2015)), it has been possible to relate fracture toughness during setting to atomic cohesion, from which fluctuations in interfacial configurations during chelation between the highly phase separated glass and the PAA polymer are observed. In this paper we show how, compared to convention, the setting of glass-ionomer cements is not monotonic. Rather, as they set, abrupt features are

found in the development of mechanical toughness which have not been previously detected. These provide clues by which mechanical performance of bio-cements might be improved.

**9:50 AM**

**(GOMD-S2-016-2016) Composition-Structure Trends of Bioactive Phosphosilicate and Borophosphosilicate Glasses Probed by Solid-State NMR and MD Simulations (Invited)**

R. Mathew<sup>1</sup>; Y. Yu<sup>1</sup>; B. Stevansson<sup>1</sup>; M. Eden\*<sup>1</sup>; 1. Stockholm University, Sweden

Silicate-based  $\text{Na}_2\text{O}-\text{CaO}-\text{SiO}_2-\text{P}_2\text{O}_5$  bioactive glasses have been used for bone regeneration applications for decades. On their contact with body fluids, they integrate with human tissues by forming a surface layer of calcium hydroxy-carbonate apatite that features a similar composition to bone mineral.  $\text{Na}_2\text{O}-\text{CaO}-\text{SiO}_2-\text{P}_2\text{O}_5$  glasses involve networks of connected  $\text{SiO}_4$  groups, whereas P may exist as ortho/di-phosphate groups, charge-balanced by the glass modifiers ( $\text{Na}^+$ ,  $\text{Ca}^{2+}$ ). Boron-bearing glasses also feature various  $\text{BO}_3$  and  $\text{BO}_4$  moieties intermixing with the silicate network. We will present an array of magic-angle-spinning (MAS) NMR experimental data, evaluated in conjunction with results from atomistic molecular dynamics (MD) simulations, to quantitatively monitor how the amounts of distinct Si, P, and B coordination polyhedra alter when the glass composition changes. Besides identifying and quantifying these basic building blocks, the intermediate-range glass structures were investigated by advanced MAS NMR experimentation, such as various multiple-quantum and heteronuclear techniques. The nature of the P distribution, the relative preferences of the glass modifiers to associate with the various Si, P and B groups, and the organization of the Si/B glass network fragments will be discussed in relation to the glass composition.

**10:20 AM**

**(GOMD-S2-017-2016) The Structure and Properties of  $20\text{Na}_2\text{O}-30[(1-x)\text{CaO}-x\text{SrO}]-50\text{P}_2\text{O}_5$  Glasses for a Biomedical Application**

P. Freudenberger\*<sup>1</sup>; R. Brown<sup>1</sup>; A. Saitoh<sup>2</sup>; H. Takebe<sup>2</sup>; S. Nakane<sup>3</sup>; H. Ikeda<sup>3</sup>; 1. Missouri University of Science & Technology, USA; 2. Ehime University, Japan; 3. Nippon Electric Glass, Japan

An optical fiber is being developed for medical applications, and phosphate glasses are the preferred materials because they are bio-resorbable. A melt process for glasses from the  $20\text{Na}_2\text{O}-30[(1-x)\text{CaO}-x\text{SrO}]-50\text{P}_2\text{O}_5$  system was developed to produce optical quality specimens. Five compositions, denoted as  $x = 0, 0.25, 0.50, 0.75,$  and  $1$ , were prepared and the effects of composition on structure and properties were investigated. When CaO replaces SrO, molar volume, refractive index, and CTE decrease, and glass transition temperature, crystallization temperature, and high temperature viscosity increase. Crystallization readily occurs across the compositional series. Shifts in the Raman peaks of modes associated with metaphosphate tetrahedra reveal systematic changes in P-O bond distances and tetrahedral symmetry.

**10:40 AM**

**(GOMD-S2-018-2016) Study of Bioglasses and Glass Ceramics by Infrared and Raman Spectroscopy (Invited)**

D. Möncke\*<sup>1</sup>; 1. Friedrich-Schiller University Jena, Germany

Raman and infrared (IR) spectroscopy are powerful tools for the structural study of glasses and glass ceramics. Bulk structures are best analysed on polished surfaces, especially when using surface sensitive IR reflectance spectroscopy. Corrosion phenomena are probed easily by measuring the same surface over time. Structural variations, inclusions or substrate-veneer interphases can be studied on cross-sections of the sample. A deeper understanding of a material's structure is helpful in the control and tailoring of its properties. By providing insight into different vibrational techniques and in regard to data evaluation, the characterisation of glasses and glass-ceramics for medical and dental uses will be attempted on

\*Denotes Presenter

examples from phosphate, silicate and borate, as well as from mixed network former bioglass systems such as Bioglass 45S5 or 13-93. IR and Raman studies on a recently developed niobate containing lithium-silicate veneer ceramic illustrate the formation of crystals within a vitreous matrix and structural variations at the interfaces. The degree of polymerization, the effect of charge-balancing cations and the influence of OH will be discussed. Also the presence of NbO<sub>6</sub> polyhedra, most probably connected to a vitreous silicate matrix, would be inferred by resolving a broad polarized Raman band into different components.

**11:10 AM**

### **(GOMD-S2-019-2016) A thermodynamic discourse on the dissolution behavior of bioactive glasses**

B. S. Pföss<sup>\*1</sup>; R. Conrad<sup>1</sup>; I. RWTH Aachen University, Germany

The dissolution behavior of bioactive glasses was found to be convenient to achieve beneficial corrosion products and therefore enable the outstanding properties of these materials for medical applications. Suitable dissociation equilibria for the oxide system of bioactive glasses were derived and used further for describing their hydrolytic stability. Ion concentrations and organic components of the medium are also considered for the calculations. The first result is the distribution of all accessible aqueous species and precipitants as a function of pH. The method of transforming the oxide composition of a glass to a set of crystalline reference phases was applied and with including the vitrification energy used to calculate the Gibbs free energy of the glasses under standard conditions. Combination of the pH dependent dissociation products and the Gibbs free energy data of the glassy state allows to estimate and compare the stability of the material in aqueous solutions. The outcome of such an approach shows an apatite precipitant as the stable phase for pH values higher than 3.5 for glass 45S5, under neutral and basic conditions Ca<sub>10</sub>(PO<sub>4</sub>)<sub>6</sub>(OH)<sub>2</sub> is the stable phase for glass 13-93. The thermodynamic argumentation confirms the well-known ability of bioactive glasses to form an apatite layer.

## **Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications**

### **Session 1: Ionic Conducting Materials**

Room: University A/B

Session Chair: Xiang-hua Zhang, Université de Rennes I

**9:20 AM**

### **(GOMD-S3-018-2016) Ion conducting oxide and sulfide glasses and development of all solid state batteries (Invited)**

A. Pradel<sup>\*1</sup>; M. Ribes<sup>1</sup>; 1. Université de Montpellier, 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 (~200-400°C compared to 900°C when ceramics are considered) could be facilitated. An overview of investigation carried out over time on lithium and sodium oxide and sulfide glasses and attempts to develop solid state batteries will be reported and the main technological issues will be discussed.

**9:50 AM**

### **(GOMD-S3-019-2016) Development and Characterization of Fast Ion Conducting Solid Electrolytes for All-Solid-State Sodium Batteries (Invited)**

S. W. Martin<sup>\*1</sup>; 1. Iowa State University, USA

Lithium batteries are important as portable energy sources, but the use of Lithium batteries in electrical grid energy storage is coming into question due to the high cost of lithium. Sodium is much cheaper than lithium, but sodium batteries operate at elevated temperatures to resolve problems of low Na<sup>+</sup> ion conductivity in solid electrolyte separators. For this reason, new higher conductivity Na<sup>+</sup> ion conducting solid electrolytes are of great interest and in this research program, we are actively exploring new glass compositions with very high conductivities. In ternary glasses which are comprised of one modifying salt, typically an alkali oxide, and two (or more) glass formers, the composition dependence of properties such as the alkali ion conductivity is a highly non-linear function of the ratio of the two glass formers at constant alkali oxide concentration. For example, in the ternary system Na<sub>2</sub>O + BO<sub>3/2</sub> + PO<sub>5/2</sub>, the Na<sup>+</sup> ion conductivity reaches a maximum nearly two orders of magnitude higher than the linear interpolation between the two end member binary glass formers. In the Na<sub>2</sub>O + BO<sub>3/2</sub> + SiO<sub>2</sub> ternary system, however, the conductivity has strongly negative Mixed Glass Former Effect. In this talk these two opposing behaviors will be described and discussed with aim of yielding new insight into the atomic level mechanisms governing these diametric behaviors.

**10:20 AM**

### **(GOMD-S3-020-2016) Characterization of a new Na bulk ionic conductor prepared from a glass reactive sintering route**

S. Chenu<sup>2</sup>; P. Bénard-Rocherullé<sup>2</sup>; R. Lebullenger<sup>1</sup>; J. Rocherullé<sup>\*1</sup>; X. Zhang<sup>1</sup>; 1. University of Rennes, France; 2. University of Limoges, France

NZP materials are a very large family of interesting inorganic phosphates based on the NaZr<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub> type-structure. These materials are stable towards temperature and also chemical composition leading to various applications and noticeably superionic conductors. However, NZP is difficult to fabricate into monoliths due to the high temperatures and long sintering times required for the synthesis. This work proposes to use the reactive sintering of a phosphate based glass to prepare a new tungsten (IV) and tin (IV) containing glass ceramic with a NZP structure. A glass powder with the appropriate composition was first pressed at room temperature. Then, the green pellet was cured at temperatures where glass reactive sintering takes place. The different parameters influencing the achievement of a single crystalline phase are the initial glass composition, the glass particle size and the curing atmosphere. The indexing of the diffraction pattern was carried out. A Rietveld refinement, combined to EDX analysis, has shown that tungsten was incorporated in a mix coordination polyhedra (M<sup>IV</sup>O<sub>6</sub>) and almost 90% of these octahedral sites were occupied by the Sn<sup>4+</sup> ions and the remaining 10% by the W<sup>4+</sup> ions. Compared to the parent glass, the glass-ceramic exhibits an important increase of ionic conduction, the residual glassy phase presenting an increase in T<sub>g</sub>.

**10:40 AM**

### **(GOMD-S3-021-2016) Transition metal oxides based glasses for solid-state batteries: Insights from a combined first-principles and classical molecular dynamics modeling approach**

G. Ori<sup>\*1</sup>; L. Sementa<sup>2</sup>; M. Boero<sup>1</sup>; C. Massobrio<sup>1</sup>; M. Montorsi<sup>2</sup>; 1. IPCMS, CNRS - University of Strasbourg, France; 2. University of Modena and Reggio Emilia, Italy

Glass-based materials containing transition metal (TM) oxides with TM in different oxidation states and modifier ions give rise to a multifunctional platform with tunable ionic-electronic conductivity properties, which are particularly suitable as electrolytes and high capacity cathodes. The absence of a long-range order allows for subtle structural adaption during ions charge/discharge processes,

which can overcome the huge capacity loss observed during the first cycles due to irreversible phase transformations occurring in other materials. Glass systems containing vanadium oxides (phosphate and tellurite for instance) are receiving a renewed attention in this field due to their tunable conductivity properties on the basis of the employed synthesis conditions. With this contribution, we show how first-principles molecular dynamics combined with density functional theory can foster our comprehension of the chemical order and chemical bonding properties of the building blocks constituting vanadophosphate glasses. The output of this work complements the structural knowledge obtained by classical molecular dynamics and represents a key step in order to disentangle the factors governing the complex scenario of the structure - conductivity properties relations for this type of glasses.

11:00 AM

**(GOMD-S3-022-2016) Structure and Physical Properties of the Glassy Solid State Electrolyte of the 0.64 Na<sub>2</sub>S+ 0.46 [xBS<sub>3/2</sub>+ (1-x) GeS<sub>2</sub>] System**

B. Curtis<sup>1</sup>; S. W. Martin<sup>1</sup>; I. Iowa State University, USA

Solid state batteries are of growing interest due to their high energy density, lifetime, and safety. As this interest grows, so does the interest for an optimal solid state electrolyte. Glassy solid state electrolytes prove to be an advantageous competitor due to the relatively low manufacturing costs and increased safety. In addition, properties of these electrolytes (i.e ionic conductivity) can be modified due to the mixed glass former effect (MGFE) which occurs when varying the ratio of glass formers from one binary system to the other through a ternary system. Physical and electrochemical properties vary in a non-linear, non-additive trend as the composition, and subsequently the structure, is changed. The structure of this glass system has been examined through various means such as infrared spectroscopy, Raman spectroscopy and nuclear magnetic resonance. The physical properties measured include the glass transition temperature, density, and ionic conductivity through differential scanning calorimetry, Archimedes method, and impedance spectroscopy, respectively. This talk will interpret the physical properties from the standpoint of short range structural models characteristic of the glass.

## **Symposium 4: Glass Technology and Cross-Cutting Topics**

### **Session 4: Glass Corrosion: Mechanisms and Rate I**

Room: Capitol B

Session Chairs: Eric Pierce, Oak Ridge National Lab; Stephane Gin, CEA

9:20 AM

**(GOMD-S4-037-2016) Corrosion Behavior of Mixed Simulated Radioactive Waste Glasses SON-68 and AFCI**

J. A. Rice<sup>1</sup>; I. Pennsylvania State University, USA

Vitrification is a common practice for the safe disposal and long-term storage of radioactive waste. However, durable, nuclear waste glass is susceptible to corrosion, and while models for the initial stages of glass corrosion have been well developed, 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. While the twenty-six component glasses studied, SON-68 and AFCI, have twenty components in common, AFCI exhibits a more rapid Stage-III transition than the more chemically durable SON-68. To help identify any critical compositional trigger(s) of Stage-III dissolution, the two glasses are studied as pure and blended compositions of 100%AFCI, 25/75, 50/50, 75/25, and 100%SON-68 (by weight). In this way the composition effects, Stage-III transition, and

crystallization events can be studied via static corrosion tests where solution analysis is monitored with (pH and ICP-AES) and solids can be probed with XRD and SEM.

9:40 AM

**(GOMD-S4-038-2016) Investigation of Alteration Gel Layers' Porosities using Positron Annihilation Spectroscopy**

J. Reiser<sup>1</sup>; J. McCloy<sup>1</sup>; M. Weber<sup>1</sup>; B. Parruzot<sup>1</sup>; L. M. Neill<sup>1</sup>; J. Ryan<sup>2</sup>; J. Neeway<sup>2</sup>; N. Wall<sup>1</sup>; 1. Washington State University, USA; 2. Pacific Northwest National Lab, USA

The safe disposal of nuclear waste is crucial for ensuring the safety of life and the environment. The current proposed methods of disposal include the immobilization of radionuclides present in waste into borosilicate glasses. The glass durability lifetime should exceed thousands of years to limit radioisotopes mobility to the accessible environment. A large body of work has been published to test the durability of nuclear waste glass forms and explain processes observed during glass alteration. A porous alteration layer is usually formed at the surface of the glass upon long term reaction of waste glass in aqueous solutions. Although some of properties of the alteration layer have been investigated, additional data are needed to propose realistic alteration layer formation mechanisms, for modeling purposes. Positron annihilation spectroscopy represents a valuable tool for investigating the porosity of the altered glass as a function of depth. Positron annihilation data will be presented for short-term and long-term static studies performed with ISG in de-ionized water.

10:00 AM

**(GOMD-S4-039-2016) Dissolution of International Simple Glass (ISG) in Sodium Chloride Brine Solution**

J. P. Icenhower<sup>1</sup>; I. Sandia National Laboratories, USA

The dissolution rate of the International Simple Glass (ISG), a six component boroaluminosilicate composition, was determined in a single-pass flow-through (SPFT) system at 90°C and pH = 9 in solution over a sodium chloride 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 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 area. The height difference is proportional to the dissolution rate. Values of the dissolution rate, based upon chemical assay of the effluent solution on the one hand, and VSI methods on the other, are compared. Results in sodium chloride solutions will be discussed in the context of rate dependency on ionic strength.

10:20 AM

**(GOMD-S4-040-2016) Corrosion behavior of ISG fibers from pH 9.5 - 12.5**

C. L. Trivelipiece<sup>1</sup>; C. G. Pantano<sup>1</sup>; I. Pennsylvania State University, USA

This study investigated the effect of initial leachate solution pH (pH<sub>i</sub> 9.5, 10.5, 11.5, 12.5) on the corrosion behavior of glass fibers synthesized from an International Simple Glass (ISG) reference ingot. Solution analyses revealed that the pH<sub>i</sub> 9.5-11.5 systems initially buffered to pH values ranging from 9.5 - 9.7, and after initial rapid dissolution associated with Stage I corrosion, the fibers corroded at a residual rate for the duration of the experiment. The pH<sub>i</sub> 12.5 system demonstrated markedly different corrosion behavior. The pH of this system remained constant until an apparent transition from Stage II to Stage III corrosion after 57 days, which resulted in a decrease in pH, an increase in the concentration of boron and silicon in solution, and consumption of Na and Al in the form of zeolite NaP2. Further solution analyses revealed that the pH<sub>i</sub> 9.5 - 11.5 systems

\*Denotes Presenter

produced excess weak acid during the experiment while the pH<sub>i</sub> 12.5 experiment produced excess strong base. These solution data, along with XRD and XPS analyses as well as SEM/TEM observations of the fibers, will be used to propose a hypothesis for a coupled solution and structural mechanism for the Stage II to Stage III corrosion transition in the pH<sub>i</sub> 12.5 experiment.

### 10:40 AM

#### (GOMD-S4-041-2016) Effect of Magnetite on Nuclear Waste Glass Alteration Layers

L. M. Neill<sup>\*1</sup>; S. Gin<sup>2</sup>; P. Jollivet<sup>2</sup>; B. Parruzot<sup>1</sup>; N. Wall<sup>1</sup>; 1. Washington State University, USA; 2. CEA, France

Understanding the effect of near-field materials such as iron corrosion products on the alteration of vitreous nuclear waste forms is essential for modeling long-term stability in a geological repository. International Simple Glass (ISG) – a six oxide borosilicate glass – was altered at 90 °C at a fixed pH of 7 in a solution initially saturated in SiO<sub>2</sub> for 3 months. Iron corrosion products are known to enhance the alteration of silicate glasses. To better understand this behavior, magnetite was added into the system to understand changes within the alteration layer of the glass. Changes in alteration were monitored by Inductively Coupled Plasma – Optical Emission Spectroscopy (ICP-OES) and Time of Flight – Secondary Ion Mass Spectrometry (TOF-SIMS). A dramatic decrease in SiO<sub>2</sub> in solution is observed when iron corrosion products are introduced into the system along with a progressive increase of the glass dissolution rate. The integration of iron into the alteration layer is also seen after several months. Methylene blue, D<sub>2</sub>O, and LiCl were also used as tracers added into the solution at room temperature after the withdrawal of each monolith to understand the porosity of the gel layer as alteration progressed under the influence of iron.

### 11:00 AM

#### (GOMD-S4-042-2016) The role played by inter-diffusion in glass dissolution: The case of basaltic and nuclear glasses

S. Gin<sup>\*1</sup>; T. Ducasse<sup>2</sup>; M. Collin<sup>2</sup>; 1. CEA, France

Inter-diffusion is a general term gathering several processes such as water diffusion in the glass, ion-exchange and in some cases hydrolysis of boron. The role of inter-diffusion during glass dissolution remains open to debate since a new model based on interfacial dissolution/precipitation reaction has been proposed, ruling out this process. Here we show new results obtained on basaltic glass and on the International Simple Glass (ISG), a six oxide borosilicate glass, showing how important is this process, especially at high reaction progress (i.e. under silica saturated conditions). We detail results obtained with ISG altered in a solution with no counter ion and solutions containing one of the following counter ions: Li, Na, K, Cs and explain, according to solid-state NMR spectroscopy, FTIR spectroscopy, TGA and ICP data why inter-diffusion is affected by the counter ion. We also explain why basaltic glass is less sensitive to inter-diffusion compare to ISG glass. This comparison contributes to reinforce the mechanistic analogy between nuclear and natural glasses.

### 11:20 AM

#### (GOMD-S4-043-2016) A Leap Towards the Quantification of Glass Dissolution Rate: An Atomic Force Microscopy Approach

Y. Gong<sup>\*1</sup>; C. L. Trivelpiece<sup>2</sup>; C. G. Pantano<sup>2</sup>; N. Mellott<sup>1</sup>; 1. Alfred University, USA; 2. Pennsylvania State University, USA

The aqueous corrosion of silicate glasses is of considerable interest given its critical role in industrial, biomedical, environmental and geological processes. Dissolution rates of silicate glasses are fundamental for predicting the long-term corrosion behavior and the understanding of its environmental impact. The measurement of glass dissolution rates is often reported by the release of elements into aqueous solution. However, assumptions associated with this method are excessive. In this study, a more direct, novel method of

measuring dissolution rates of glasses via atomic force microscopy is presented. In addition to the measurement of dissolution rates, derived from step recession of melt surfaces of an aluminoborosilicate glass at pH 2, 7, and 10 for up to 960 hours, the morphology, chemical composition and roughness was also investigated. Particular attention will be focused on the overall validation and errors associated with this strategy.

### 11:40 AM

#### (GOMD-S4-044-2016) Role of zirconium in nuclear waste glass and in the corresponding alteration gels

L. Galois<sup>\*1</sup>; G. Calas<sup>2</sup>; P. Jollivet<sup>2</sup>; F. Angeli<sup>2</sup>; S. Gin<sup>2</sup>; 1. UPMC, France; 2. LCLT, CEA-Marcoule, France

Vitrification of radioactive waste in borosilicate glasses receives important attention in several countries. The fundamental properties are chemical and mechanical durability that governs radionuclide release and the safety of the disposal. In geological repository, glass leaching by water severely affects the long-term evolution of borosilicate glasses. We will present the evolution of the french SON 68 glass and simplified glasses under forcing conditions. The durability of the gel and its properties depend on the structural role played by elements such as Zr<sup>4+</sup>. Short- and medium-range environment of zirconium in these glasses was determined by Zr L<sub>2,3</sub>-edges and K-edge XANES and by K-edge EXAFS. In the SON 68 glass, under saturated conditions of alteration, Zr<sup>4+</sup> remains in octahedral sites, in a protective gel. In open alteration conditions, Zr<sup>4+</sup> coordination changes to 7, in a non-protective gel and the dissolution rate of the glass increases. New generations of spent fuels require high content of Zr<sup>4+</sup> in glasses. The modifications of Zr<sup>4+</sup> environment in the glass and gel has been investigated in simplified 5-oxide glasses with 1 to 8 mol% Zr. The structural modifications illustrate the molecular-scale origin of the processes of the glass-to-gel transformation.

## Symposium 5: Festschrift for Professor Donald R. Uhlmann

### Models and Connections

Room: Madison

Session Chair: Lisa Klein, Rutgers University

### 9:20 AM

#### (GOMD-S5-004-2016) Modeling of Glass-Ceramics with Anisotropic Crystallization (Invited)

D. P. Birnie<sup>\*1</sup>; 1. Rutgers University, USA

Many anisotropic phases form during crystallization in various glass-ceramic systems. These anisotropic grains grow into interesting morphologies that exhibit interconnected textures, which can have beneficial mechanical, electrical or other properties. Anisotropic shapes result from rapid growth in certain crystal directions or by crystals being bounded by low surface energy crystallographic facets. In either case the kinetics of the transformation and the morphology of the final product are strongly influenced by these shape effects. This paper reviews various kinetic and morphological analyses of such anisotropic transformations. Interestingly, the faster growing directions interact with neighboring particles sooner in the transformation and result in grain morphologies that appear less elongated and the JMAK transformation exponents are reduced from what would be extracted from the earliest stages of a transformation.

### 9:50 AM

#### (GOMD-S5-005-2016) Connections: From metallurgy, to glass science, to phase separation, to localization of light (Invited)

T. P. Seward<sup>\*1</sup>; 1. Retired, USA

This talk illustrates how faculty advisors and scientific colleagues, both in university and industry, through generating ideas, stimulating curiosity and providing strong encouragement can propel

one into new research areas, open career path opportunities and sometimes lead to useful new products. Don Uhlmann and I each began our graduate work in metallurgy, then moved into glass science under the guidance and encouragement of Professor David Turnbull. Don was the first to interest me in phase separation and the mechanisms by which its microstructure evolves. He continued to encourage me in related investigations long after graduate school. I hope to show how understanding of solidification in metal systems and phase separation in glasses can come together to yield better understanding and control of unusual optical behavior of glasses, such as photochromism and photo-adaptation, and how mechanical elongation of viscous phase-separated glass melts can lead to even more unusual optical behavior, such as light polarization, image transfer and light localization.

**10:20 AM**

**(GOMD-S5-006-2016) The Spherical Cow and Associated Technological Breakthroughs: A tribute to Don Uhlmann**

G. W. Scherer<sup>\*1</sup>; 1. Princeton, USA

Creative approximation is essential to modeling of complex physical phenomena, even when numerical methods are applied. A few examples, inspired by the tutelage of DRU, will be offered to illustrate the advantages and pitfalls of such analyses. The particular case of crystal growth in a porous network will be considered in detail.

**10:40 AM**

**(GOMD-S5-007-2016) Cigars and Tiny Bubbles (Invited)**

G. Wicks<sup>\*1</sup>; 1. Wicks Consulting Services, LLC, USA

Prof. Don Uhlmann is one of the top glass scientists in the world and has served as major professor and mentor to many students during his illustrious career. We have all benefited from his many contributions and will also remember with fondness his unique 'signatures', including cigars and love of the 'bubbly', especially fine wines. A presentation will be given by a former student and include antidotes of Don from 40 years ago, and will also focus on an expanded view of 'tiny bubbles' .... not those to drink, but instead, a new class of materials called Porous Wall Hollow Glass Microspheres (PWHGMs). These tiny glass micro-balloons are about one-half the diameter of a human hair and range in size from 2 to about 100 microns, and were featured on the covers of Ceramic Bulletin and IJAGS. The thin outer shells are about one micron thick and what makes these microspheres one-of-a-kind is that an interconnected, through-wall porosity was induced and controlled on a scale of 100 to 1,000 Å. This porosity is then used to fill the microspheres with a variety of materials, including solids, liquids and gases, which result in new composites having unique properties and payloads. This microsphere technology has been involved in more than a dozen different programs and applications in areas of energy, environmental remediation, defense and medicine. PWHGMs have been patented, licensed, and are now being further advanced at the Applied Research Center in SC.

**11:10 AM**

**(GOMD-S5-008-2016) Applications of the Uhlmann Conjecture in Non-Traditional Domains (Invited)**

B. Fabes<sup>\*1</sup>; 1. Civic Consulting Alliance, USA

In 1984, Don Uhlmann described a generalizable formula (the Uhlmann Conjecture) for choosing problems to explore in materials science:  $\Sigma = f(Cx\Delta)$ , where  $\Sigma$  is the satisfaction derived from exploration,  $C$  is the degree of complexity in solving any particular problem, and  $\Delta$  is the depth of engagement with interesting people necessary for the problem's successful exploration. Just as Don's contributions have been seminal in traditional and non-traditional glasses, the Uhlmann Conjecture has proven, through more than three decades of experimentation, to be highly relevant in traditional and non-traditional career domains. This talk will explore applications of the Uhlmann Conjecture to minor fields outside of materials

science, including business, university administration, non-profit management, and life in general, establishing an empirical basis for the initial Conjecture. Point solutions for specific cases will be presented, and at least one extension of the general formula will be proposed.

**Norbert J. Kreidl Award Lecture**

Room: Madison

**12:00 PM**

**(GOMD-AW-003-2016) Materials and devices for mechanically flexible integrated photonics (Invited)**

L. Li<sup>\*1</sup>; 1. Massachusetts Institute of Technology, USA

Flexible integrated photonics is a new technology that has only started to burgeon in the past few years, which opens up emerging applications ranging from flexible optical interconnects to conformal sensors on biological tissues. In this talk, we will discuss the synthesis and characterization of chalcogenide glass (ChGs) and amorphous titanium dioxide materials for flexible integrated photonics. Our technology capitalizes on the exceptional properties of these amorphous materials including broadband infrared (IR) transparency, wide accessible range of refractive indices, as well as low deposition temperature to realize monolithic photonic integration on plastic substrates. High-index-contrast multi-layer 2.5-D photonic devices with record optical performance were fabricated using simple, low-cost contact lithography. A novel multi-neutral-axis design is implemented to render the structure highly mechanically flexible, allowing repeated bending of the devices down to sub-millimeter bending radius without measurable optical performance degradation. We further demonstrated hybrid integration of active optoelectronic components onto the flexible photonic platform, which potentially enables complete system-on-a-flexible-chip solutions for a wide cross-section of applications.

**Symposium 1: Fundamentals of the Glassy State**

**Session 1: Glass Formation and Relaxation II**

Room: Capitol A

Session Chair: Sabyasachi Sen, UC Davis

**1:20 PM**

**(GOMD-S1-014-2016) Structural relaxation of organic and metallic glasses: A new mechanism for relaxation in glasses of high kinetic stability (Invited)**

M. D. Ediger<sup>\*1</sup>; 1. University of Wisconsin-Madison, USA

Here we describe recent studies of structural relaxation in organic and metallic glasses. Gold-based metallic glasses were cooled very rapidly from the liquid; the impact of aging on the enthalpy and the kinetic stability was tracked during seven decades of physical aging. The onset temperature increased by nearly 30 K as a result of annealing. Organic glasses of high stability were prepared by physical vapor deposition. Both the metallic and organic glasses were subjected to temperature up-jump experiments in which structural relaxation occurs into the supercooled liquid. Glasses with very high kinetic stability transform into the supercooled liquid via a constant velocity front. In this respect, glasses with high kinetic stability show a new mechanism for structural relaxation. Transformation via front propagation has also been observed in recent computer simulations of high stability glasses. The aged metallic glasses show no evidence for front propagation and a quantitative comparison is made between the organic and metallic systems.

\*Denotes Presenter

1:50 PM

## (GOMD-S1-015-2016) Microscopic Theory of Elasticity-Mediated Activated Relaxation in Glass-Forming Liquids (Invited)

K. Schweizer<sup>\*</sup>; 1. University of Illinois, USA

We formulate and apply a predictive, quantitative, force-level, statistical mechanical theory of activated relaxation in real space that covers in a unified manner the Arrhenius, dynamic crossover and deeply supercooled regimes. The elementary irreversible re-arrangement event is of a mixed local-nonlocal character which involves coupled cage-scale large amplitude hopping and a longer range collective spontaneous elastic distortion of the surrounding liquid. The more strongly temperature and density dependent collective process is associated with a growing length scale, the transient localization length, and density fluctuation amplitude. Chemical complexity in specific molecular and polymeric liquids is addressed based on an a priori mapping to an effective spherical particle fluid with an identical thermodynamic state dependent amplitude of long wavelength dimensionless density fluctuations. The theory is devoid of fit parameters, has no divergences at finite temperature or below jamming, and captures the key features of the mean alpha relaxation time in colloidal suspensions, molecular liquids and polymer melts. Predictions for connections between short and long time dynamics, fragility and the glassy elastic shear modulus have also been made. The approach can be generalized to treat spatial mobility gradients and vitrification temperature shifts in thin films.

2:20 PM

## (GOMD-S1-016-2016) Viscosity of hydrous borate and silicate glasses

J. Deubener<sup>\*1</sup>; H. Behrens<sup>2</sup>; R. Müller<sup>3</sup>; 1. Clausthal University of Technology, Germany; 2. Institute of Mineralogy, Leibniz University of Hannover, Germany; 3. Federal Institute for Materials Research and Testing (BAM), Berlin, Germany

Borate and silicate glasses with different water content using wet condition of melting under external pressure up to 6 kbar were studied. Experiments on hydrous melts and glasses were conducted to determine the effect of total water content on viscous flow, glass transition temperature and kinetic fragility as well as the influence of the water speciation on the boron and silicon speciation, respectively. The findings indicate that water dissolves in borate glasses quasi exclusively as OH-group, which primarily causes breaking of B-O-B bonds rather than supporting 4-fold coordinated boron while in hydrous silicate glasses besides OH-groups H<sub>2</sub>O molecules are present leading to a more complex change in viscous behavior.

2:40 PM

## (GOMD-S1-017-2016) Role of Structural Relaxation in the Network Dilation of Ion-Exchanged Glasses

E. A. King<sup>\*1</sup>; D. C. Allan<sup>1</sup>; J. C. Mauro<sup>1</sup>; 1. Corning Incorporated, USA

Chemically strengthened glasses produced via ion exchange processes are currently of great interest due to their high strength and damage resistance. Such strengthening is the result of an atomic size mismatch between exchanged alkali ions, leading to elastic strain within the glass network and ultimately changes in the glass dimensions. Dilation of the glass network during such processes is captured by the linear network dilation coefficient (B), defined as the strain per molar concentration of exchanged alkali ions, and is critical to understanding the fundamental strengthening mechanisms during ion exchange processes. Previously we have shown how to directly access B via direct strain measurements, allowing us to track the dimensional changes associated with the elastic strain in the network. These dimensional changes were found to be linearly proportional to the fractional weight gain (a measure of the number of atoms exchanged) of the glass during the ion exchange process at low temperatures. Departures from linearity are observed at higher ion exchange temperatures due to the presence of structural relaxation. Linearity is restored when structural relaxation is taken into

account. Here we extend our past study to consider both compositional effects in varying alkali aluminosilicate glasses and a wider range of thermal histories.

3:00 PM

## (GOMD-S1-018-2016) Structural Relaxation Time of Supercooled Pt<sub>57.5</sub>Cu<sub>14.7</sub>Ni<sub>5.3</sub>P<sub>22.5</sub> Nanowires in the Supercooled Liquid State from Electron Correlation Microscopy

P. Zhang<sup>\*1</sup>; L. He<sup>1</sup>; Z. Liu<sup>2</sup>; J. Schroers<sup>2</sup>; P. Voyles<sup>1</sup>; 1. University of Wisconsin-Madison, USA; 2. Yale University, USA

We have developed electron correlation microscopy (ECM), the coherent electron scattering equivalent of photon correlation spectroscopy, as a way to measure structural relaxation times of liquids with nanometer-scale spatial resolution. ECM uses a time series of electron nanodiffraction patterns measured with a nanometer-diameter coherent probe beam in a field-emission scanning transmission electron microscope (STEM) to measure the time autocorrelation function  $g_2(t)$ , which we fit to the Kohlrausch-Williams-Watt function to obtain the structural relaxation time  $\tau$  and stretching exponent  $\beta$ . We have applied ECM with a 3.5 nm diameter probe to glassy Pt<sub>57.5</sub>Cu<sub>14.7</sub>Ni<sub>5.3</sub>P<sub>22.5</sub> nanowire heated inside the STEM into the supercooled liquid region. The measured  $\tau$  shows a continuous decrease from  $T_g$  to  $T_g + 28$  °C.  $\beta$  also decreases when nanowire was heated from metastable glassy state to supercooled liquid. These data also demonstrate the limits of applicability of the ECM technique: the time series must be at least 30t to obtain a well-converged  $g_2(t)$ , and the time per frame must be less than 0.1t to obtain sufficient sampling. Using a fast (2.5 ms frame time) direct electron detection camera on a modern, stable STEM instrument, we can obtain reliable data over whole measured temperature regime, covering t from 0.2s to 4.4s.

3:40 PM

## (GOMD-S1-019-2016) Enthalpy relaxation in melt-quenched metal-organic framework glasses (Invited)

Y. Yue<sup>\*1</sup>; 1. Aalborg University, Denmark

The metal-organic framework (MOF) glass is a new member of the family of melt-quenched glasses (MQG) besides organic glass, inorganic non-metallic glass and metallic glass. It is hybridized between metal atoms and organic molecules. Original MOFs are microporous materials of special interest for gas storage and separation, catalysis and drug delivery. It has been found that upon heating some of MOFs can be melted and then quenched to bulk glass. As the MOF glass is of recent origin, numerous fundamental problems need to be explored. In the present work we explore the enthalpy relaxation in MOF glasses. The focus is placed on ZIF-4 (Zn(C<sub>3</sub>H<sub>3</sub>N<sub>2</sub>)<sub>2</sub>) - a kind of zeolitic imidazolate frameworks (ZIFs). We investigate both alpha- and beta-relaxation behaviors of ZIF-4 MQG by varying quenching rate and performing long time sub- $T_g$  annealing. The stability of the medium-range order structure of ZIF-4 MQG upon annealing is studied using both DSC and small angle XRD methods. The structural heterogeneity in ZIF-4 MQG is revealed in terms of the non-exponentiality of enthalpy relaxation, and then is compared with that of HDAP. Our enthalpy relaxation study also provides insights into the polyamorphic transition in collapsed ZIF-4.

4:10 PM

## (GOMD-S1-020-2016) Which equation best describes the equilibrium viscosity of glass-forming liquids?

D. R. Cassar<sup>\*3</sup>; M. L. Nascimento<sup>1</sup>; A. M. Rodrigues<sup>3</sup>; T. D. Fragoso<sup>2</sup>; F. Louzada Neto<sup>2</sup>; E. Dutra Zanotto<sup>3</sup>; 1. Institute of Humanities, Arts & Sciences, Federal University of Bahia, Brazil; 2. Institute of Mathematical and Computational Sciences, University of São Paulo, Brazil; 3. Department of Materials Engineering, Federal University of São Carlos, Brazil

We report results of the ability of 18 existing equations to describe the equilibrium viscosity versus temperature curve of glass-forming liquids. We analyzed reported data for 42 inorganic,



metallic, and organic liquids, covering a wide range of fragility indexes. We selected only compositions having at least five data points with viscosity below  $10^4$  Pa.s as well as at least five data points above  $10^8$  Pa.s (“low” and “high” viscosity, respectively). Some of the tested equations were the Vogel–Fulcher–Tammann (VFT), Avramov–Milchev (AM), Cukierman–Lane–Uhlmann (CLU), Bendler–Shlesinger (BS), Angell–Bressel (AB), Demetriou–Harmon–Tao–Duan–Samwer–Johnson (DHTDSJ), and Mauro–Yue–Ellison–Gupta–Allan (MYEGA) with two and three adjustable parameters. We carried out statistical tests using 2,000 bootstrap sub-samples for each composition by fitting all the equations for each sub-sample and computing the mean squared error penalized by the Akaike information criterion, which allowed us to compare equations having different numbers of adjustable parameters. It is relevant to note that the best equations do not predict a viscosity divergence at  $T > 0$  K. We also tested which ones of those 18 equations were best at predicting high viscosity data, and the same trend was observed. We plan to increase the number of analyzed liquids until the presentation in May.

**4:30 PM**

**(GOMD-S1-021-2016) Connectivity Patterns in the Fragility of Network-forming Glasses**

D. Sidebottom<sup>\*1</sup>; I. 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, highlight recent efforts to include additional systems and propose a theoretical interpretation for the universal pattern. Our interpretation is based on the Adam-Gibbs viscosity model and incorporates elements of rigidity percolation. We suggest that the fragility pattern is connected to changes in entropy associated with bond breaking that take two forms: one configurational (that vanishes for connectivities in excess of the rigidity percolation threshold) and the other vibrational.

**Session 3: NMR**

Room: Capitol B

Session Chair: Randall Youngman, Corning Incorporated

**3:40 PM**

**(GOMD-S1-022-2016) Connecting NMR Spectroscopy Results and MD Simulations of Ba-Silicate Glasses**

T. M. Alam<sup>\*1</sup>; T. Zeitler<sup>2</sup>; K. Ewsuk<sup>3</sup>; B. A. Hammann<sup>2</sup>; 1. Sandia National Laboratories, USA; 2. Washington University in St. Louis, USA

Solid state NMR is an important tool for the characterization of glasses, while molecular dynamics (MD) simulations have become crucial in understanding the impact of constituents on glass structure and properties. NMR probes the local and intermediate structures allowing the coordination, bond angle and distances to be determined. Unfortunately extracting this information requires correlations between the NMR results and glass structure to be developed, and in many instances proves difficult to establish with known reference materials. In this presentation, we discuss recent efforts in modeling the variation of the  $^{29}\text{Si}$  MAS NMR spectra for Ba-silicate glasses being developed for advanced glass composites, by predicting the NMR chemical shifts directly from MD generated glass structures. By combining empirical relationships with first principle GIPAW (gauge including projected augment wave) periodic system NMR calculations, it was possible to predict NMR chemical shifts for MD simulations containing a very large number of atoms (between 3,000 and 30,000), thus improving the correlation statistics in these amorphous structures. The combined MD-NMR

calculations allowed the impact of different network modifying cations, low concentration constituents and the presence of surface boundaries on the local glass structure to be individually addressed.

**4:00 PM**

**(GOMD-S1-023-2016) Temperature effects on the distribution of non-bridging oxygens on Si and Al in aluminosilicate glass**

E. I. Morin<sup>\*1</sup>; J. Stebbins<sup>1</sup>; I. Stanford University, USA

Non-bridging oxygen (NBO) join one network former to one or more network modifiers. The NBO concentration and distribution influences many properties, including viscosity. In conventional models, NBO are found on  $\text{SiO}_4 = ^{14}\text{Si}$  groups, and are not found on  $^{14}\text{Al}$  or  $^{14}\text{B}$ . However, significant Al-NBO do exist in some aluminosilicates that have high Al/Si ratios and high modifier oxide concentration, such as “CAS10” with Al/Si of ~6 and ~60 mol% calcium oxide (Allwardt et al. 2003). The Al-NBO species is stabilized by high field strength cations, such as  $\text{Y}^{3+}$  (Jaworski et al. 2015). The presence of both Al-NBO and Si-NBO allows for effects of temperature and composition on their relative proportions. Upon comparing annealed glass to a glass with a higher fictive temperature, we obtained the first measurements of a T effect on Al-NBO in a  $^{17}\text{O}$ -enriched yttrium aluminosilicate with an Al/Si of 1 (Schaller et al. 1998). Using  $^{17}\text{O}$  MAS NMR, we see more Al-NBO at high fictive temperature, as expected by greater contribution to configurational entropy and by the likelihood of a  $\Delta H > 0$  for the reaction:  $\text{Si-O-Al} + \text{Si-O-NBO} = \text{Si-O-Si} + \text{Al-O-NBO}$ .

**4:20 PM**

**(GOMD-S1-024-2016) Oxygen Speciation in Calcium Aluminosilicate and Aluminoborosilicate Glasses as Quantified Through  $^{17}\text{O}$  Double-Resonance NMR**

M. M. LaComb<sup>\*1</sup>; D. M. Rice<sup>1</sup>; J. Stebbins<sup>1</sup>; I. Stanford University, USA

$^{17}\text{O}$ ,  $^{27}\text{Al}$  and  $^{11}\text{B}$  NMR have widely been used to quantify numerous aspects of oxide glass structure, but many issues remain to be resolved, including basic issues of assignment of overlapping  $^{17}\text{O}$  resonances. Double resonance NMR, involving cation spin pairs such as  $^{27}\text{Al}$  and  $^{11}\text{B}$ , has provided further details of network connectivities in some multicomponent glasses; very recent work on  $^{27}\text{Al}$ - $^{17}\text{O}$  has allowed unique identification of non-bridging oxygen (NBO) on aluminum cations in lanthanum aluminoborosilicate glasses (Jaworski et al. 2015). We have explored  $^{17}\text{O}\{^{27}\text{Al}\}$  and  $^{17}\text{O}\{^{11}\text{B}\}$  TRAnSfer of Population in DOuble-Resonance (TRAPDOR) NMR experiments in several calcium aluminosilicate and aluminoborosilicate glasses. We have demonstrated clear distinction among resonances for  $^{17}\text{O}$  associated with boron and/or aluminum, including quantification of NBO associated with boron, aluminum and silicon in multicomponent glasses. Spectral components for bridging oxygens with aluminum and boron can also be at least in part separated.

**4:40 PM**

**(GOMD-S1-025-2016) Measuring bond angle distribution in silicate glasses with 2D J PIETA NMR**

D. Srivastava<sup>\*1</sup>; P. Florian<sup>2</sup>; P. Grandinetti<sup>1</sup>; J. Baltisberger<sup>3</sup>; 1. Ohio State University, USA; 2. CEMHTI-CNRS UPR3079, France; 3. Berea College, USA

The importance of measuring the distribution of Si-O-Si angles in silicate glasses cannot be overstated. It is the first broken structural constraint and the variation in these angles is considered to be one of the main sources of disorder in silicate glasses. The  $^2J_{\text{Si-O-Si}}$  coupling in NMR spectroscopy can be used as a probe of structure in the Si-O-Si linkage, although the size of this coupling in silicates is on the order of 0 to 15 Hz. The greatest utility of the  $^2J_{\text{Si-O-Si}}$  coupling, to date, has been in establishing through-bond connectivities between  $\text{Q}^{(n)}$  units, forming the basis of a number of successful INADEQUATE NMR studies. We recently developed the Phase Incremented Echo Train Acquisition (PIETA) method for more accurate measurement of

\*Denotes Presenter

transverse relaxation behavior and J coupling evolution during echo train acquisition. In this three-dimensional experiment we separate and correlate the  $^{29}\text{Si}$  chemical shift to the  $^{29}\text{Si}$ - $^{29}\text{Si}$  J coupling spectrum to the  $^{29}\text{Si}$   $T_2$  relaxation "spectrum". Our results on silica glass show a Si-O-Si bond angle distribution similar to previous  $^{17}\text{O}$  DAS NMR results with a distribution peak at  $147^\circ$  and extending from  $140^\circ$  to  $154^\circ$ . We will also present results on mesoporous silica with 4 nm ordered pores. Interestingly, we observe little variation in the distribution of  $^2J_{\text{Si-O-Si}}$  couplings for the  $Q^{(3)}$  site, consistent with the  $Q^{(3)}$  residing on the walls of the ordered pores.

### 5:00 PM

#### (GOMD-S1-026-2016) Network Structure and Rare-earth Ion Local Environments in Fluorophosphate Photonic Glasses Studied by Solid State NMR and EPR Spectroscopies

M. de Oliveira<sup>\*1</sup>; T. Uesbeck<sup>2</sup>; T. Gonçalves<sup>1</sup>; C. Magon<sup>1</sup>; P. S. Pizani<sup>3</sup>; A. de Camargo<sup>1</sup>; H. Eckert<sup>1</sup>; 1. University of Sao Paulo, Brazil; 2. Westfälische Wilhelms-Universität Münster, Germany; 3. Federal University of Sao Carlos, Brazil

Currently, glasses and glass ceramics doped with trivalent rare earth ions ( $\text{RE}^{3+}$ ) represent the most important class of materials for laser and other optical applications in the visible and near-infrared spectral regions. In this context, one of the challenges is to find host matrices that assure good optical quality and optimum performance of the dopant ions, while still maintaining thermal and mechanical stabilities. Therefore, fluorophosphates have been explored with the promise to combine the merits of fluorides (low phonon energies and refractive index, extensive optical window) and of phosphates (good mechanical properties). In this work we present a detailed structural investigation of fluorophosphate laser glasses in the series  $\text{BaF}_2\text{-SrF}_2\text{-Al}(\text{PO}_3)_3\text{AlF}_3\text{-YF}_3$  doped with Yb or Eu, using Raman, NMR and EPR spectroscopies. The network structure is dominated by the preferred formation of Al-O-P linkages, which have been quantified by means of  $^{27}\text{Al}/^{31}\text{P}$  NMR double resonance techniques. The EPR and optical spectroscopic properties indicate that the local environment of the  $\text{RE}^{3+}$  ions is characterized by a mixed P/F environment, and a preference for fluoride ligation, which evolves with composition in the expected manner. Nevertheless, even at the highest fluoride levels the data suggest residual  $\text{RE}^{3+}$ -phosphate coordination.

## Session 4: Predicting Glass Properties from Simulations

Room: University C/D

Session Chairs: Carlo Massobrio, CNRS-IPCMS-UNR 7504;

Jincheng Du, University of North Texas

### 1:20 PM

#### (GOMD-S1-027-2016) Molecular dynamics simulations study on the relation between dynamical heterogeneity, structural relaxation, and self diffusion in viscous silica (Invited)

M. Vogel<sup>\*1</sup>; P. Henritzi<sup>1</sup>; F. Klameth<sup>1</sup>; A. Bormuth<sup>1</sup>; J. Geske<sup>1</sup>; B. Drossel<sup>1</sup>; 1. Institute of Condensed Matter Physics, TU Darmstadt, Germany

We investigate the relation between dynamical heterogeneity, structural relaxation, and self diffusion in a model of viscous silica. Furthermore, we ascertain the connection between the temperature-dependent dynamical properties of viscous silica, in particular, a high temperature fragile-to-strong transition, and the emergence of tetrahedral order of the silica glass network upon cooling. We characterize the space-time characteristics of dynamical heterogeneity by the degree of deviations from Gaussian displacement statistics ( $\alpha_s$ ), the size of clusters comprising highly mobile particles ( $S_w$ ), and the length of strings consisting of cooperatively moving particles ( $L_w$ ). Comparison with simulation results for a large variety of viscous liquids, reveals a nearly universal decoupling between the time scale of maximum non-Gaussian parameter ( $\tau_{\alpha 2}$ ) and the time constant of structural relaxation ( $\tau_\alpha$ ) upon cooling, explicitly,  $\tau_{\alpha 2} \propto \tau_\alpha$

$^{3/4}$ , while such uniform relation does not exist for the peak times of  $S_w$  or  $L_w$ . On the other hand, the time scale of maximum string length follows the inverse of the self-diffusion coefficient of various viscous liquids, i.e.,  $\tau_1 \propto D^{-1}$ . In addition, we study to which extent relations between dynamical and structural properties of the model silica melt are affected by confinement.

### 1:50 PM

#### (GOMD-S1-028-2016) Glass surface properties design with thermal poling: A Molecular Dynamics study (Invited)

A. Tandia<sup>\*1</sup>; 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 simulations are based on a wide range of glass compositions with and without different types of alkalis and alkaline earth, under 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, and poling conditions. Most of the compositions in depleted layers correspond to forbidden compositions that normally could not be achieved through melting. Detailed characterizations of the chemistry of the depleted surface from thermal poling include calculation of binding energies of these glasses with a water layer before and after the poling, surface response to nano-indentation, coordination and  $Q^n$  speciation variation. 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.

### 2:20 PM

#### (GOMD-S1-029-2016) Atomic-Scale Study of High-Frequency Energy Dissipation in Oxide Glasses

T. Damart<sup>\*1</sup>; A. Tanguy<sup>2</sup>; D. Rodney<sup>1</sup>; 1. Institut Lumière Matière, Université Lyon 1, France; 2. LAMCOS, INSA de Lyon, France

The attenuation of high-frequency sound waves in glasses is still poorly understood, partly because the underlying mechanism strongly depends on the frequency of the incident wave and the ratio between its wavelength and the characteristic length scales in the glasses. A better understanding would however highly benefit a number of applications. One example is the coatings of the mirrors used in the interferometers of gravitational wave detectors. The coatings, made of a multilayer of oxide glasses ( $\text{SiO}_2$  and  $\text{Ta}_2\text{O}_5$ ), are the main sources of dissipation that limit the precision of measurement of the entire detectors. Here, we investigate energy dissipation in model oxide glasses using atomic-scale simulations. We first study the structural and vibrational properties of  $\text{SiO}_2$  and  $\text{Ta}_2\text{O}_5$  glasses. We then employ Molecular Dynamics to measure energy dissipation using simulated mechanical spectroscopy in the GHz and THz regimes. We find that the numerical models compare favorably with existing experimental data. We also show that when the frequency of the loading lies within the frequency range of the normal modes of the system, dissipation is mainly harmonic and arises from the coupling between the loading and the collective excitations of the system, rather than individual atomic motions. At lower frequencies, anharmonicity is measured and analyzed.

### 2:40 PM

#### (GOMD-S1-030-2016) Influence of Deformation Induced Topological Anisotropy on Mechanical Properties of Silica Glass: An Atomistic Study

V. Ganiseti<sup>\*1</sup>; E. Bitzek<sup>1</sup>; 1. Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Glasses are generally believed to be isotropic materials. However, it is well known that anisotropy can be introduced in silica glass, e.g., by wire drawing, and that the mechanical properties are subsequently

anisotropic. Since topology plays an important role for the mechanical properties, it is necessary to understand the physics behind the development of topological anisotropy on the atomic scale. Here we present the results of atomistic simulations using an ab-initio based polarisable force field. Isotropic silica glass was prepared by the melt quenching method. Anisotropy was introduced by either elongating, compressing or shearing the glass. During load, transient anisotropy is observed, as characterized by the anisotropy factor. Significant persistent anisotropy, which remains after removal of load, could only be introduced by compression and shear. Samples with persistent topological anisotropy show also a pronounced anisotropy in the mechanical properties, in particular on the elastic constants and fracture strain. By detailed structural analysis we could relate the changes in properties to topological changes. The results are further discussed in the context of novel processing routes towards ultra-strong glasses.

**3:00 PM**

**(GOMD-S1-031-2016) Dispersion and pressure-dependence of photoelastic response in inorganic glass (Invited)**

J. Zwanziger\*<sup>1</sup>; 1. Dalhousie University, Canada

We present recent results on the dispersion and pressure-dependence of the photoelastic response in typical inorganic glass systems. We take advantage of the similarity in electronic structure between glasses and crystals to simplify the problem and focus on model crystallites. Then the stress-optic response is computed both with density functional perturbation theory, for the pressure case, and from the Bethe-Salpeter equation, for the dispersion. Both types of computations are carried out using density functional theory, in a planewave/pseudopotential implementation. We then connect our computational findings with recent work in our lab that showed distinct qualitative differences in the dispersion depending on the nature of the additive used.

**3:50 PM**

**(GOMD-S1-032-2016) Stretched Exponential Relaxation of Glasses at Low Temperature (Invited)**

Y. Yu<sup>1</sup>; M. Wang<sup>1</sup>; D. Zhang<sup>1</sup>; B. Wang<sup>1</sup>; G. Sant<sup>1</sup>; M. Bauchy\*<sup>1</sup>; 1. University of California, Los Angeles, USA

While it is indeed commonly believed that, as frozen supercooled liquids, glasses should continue to flow over the years (e.g., in the case of the stained-glass windows of medieval cathedrals), the dramatic increase of their viscosity below the glass transition temperature  $T_g$  suggests, on the contrary, that their relaxation time is on the order of  $10^{32}$  years at room temperature. However, a recent study conducted by Mauro et al. reported the intriguing dynamics of the relaxation of a commercial Corning® Gorilla Glass® at room temperature, over 1.5 years. Here, we report a novel atomistic simulation method allowing us to directly access the long-term (years) dynamics of glass relaxation at room temperature. We find that the potential energy relaxation follows a stretched exponential decay, with a stretching exponent  $\beta = 3/5$ , as predicted by Phillips' diffusion-trap model. Interestingly, volume relaxation is also found. However, it is not correlated to the energy relaxation, but it is rather a manifestation of the mixed alkali effect. Beyond glasses, being able to predict and tune the relaxation and aging of materials could improve the understanding of memory encoded materials or protein folding.

**4:20 PM**

**(GOMD-S1-033-2016) Atomic-scale calculation of thermal properties via the "approach-to-equilibrium" methodology**

E. Lampin\*<sup>1</sup>; P. Palla<sup>1</sup>; F. Cleri<sup>1</sup>; G. Ori<sup>2</sup>; A. Bouzid<sup>2</sup>; C. Massobrio<sup>2</sup>; M. Boero<sup>2</sup>; 1. IEMN, France; 2. IPCMS, France

The thermal conductivity of phase change materials (PCM) is a key property that controls the heat transport and dissipation during the writing/reading processes of memories. Since nanoscale

effects impact the value of this property, atomic-scale theoretical approaches are ideally suited to address its microscopic foundations. Recently, we developed a new method to study thermal properties, the approach-to-equilibrium (AE) molecular dynamics, based on the analysis of the temperature transient during the approach to equilibrium in the presence of an initial temperature difference. It would be highly desirable to employ this method to tackle heat transfer in systems as PCM's for which a first-principles treatment is necessary to account realistically for the interatomic forces. In this presentation, we will show our preliminary results obtained when applying the AE approach in the framework of first-principles molecular dynamics for a PCM material. The amorphous phase of GeTe<sub>4</sub> will be investigated and the limitations inherent in the time and space scales of FPMD when applied to thermal properties through the AE method will be explicitly discussed.

**4:40 PM**

**(GOMD-S1-034-2016) Multiscale cohesive zone model for simulation of brittle glass material**

S. Urata\*<sup>1</sup>; S. Li<sup>2</sup>; 1. Asahi Glass Co., Ltd., Japan; 2. University of California, Berkeley, USA

In this work, the multiscale cohesive zone model (MCZM) is applied to simulate crack propagation in brittle materials. MCZM model assumes existence of an extremely thin cohesive zone element between bulk elements to represent an evolving process zone in material damage. Because the model estimates stress in each element by using atomistic potentials with the Cauchy-Born rule, it is possible to simulate crack propagation from first principle without any experimental information and ad hoc assumptions for the cohesive traction. In this study, we employed higher order Cauchy-Born rule to capture nonlinear deformation in the material, and as a result, we found that the cohesive zone can represent nonlinear and inhomogeneous deformation, which makes cohesive zone more prone to damage than the rest of bulk material. Consequently, the cohesive zone, which may have some causes of fracture, such as voids, inhomogeneous stress distribution and atomistic discontinuity, can be modeled by using interatomic potentials without modification. We will compare our simulation results with experimental data of fracture toughness measured by single-edge-notched tension specimen of silicon. Tersoff potential, which is three body interaction, was utilized to evaluate stress distribution in the specimen. Moreover, we shall discuss how to extend our model to amorphous materials to simulate glass substrates.

**5:00 PM**

**(GOMD-S1-035-2016) Network modeling and Simulation of Amorphous Silicon Boron Nitride (SiBN)**

A. Dasmahapatra\*<sup>1</sup>; Y. Ni<sup>2</sup>; T. Dumitrica<sup>2</sup>; P. Kroll<sup>1</sup>; 1. The University of Texas at Arlington, USA; 2. University of Minnesota, USA

Amorphous silicon boron nitride (SiBN) is a refractory material with an expected glass transition temperature above its thermal degradation temperature (~1700°C). Besides its high thermal stability the material is also resistant to oxidation at 1400°C. Here we investigate SiBN materials with compositions between Si<sub>3</sub>N<sub>4</sub> and BN. For each composition, several independent models comprising 100-200 atoms are generated via a network algorithm followed by a simulated annealing procedure using ab-initio molecular dynamic simulations. Within Density-Functional Theory we compute vibrational spectra and elastic constants for all models to extract the minimum lattice thermal conductivity ( $\kappa_{\min}$ ) at high temperatures using the phenomenological model of Clarke. Additionally, we study temperature dependence of thermal conductivity of SiBN via equilibrium molecular dynamics (MD) and the Green-Kubo (GK) method using a Tersoff potential to describe the interatomic potential between Si, B, and N atoms. We find that thermal conductivity is impacted by the dispersion and extend of BN domains inside the SiBN structure. While small BN units act as scattering centers and reduce the

phonon transport (e.g. in Si<sub>3</sub>BN<sub>5</sub>), large extended BN segregations lead to higher thermal conductivity.

**5:20 PM**

### **(GOMD-S1-036-2016) Molecular Dynamics Simulation of Glasses for Photomultiplier Tubes in Neutrino Detection**

R. Dongol<sup>\*1</sup>; S. K. Sundaram<sup>1</sup>; A. Tandia<sup>2</sup>; 1. Alfred University, USA; 2. Corning Inc., 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 classical molecular dynamics (MD) simulation to investigate the structural and mechanical properties for PMT glass composition range (wt%): SiO<sub>2</sub> = 65-70, Na<sub>2</sub>O = 6-9, Al<sub>2</sub>O<sub>3</sub> = 4-7, B<sub>2</sub>O<sub>3</sub> = 15-18, BaO = 0-3, ZnO = 0-3, and CaO = 0-1. In particular, we will use molecular dynamics to study the relative changes of the glass surface structure and property such as: bond length and angle, chemical species, coordination number, Young's, bulk, shear modulus, stress-strain ratio Young's, shear, bulk moduli, stress-strain analysis 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 optimized glass composition with mechanical properties. The selected glass composition will be used for further experimental study of performance of the glass for neutrino application.

## **Session 5: Mechanical Properties of Glasses I**

Room: Wisconsin

Session Chair: Tanguy Rouxel, Université de Rennes 1

**1:20 PM**

### **(GOMD-S1-037-2016) Water-Enhanced Swelling of Silica Glass: Role of Applied Stress (Invited)**

S. Wiederhorn<sup>\*1</sup>; G. Rizzi<sup>2</sup>; M. Hoffmann<sup>2</sup>; T. Fett<sup>2</sup>; 1. National Institute of Science and Technology, USA; 2. Karlsruhe Institute of Technology, Germany

We applied the theory of Le Chatelier to study the reaction of water with silica glass simultaneously subjected to high external tensile stresses. We show that an applied tensile stress in the GPa range can change the equilibrium constant of the water/silica reaction sufficiently to enhance the concentration of ≡SiOH approximately ten-fold, and the residual swelling stress by a similar amount. Using ≡SiOH data obtained by either I-R Analysis or Nuclear Reaction Analysis, we found that stresses applied during the exposure of silica glass to water vapour at temperatures ranging from 200°C to 500°C enhanced water penetration into the silica glass and substantially strengthened the glass. Our results support the idea that the water migration into silica glass strengthens the glass sufficiently at elevated stresses and temperatures to justify the strengthening results obtained recently by Lezzi et al.

**1:50 PM**

### **(GOMD-S1-038-2016) Glass Strength and Water (Invited)**

M. Tomozawa<sup>\*1</sup>; 1. Rensselaer Polytechnic Institute, USA

It has been well known that water and water vapor reduce the mechanical strength of oxide glasses. Also, in some cases, glass strength increases by the interaction with water. In spite of numerous proposed models, it is still not clear exactly how water influences mechanical strength of glasses. It is a high time to review various models and compare them with the accumulated experimental data, especially those of silica glass, prototype of oxide glasses. In particular, the effect of stress on silica glass and water interaction as well as the effect of glass-water interaction on the stress on silica glass will be discussed.

**2:20 PM**

### **(GOMD-S1-039-2016) Effect of Water on Aging and Fatigue of Soda-Lime-Silicate Glass**

E. Ronchetto<sup>\*1</sup>; R. Brow<sup>1</sup>; 1. Missouri University of Science and Technology, USA

Melts of a commercial flint soda-lime-silicate (SLS) container glass were prepared under dry or wet conditions, and fibers drawn from these melts were aged either in 80%RH / 50°C or 1%RH / 50°C air for at least 30 days. Failure strain distributions were measured in liquid nitrogen and in room temperature air at 40% relative humidity using a two-point bend (TPB) test to evaluate the effects of aging and fatigue. Failure strains of fibers drawn from wet melts were lower than those drawn from dry melts, and failure strains from both sets of fibers decreased with aging time. The fatigue parameter, which is used to determine a materials susceptibility to fatigue, was determined by measuring the differences in average failure strain at varying faceplate velocities during the TPB tests, and increased from a value of 15 for pristine glasses to 25 after 28 days of aging in 80%RH/50°C conditions. The glass surfaces were examined with Raman and FTIR spectroscopy, scanning electron microscopy, and atomic force microscopy, which revealed the development of Na-carbonate crystallites on the aged glasses.

**2:40 PM**

### **(GOMD-S1-040-2016) Origin of the Fatigue Limit in Oxide Glasses: Fracture Mechanics Modelling**

J. H. Seaman<sup>\*1</sup>; T. Blanchet<sup>1</sup>; M. Tomozawa<sup>1</sup>; 1. Rensselaer Polytechnic Institute, USA

When loaded in tension, glasses fail due to crack initiation, slow crack growth, and then rapid crack growth as the crack length and loading condition combine to meet the material fracture toughness. It has been observed that below a threshold stress intensity factor,  $K_{IS}$ , also known as the static fatigue limit, cracks appear to not grow. The origin of the fatigue limit has been attributed to crack tip rounding/blunting and water diffusion and swelling. However, both of these concepts have limitations and there is no satisfactory explanation. It is proposed that the fatigue limit of oxide glass is due to the newly observed surface stress relaxation that may relax crack tip tensile stresses. For slowly growing cracks, a correlation exists between the diffusivity of surface stress relaxation and the slow crack growth rate at the fatigue limit. A fracture mechanics model has been developed to predict crack growth behavior near the fatigue limit. The prediction is that cracks growing near the fatigue limit will decrease in velocity under a constant stress intensity, eventually becoming immeasurably small. DCB slow crack growth experiments were performed to prove the validity of this theory. The focus of this talk will be on the fracture mechanics modelling techniques used to make these predictions, including the analogy between plastic deformation and surface stress relaxation.

**3:00 PM**

### **(GOMD-S1-041-2016) The Size Effect of Surface Stress Relaxation**

E. Aaldenberg<sup>\*1</sup>; J. H. Seaman<sup>1</sup>; M. Tomozawa<sup>1</sup>; 1. Rensselaer Polytechnic Institute, USA

It was shown that glass surfaces experience faster structural relaxation kinetics than the bulk when exposed to an atmosphere containing water vapor. Furthermore, the relaxation kinetics were found to depend on the sample size, where faster relaxation was observed for larger surface area to volume ratios. The surface stress relaxation kinetics of silica glass fibers have also been found to be faster than the bulk at temperatures far below the glass transition temperature. Surface stress relaxation has been characterized as a diffusion controlled process, leveraged to create stronger glass fibers, and used to explain other mechanical phenomena in glass. In the present study, the size effect of surface stress relaxation was investigated. Silica glass fibers of varying diameters were fabricated using a

microheater and motorized translation stages. The fibers were then heat-treated in a two-point bend configuration and the residual curvature was measured. From these measurements, it was determined that the relaxation kinetics are dependent on the size of the fiber.

### Session 5: Mechanical Properties of Glasses II

Room: Wisconsin

Session Chair: Minoru Tomozawa, Rensselaer Polytechnic Institute

3:40 PM

#### (GOMD-S1-042-2016) Structural origin of the flaw sensitivity in glasses from different chemical systems: Interatomic bonding character and medium-range order

T. Rouxel<sup>\*1</sup>; 1. University of Rennes 1, France

It is usually said that stiffness comes with strength and hardness, while softness comes with toughness! On the contrary to this common belief which indeed reflects global trends, such as those observed by comparing polymers with metals and further metals with ceramics, the fine details within a class of materials are much more complicated, and thus interesting. For example there are stiff glasses, such as silicon oxynitride ones, that are weak toward indentation cracking, and soft glasses, such as chalcogenide ones, that exhibit a low toughness. The source for the flaw sensitivity lies in the atomic network structure, at the scales of both the atomic bonding and at the medium range order. The ability of structural units to leave some room for shear or for densification is a key factor. The presence of low energy paths for shear and the ease for structural re-combination governs the shear ductility, as is illustrated in the cases of metallic glasses and oxide glasses with large contents of transition metals (d-type). In this regard, temperature and pressure are usually effective in changing the situation.

4:00 PM

#### (GOMD-S1-043-2016) Mechanical Properties of Tectosilicate Calcium-Aluminosilicate, Magnesium-Aluminosilicate, and Calcium-Galliosilicate Glasses

L. Lamberson<sup>1</sup>; R. Youngman<sup>2</sup>; S. P. Baker<sup>\*1</sup>; 1. Cornell University, USA; 2. Corning Incorporated, USA

Aluminosilicate glasses are widely used in applications such as LCD glass, touchscreens for hand held devices and car windows. We have shown that the tectosilicate compositions exhibit an interesting non-monotonic variation in hardness with increasing SiO<sub>2</sub> content. Hardness and indentation modulus both decrease as SiO<sub>2</sub> content increases from 40% to 85 mol%. Above 85 mol% hardness increases while indentation modulus continues to decrease. The modulus correlates well with density. At low SiO<sub>2</sub> contents, hardness was consistent with the topological constraint theory, while glasses above 85 mol% SiO<sub>2</sub> are consistent with a plastic deformation mechanism switch from shear to densification. Substituting Mg for Ca or Ga for Al results in similar behavior with slightly higher and significantly lower hardnesses for magnesium-aluminosilicate and calcium-galliosilicate glasses, respectively. The hardness minimum is shifted to lower silica contents in both variants. We describe variations in possible plastic deformation mechanisms based on various species in the glass determined by NMR. Linking unit deformation mechanisms to hardness is key to developing glasses that exhibit more desirable mechanical properties.

4:20 PM

#### (GOMD-S1-044-2016) Mechanical Properties of Denisified Tectosilicate Calcium-Aluminosilicate Glasses

N. Johnson<sup>\*1</sup>; L. Lamberson<sup>2</sup>; M. M. Smedskjaer<sup>3</sup>; S. Baker<sup>1</sup>; 1. Cornell University, USA; 2. Corning Incorporated, USA; 3. Aalborg University, Denmark

Aluminosilicate glasses are widely used in applications such as LCD glass, touchscreens for hand held devices and car windows. We have

shown that the tectosilicate compositions exhibit an interesting non-monotonic variation in hardness with increasing SiO<sub>2</sub> content. From 40% to 85 mol% SiO<sub>2</sub>, hardness and indentation modulus both decrease, consistent with the topological constraint theory. Above 85 mol% SiO<sub>2</sub>, hardness increases rapidly with increasing SiO<sub>2</sub> content while modulus continues to decrease. A switch from shear to densification based on the species present in the glass has been proposed to explain this behavior. To reduce densification and study shear deformation independently, a series of calcium aluminosilicate glasses with tectosilicate compositions were densified by isostatic compression in a gas pressure chamber at elevated temperatures. The compressed glasses have increased elastic modulus and hardness in comparison to their uncompressed counterparts. Structural changes during compression can inform mechanisms of deformation at the atomic scale, and linking unit deformation mechanisms to hardness is key to developing glasses that exhibit desirable mechanical properties like resistance to brittle fracture.

4:40 PM

#### (GOMD-S1-045-2016) Vickers Indentation of Ion-Exchanged Glasses at Quasi-Static and Dynamic Loading Rates

T. M. Gross<sup>\*1</sup>; 1. Corning Incorporated, USA

The resistance to the formation of strength limiting flaws (median/radial cracks) by contact in ion-exchanged alkali aluminosilicate glasses is commonly measured using Vickers indentation under quasi-static loading conditions. With similar ion-exchange compressive stress profiles, a normal glass composition has a quasi-static Vickers cracking threshold of 7 kilograms force (kgf), while an intermediate glass composition deforming with more densification and less shear has a cracking threshold exceeding 30 kgf. Under dynamic loading conditions, the Vickers cracking thresholds exceed 50 kgf and 150 kgf for the normal and intermediate glasses, respectively. The rate dependence on the cracking thresholds is discussed in terms of rate dependence of deformation mechanisms for these different glass types. The water interaction with glass during indentation and its role in the formation of cracking systems is also discussed.

5:00 PM

#### (GOMD-S1-046-2016) Surface deformation and indentation-induced stress in various nanocrystallized glasses

K. Shinozaki<sup>\*1</sup>; T. Honma<sup>1</sup>; T. Komatsu<sup>1</sup>; 1. Nagaoka University of Technology, Japan

Nowadays, glasses are widely used in various fields such as structural, optical, and electronic applications. Glasses have brittle nature, but the requirement for reducing thickness has increased, so that reduction of brittleness of glass is important to use for practical applications. It has been proposed the relationship between brittleness and physical property of glass (density, poisons ratio) or deformation behavior (ratio of densification and plastic deformation). On the other hand, the role of nanocrystals on clack initiation and propagation in nanocrystallized glasses is really complicated, so it has not been understood well. We focused our attention on the effect of nanocrystals on surface deformation behavior and formation of residual stress field in various optical functional transparent glass-ceramics with silicates, borates, germinates, tellurites, and oxyfluorides. Surface deformation behavior was investigated with using nanoindentation technique and residual stress fields around indents were observed by using birefringence imaging system. The relationship of clack propagation around Vickers indents, residual stress field around indents, and deformation behavior under nanoindentation has been proposed in this work.

\*Denotes Presenter

5:20 PM

**(GOMD-S1-047-2016) Influence of mechanical properties on the dimple formation of non-alkaline glass substrate during the chemical thinning process**

H. Tokunaga<sup>\*</sup>; K. Hayashi<sup>1</sup>; I. Asashi Glass Co.,Ltd, Japan

Chemical thinning is one of the significant processes to obtain thin display panels. During this process, small circular dimples were formed and recognized as defects. In this study, dimple formation behavior during chemical thinning process of non-alkaline glasses was investigated. Vickers indentation was performed on the surface of the glasses as a typical mechanical damage. Then the glasses were etched with HF. After that, indents were observed using laser microscope. As indented at less than 100gf load in the ambient atmosphere, no cracks were observed. However, after immersing into HF solution to etch 5 $\mu$ m in thickness, grooves were observed along with the diagonal direction of the impression. The reason of groove formation is considered that reaction with HF weakened the bonding of glass network and residual stress caused the crack formation. With further etching up to around 300 $\mu$ m, round-shaped dimples were formed. The final dimple size of the glass with higher Young's modulus was smaller than that of conventional non-alkaline glass. Since measured fracture toughness of the higher Young's modulus glass is larger than of the conventional glass, the length of initial crack for higher Young's modulus glass showed smaller dimple size. The dimple formation behavior using indenters with various tip geometry also will be discussed in the presentation.

### **Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications**

#### **Session 1: Electronic Conducting Materials I**

Room: University A/B

Session Chair: Ruud Schropp, Eindhoven University of Technology (TU/e)

1:20 PM

**(GOMD-S3-023-2016) Electron-conducting Filaments in Ion-conducting Ag-Ge-Se Glasses (Invited)**

G. Chen<sup>\*</sup>; M. Sundarajan<sup>1</sup>; L. Zella<sup>1</sup>; H. Abu Jeib<sup>1</sup>; D. Drabold<sup>1</sup>; M. Kordesch<sup>1</sup>; D. Ingram<sup>1</sup>; I. Ohio University, USA

Ag doped chalcogenide glasses exhibit extremely high ionic conductivity but very low electrical conductivity. Under a strong external electric field, an electron-conducting path can be created or annihilated inside the glasses, depending on the polarity of the electric field. This interesting phenomenon is the basis of Conductive Bridging Random Access Memory. However, little is known about the structure and properties of the electron-conducting filaments. To shed light on the structural origin of the filaments, we selected Ag-Ge-Se ternary glasses as a model system. Ag<sub>x</sub>(GeSe<sub>2</sub>)<sub>1-x</sub> and Ag<sub>x</sub>(GeSe<sub>3</sub>)<sub>1-x</sub> thin films were prepared by physical vapor deposition. Structure of the Ag-Ge-Se glasses was characterized by various X-ray techniques and correlated with their optical and electrical properties. The experimental results were compared with theoretical calculations based on ab-initio simulations. Our study provides atomistic insight into structure-property relations of the electron-conducting filaments in Ag-Ge-Se glasses.

1:50 PM

**(GOMD-S3-024-2016) Relation between hydrogen-bonding environment and high frequency Si-H stretching vibrations in hydrogenated amorphous silicon (Invited)**

P. Biswas<sup>\*</sup>; D. Drabold<sup>2</sup>; I. The University of Southern Mississippi, USA; 2. Ohio University, USA

Recent experiments on vibrational transient-grating measurements using picosecond infrared pulses from free electron lasers have demonstrated the presence of highly localized modes in the high-frequency band of hydrogenated amorphous silicon around 2000 cm<sup>-1</sup> with the flow of vibrational energy to the bending modes. Motivated by this observation, we have addressed the problem from a first-principles density-functional approach using the models of hydrogenated amorphous silicon obtained via the experimental constraint molecular relaxation (ECMR) method. The localized nature of the high-frequency vibrational modes has been studied using the inverse participation ratio of the vibrational eigenstates. Our study indicates that isolated Si-H bonds give rise to the localized modes near the frequency 2000 cm<sup>-1</sup>. Analysis of vibrational eigenvectors, obtained from the first-principles DFT calculations, suggests that the isolated high-frequency modes are mostly stretch modes, whereas the low-frequency modes predominantly exhibit a bending character. Further, the local hydrogen microstructure is found to influence the exact frequency and the nature of these localized modes. The frequency shift associated with the high-frequency localized modes, and its relation to the local hydrogen environment has been also addressed from a first-principles point of view.

2:20 PM

**(GOMD-S3-025-2016) Electron-phonon couplings for disordered systems**

D. Drabold<sup>\*</sup>; K. Prasai<sup>1</sup>; I. Ohio University, USA

We have pointed out that the electron-lattice coupling is large for localized states, manifesting itself in many interesting physical processes among them light-induced structural rearrangements such as the Staebler-Wronski effect in amorphous silicon, analogous phenomena in chalcogenide glasses, and applications like thermal imaging. In this talk, we describe updated calculations of these couplings including surface plots of the coupling for amorphous selenium (a-Se), simulations of photoresponse of a-Se, and new evidence for the remarkable correlation between localization gauged by inverse participation ratio (a strictly static quantity) and the thermally-induced root-mean-square fluctuation in Kohn-Sham eigenvalues near the Fermi level (a dynamical quantity). We point out the utility of Hellmann-Feynman forces (employed as a sort of artificial electron-phonon coupling) as a tool to engineer materials with desired electronic properties.

2:40 PM

**(GOMD-S3-026-2016) Vibrations in amorphous silica**

B. Bhattacharai<sup>\*</sup>; D. Drabold<sup>1</sup>; I. Ohio University, USA

In this talk, we describe the vibrational properties of a realistic 648-atom model a-SiO<sub>2</sub>. The normal modes of a 648-atom model are computed with the ab initio density functional code SIESTA. The static structure factor and the electronic density of states are in good agreement with the experimental data. The vibrational density of states is analyzed by evaluating the partial density of states and localization. The vibrational modes were further investigated by calculating phase quotient and stretching character, and constructing animations of specific nodes of interest. We have obtained a low temperature specific heat in qualitative agreement with experiments, including a feature resembling the Boson peak, and the modes that give rise to this feature. This talk is of some interest as the largest (648-atom) ab initio study of vibrations in amorphous silica presented to date. The vibrations occurring at different specific modes are visually analyzed and presented.

3:00 PM

**(GOMD-S3-027-2016) Gap engineering using Hellmann-Feynman forces: method and applications**K. Prasai<sup>\*1</sup>; P. Biswas<sup>2</sup>; D. Drabold<sup>1</sup>; 1. Ohio University, USA; 2. The University of Southern Mississippi, USA

Materials with optimized band gap are needed in many specialized applications. In this talk, we demonstrate that Hellmann-Feynman forces associated with the gap states can be used to find atomic coordinates that yield desired electronic density of states. Using tight-binding models, we show that this approach may be used to arrive at electronically designed models of amorphous silicon and carbon. We provide a simple recipe to include *a priori* electronic information in the formation of computer models of materials, and prove that this information may have profound structural consequences. We'll briefly discuss implementation of the method in *ab-initio* molecular dynamics simulations and highlight the latest feats of the method ranging from modeling amorphous semi-conducting materials to understanding the structure and properties of memory materials.

**Session 1: Electronic Conducting Materials II**

Room: University A/B

Session Chair: Partha Biswas, The University of Southern Mississippi

3:40 PM

**(GOMD-S3-028-2016) Advanced electronic quality of narrow-gap amorphous silicon-germanium (Invited)**R. E. Schropp<sup>\*1</sup>; Y. Kuang<sup>1</sup>; L. W. Veldhuizen<sup>1</sup>; 1. Eindhoven University of Technology (TU/e), Netherlands

Hydrogenated amorphous silicon-germanium (a-SiGe:H) is an attractive direct-bandgap absorber material for thin film solar cells. We have investigated this material for application in multibandgap tandem solar cells, where it could replace the rather thick (1-2  $\mu\text{m}$ ) microcrystalline silicon ( $\mu\text{c-Si:H}$ ) thin films. a-SiGe:H with an order of magnitude smaller thickness can absorb the same amount of light, but it has been difficult to obtain this alloy with sufficient electronic quality using conventional deposition techniques. As an alternative we studied the hot wire CVD technique, which has the potential to deposit higher electronic quality films due to its fundamentally different decomposition method and growth ambient. We have developed chemically isotropic a-SiGe:H materials with excellent electronic quality. In solar cell devices the photocurrent generation of a 150-nm a-SiGe:H layer with a band gap of 1.54 eV is as high as that of a 1.8- $\mu\text{m}$  microcrystalline silicon layer. Moreover, this layer is deposited within only six minutes, thus facilitating production in substantially smaller vacuum systems. As the hot wire is a linear source of growth radicals, the HWCVD technique is perfectly suitable for roll-to-roll fabrication. We will show that the conformal nature of HWCVD facilitates deposition of defect-free layers over highly corrugated nano-pillar shaped surfaces for additional light trapping.

4:10 PM

**(GOMD-S3-029-2016) The amorphous structure of prototypical phase change materials revisited: New first-principles molecular dynamics insights (Invited)**A. Bouzid<sup>\*1</sup>; 1. Institut de physique et chimie des matériaux de Strasbourg, France

Chalcogenide memory materials or phase change materials (PCM) are based on the fast and reversible switching between the crystalline and amorphous states. This property allows for their incorporation in a wide range of technological devices. Within the family of chalcogenides used to make PCM devices,  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  (GST) is considered as the prototypical system due to its high switching speed and to its good optical contrast. Focusing on its glassy state, theory

and experiments provided insights into its atomic scale structure by resorting to different models. However, the structure of this system is controversial and optimal agreement with experimental data remains to be achieved. In this work, I will first focus on the impact of different theoretical schemes (different exchange and correlation functionals and the inclusion of the van der Waals dispersion forces) on the structure of glassy  $\text{GeTe}_4$ . This compound is a recurrent subsystem on many  $\text{GeSbTe}$  phase change alloys. Second, interest will be devoted to recent structures of GST obtained by first-principles molecular dynamics. Systematic comparison with experimental findings and previous simulation results will be carried out.

4:40 PM

**(GOMD-S3-030-2016) Force-enhanced Atomic Refinement (FEAR): A structural modeling technique for disordered and glassy materials**A. Pandey<sup>\*1</sup>; P. Biswas<sup>2</sup>; D. Drabold<sup>1</sup>; 1. Ohio University, USA; 2. The University of Southern Mississippi, USA

We introduce a structural modeling technique, dubbed force-enhanced atomic refinement (FEAR)[1]. The technique incorporates interatomic forces within reverse Monte Carlo (RMC) simulations for structural refinement by fitting experimental diffraction data using the conventional RMC algorithm and periodically minimizes the total energy and forces from an interatomic potential. The inclusion of forces generated from a potential ameliorates shortcomings of RMC and produce more realistic models. The technique minimizes the number of force calls, making it more efficient than existing conventional molecular dynamics techniques. We illustrate the approach by studying a typical glass forming material amorphous silica (a- $\text{SiO}_2$ ) and amorphous silicon (a-Si). The structural and electronic properties of the FEAR models agree well with experimental neutron and x-ray diffraction data and the results obtained from previous molecular dynamics simulations of a- $\text{SiO}_2$  and a-Si. The computational time in FEAR has been observed to scale quadratically with the number of atoms. We present first results of the method with *ab initio* interactions.

**Symposium 4: Glass Technology and Cross-Cutting Topics****Session 4: Glass Corrosion: Mechanisms and Rate II**

Room: Capitol B

Session Chairs: Eric Pierce, Oak Ridge National Lab; Stephane Gin, CEA

1:20 PM

**(GOMD-S4-045-2016) Interfacial behavior and dissolution gel structures of silicate glasses from ReaxFF and *ab initio* based computer simulations**J. M. Rimsza<sup>\*1</sup>; J. Du<sup>1</sup>; 1. The University of North Texas, USA

Identification of the reactions and processes at water-silica interfaces are critical to predicting the chemical durability of silicate glasses, including nuclear waste glasses. Of particular interest is how intermediate phases, such as silica gels or alternation layers, affect the diffusion of water through the system and the dissolution rate. However, atomistic level information of the structure and dynamics at the glass-water interface is still missing, even for pure silica glasses. Simulations provide a unique opportunity to probe the processes which are responsible for the varying stability of interfaces and gel structures which form during dissolution. In this work, a series of atomistic interfacial models, including the dense silica-gel and gel-water interfaces, were developed to investigate the stabilities of the silica byproducts which govern dissolution. A classical molecular dynamics simulation method with an improved reactive force field (ReaxFF), which was validated with *ab initio* simulations, was implemented to investigate the interfacial structure of the silica gel layer

\*Denotes Presenter

as well as the diffusion of water and silica species into the aqueous solution. This new interface model provides the opportunity to investigate how the development of interfacial gel layers can affect the kinetics of silica glass dissolution in aqueous environments.

**1:40 PM**

### **(GOMD-S4-046-2016) Composition and Structural Trends in Static Corrosion of Calcium Aluminosilicate Glasses**

N. J. Smith<sup>\*1</sup>; R. Schaut<sup>1</sup>; J. Hamilton<sup>1</sup>; J. Klotz<sup>1</sup>; E. Bakowska<sup>1</sup>; A. Li<sup>1</sup>; K. Murphy<sup>1</sup>; 1. Corning Incorporated, USA

In the development of technical glasses for industrial applications, the link between glass structure and chemical durability represents an area of great practical significance—in some cases impacting functional performance of a surface in end use, but also potentially affecting ability to clean or otherwise treat surfaces in aqueous chemistries during production. In an effort to better understand the effect of composition and structure on these attributes (and particularly over relatively short corrosion timeframes), here we investigate the static corrosion response of a wide series of model glasses in the calcium aluminosilicate system. Through evaluations of static extraction rates in acidic, basic and neutral-pH media under low surface-area-to-volume ratio conditions, we highlight notable trends in this space as a function of composition/structure, as well as discuss some experimental considerations.

**2:00 PM**

### **(GOMD-S4-047-2016) Topological Control on Silicates Dissolution Kinetics**

I. Pignatelli<sup>1</sup>; A. Kumar<sup>1</sup>; B. Wang<sup>\*1</sup>; M. Bauchy<sup>1</sup>; G. Sant<sup>1</sup>; 1. University of California, Los Angeles, USA

Silicate solids, e.g. silicate minerals and glasses, dissolve when placed in contact with water. In a given aqueous environment, the dissolution rate depends highly on the composition and the structure of the solid, and can span several orders of magnitude. Although the kinetics of dissolution depends on the complexities of both the dissolving solid and the solvent, a clear understanding of which critical structural descriptors of the solid control its dissolution rate is lacking. Through pioneering dissolution experiments and atomistic simulations, we correlate the dissolution rates - ranging over four orders of magnitude - of a selection of silicate glasses and crystals, to the number of chemical topological constraints acting between the atoms of the dissolving solid. The number of such constraints serves as an indicator of the effective activation energy, which arises from steric effects, and prevents the network from reorganizing locally to accommodate intermediate units forming over the course of the dissolution.

## **Session 4: Glass Corrosion: Analytical Techniques**

Room: Capitol B

Session Chairs: Jonathan Icenhower, Sandia National Laboratories; S. Sundaram, Alfred University

**2:20 PM**

### **(GOMD-S4-048-2016) Towards an Understanding of Surface Layer Formation, Growth, and Transformation at the Glass-Fluid Interface**

J. Hopf<sup>1</sup>; J. R. Eskelsen<sup>1</sup>; D. N. Leonard<sup>1</sup>; E. M. Pierce<sup>\*1</sup>; 1. Oak Ridge National Lab, USA

Describing the reactions that occur at the glass-water interface and control the development of altered layer constitutes one of the main scientific challenges impeding existing models from providing accurate radionuclide release estimates. Radionuclide release estimates are a critical component of the safety basis for geologic repositories. The altered layer (i.e., amorphous hydrated surface layer and crystalline reaction products) represents a complex region, both physically and chemically, sandwiched between two distinct

boundaries—pristine glass surface at the inner most interface and aqueous solution at the outer most interface. Silica-rich altered layers, similar to inorganic coatings on natural minerals, can affect the microscopic processes (e.g., ion diffusion, adsorption, etc.) that impact elemental release rates. This presentation will highlight a newly developed atomic force microscopy technique (Quantitative Nanomechanical Peak Force<sup>®</sup> [PF-QNM]) for simultaneously measuring thickness and mechanical properties of the altered layer. The PF-QNM thickness results presented will be combined with other measurements (e.g., elemental release and scanning transmission electron microscopy) and used to demonstrate that altered layer formation and growth can be described with the polynuclear model, which is based on classical nucleation and growth theory.

**2:40 PM**

### **(GOMD-S4-049-2016) The influence of transition metal oxides induced absorption on LEAP detection efficiency and its glass alteration behaviors of ISG glasses**

X. Lu<sup>\*1</sup>; D. Schreiber<sup>2</sup>; J. Neeway<sup>2</sup>; J. Ryan<sup>2</sup>; J. Du<sup>1</sup>; 1. University of North Texas, USA; 2. Pacific Northwest National Lab, USA

Atom probe tomography has been successfully applied to understand glass dissolution mechanisms in atomic level. In this paper, the effect of optical absorption of glass samples on the detection efficiency of local electrode atom probe (LEAP) tomography with different lasers has been studied on international simple glass (ISG), a model nuclear waste glass system. Influences of optical absorption of pristine ISG, Co and V doped ISG and SON68 for optimal performance in two laser assisted LEAP systems are studied. It was found that laser spot size played a key role of optimum performance in atom probe tomography on the glass samples. Better optical absorption of laser wavelength had also affected the performance in terms of improving mass resolution, reducing chances of ruptures, and better chemical identification. Static chemical durability tests were performed at 90 °C with a PH value of 7 and a surface-area-to-solution-volume of 200 m<sup>-1</sup> for 112 days. Solution analysis showed both doping with V and Co could reduce the leaching rate and normalizes mass loss of Na and B comparing with undoped ISG. In addition, differential scanning calorimetry (DSC) curves showed that V doping could reduce the transition temperature (T<sub>g</sub>) of ISG and the effect became significant with increasing dopant amount, while Co doping slightly increased the T<sub>g</sub> of ISG.

**3:00 PM**

### **(GOMD-S4-050-2016) Nanoscale Imaging of Li and B in Nuclear Waste Glass using APT, ToF-SIMS, and NanoSIMS**

Z. Zhu<sup>\*1</sup>; Z. Wang<sup>1</sup>; J. Liu<sup>1</sup>; J. Neeway<sup>1</sup>; D. Schreiber<sup>1</sup>; J. V. Crum<sup>1</sup>; J. Ryan<sup>1</sup>; F. Wang<sup>2</sup>; 1. Pacific Northwest National Laboratory, USA; 2. Institute of Chemistry, Chinese Academy of Sciences, China

Nanoscale imaging of Li and B in glass samples has long been of great interest, but difficult to achieve. In this study, atom probe tomography (APT), time-of-flight secondary ion mass spectrometry (ToF-SIMS), and nanoscale secondary ion mass spectrometry (NanoSIMS) were used to image the distribution of Li and B in two representative glass samples. APT can provide three-dimensional Li and B imaging with very high spatial resolution ( $\leq 2$  nm). In addition, absolute quantification of Li and B is possible, though room remains to improve accuracy. However, the major drawbacks of APT include limited field of view (normally  $\leq 100 \times 100 \times 500$  nm<sup>3</sup>) and poor sample compatibility. As a comparison, ToF-SIMS and NanoSIMS are sample-friendly with flexible field of view (up to  $500 \times 500 \mu\text{m}^2$  and image stitching is feasible); however, lateral resolution is limited to only about 100 nm. Therefore, SIMS and APT can be regarded as complementary techniques for nanoscale imaging Li and B in glass and other novel materials.



## **Symposium 5: Festschrift for Professor Donald R. Uhlmann**

### **Gels and Applications**

Room: Madison

Session Chair: Lisa Klein, Rutgers University

**1:20 PM**

#### **(GOMD-S5-009-2016) How I took Don's Advice and Signed up for Organic Chemistry (Invited)**

L. C. Klein\*<sup>1</sup>; 1. Rutgers University, USA

The first time, I took a class with Don at MIT, it was Spring 1972, and the class was 3.06 "Glass". The topics ranged from classical nucleation theory to visiting a light bulb factory in Rhode Island. That course led to a summer UROP Project looking at glass samples recently returned from the surface of the Moon. In my senior year, I had one last class that I could take Pass/Fail, so I took organic chemistry on Don's advice. Little did I know at the time how useful this would be in making the transition from conventional glass forming to sol-gel processing. When it became clear that this was a new trend in glass and ceramic research, it was easy to make the transition to reactions in a flask, rather than high temperature treatment. For this, I thank Don.

**1:50 PM**

#### **(GOMD-S5-010-2016) Strong gels and glass science (Invited)**

P. Calvert\*<sup>1</sup>; 1. NMT, USA

The development of tissue engineering has led to a need for tougher hydrogels to act as matrices for embedded cells. In principle a cell matrix ought to be able to withstand stitching during surgery or be rugged enough to be undamaged over long periods in a bioreactor. Many biological gels, from seaweeds to cartilage, are quite tough but most synthetic gels are brittle in the sense that they readily tear when notched. The approaches that lead to tough gels are very similar to those that lead to toughening of glasses or ceramics and I will discuss some examples. Really tough gels may allow us to start building soft wet machines and devices.

**2:20 PM**

#### **(GOMD-S5-011-2016) Fibers and Non-Wovens from Long Carbon Nanotubes: A Model for Extended Chain Polymers Process, Structure and Applications (Invited)**

M. Jaffe\*<sup>1</sup>; 1. New Jersey Institute of Technology, USA

It has been more than a decade since the first reports of continuous production of carbon fibers comprised of long carbon nanotubes from the gas phase was reported (YL Li, I. A. Kinloch & A. H. Windle, "Direct spinning of carbon nanotube fibers from chemical vapor deposition synthesis" *Science* **304**, 276-278 (2004)). Since the initial discovery much progress has been made in process understanding, materials characterization and application development. Mechanical properties of the fibers or mats bracket the properties of other high performance fibers with the exception that knot efficiency, very low in most high performance fibers (~10%) approaches 95% in these CNT C fibers. Non-woven mats of CNT fibers have electrical conductivity within an order of magnitude of copper and thermal conductivity 3 times that of copper. Applications range from unique non-fouling water purification membranes to EMI shielding to composite materials with a unique balance of properties.

**2:50 PM**

#### **(GOMD-S5-012-2016) From random glass networks to random silica gel networks and their use as host for biocatalytic applications (Invited)**

A. C. Pierre\*<sup>1</sup>; 1. Retired, Université Claude Bernard Lyon 1, France

Silica aerogels have in common with silica glass to present a random 3-dimensional network, for aerogels of SiO<sub>2</sub> nano-particles, for glass of Si(-O-)<sub>4</sub> atomic tetrahedrons. One main difference is the presence of a range of pores in the aerogels, resulting in a porosity which may exceed 90% by volume, while a glass is dense. Consequently, an aerogel can entrap relatively big macromolecules in its pores. Presently, the work done on the encapsulation of 2 types of enzymes is summarized. A first one is lipases, used as biocatalysts of esterification reactions in organic solvents. The aerogels were dried by the CO<sub>2</sub> supercritical method after lipase encapsulation. The second one is carbonic anhydrase, applicable in the capture of CO<sub>2</sub> and used as aqueous un-dried wet gels. The influence of the gel network on the enzyme activity and of the enzymes on the gel network structure, are both discussed.

### **Legacy**

Room: Madison

Session Chair: Lisa Klein, Rutgers University

**3:40 PM**

#### **(GOMD-S5-013-2016) A Novel Cancer Therapy Utilizing Alternating Electric Fields Delivered via Lead Magnesium Niobate - Lead Titanate Transducers**

W. F. Doyle\*<sup>1</sup>; 1. Novocure Ltd., USA

Tumor Treating Fields (TTFields) is a novel cancer treatment modality utilizing 100-1000kHz, electric fields to exert forces on charged intracellular proteins interrupting cell division and causing cancer cell death. In 2015 the FDA approved TTFields for the treatment of newly diagnosed glioblastoma, the most common primary brain cancer, based on the results of a phase 3 clinical trial demonstrating significant improvements in progression free and overall survival. TTFields therapy requires tumor exposure to electric fields of 1-3 volts per centimeter for at least 18 hours per day for a period of up to two years. Exposure is accomplished with a portable electric field generator and transducer arrays attached to the skin surrounding the tumor region. These arrays are insulated by a high dielectric constant ( $\epsilon > 5,000$ ), non-porous, Lead Magnesium Niobate - Lead Titanate (PMN-PT) ceramic layer to provide maximum electric field intensity while minimizing tissue damage at the sites of application.

**4:00 PM**

#### **(GOMD-S5-014-2016) Review of Anti-Reflection Sol-Gel Coatings in High Energy Lasers**

T. I. Suratwala\*<sup>1</sup>; 1. Lawrence Livermore National Laboratory, USA

The following presentation is in honor of Prof. Don Uhlmann for his large contributions to many areas in materials science, including sol-gel coatings. Sol-gel derived colloidal silica (derived by the Stober process) as films on optical surfaces have served as excellent anti-reflection (AR) coatings for use in high power & energy laser systems. Since its initial development over 30 years ago by I.M. Thomas, it is still the coating of choice due to its superb laser damage resistance. In the following review, progress over the last decade both on novel variations of the original sol formulation and on detailed understanding of their behavior are described. Some specific topics include: 1) understanding the kinetics of hydrolysis and condensation of the colloid formation; 2) understanding & controlling the surface chemistry leading to novel coating formulations; 3) development of a hydrophobic AR coating with trimethylsilyl functionalized colloidal silica for use in niche applications; 4) understanding the relationship coating microstructure changes and AR properties

during dip & spin coating; and 5) understanding the environmental behavior (absorption isotherms) and the stability of the AR coatings during use. Finally, some unique AR coating applications on novel optics enabling greater functionality, higher laser power, and/or increased optics lifetime are described.

**4:20 PM**

**(GOMD-S5-015-2016) Glass formation, crystallization, and Don (Invited)**

J. McCloy\*<sup>1</sup>; 1. Washington State University, USA

From ~1970~2000, Don Uhlmann and his students studied the kinetics of glass formation and crystallization. Before, after, and during, Don was interested in a great many other topics, including polymer behavior, ferroelectric thin films, and biomaterials. I came to Don as an older, nontraditional student working in industry, and he agreed to advise me through the PhD process at University of Arizona 2005-2008. My work at the time was NOT focused on glasses, and it was not until years later that I appreciated the tremendous contributions he and his legacy have made towards understanding crystallization and the prevention thereof. It is somewhat interesting, therefore, that my current research has led me in the direction that much of Don's life took him, even though he and I never discussed it in those days. I therefore dedicate this talk to him, focusing on some of the work my group has done in the last several years on phase separation, crystallization, and glass chemistry, particularly applied to optical and nuclear glasses and glass ceramics. Along the way, I share a few life lessons that Don taught me, knowingly or unknowingly.

## Wednesday, May 25, 2016

### Varshneya Frontiers of Glass Science Lecture

Room: Madison

**8:00 AM**

**(GOMD-AW-004-2016) Multiscale investigation of stress-corrosion crack propagation mechanisms in oxide glasses (Invited)**

M. Ciccotti\*<sup>1</sup>; 1. ESPCI, France

Fracture propagation involves the coupling of many length scales ranging from the sample loading geometry to the molecular level. In brittle materials, the length scales of the damage process zone are reduced to a submicrometric scale and the coupling with the macroscopic scale is expected to be the domain of linear elastic fracture mechanics (LEFM). However, although 2D elastic analyses are generally adequate to describe the sample deformation at macroscopic scales, a micromechanical analysis requires the use of 3D mechanical tools due to the crack front local curvature and to the corner point singularities at the intersection between the crack front and the external surfaces of the sample. In this lecture we will present a thorough investigation of the slow crack growth of a sharp crack in oxide glasses in the stress-corrosion regime, combining numerical and experimental analyses from the millimetre scale to the nanoscale range. The principal aim of the study is identifying the length and time scales of the mechanisms of damage and interaction between water and glass, which have been the subject of an extensive debate in last decades.

## Symposium 1: Fundamentals of the Glassy State

### Session 1: Glass Formation and Relaxation III

Room: Capitol A

Session Chair: Ozgur Gulbiten, Corning Incorporated

**9:20 AM**

**(GOMD-S1-048-2016) Linking Equilibrium and Nonequilibrium Dynamics in Glass-Forming Systems**

J. C. Mauro\*<sup>1</sup>; X. Guo<sup>1</sup>; M. M. Smedskjaer<sup>2</sup>; 1. Corning Incorporated, USA;

2. Aalborg University, Denmark

Understanding nonequilibrium glassy dynamics is of great scientific and technological importance. However, prediction of the temperature, thermal history, and composition dependence of nonequilibrium viscosity is challenging due to the noncrystalline and nonergodic nature of the glassy state. Here, we show that the nonequilibrium glassy dynamics are intimately connected with the equilibrium liquid dynamics. This is accomplished by deriving a new functional form for the thermal history dependence of nonequilibrium viscosity, which is validated against experimental measurements of industrial silicate glasses and computed viscosities for selenium over a wide range of conditions. Since the temperature and composition dependence of liquid viscosity can be predicted using temperature-dependent constraint theory, our work also opens the possibility to improve understanding of the physics of nonequilibrium viscosity.

**9:40 AM**

**(GOMD-S1-049-2016) Viscosity for low alkali binary silicate melts**

J. Wu\*<sup>1</sup>; 1. Corning Incorporated, USA

To understand how cation field strength affects the viscosity of silicate melts, two series of alkali silicate glasses (5 and 10 mol% of alkali oxide [R<sub>2</sub>O] with the following cation field strength order: Li > Na > K > Rb > Cs) have been made. Viscosity was measured with beam-bending (BBV), parallel plate (PPV) and rotation viscometers. From all three types of viscometers data, the isothermal viscosity for both series of alkali silicates decreases in the order of Cs > Rb > K. The amounts of non-bridging oxygens (NBOs) are the same for each series of glasses. If viscosity is directly related with breaking the weakest bonds in these glasses, the higher viscosity for the larger modifier may due to larger numbers of bonds need to be broken, since larger cation has higher coordination number and connects with more oxygen atoms. The differences in isothermal viscosity for 5mol% alkali silicate glasses are much smaller than the 10mol% ones. The viscosity of Na glasses (from BBV and PPV data) are much higher than other glasses in both series (viscosity for Li glasses are not available due to crystallization and severe phase separation). The high viscosities for sodium glasses are due to phase separations, which hinted by the big discrepancy of glass transition temperature measured by BBV and differential scanning calorimeter (DSC).

**10:00 AM**

**(GOMD-S1-050-2016) Near-Tg and sub-Tg structural relaxation in window glass: precise experiment vs. known models**

A. Priven\*<sup>1</sup>; 1. Corning Korea, Republic of Korea

Although multiple approaches and models of structural relaxation in glass have been suggested during the last decades, the problem of accurate description and prediction of glass behavior during heat treatment still exists. The problem is especially important for the temperature range below the glass transition temperature (T<sub>g</sub>) where the measurements of structural relaxation are difficult because of very small effects on physical properties - but these effects are sometimes very important. In this presentation, the results of precise dilatometric experiments on the window glass are compared with

predictions of several different models. The results show that none of these models accurately describes all experiments near and below  $T_g$ , although most of them are able to describe each experiment separately, with the use of specially fitted model constants. In other words, the known models in the sub- $T_g$  range are descriptive rather than predictive. Some reasons of this model behavior are discussed and some directions of improving the models suggested.

#### 10:20 AM

##### (GOMD-S1-051-2016) Preparing organic glasses with high kinetic stability via physical vapor deposition: Role molecular structure

M. Tylinski\*<sup>1</sup>; M. Beasley<sup>1</sup>; Y. Chua<sup>2</sup>; C. Schick<sup>2</sup>; M. D. Ediger<sup>1</sup>; 1. University of Wisconsin - Madison, USA; 2. University of Rostock, Germany

Glasses are often prepared by cooling the liquid. Small changes to their properties can be made by changing the cooling rate or by aging the material. The past decade has seen increased research into preparing glasses by physical vapor deposition (PVD). Organic glasses prepared by PVD have shown increased kinetic stability compared to their liquid-cooled counterparts. At high temperatures, the vapor-deposited glasses can take thousands of times longer than a liquid-cooled glass to relax into the supercooled liquid. It is thought that the mechanism allowing for the preparation of these stable glasses is fast surface mobility at temperatures below  $T_g$  which enables molecules to find low energy configurations during deposition. This hypothesis is supported by surface diffusion measurements near  $T_g$  and the dependence of stability on substrate temperature and deposition rate during preparation. We have found that molecular structure can also significantly affect the kinetic stability of a vapor-deposited glass. By depositing a variety of molecules, we have found that hydroxyl groups and aliphatic chains tend to hinder a molecule's ability to form stable glasses. We prepare 2-ethyl-1-hexanol glasses using a wide range of deposition rates to investigate why this molecule does not form glasses with high kinetic stability and to test our hypothesis of stable glass formation.

#### 10:40 AM

##### (GOMD-S1-052-2016) Effect of network structure on the mixed cation phenomenon in lithium-calcium borosilicate glasses

Y. Shih\*<sup>1</sup>; J. Jean<sup>1</sup>; 1. National Tsing Hua University, Taiwan

This research deals with the variation of mixed cation effect (MCE) in lithium-calcium borosilicate glasses. The glass system investigated is  $0.4[x\text{CaO}(1-x)\text{Li}_2\text{O}]0.6[y\text{B}_2\text{O}_3(1-y)\text{SiO}_2]$  with  $x$  varying in the range of 0-1 and  $y$  in the range of 0.33-0.83. The MCE manifests itself in a non-additive deviation when lithium ion is replaced by calcium ion, especially in those properties which are related to ion transportation including glass transition temperature, dilatometric softening temperature, fragility, hardness, dielectric constant and dielectric loss. Moreover, the deviation exhibits a maximum near  $[\text{CaO}]/([\text{CaO}]+[\text{Li}_2\text{O}])=0.5$ , and increases with increasing  $[\text{SiO}_2]/[\text{B}_2\text{O}_3]$  ratio ( $K$ ). According to the  $^{11}\text{B}$  NMR results, increasing  $K$  improves the formation of non-bridging oxygen (NBO), which suggests to limit the ability of cation transportation, resulting in enhancing the deviation.

#### 11:00 AM

##### (GOMD-S1-053-2016) Silica network modification during multicomponent diffusion in the soda-lime glass

E. Burov\*<sup>1</sup>; E. Gouillart<sup>1</sup>; W. Woelffel<sup>1</sup>; M. Toplis<sup>2</sup>; 1. Saint-Gobain, France; 2. Observatoire Midi-Pyrénées, France

In this study, to improve our understanding of the multicomponent diffusion mechanism in glass at the atomistic scale, we have collected Raman spectra along diffusion profiles of three couples of soda-lime glasses centered around an average composition of 70.0 wt%  $\text{SiO}_2$ , 12.5 wt%  $\text{CaO}$ , 16.3 wt%  $\text{Na}_2\text{O}$ . The temperature-time range (1000 °C for 1 h) was selected such that compositional variation generated by diffusion were on the order of a couple of millimeters, which gives the possibility to obtain both, good spatial resolution for the

Raman spectra collection, and the Electron Probe Micro-Analysis profile. In total, 169 Raman spectra and composition points have been obtained. For the diffusion matrix and eigenvectors definition the three composition profiles have been fitted simultaneously. The shape variations of the Raman spectra along the diffusion profile are analyzed using a combination of principal components analysis (PCA) and sparse non-negative matrix factorization (NMF). Obtained result implies a link between Qn species modification and the shift of the medium-range network features in the main band of the Raman spectra along the diffusion profile. The correlation between the principal component variation along the diffusion profile and the diffusion eigenvector will be also discussed

### Session 3: Scattering Techniques

Room: Capitol B

Session Chair: Paul Voyles, University of Wisconsin

#### 9:20 AM

##### (GOMD-S1-054-2016) Local density changes of deformed metallic glasses (Invited)

V. Schmidt\*<sup>1</sup>; H. Rösner<sup>1</sup>; M. Peterlechner<sup>1</sup>; P. Voyles<sup>2</sup>; G. Wilde<sup>1</sup>; 1. University of Münster, Germany; 2. University of Wisconsin, USA

Metallic glasses (MGs) exhibit superior mechanical properties such as high yield strength, extended elasticity, high wear and corrosion resistance. However, after a large apparently elastic regime MGs are prone to catastrophic failure, especially under tensile load due to shear localization enabling plastic flow in narrow regions called shear bands. The limited ductility is a major obstacle for MGs as structural materials. This motivates generally an interest in understanding the deformation behavior of MGs in more detail. In my talk, I will present a new method for quantitative local density measurement in amorphous materials combining electron scattering signals such as high angle annular dark field scanning transmission electron microscopy and low-loss electron energy loss spectroscopy to determine the local normalized density changes. Applying this approach to shear bands in different MGs ( $\text{Al}_{88}\text{Y}_7\text{Fe}_5$ ,  $\text{Pd}_{40}\text{Ni}_{40}\text{P}_{20}$  and Vitreloy 105) shows common structural features; that is, alternating high and low density regions. The density changes are correlated with small deflections in the propagation direction, variations in short or medium range order and chemical composition. Similar behavior has been reported for granular media, but not for amorphous solids suggesting fundamental connections to the physics of granular materials and jammed systems.

#### 9:50 AM

##### (GOMD-S1-055-2016) Isotope substitution neutron scattering of $\text{MgTiO}_3$ in the stable liquid supercooled liquid and crystalline state

J. Neuefeind\*<sup>1</sup>; C. J. Benmore<sup>2</sup>; R. Weber<sup>3</sup>; O. L. Alderman<sup>3</sup>; L. Skinner<sup>3</sup>; 1. Oak Ridge National Lab, USA; 2. Argonne National Lab, USA; 3. Materials Development, USA

$\text{MgTiO}_3$  samples enriched in the Ti isotopes  $^{46}\text{Ti}$  and  $^{48}\text{Ti}$  for use in an aerodynamic levitator have been prepared. The samples were measured with neutron scattering at the Nanoscale Ordered Materials Diffractometer in three thermodynamic states, in the stable solid at RT, in the stable liquid at 1800 C and in the supercooled liquid at 1500 C. Two groups of partial pair distribution functions can be isolated: The Ti first order difference (FOD) isolates the local environment of the Ti atom and is dominated by the TiO partial. A different linear combination eliminates the TiX partials and is dominated by the MgO and OO partial. The Ti coordination decreases from sixfold to fivefold and the TiO bond distance contracts in the liquid states in agreement with previous results for similar systems. The inter-oxygen distances on the other hand expand accounting for the decreased overall density in the liquid.

10:10 AM

## (GOMD-S1-056-2016) Local structural changes on melting and glass formation in alkali-free titanates

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We extend our earlier work on molten TiO<sub>2</sub> and alkaline earth metatitanates, to include i) glass forming titanate systems and ii) in-situ Ti K-edge x-ray absorption fine structure (XANES) spectroscopy, in addition to in-situ high-energy x-ray and neutron diffraction. Glass forming systems studied include BaTi<sub>2</sub>O<sub>5</sub>, rare earth titanates 17RE<sub>2</sub>O<sub>3</sub>.83TiO<sub>2</sub> (RE = La, Nd), CaSiO<sub>3</sub>-TiO<sub>2</sub> and alkali-free synthetic basalts. Non-glass-forming systems include alkaline earth metatitanates, MTiO<sub>3</sub>, 17RE<sub>2</sub>O<sub>3</sub>.83TiO<sub>2</sub> (RE = Y, Sc) and high-alumina Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub>. Measurements were made using an aerodynamic levitation system combined with CO<sub>2</sub> laser heating. Results clearly demonstrate that Ti<sup>4+</sup>-O coordination in the melts ranges between 4 and 5, i.e. lower than 6, as found in most of the isocompositional crystal structures. Furthermore, significant increases in Ti-O coordination were found on cooling through the glass transition. Various levitation gas compositions were used to vary oxygen partial pressure. Largely transparent glasses formed under oxidizing conditions, whilst under reducing conditions they became black. Despite this optical change, no changes in local structure were detectable, suggesting only a small fraction of Ti<sup>3+</sup> ions. Nonetheless, this small fraction of Ti<sup>3+</sup> were sufficient to prevent glass formation in the poor glass-former BaTi<sub>2</sub>O<sub>5</sub>.

10:30 AM

## (GOMD-S1-057-2016) Structure of lithium germanate glasses by neutron diffraction with isotopic substitution

A. C. Hannon<sup>\*1</sup>; 1. ISIS Facility, United Kingdom

The thermophysical properties of germanate glasses show a minimum or maximum as increasing amounts of modifier are added to the glass, and this behaviour is known as the germanate anomaly. One of the factors involved in the germanate anomaly is the Ge-O coordination number, which initially increases above a value of 4 for pure GeO<sub>2</sub>, and then decreases back towards 4 for high modifier contents. A report is given of a high resolution neutron diffraction study of lithium germanate glasses, with the use of lithium isotopic substitution. The use of lithium isotopes enables the Ge-O coordination number to be determined without interference from the Li-O bonds in the glass. Furthermore, the Li-O coordination number is also determined due to the use of lithium isotopes.

10:50 AM

## (GOMD-S1-058-2016) Combining X-ray Scattering and Optical Techniques to Characterize the Structure of Organic Glasses formed by Physical Vapor Deposition

A. Gujral<sup>\*1</sup>; J. Jiang<sup>1</sup>; J. Gomez<sup>1</sup>; D. M. Walters<sup>1</sup>; C. Huang<sup>1</sup>; K. A. O'Hara<sup>2</sup>; M. F. Toney<sup>3</sup>; L. Yu<sup>1</sup>; M. L. Chabiny<sup>2</sup>; M. D. Ediger<sup>1</sup>; 1. University of Wisconsin, USA; 2. University of California, Santa Barbara, USA; 3. Stanford Synchrotron Radiation Lightsource, USA

Organic glasses formed by quenching inherit the bulk structure of the equilibrium liquid they are cooled from. On the other hand, organic glasses prepared by physical vapor deposition may be trapped in structural configurations not found in bulk equilibrium materials. By tuning certain conditions during the deposition process, such as the substrate temperature and the rate of deposition, the same molecule can form a variety of glasses with anisotropic structures. In this work, we will illustrate how x-ray scattering along with infrared spectroscopy and spectroscopic ellipsometry can be used to characterize the structures formed in vapor-deposited glasses. Two systems will be described to elucidate the strength of combining these techniques: itraconazole, a liquid crystal-former, and TPD, a non-liquid crystalline small organic molecule. In both

cases, it is found that average molecular orientation in the film can be altered by controlling substrate temperature during deposition. Itraconazole, however, also exhibits tunable smectic-like layering as a function of substrate temperature.

11:10 AM

## (GOMD-S1-059-2016) Subsurface structure of soda lime float glass and thermodynamics of water-glass interactions studied with vibrational sum frequency generation (SFG) spectroscopy

J. Luo<sup>\*1</sup>; J. Banerjee<sup>1</sup>; C. G. Pantano<sup>1</sup>; S. H. Kim<sup>1</sup>; 1. Pennsylvania State University, USA

Understanding the chemical structure in the surface region of commercial soda lime float glass is crucial to expand its areas of application by strengthening the glass through surface modification like coatings, ion-exchange, etc. To be specific, the interplay between hydrous species (molecular water and silanol groups) and silica network structure characterized with rich sodium content and non-bridging oxygen (NBO) in the surface region of the soda lime float glass, have been suggested to play vital roles in its surface mechanical responses to different environment. SFG spectroscopy has been recently developed to study the speciation of hydrous species in the surface region of the glass. Unlike the glasses without leachable ions, the soda lime float glass show multiple sharp OH peaks. The thermodynamics of each individual peak are then investigated with SFG to reveal the nature of them compared with the results from SR-IR and ATR-IR spectroscopy. It turns out that the multiple peaks mainly come from the water molecules in the subsurface region where a concentration gradient of sodium was created and water molecules ingressed into the glass network during the commercial SO<sub>2</sub> dealcalization process. SFG spectra reveal the different chemistry environment where these water molecules are resided in the subsurface region.

## Session 4: First Principles Methods and ab initio MD Simulations of Glasses

Room: University C/D

Session Chairs: Jincheng Du, University of North Texas; Carlo Masobrio, CNRS-IPCMS-UNR 7504

9:20 AM

## (GOMD-S1-060-2016) Second Generation Car-Parrinello-type Molecular Dynamics: Advantages and Disadvantages (Invited)

M. Boero<sup>\*1</sup>; 1. University of Strasbourg and CNRS, France

We present an overview of one of the most advanced computational approaches used nowadays in the field of first-principles simulations for the modeling of amorphous and liquid materials. The scope is to bring attention on advances in DFT-based techniques to extend the time and size scale of the simulations to a more realistic modeling. The basic idea of what it is called nowadays "second generation Car-Parrinello" (SGCP) method is to join together the advantages of the Born-Oppenheimer (BO) approach and those of the Car-Parrinello molecular dynamics (CPMD), namely avoiding electronic structure re-optimization and Hamiltonian diagonalization at each simulation step, typical of BO but not required in CPMD, while having a good conservation of the constant of motion (as in CPMD) and an integration step at least one order of magnitude bigger than CPMD (as in BO). After inspecting the basic methodology, we shall focus on its practical applications and on its advantages and disadvantages. Specifically, we shall focus on the improvements in the modeling of an amorphous material made possible by the use of slower quenching rates from a melt but also on the intrinsic problems arising from long time steps and not fully converged wavefunctions.

9:50 AM

**(GOMD-S1-061-2016) Large Scale Simulation of Structure and Properties of Metal-Organic Frameworks Hybrid Glasses: ZIF-4 (Invited)**N. Li<sup>\*1</sup>; 1. Wuhan University of Technology, China

In this work, we generated the amorphous ZIF-4 (a-ZIF-4) based on a larger continuous random network (CRN) model of amorphous SiO<sub>2</sub> (a-SiO<sub>2</sub>) glass with 1296 atoms, using TOBUNPOROUS.3,4. For the CRN a-ZIF-4, there is no broken bonds or over-/under-coordinated Zn atoms or organic group. The large periodic models were first relaxed by using VASP with high accuracy and their physical properties are calculated using the first-principles OLCAO method. The full spectrum of properties of a-ZIF-4 and crystal ZIF-4 including atomic structure, bonding characteristics, effective charges, bond order values, electron density of states, localization of wave functions, elastic and mechanical properties, and inter-band optical absorption are discussed. Moreover, the properties of a-ZIF-4 with high pressure and temperature will also be discussed in the work. Based on our results, we are trying to provide evidence that the wide-ranging melting temperatures of zeolitic MOFs are related to their network topologies and opens up the possibility of 'melt-casting' MOF glasses.

10:20 AM

**(GOMD-S1-062-2016) Structure Modeling and Thermochemical Properties of Tantalum-Silica Glasses**I. Ponomarev<sup>1</sup>; A. Dasmahapatra<sup>1</sup>; P. Kroll<sup>\*1</sup>; 1. UT Arlington, USA

We study Ta<sub>2</sub>O<sub>5</sub>-SiO<sub>2</sub> glass systems using Density Functional Theory calculations and ab-initio Molecular Dynamic simulations. Glass structures through the complete composition range from SiO<sub>2</sub> to Ta<sub>2</sub>O<sub>5</sub> are generated via a melt-quench procedure with additional sequences of simulated annealing. At low Ta<sub>2</sub>O<sub>5</sub>-concentration, Ta is integrated into the network in five-fold coordination. With increasing Ta<sub>2</sub>O<sub>5</sub> content a gradual change to higher coordinated Ta happens, and TaO<sub>6</sub>-polyhedra appear together with three-coordinated O atoms. We estimate the enthalpy of formation of pure amorphous Ta<sub>2</sub>O<sub>5</sub> to be 0.6 eV/Ta<sub>2</sub>O<sub>5</sub> with reference to the monoclinic crystal structure of Ta<sub>2</sub>O<sub>5</sub>. At low Ta<sub>2</sub>O<sub>5</sub>-concentration, we calculate an enthalpy of mixing Ta<sub>2</sub>O<sub>5</sub> into SiO<sub>2</sub> of 0.4 eV/Ta<sub>2</sub>O<sub>5</sub>. The thermochemical data through the complete composition range from SiO<sub>2</sub> to Ta<sub>2</sub>O<sub>5</sub> can be approximated using a regular mixing model.

10:40 AM

**(GOMD-S1-063-2016) Computational Studies of the Glass Phase in Hydrogrossular Mineral Series**P. Adhikari<sup>\*1</sup>; C. C. Dharmawardhana<sup>1</sup>; W. Ching<sup>1</sup>; 1. University of Missouri, Kansas City, USA

The mineral hydrogrossular series (Ca<sub>3</sub>Al<sub>2</sub>(SiO<sub>4</sub>)<sub>3-x</sub>(OH)<sub>4x</sub>; 0 ≤ x ≤ 3) are important water bearing minerals found in the Earth's mantle. They are vital to the planet's hydrosphere under different hydrothermal conditions. The composition and structure of this mineral series are important in geoscience and share many commonalities with glass, cement and clay materials. Other than the end members of the series x = 0 (grossular) and x = 3 (katoite) which have a cubic garnet structure, the structure of the series is totally unknown. We used large-scale ab initio modeling to investigate the structures and properties for hydrogrossular series for x = 0, 0.5, 1, 1.5, 2, 2.5, 3. Results indicate that for x > 0 and x < 3, the structures are non-crystalline and considered as an amorphous glass. This shows lowering of overall symmetry associated with changes in the composition of SiO<sub>4</sub> tetrahedra and AlO<sub>6</sub> octahedra. The electronic structure, mechanical and optical properties of the hydrogrossular series are calculated and the results for grossular and katoite are in good agreement with the available experimental data.

11:00 AM

**(GOMD-S1-064-2016) First Principles study of silicate glasses: interplay between structural and vibrational properties (Invited)**S. Ispas<sup>\*1</sup>; D. A. Kilymis<sup>1</sup>; J. Delaye<sup>2</sup>; B. Hehlen<sup>1</sup>; 1. University of Montpellier, France; 2. CEA Marcoule, France

In recent years, Raman spectroscopy has become a tool of choice for the structural analysis of glasses, due to its simplicity and the low cost of acquisition. However, the broad and overlapping peaks observed in the spectra result in a phenomenological and often qualitative interpretation. In order to improve the analysis of Raman spectra, and to start to obtain a more quantitative interpretation, one needs to identify the exact contributions arising from individual structural units. We have used first-principles and combined classical/first-principles approaches to create representative atomistic models of some simple binary soda- and lime-silicates, as well as for some ternary aluminosilicates. Within the density functional theory framework, we have calculated the vibrational density of states as well as the IR and Raman spectra of these glass models, and we have found a good agreement with the experimental spectra. The knowledge of the theoretical spectra and the atomic structure has made possible to identify the signatures of the various constituents of the glasses in the spectra, as for example the Qi species. The obtained correlations can be then used to better assign the main bands present in the spectra of more complex silicate glasses.

11:30 AM

**(GOMD-S1-065-2016) Electronic structures, interatomic bonding and physical properties of Si<sub>x</sub>Ge<sub>1-x</sub>O<sub>2</sub> glass (x = 0 to 1)**K. Baral<sup>\*1</sup>; P. Adhikari<sup>1</sup>; W. Ching<sup>1</sup>; 1. University of Missouri, Kansas City, USA

The amorphous silica (a-SiO<sub>2</sub>) and germania (a-GeO<sub>2</sub>) have a wide range of applications in glass industry. We present the computational results of Si<sub>x</sub>Ge<sub>1-x</sub>O<sub>2</sub> glass models constructed using a nearly perfect continuous random network (CRN) model with 1296 atoms and periodic boundary conditions. We have calculated the structural, electronic, mechanical and optical properties for the series by using the orthogonalized linear combination of atomic orbital (OLCAO) method and the calculated values are compared with available experimental values. The x-dependence of the variations of the properties are analyzed. In addition for x = 0.5, we have constructed six different kinds of models which include glass spheres of different radii in the medium of the other glass and their physical properties are compared and contrasted.

11:50 AM

**(GOMD-S1-066-2016) Structure Modeling and DFT Calculations of Hafnia Soda Silicate Glasses**I. Ponomarev<sup>\*1</sup>; A. Dasmahapatra<sup>1</sup>; J. P. Nimmo<sup>1</sup>; P. Kroll<sup>1</sup>; 1. University of Texas, Arlington, USA

We investigate the impact of mixing hafnia (HfO<sub>2</sub>) into soda silicate glasses (Na<sub>2</sub>O-SiO<sub>2</sub>) by density functional calculations. Models with up to 10 mol% HfO<sub>2</sub> are generated via a melt-quench procedure with additional annealing sequences. Optimized models are analyzed for their structure, thermochemistry, elastic properties, and subsequently <sup>29</sup>Si-NMR chemical shifts are computed within the gauge-including projector augmented wave (GIPAW) method. In all models, HfO<sub>6</sub>-octahedra are surrounded by tetrahedral SiO<sub>4</sub>-units and no HfO<sub>x</sub>-clusters are observed at these concentrations. We find a negative enthalpy of mixing (-15 kJ/mol) for adding HfO<sub>2</sub> to Na<sub>2</sub>O•3SiO<sub>2</sub>, which agrees very well with experimental calorimetric studies. Addition of HfO<sub>2</sub> to the soda-silicate glass increases elastic constants and yields increased hardness as well. <sup>29</sup>Si- and <sup>17</sup>O-NMR chemical shifts can be related to the various environment of O atoms, which form the network with Si and Hf, which is then modified by adjacent Na atoms.

## Session 5: Mechanical Properties of Glasses III

Room: Wisconsin

Session Chair: Satoshi Yoshida, The University of Shiga Prefecture

9:20 AM

### (GOMD-S1-067-2016) Fracture-induced amorphization of polycrystalline SiO<sub>2</sub> stishovite: nanoscale transformation toughening in the hardest oxide (Invited)

N. Nishiyama<sup>\*1</sup>; F. Wakai<sup>2</sup>; 1. Deutsches Elektronen-Synchrotron, Germany; 2. Tokyo Institute of Technology, Japan

Silicon dioxide (silica) is the most abundant oxide component on the Earth's surface and has been widely used in industry. Stishovite is a high-pressure polymorph of silica stable above 9 GPa. This material has been known as the hardest oxide at ambient conditions ( $H_V \sim 30$  GPa). A previous study reported synthesis of nanocrystalline bulk stishovite from a bulk silica glass rod. Fracture toughness of this material was reported to be  $\sim 10$  MPa m<sup>0.5</sup>, whereas single crystal stishovite is known as a very brittle material ( $K_{Ic} = 1.6$  MPa m<sup>0.5</sup>). Nanocrystalline bulk stishovite is a very hard and toughed material. In order to understand an active toughening mechanism in this material, we performed Si-K XANES measurements and TEM observations for fracture surfaces of nanocrystalline bulk stishovite. Our experimental results show that amorphous silica exists on the outermost fracture surfaces. These results indicate that huge tensile stress at the crack tip induces solid-state amorphization from stishovite to amorphous silica. This transformation accompanies a huge volume expansion of 95%. This volume expansion causes transformation toughening. In addition, this volume expansion is much larger than that of tetragonal to monoclinic transition in zirconia (4%), resulting in a thinner transformed region whose thickness is several tens of nanometers.

9:50 AM

### (GOMD-S1-068-2016) Mechanical properties of hard oxide glasses prepared by a levitation technique (Invited)

A. Masuno<sup>\*1</sup>; 1. The University of Tokyo, Japan

Containerless processing using an aerodynamic levitation furnace allows us to fabricate unconventional glasses with very low glass forming ability because it can suppress heterogeneous nucleation at the boundary between a melt and a container. Recently, we have successfully obtained new glasses with fascinating properties by using the levitation technique. We have found that some of them, Al<sub>2</sub>O<sub>3</sub>-Ta<sub>2</sub>O<sub>5</sub> binary glasses, have high elastic moduli (Young's modulus of 158.3 GPa) and hardness (Vickers hardness of 9.1 GPa). Furthermore, Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> binary glasses showed higher crack resistance with an increase of Al<sub>2</sub>O<sub>3</sub> content. Recent progress on hard oxide glasses will be shown.

10:20 AM

### (GOMD-S1-069-2016) Surface indentation topometry and fracture behavior of Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> glasses with high cracking initiation load

G. A. Rosales Sosa<sup>\*1</sup>; A. Masuno<sup>1</sup>; Y. Higo<sup>2</sup>; T. Ishikawa<sup>3</sup>; H. Inoue<sup>1</sup>; 1. The University of Tokyo, Japan; 2. Japan Synchrotron Radiation Research Institute, Japan; 3. Japan Aerospace Exploration Agency, Japan

Obtaining a glass that combines high hardness and cracking resistance has always been on great importance in glass science and technology. The hardness and the elastic moduli of oxide glasses can be improved with the addition of Al<sub>2</sub>O<sub>3</sub> because it enhances the overall dissociation energy per unit volume of the glass and the atomic packing density. However, the glass yield using conventional melting techniques is usually limited to 30% mol of alumina due to easy crystallization from the melts and high melting temperatures. Recently, we reported a family of transparent Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> glasses with high alumina content obtained via aerodynamic levitation. Particularly, a glass with composition same to mullite (60Al<sub>2</sub>O<sub>3</sub>-40SiO<sub>2</sub>) was found to combine high hardness, elastic modulus and

high cracking initiation load. In this work, the surface topometry and the fracture behavior at the atomic scale of xAl<sub>2</sub>O<sub>3</sub>-(100-x)SiO<sub>2</sub> glasses with x = 30-60 were investigated by means of laser microscopy and molecular dynamics simulations respectively. The relationship between the topometry, fracture behavior of these glasses will be discussed.

10:40 AM

### (GOMD-S1-070-2016) New route to ultra-stiff glass material composition

Y. Yu<sup>\*1</sup>; Z. Maw<sup>1</sup>; B. Wang<sup>1</sup>; M. Wang<sup>1</sup>; M. Bauchy<sup>1</sup>; 1. University of California, Los Angeles, USA

Elastic properties (Young's modulus E, bulk modulus K, shear modulus G, and Poisson's ratio  $\nu$ ) are of primary interest for applications such as accelerated devices, including hard discs and surgery equipment, lightweight construction and composite materials. As such, it is of primary importance to understand and predict the relation between elastic properties and composition. However, as elastic properties are typically not a linear function of the composition, empirical models lacking a physical basis are usually limited to a narrow range of compositions. In addition, as the number of potential glass compositions is virtually infinite, conventional brute-force experimental or simulation-based approach will not enable the development of an accurate and transferrable model of elasticity. Here, based on molecular dynamics simulations (MD) of calcium aluminosilicate glasses coupled with topological constraints theory (TCT), we present a new model of elasticity based on the number of bond-stretching and bond-bending constraints created by each atomic species. We demonstrate that our model offers a better agreement than previous conventional models based on additive approaches or the fitting of experimental data. The presented approach serves to bridge the gap between structure and macroscopic property, and promotes the design of ultra-stiff glasses for advances applications.

11:00 AM

### (GOMD-S1-071-2016) Calculating elastic moduli from composition

K. Philipps<sup>\*1</sup>; R. Conrad<sup>1</sup>; 1. RWTH Aachen University, Institute of Mineral Engineering, Germany

Calculating elastic moduli of oxide glasses from the composition is still a great challenge. A well-known approach by Makishima and Mackenzie [1973] is taking the dissociation energies of various oxides and the atomic packing density to calculate the Young's modulus. This approach is successful for glasses with compositions in the range of normally applied mass glasses. Going beyond these compositions, the Makishima-Mackenzie model loses its accuracy; Young's moduli of glasses from the system CMAS for example are underestimated by the model up to 10%. The constitutional approach to glasses, which is well-established in thermodynamics, is used to further improve the results of the Makishima-Mackenzie model for a broader range of compositions and to significantly enhance the accuracy of its predictions.

11:20 AM

### (GOMD-S1-072-2016) Tribochemical Wear of Phosphate Laser Glass

J. Yu<sup>\*1</sup>; 1. Southwest University of Science and Technology, China

The wear resistance of glass is not only depended on the environment that it is exposed to, but also the effects of counter-surface (ball) chemistry. Upon a reciprocating ball-on-flat tribometer, the effects of liquid water and counter-surface chemistry on the friction and wear behaviors of phosphate laser (PL) glass were investigated. The wear volume and friction coefficient of PL glass were lower in water than in dry air, which suggested the tribochemical wear of PL glass in water were not limited to the effect of stress corrosion. In contrast, the wear of PL glass in water was more severe than in

dry air when rubbing other ball materials ( $\text{Si}_3\text{N}_4$ ,  $\text{ZrO}_2$  and  $\text{Al}_2\text{O}_3$ ), that implied stress corrosion could dominate the tribochemical wear in these cases. The analysis for pH, ions concentration, and FT-IR spectra of the solution after wear of PL glass against silica ball suggested that the unique suppressed tribochemical wear of PL glass in water by rubbing with silica ball must be the consequence of tribochemical reactions involving glass substrate, water and counter-surfaces chemistry. These results provide new insights into the wear of glass materials, which would be helpful for understanding the mechanisms of material removal in glass machining.

**11:40 AM**

**(GOMD-S1-073-2016) In-situ observation of crack growth in LCD glass substrate during wheel scribing**

N. Tomei<sup>1</sup>; K. Murakami<sup>1</sup>; T. Fukunishi<sup>1</sup>; S. Yoshida<sup>2</sup>; J. Matsuoka<sup>2</sup>;  
1. Mitsubishi Diamond Industrial Co., Ltd, Japan; 2. The University of Shiga Prefecture, Japan

Wheel scribing and breaking method has been widely adopted for cutting of LCD panels. When scribing a glass, it is important to create much deeper median cracks in order to reduce the breaking force. Unfortunately, however, there were very limited data about scribing a glass. Therefore, in this study, in-situ observation of the median crack propagation in the glass was performed using a high speed camera in order to get a deeper insight into the wheel scribing of glass. As a result, it was found that a median crack was initiated beneath the wheel, then arrested, and re-propagation of the crack occurred after passing through the wheel. From in-situ photoelastic measurements during static wheel indentation, it was found that the maximum tensile stress was generated beneath the wheel. The tensile stress was also obtained from FE analysis. It is concluded that this tensile stress causes the median crack during wheel scribing.

**Session 6: Carbide and Nitride Glasses**

Room: Senate A/B

Session Chair: Tanguy Rouxel, Université de Rennes 1

**9:20 AM**

**(GOMD-S1-074-2016) High-Temperature Creep Behavior of SiOC Glasses and Glass Ceramics (Invited)**

C. Stabler<sup>1</sup>; M. Narisawa<sup>2</sup>; M. Heilmaier<sup>3</sup>; H. Kleebe<sup>1</sup>; R. Riedel<sup>1</sup>; E. Ionescu<sup>\*1</sup>;  
1. Technical University Darmstadt, Germany; 2. Osaka Prefecture University, Japan; 3. Karlsruhe Institute of Technology, Germany

Several silicon oxycarbide glasses with different carbon contents were analyzed in the present study with respect to their high-temperature creep behavior. The tests were performed in compression at 1100, 1200 and 1300 °C; in this temperature range the mechanism of creep relies on viscoelastic flow within the samples. After the release of the applied mechanical stress, a viscoelastic recovery behavior was observed in all samples. The creep behavior of the investigated glasses was rationalized by using the Jeffreys viscoelastic model, indicating two distinct contributions to the high temperature creep in SiOC: (i) a viscous contribution, coming from the silica rich network, and (ii) an elastic response from the segregated carbon phase present in the samples; this is in agreement to the previously proposed nano-heterogeneous network topology of SiOC glasses. Furthermore, two distinct effects of the carbon phase on the HT creep behavior of SiOC were identified and will be discussed: the effect of the carbon present within the SiOC network (the "carbide" carbon), which induces a significant increase of the viscosity and a strong decrease of the activation energy for creep as compared to vitreous silica; and the influence of the segregated carbon phase, which has been shown to affect the viscosity and the activation energy of creep and dominates the creep behavior in phase-separated silicon oxycarbides.

**9:50 AM**

**(GOMD-S1-075-2016) Silicon Oxycarbide Glasses: Synthesis, Structure and Properties (Invited)**

G. Soraru<sup>\*1</sup>; 1. University of Trento, Italy

Silicon oxycarbide glasses (Si-O-C) are anionic modification of silica glass where divalent oxygen atoms are replaced by tetravalent carbon atoms forming  $\text{CSi}_4$  tetrahedral sites. They emerged in the scientific literature at the end the 80s for their potential high temperature structural application as matrices for CMC. Si-O-C can be processed by pyrolysis of crosslinked siloxane resins and accordingly they belong to the wider family of Polymer Derived Ceramics. The substitution of O with C in the amorphous silica network leads to a unique set of properties i.e. more than 50% increase of the elastic modulus, the lowest poisson ratio measured for glasses,  $T_g$  above 1350°C and exceptionally high devitrification stability. However, the structure of Si-O-C is far more complicated than the simple one which could result from the O to C substitution. Indeed the presence of mixed silicon oxycarbide units,  $\text{SiC}_x\text{O}_{4-x}$  and heterogeneity at the nanometer level leading to C-rich and silica-rich clusters have been clearly shown. Moreover a network of  $\text{sp}^3$  C layers can also be part of the structure. In this presentation it will be shown how the composition and the phase assemblage of the Si-O-C materials can be controlled by the appropriate choice of the starting molecular precursors. The Si-O-C nanostructure will be related to the new functional properties (optical, electrical and electrochemical) which have been recently reported.

**10:20 AM**

**(GOMD-S1-076-2016) Nitrogen rich oxynitride glasses – Difficulties and Opportunities (Invited)**

S. Ali<sup>\*1</sup>; 1. Linnæus University, Sweden

Oxynitride glasses are a group of specially glasses, obtained by incorporation of nitrogen atoms into oxide glass network. Oxynitride glasses and glass ceramics are increasingly recognized as potential materials in specialist applications in modern industrial sectors. These glasses have superior mechanical, chemical and optical properties to their oxide glass counter partner. Properties of these glasses can be tailored by changes in nitrogen content and additions of various alkaline-earth and/or rare-earth elements. However, to date, the gains in properties are not significant enough to compensate for the increased production costs arising from the more difficult preparative processes involved. Furthermore, these glasses are less transparent and are often grey or black and translucent only in thin sections, due to inclusions of other phases. Poor transparency in the visible region of the oxynitride glasses is the main obstacle to their utilization. The most common reasons for the diminished transparency are precipitation of elemental silicon and silicides. This presentation provide an overviewed of previous work on oxynitride glasses containing high amount of nitrogen and modifiers, outlines the effect of glass composition on properties and discusses the difficulties and opportunity associated with these glasses.

**Session 6: Metallic Glasses**

Room: Senate A/B

Session Chair: Emanuel Ionescu, Technical University Darmstadt

**10:50 AM**

**(GOMD-S1-077-2016) An Alternative View on the Fundamental Structural Units in Bulk Metallic Glasses (Invited)**

W. Ching<sup>\*1</sup>; 1. University of Missouri-Kansas City, USA

Based on the data obtained from high precision ab initio calculations of electronic structure and bonding in a large number of binary ( $\text{Zr}_x\text{Cu}_y$ ), ternary ( $\text{Zr}_x\text{Cu}_y\text{Al}_z$ ) and multicomponent (Vitreloy:  $\text{Zr}_{41.2}\text{Ti}_{13.8}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$ ) bulk metallic glasses (BMG), it is demonstrated that the long-standing notion of using icosahedron as the basic structural unit to describe both the short range order (SRO)

and intermediate range order (IRO) in BMG is questionable. Such pure geometric analysis requires the definition of “bond length” between different pairs of metallic atoms which is generally ill-defined and unprecise. In this talk, I advocate the use of total bond order density (TBOD) as a quantum mechanically derived metric to characterize BMGs. This new concept is supported by the results from calculations on large models of 1024 atoms with periodic boundaries and the evaluations of bond order (BO) values between all pairs of atoms. The TBOD is obtained as the sum of all BO values normalized by cell volume. Detailed analysis of the distribution of TBOD reveals intimate details and correlations between TBOD and fundamental physical properties including the glass forming ability, chemical composition, density of states (DOS) at the Fermi level etc.

**11:20 AM**

**(GOMD-S1-078-2016) Elastic properties and atomic bonding character in inorganic glasses: Metallic, oxide, and non-oxide**

T. Rouxel<sup>\*1</sup>; 1. University of Rennes 1, France

The elastic properties of glasses from different chemical systems were studied in the light of the atomic packing density and bonding character. We found that the electronegativity mismatch ( $\Delta e$ ) between the host- and the major solute - elements provides a plausible explanation to the large variation observed for Poisson's ratio ( $\nu$ ) among metallic glasses (MGs) (from 0.28 for Fe-based to 0.43 for Pd-based MGs) notwithstanding a similar atomic packing efficiency (Cg). This correlation also holds for monoconstituent oxide glasses and hence provides an explanation to the variation of  $\nu$  observed for seemingly “isostructural” glasses. Ductility is favored in glasses exhibiting a weak bond directionality in average and opposing a strong resistance to volume change.

### Session 7: Synthesis, Structure and Properties of Glass under Extreme Conditions

Room: Madison

Session Chair: Mathieu Bauchy, University of California, Los Angeles

**9:20 AM**

**(GOMD-S1-079-2016) Structural changes in glass-forming silicates at high pressures, temperatures and extremes of composition: What's known and what's to be learned (Invited)**

J. Stebbins<sup>\*1</sup>; 1. Stanford University, USA

Glasses (or more precisely glass-forming molten silicates) at 'extremes' of temperature (e.g. >2000 C), pressure (e.g. to >100 GPa) and composition (perhaps not even glass-forming) have long been of major importance in the Earth sciences, as most of the planet finds such conditions 'routine'. Recently there has been considerable convergence of interest among geoscientists, glass scientists, and physical chemists on experimental and theoretical work on structure and dynamics at high P/T, as well on compositions outside of the usual technological range. This talk will provide milestones of key findings on pressure and temperature effects, and highlight directions for the future. One example to be discussed will be the controversial “free” oxide species, which for decades has been considered important only in models of very low-silica, non-glass-forming liquids of most interest in metallurgical slag chemistry. There is now definitive, direct observation of this species in what are to glass scientists ‘extreme’ compositions (silicate glasses very high PbO, HfO<sub>2</sub>, or MgO). However, simple thermodynamic considerations suggest that the concentrations of “free” oxide may be much higher at and above liquidus temperatures in these and other, more technologically and geologically relevant, compositions.

**9:50 AM**

**(GOMD-S1-080-2016) Anomalous dynamics during glass transition linked with rigidity properties (Invited)**

M. Micoulaut<sup>\*1</sup>; M. Bauchy<sup>2</sup>; 1. UPMC, France; 2. UCLA, USA

We present results from the investigation of simulated densified supercooled silicate liquids (2SiO<sub>2</sub>-Na<sub>2</sub>O). A cascade of dynamic anomalies are found which lead to extrema (maxima or minima) with pressure: diffusivity, activation energies, viscosity, volume recovery during a heating-colling cycle across the glass transition region. An analysis from topological rigid constraints indicates that the region of anomalous behavior corresponds to isostatic liquids, and is identified as the pressure analogue of the stress-free intermediate phase in rigidity driven by composition, found between flexible/low-connected and stressed rigid/highly cross-linked network glasses. Connections with the well-known water-like anomalies and dynamic heterogeneities will also be discussed.

**10:20 AM**

**(GOMD-S1-081-2016) Chemical durability of ‘forbidden’ glasses: Separating the effects of glass structure and chemistry**

R. Schaut<sup>\*1</sup>; S. Tietje<sup>1</sup>; 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. Previously we showed for one glass family that the potassium-rich surface produced by ion-exchange has indistinguishable durability (at high pH) from the parent sodium-rich glass. This suggested that the durability was driven by the structure of the glass rather than by the specific chemistry. Here, we apply the same approach to broader glass composition space and chemical durability tests (acid and base). The results will be discussed with respect to the structure of the parent glasses (Q<sub>3</sub>, Q<sub>4</sub>, NBO, B<sup>III</sup>, B<sup>IV</sup>, etc.).

**10:40 AM**

**(GOMD-S1-082-2016) Structure-Property Transformations in Oxide and Non-Oxide Glasses and Supercooled Liquids Subjected to Extreme Conditions (Invited)**

S. Sen<sup>\*1</sup>; 1. UC Davis, USA

Most of what we know about structure-property relations in glasses and glass-forming liquids comes from one atmosphere experimental measurements. Nevertheless, fundamental understanding of the effects of extreme pressure, temperature and strain rate conditions is often crucial to model a wide range of processes including, for example, extrusion or fiberization of glass to magma transport in earth's interior. Recent studies in our group have focused on three such areas, namely: (i) investigation of structural mechanisms of pressure induced densification in silicate glasses and liquids; (ii) structural nature of pressure induced, polyamorphic molecule-to-network and semiconductor-to-metal transformation in chalcogenide glasses and (iii) investigation of atomistic mechanism of shear thinning at high strain rates in chalcogenide liquids. The results obtained in these studies from structure and property measurements, performed in situ in diamond anvil cell and ex situ on samples quenched from high pressure and temperature in multi-anvil cell or subjected to high strain rate in a capillary rheometer will be presented. Structural models of densification, polyamorphic transformation and non-Newtonian rheology, built on the basis of these results, will be discussed.



11:10 AM

**(GOMD-S1-083-2016) Glasses under compression and surface confinement (Invited)**S. Lee\*<sup>1</sup>; 1. Seoul National University, Republic of Korea

We provide an overview of the recent progress that we have made into structures of iron-bearing, multi-component oxide glasses with varying pressure, composition (fluid contents), and surface confinement using solid-state NMR and synchrotron x-ray techniques. Despite the pronounced paramagnetic effect, detailed structural changes in the cold-compressed iron-bearing Mg-silicate glasses can now be probed using solid-state NMR techniques, revealing an increase in Al coordination number with increasing pressure up to 25 GPa. These results, along with new structural insights made by carbon-bearing silicate glasses at high pressure provide atomistic insights into the complex and non-linear variations of melt-properties and distribution of B and C in the earth's interior. We also show that the coordination environments in the surface confined oxide glasses are distinct from those of bulk, highlighted by a decrease in the fractions of high-energy clusters (and thus the degree of disorder) near interface. We also report NMR results that shows the structure of glass surfaces is also affected by the types of interfaces (e.g. crystalline vs. non-crystalline). The result implies that a wide range of variations in amorphous states can be identified by controlling its dimensionality and interfaces.

11:40 AM

**(GOMD-S1-084-2016) Raman spectroscopy of v-SiO<sub>2</sub> under rare gas compression**C. Weigel<sup>1</sup>; B. Hehlen<sup>1</sup>; A. Polian<sup>2</sup>; B. Rufflé<sup>1</sup>; R. Vacher<sup>1</sup>; M. Foret\*<sup>1</sup>; 1. University of Montpellier, France; 2. University Paris 6, France

We present accurate measurement of the VV- and VH-polarized Raman spectra of vitreous SiO<sub>2</sub> pressurized in the range 0 – 8 GPa in argon or helium atmosphere by means of diamond anvil cell. A fine quantitative analysis of the behavior of the Raman modes in function of pressure is achieved with the help of an old central-force model by Sen and Thorpe describing the dynamics of covalently bonded networks. The model predicts the effect of changes in force constants and bond angles on the vibrational frequencies of the coupled SiO<sub>4</sub> tetrahedral network. We show that the pressure shift of the Raman bands cannot be understood without encompassing the variations of both parameters. Investigating two different pressurizing fluids including He which is adsorbed into the silica network, allows revealing the role of each parameter in the compression mechanism of the glass.

**Session 2: Fundamentals**

Room: Capitol A

Session Chair: Edgar Dutra Zanotto, Federal University of Sao Carlos

1:20 PM

**(GOMD-S1-085-2016) Role of structural relaxation in crystal nucleation kinetics (Invited)**P. Gupta\*<sup>1</sup>; D. R. Cassar<sup>2</sup>; E. Dutra Zanotto<sup>2</sup>; 1. Ohio State University, USA; 2. Federal University of Sao Carlos, Brazil

The dramatic failure of the classical nucleation theory to describe crystal nucleation kinetics in super-cooled liquids is well documented. In this talk, we discuss a proposal that nucleation kinetics at low temperatures are significantly influenced by the rapid slowing down of the structural relaxation processes in the liquid. The cooperative nature of structural relaxation in a super-cooled liquid suggests that, at sufficiently low temperatures (close to the laboratory glass transition range), structural rearrangements needed to form a critical nucleus cannot take place because the critical nucleus size is too small and is unable to provide needed cooperativity. We analyze this proposal using published data for the stoichiometric lithium

disilicate system for which homogeneous nucleation has been well documented and relevant thermodynamic and kinetic data are available. Our results support the notion that structural relaxation effects slow down nucleation kinetics at low temperatures.

1:50 PM

**(GOMD-S1-086-2016) Synthesis of Nanostructures during Devitrification of Metallic Glass Alloys (Invited)**J. H. Perepezko\*<sup>1</sup>; Y. Shen<sup>1</sup>; 1. University of Wisconsin, USA

While the nanocrystalline state is often viewed in terms of isolated nanocrystalline particles, an equally important form of nanostructured alloys is based upon a dispersion of a high number density of nanocrystals within an amorphous matrix. For example, from amorphous precursors based upon marginal glass forming alloys with compositions that limit the solute content to <15 at%, primary crystallization can yield nanocrystals with sizes of 10-20 nm and densities of 10<sup>21</sup>-10<sup>22</sup> m<sup>-3</sup>. It is now established in Fe and Al base systems that the primary nanocrystallization reaction yields single crystal nanocrystals with little retained solute and that the nanocrystals are enveloped in a solute-rich layer that develops during diffusion-controlled growth. Recent crystallization kinetics analysis and microstructure examination provide new evidence for the role of the structural heterogeneities based upon medium range order (MRO) that can act as nucleation sites for nanocrystal synthesis and promote transient kinetics behavior. At the same time, the primary crystallization reaction can be controlled by suitable doping with either soluble or insoluble solute to enhance or reduce the nanocrystal densities. These are new developments that offer exciting possibilities for control of nanoscale microstructures as well as challenges for the fundamental understanding of the reaction mechanisms.

2:20 PM

**(GOMD-S1-087-2016) The Investigation of the Nucleation Delay Time in Al-based Metallic Glasses by the High Rate Calorimetry**Y. Shen\*<sup>1</sup>; J. H. Perepezko<sup>1</sup>; 1. University of Wisconsin-Madison, USA

Upon annealing at temperatures lower than the crystallization onset temperature, the Al<sub>88</sub>Y<sub>7</sub>Fe<sub>5</sub> metallic glass undergoes a period of delay time ( $\tau$ ) before the primary crystallization reaction. The delay time is an important parameter, which is closely related with the transport behavior and can be used to calculate the diffusion coefficient and steady state nucleation rate. Previously,  $\tau$  was usually determined by the crystalline number density vs. annealing time plot through the tedious TEM measurements. Now, we have developed a more convenient approach to measure  $\tau$  by analyzing the glass transition temperature ( $T_g$ ) shift with FlashDSC. With the increase of annealing time,  $T_g$  shifts to higher temperatures and in the  $T_g$  vs.  $t_{\text{annealing}}$  plot, there is a break point corresponding to  $\tau$ . Before this break point, no Al nanoparticles could be detected but after this break point, they were identified. The underlying mechanism is unveiled through the crystallization enthalpy analysis by FlashDSC and matrix composition measurement by EDS. The analysis reveals that before the break point,  $T_g$  shifts solely due to the increased glass stability through a relaxation process. After the break point, the precipitation of Al nanoparticles induces a composition change in the amorphous matrix so that  $T_g$  shifts to higher temperatures because of both the relaxation and composition change effects.

2:40 PM

**(GOMD-S1-088-2016) Crystallization of nepheline (Na<sub>2</sub>O•Al<sub>2</sub>O<sub>3</sub>, 2SiO<sub>2</sub>) based glasses – Impact of cation mixing**A. Deshkar<sup>1</sup>; J. Marcial<sup>3</sup>; S. Southern<sup>2</sup>; L. Kobera<sup>2</sup>; D. Bryce<sup>2</sup>; J. McCloy<sup>3</sup>; A. Goel\*<sup>1</sup>; 1. Rutgers University, USA; 2. University of Ottawa, Canada; 3. Washington State University, USA

Understanding the molecular basis of nucleation and crystallization in nepheline based glasses has high technological implications. On one hand, controlled crystallization in these glasses results in

\*Denotes Presenter

glass-ceramics with high mechanical strength. On the other hand, nepheline crystallization in high level nuclear waste glasses (at Hanford site in Washington State) results in severe deterioration of the chemical durability of the final waste form, providing a challenge for long-term repository stability of the waste form. The present study focuses on investigating the impact of cation mixing ( $\text{Na}^+ \leftrightarrow \text{Ca}^{2+}$ ) on the crystallization of nepheline based glasses, as a function of their chemical composition and molecular structure. Accordingly, the structure and crystallization behavior of glasses with varying  $\text{Na}_2\text{O}/\text{CaO}$  and  $\text{SiO}_2/\text{CaO}$  ratio have been studied using NMR, DSC, quantitative XRD and SEM. The as obtained results will be discussed at the conference.

**3:00 PM**

**(GOMD-S1-089-2016) Characterization of CMAS and CMAS-TiO<sub>2</sub> crystallization behavior from the melt for EBC applications**

R. Webster<sup>\*1</sup>; E. Opila<sup>1</sup>; 1. University of Virginia, USA

Calcium magnesium aluminosilicate (CMAS) attack is a pressing issue in the development of Environmental Barrier Coatings (EBCs) for Ceramic Matrix Composites (CMCs). At temperatures greater than  $\sim 1200^\circ\text{C}$ , CMAS becomes molten and can penetrate EBC materials, causing premature coating failure. Inducing crystallization of these glassy deposits has been suggested in the literature as a mitigation strategy. In this study, the crystallization behavior of CMAS and CMAS with the addition of titania ( $\text{TiO}_2$ ) was investigated from melts equilibrated at 1300 and 1500 $^\circ\text{C}$ . Samples were exposed in both a stagnant air furnace and a Differential Scanning Calorimeter (DSC). Resulting glass and crystalline phases were characterized after cooling from the melt at 10 $^\circ\text{C}/\text{min}$  as well as after holding at temperatures between 800-1000 $^\circ\text{C}$ . Results suggest that  $\text{TiO}_2$  additions between approx. 12.5-20 wt % aid in the crystallization of CMAS melts and that holding at temperatures between 850-1000 $^\circ\text{C}$  increases the amount of crystalline product formed. Preliminary studies have also been carried out assessing CMAS interactions with possible coating constituents, RE (Rare Earth)-mono- and di-titanates ( $\text{RE}_2\text{TiO}_5$  and  $\text{RE}_2\text{Ti}_2\text{O}_7$ , respectively), under similar conditions.

**3:40 PM**

**(GOMD-S1-090-2016) Nucleation Mechanisms Revealed by Molecular Dynamics Simulations (Invited)**

H. Fang<sup>1</sup>; Y. Zhang<sup>1</sup>; R. Newman<sup>1</sup>; J. Kieffer<sup>\*1</sup>; 1. University Of Michigan, USA

The direct observation of the crystallization process in molecular dynamics (MD) simulations requires simulation ensembles that are sufficiently large and tracked over sufficiently long times, to allow for nuclei of critical size to form. This probability is quite accurately described by classical nucleation theory. Furthermore, the nucleation rates are highest for materials with simple chemical composition and that form densely packed high-symmetry crystal configurations. For example, in elemental metallic systems and 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. The nucleation rate decreases dramatically, as the underlying mechanism changes. Systematic study of such a 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 factors such as impurity diffusion that control the nucleation process. We also examine the effect of structural complexity on the nucleation process. Acknowledgement: NSF-DMR 1106058

**4:10 PM**

**(GOMD-S1-091-2016) Crystallization of liquids and glasses: learning from molecular simulations (Invited)**

M. Micoulaut<sup>\*1</sup>; 1. UPMC, 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.

**4:40 PM**

**(GOMD-S1-092-2016) Crystallization of molecular glasses: A central role for surface mobility (Invited)**

L. Yu<sup>\*1</sup>; C. Powell<sup>1</sup>; Y. Chen<sup>1</sup>; W. Zhang<sup>1</sup>; M. D. Ediger<sup>1</sup>; 1. University of Wisconsin, USA

Crystallization of glass-forming liquids is important for developing stable amorphous materials and exhibits surprising phenomena still poorly understood. Our recent work showed that surface diffusion is extremely fast on molecular glasses, outpacing bulk diffusion by a factor of  $10^5$  to  $10^8$  at  $T_g$ . This high surface mobility enables fast crystal growth on free surfaces at velocities that scale with surface diffusivity. High surface mobility also suggests an explanation for the surprisingly fast crystal growth in the bulk. Molecular glasses are easy to fracture and fracture surfaces can support fast crystal growth. This mechanism may underlie the mysterious "glass-to-crystal" growth mode in molecular glasses.

**5:10 PM**

**(GOMD-S1-093-2016) Fast Crystal Growth in Organic Glasses: A Possible Role for Fracture and Surface Mobility**

C. T. Powell<sup>\*1</sup>; Y. Chen<sup>1</sup>; M. D. Ediger<sup>1</sup>; L. Yu<sup>1</sup>; 1. University of Wisconsin-Madison, USA

The amorphous phase of small-molecule organic materials can develop an unexpectedly fast mode of crystal growth near and below the glass transition temperature. This crystal growth phenomenon termed "GC growth" for its glass-to-crystal phase transition remains imperfectly understood with several explanations proposed. We report that GC growth in the model system ortho-terphenyl conserves the overall system volume, despite a 5% higher density of the crystal, and produces fine crystal grains with the same unit cell as normally grown crystals. These results indicate that GC growth continuously creates voids and free surfaces, possibly by fracture. Given the existence of even faster crystal growth on the free surface of molecular glasses, we consider the possibility that GC growth is facilitated by fracture and surface mobility. This notion has support from the fact that GC growth and surface growth are both highly correlated with surface diffusivity and with fast crystal growth along preformed cracks in the glass.

**5:30 PM**

**(GOMD-S1-094-2016) Computational modeling of synthesis of amorphous serpentine from olivine: Implications for planetary water delivery and formation of hydrous minerals in the solar nebula**

A. Asaduzzaman<sup>1</sup>; K. Muralidharan<sup>\*1</sup>; J. Ganguly<sup>1</sup>; 1. University of Arizona, USA

Formation of hydrous phyllosilicates such as serpentine and talc has been a subject of debate in the planetary sciences community; characterizing the timescale of phyllosilicate formation will have fundamental implications for understanding the origin of planetary water. Based on a model derived from the simple collision theory, it was assumed that under solar nebular conditions, the timescale for

formation of serpentine (obtained when olivine reacts with water) was longer than the solar nebular lifetime. Contrary to this model, using computational techniques (density functional theory and kinetic Monte Carlo) we demonstrate that the formation of serpentine can indeed occur well within nebular timescales. The formation of serpentine is initiated through the chemisorption of water molecules on olivine surfaces. This is followed by the formation of a surface amorphous phase that is chemically representative of serpentine, which serves as the precursor for the gradual serpentinization of the olivine sub-surface. Interestingly recent experiments have detected amorphous silicates in minimally altered carbonaceous chondrites. From textural analysis it has been suggested that the serpentine/saponite areas of the chondrites were formed from these amorphous silicates, corroborating our findings.

### Session 3: New Techniques and Applications

Room: Capitol B

Session Chair: Dominique de Ligny, University Erlangen-Nürnberg

1:20 PM

#### (GOMD-S1-095-2016) Atom-probe tomography in the glass sciences (Invited)

J. Ryan<sup>\*1</sup>; D. Schreiber<sup>1</sup>; 1. Pacific Northwest National Lab, USA

Atom-probe tomography (APT) is an emerging experimental microstructural analysis technique in the field of glass science. Although not a new technique, the introduction of laser-pulsed APT systems over the last 8 years has opened the door to APT examinations of insulating materials systems such as oxide glasses. Put simply, APT combines field ion microscopy with time-of-flight mass spectrometry, where individual atoms are evaporated from the surface of a FIB-produced sample specimen one-by-one, accelerated through a field, and collected with a position-sensitive detector. Together, the time-of-flight mass spectrum and 3D position information are used to generate a 3D elemental map (single-atom sensitivity) with near-atomic resolution in depth and sub-nm lateral resolution. This powerful combination of spatial and compositional information has enabled many novel experiments in the field of glass science. The talk will present a thorough introduction to the technique, including theory, typical instrumentation, data analysis, and a literature review of recent applications. Specific case studies will be presented to illustrate the potential of the technique to common problems in glass science, including interfaces in corroded glasses, nanoparticles, crystallization, dopant dispersion, and phase separation. The talk will conclude with a discussion on prospective future areas of glass research where APT could be very useful.

1:50 PM

#### (GOMD-S1-096-2016) Usable Strength of Glass - Surface Science Perspective

N. Sheth<sup>\*1</sup>; J. Luo<sup>1</sup>; C. G. Pantano<sup>1</sup>; S. H. Kim<sup>1</sup>; 1. Pennsylvania State University, USA

Glass surface composition, specifically variation in alkali modifier content, may alter the surface reactivity. Dealkalization treatments improve the chemical durability and mechanical strength by permanently altering the glass surface chemistry. To probe changes in glass surface chemistry due to dealkalization processing, the mechanisms of modifier replenishment into the depleted layer are studied. In this study, heat-induced replenishment of the depletion layer is used to probe dealkalization effects on surface chemistry. Surface-sensitive characterization tools (SFG, FTIR, XPS) are vital for investigating how dealkalization processing alters glass surface composition, structure and adsorbed molecules; Glass surface chemistry is then correlated with mechanical wear behavior and surface defects distribution probed from crack initiation load. By understanding how dealkalization processing modifies glass surface properties, the relationship between modifiers, surface defect formation and mechanical performance can be better understood. This work was

supported by the Usable Glass Strength Coalition (UGSC) and the National Science Foundation Graduate Student Fellowship (NSF-GRFP).

2:10 PM

#### (GOMD-S1-097-2016) Structural characterization of mirror coating for gravitational waves detection

V. Martinez<sup>\*1</sup>; C. Elodie<sup>1</sup>; G. Massimo<sup>2</sup>; M. Christine<sup>1</sup>; V. Dolique<sup>2</sup>; A. Mermet<sup>1</sup>; G. Cagnoli<sup>2</sup>; 1. ILM, France; 2. LMA, France

The detection of gravitational waves is essential to get a better understanding of the Universe and constitute one of the ultimate tests of the General Relativity. The current important limitation of gravitational wave detectors (GWD) is that the signal is of the same order of magnitude of the thermal noise from the mirror amorphous coating (alternative layers of SiO<sub>2</sub> and TiO<sub>2</sub>-doped Ta<sub>2</sub>O<sub>5</sub>). This study is focused on amorphous silica films whose mechanical losses (which are directly connected to thermal noise) can be reduced by annealing. The aim is to clarify the link between this reduction and the film structure at short and medium range order probed by Raman spectroscopy. Thin silica films were synthesized by Ion Beam Sputtering. The Raman spectroscopic signature study indicates that this high energy ion deposition process leads to a dense and stressed silica glass film. Moreover the Raman D2 line, assigned to breathing mode of three-membered rings, is about six times larger for our deposited films than silica. Formation of small rings is favored by the deposition process. Different annealing times were performed on these amorphous silica films at a temperature much lower than glass transition temperature. The evolution of the different spectroscopic signatures as a function of annealing time will be presented and the correlation between mechanical losses and these signatures will be discussed.

2:30 PM

#### (GOMD-S1-098-2016) Densification Mechanisms in Vitreous Ge<sub>x</sub>Se<sub>1-x</sub>

C. Yildirim<sup>\*1</sup>; M. Micoulaut<sup>1</sup>; J. Raty<sup>2</sup>; 1. University Paris 6, France; 2. Université de Liège, Belgium

Pressure induced structural modifications in vitreous Ge<sub>x</sub>Se<sub>1-x</sub> (where 0.10 ≤ x ≤ 0.25) are investigated using X-ray absorption spectroscopy (XAS) along with supplementary X-ray diffraction (XRD) experiments and ab initio molecular dynamics (AIMD) simulations. All the compositions studied are observed to remain amorphous under pressure values up to 42 GPa. The Ge-Se bond distances extracted from XAS data show a two-step response to the applied pressure; a gradual decrease followed by an increase at around 15-20 GPa, depending on the composition. This increase is attributed to the metallization event that can be traced with the red shift in Ge K edge energy which is also identified by the principle peak position of the structure factor. The densification mechanisms are studied in details by means of AIMD simulations and compared to the experimental results. The evolution of bond angle distributions, neighbor distances, standard deviations, coordination numbers and topological constraints are examined. Universal changes in distances and angle distributions are observed when scaled to reduced densities. The interplay between the structural motifs, transition of tetrahedral to octahedral geometry and reversibility of the structural changes under pressure is discussed.

2:50 PM

#### (GOMD-S1-099-2016) Tunable Molecular Orientation in Vapor-Deposited Molecular Glasses

D. M. Walters<sup>\*1</sup>; S. S. Dalal<sup>1</sup>; N. D. Johnson<sup>1</sup>; M. D. Ediger<sup>1</sup>; 1. University of Wisconsin-Madison, USA

Physical vapor deposition can prepare molecular glasses with highly anisotropic orientation unseen in traditional, liquid-cooled glasses. This feature is harnessed for applications in organic electronics, and while previous studies have shown that molecular shape and

\*Denotes Presenter

substrate temperature influence molecular orientation, the origin of this anisotropy is not fully understood. To gain fundamental insight, we apply high-throughput techniques to investigate the effect of the substrate temperature on vapor-deposited glasses with a variety of molecular shapes. Using spectroscopic ellipsometry, we characterize the average molecular orientation. We find that rod and disc-shaped molecules, such as TPD and m-MTDATA, and can be highly anisotropic and have continuously tunable molecular orientation over a wide range of substrate temperatures, while a spherical molecular, Alq<sub>3</sub>, is optically isotropic. The limits of molecular shape are explored as a compact molecule, p-TTP, shows tunable orientation intermediate spheres and rods, while, surprisingly, several rod-shaped molecules with a wide range of aspect ratios show the same orientation trend. Simulations of rod-like TPD offer an explanation for the orientation based on surface mobility and structure at the equilibrium liquid surface. These results shed light on the origin of anisotropy in vapor deposited glasses.

### Session 3: Optical and Vibrational Measurements

Room: Capitol B

Session Chair: Mario Affatigato, Coe College

3:40 PM

#### (GOMD-S1-100-2016) Structural Studies by Vibrational Spectroscopy of Glasses Based on Less-conventional Glass Formers: from Sulfates to Tungstates (Invited)

D. Möncke<sup>\*1</sup>; E. I. Kamitsos<sup>2</sup>; I. Friedrich-Schiller University Jena, Germany; 2. National Hellenic Research Foundation, Greece

The complementary methods of Raman and infrared (IR) spectroscopy are powerful tools in the structural analysis of glasses. Vibrational bands shift in position as the polyhedral cation changes (SiO<sub>4/2</sub><sup>0</sup> and TiO<sub>4/2</sub><sup>0</sup> / SO<sub>4</sub><sup>2-</sup>, PO<sub>4</sub><sup>3-</sup>, SiO<sub>4</sub><sup>4-</sup>), with the degree of polymerization, (SiO<sub>4</sub><sup>4-</sup>, to SiO<sub>2</sub><sup>0</sup>), or with the type of modifier cation which charge-balances a non-bridging oxygen atom (Li<sup>+</sup> to Rb<sup>+</sup>). Via the cation motion bands, far infrared spectra give information on the number and type of various site environments. The coordination of glass forming polyhedral, as well as their connectivity, has a large impact on band assignments (e.g., BO<sub>3</sub> versus BO<sub>4</sub>). Sometimes additional information is needed: bands of highly depolymerized niobate octahedra might overlap with bands of niobate tetrahedra, the Sb<sup>3+</sup>/Sb<sup>5+</sup> ratio needs to be considered for antimonate glasses. In this work, IR and Raman spectroscopy were used in the evaluation of less conventional glass systems ranging from fluoride-sulfate to Sb-, Mo-, W-, Ga-, or In-containing glasses. The glass forming role of MnO, ZnO, Eu<sub>2</sub>O<sub>3</sub> is discussed for highly modified glass systems. It will be shown how the combination of IR and Raman data, as well as the comparison with polarized Raman spectra, allows for well-founded vibrational assignments of various vibrational modes of the less conventional glass former polyhedra.

4:10 PM

#### (GOMD-S1-101-2016) Structural control of optical properties linked to transition elements in borate glasses

G. Calas<sup>\*1</sup>; N. Capobianco<sup>1</sup>; L. Cormier<sup>1</sup>; L. Galoisy<sup>1</sup>; M. Hunault<sup>1</sup>; G. Lelong<sup>1</sup>; 1. University P&M Curie, Paris, France

The presence of transition elements in alkali borate glasses is at the origin of one of the most important chemical dependence of the color of oxide glasses. We present a set of high-quality optical absorption spectra of borate glasses containing Cr<sup>3+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup> and Cu<sup>2+</sup>. It is noteworthy that the variations in glass composition cause different modifications in the speciation of the transition elements in these glasses: crystal-field variations, site distribution or distortion of the site geometry. Such differences depend on the existence of either only one or more sites occupied by the transition element. These spectroscopic properties will be discussed at the light of recent findings on the medium-range organization in borate glasses, in particular B coordination and the geometry of super-units. The

local rigidity induced by these latter also explains the formation of ordered element clusters, already demonstrated in low-alkali borate glasses containing Ni, Co or Zn.

4:30 PM

#### (GOMD-S1-102-2016) Boson Mode, Topological Phases, Immiscibility Window, and Glass Structure in Ba-Borate glasses

C. Holbrook<sup>\*1</sup>; R. Chbeir<sup>2</sup>; A. Czaja<sup>2</sup>; P. Boolchand<sup>2</sup>; 1. Air Force Research Lab, USA; 2. University of Cincinnati, USA

Raman scattering of B<sub>2</sub>O<sub>3</sub> glass display a strongly excited Boson peak. In Li-, Na- or Ba-modified Borates the scattering strength of the Boson mode and the Boroxyl Ring (BR) mode decreases almost linearly with modifier content. Scaling of scattering strengths suggests that the Boson mode is due to weak off-planar interactions that stabilize the BRs in these glasses. Strikingly, a thermally reversing window (RW) manifests in the 24% < x < 32% range of BaO. The RW fixes the three topological phases; compositions at x < 24% are stressed-rigid, those at x > 32% flexible, while those in the RW are isostatically rigid. Raman scattering also reveals a triad of modes (770 cm<sup>-1</sup>, 750 cm<sup>-1</sup>, 705 cm<sup>-1</sup>) on the low frequency side of the BR mode, which are due to mixed-rings. These modes are not observed at x < 15%, the immiscibility range. At x > 15 mol%, the 770 cm<sup>-1</sup> mode scattering strength grows precipitously to display a maximum near x<sub>c</sub> = 20%, correlating with presence of Ba-Tetraborates. At x > 15%, we also observe scattering strength of the 750 cm<sup>-1</sup> mode to increase with x and show a maximum near x<sub>c</sub> = 33%, which correlates with formation of Ba-Diborates. The location of the RW between the two established SGs (x<sub>c</sub> = 20% and 33%) where T<sub>g</sub>(x) shows a broad maximum is not accidental. It is consistent with the count of bonding constraints of the two SGs modified by the presence of NBO.

4:50 PM

#### (GOMD-S1-103-2016) Structural modification of titanosilicate glasses with change of fictive temperature

D. Wenzel<sup>1</sup>; A. Veber<sup>1</sup>; M. Cicconi<sup>1</sup>; D. de Ligny<sup>\*1</sup>; 1. University Erlangen-Nürnberg, Germany

Titanosilicates have a very large set of application due to their higher refractive index and very low thermal expansion. Moreover they present also anomalies as a decrease of their heat capacity just above their glass transition. The origin of such anomalies were associated to flexible oxygen coordination of the titanium and a mainly network former role. The local structure of titanium can be easily followed by vibrational spectroscopy. A recent study has also shown an unusual relationship between the packing density of these glasses and their Poisson ratio inducing a good damage resistance (Scannell, Huang and Rouxel 2015). A series of glass in the system Na<sub>2</sub>O-TiO<sub>2</sub>-SiO<sub>2</sub> were here synthesized from regular quenching method. An ULE glass was added as a sodium free endmember. The effect of the fictive temperature was observed both on volume and index of refraction. The evolution of the structure of the glass was investigated on all range order from short to long. Both Raman and Brillouin spectroscopy was used to characterized the glass samples equilibrated at different temperatures. The sensitivity of the short range order is strongly correlated to the content of sodium. At the opposite the high amount of titanium enhances structural evolution in the long range order with the fictive temperature.

## Session 4: Simulations of Chalcogenide and Metallic Glasses

Room: University C/D

Session Chairs: Carlo Massobrio, CNRS-IPCMS-UNR 7504; Walter Kob, Laboratoire Charles Coulomb

1:20 PM

### (GOMD-S1-104-2016) Density functional/molecular dynamics simulations of functional chalcogenide materials (Invited)

J. Akola<sup>\*1</sup>; 1. Tampere University of Technology, Finland

Simulations of amorphous chalcogenide materials have been performed for two classes of materials which are important for nonvolatile computer memory: phase-change materials (DVDs, phase-change RAM) and Ag-containing Ge/As sulphides (conductive-bridging RAM). For the first case, we have carried out extensive DF/MD simulations for the amorphous-to-crystalline transition of Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> up to 6.5 ns in order to elucidate the atomistic details. Our simulations demonstrate the stochastic property of the crystallisation process, and how one can bias the crystallization process by embedding crystalline templates (“seeds”) inside the amorphous starting structures. Aspects in percolation and voids (free volume) turn out useful in interpreting the MD data and structural transitions. In the latter case, we have focused in determining structural and other properties of amorphous Ag/Ge/S and Ag/As/S alloys which have high ionic (Ag) conductivity. For atomic structure, we find excellent agreement between the experimental results and large-scale simulations. The calculated electronic structures, vibrational densities of states, ionic mobilities, and cavity distributions of the amorphous materials are discussed. The high mobility of Ag in solid state electrolyte applications is related to the presence of cavities and can occur via jumps to a neighbouring vacant site.

1:50 PM

### (GOMD-S1-105-2016) Role of Van der Waals interactions in determining the structure of liquid tellurides

M. Micoulaut<sup>\*1</sup>; H. Flores-Ruiz<sup>1</sup>; A. Piarristeguy<sup>2</sup>; V. Coulet<sup>4</sup>; M. Johnson<sup>3</sup>; G. Cuello<sup>3</sup>; A. Pradel<sup>3</sup>; C. Bichara<sup>4</sup>; 1. UPMC, France; 2. Université Montpellier II, France; 3. Institut Laue Langevin, France; 4. Université Aix-Marseille, France

The simulation of tellurides using standard density functional (DFT) theory based molecular dynamics usually leads to an over-estimation of the bond distances and a noticeable mismatch between theory and experiments when e.g. structure functions are being directly compared. Here, the structural properties of several compositions of Ge-Te and Ge-Sb-Te liquids are studied from a combination of neutron diffraction and DFT-based molecular dynamics. Importantly, we find an excellent agreement in the reproduction of the structure in real and reciprocal spaces, resulting from the incorporation of dispersion forces in the simulation. We then investigate structural properties including structure factors, pair distribution functions, angular distributions, coordination numbers, neighbor distributions, and compare our results with experimental findings.

2:10 PM

### (GOMD-S1-106-2016) Atomic scale modeling of glassy chalcogenide surfaces: insights into their adsorption and gas separation properties (Invited)

G. Ori<sup>\*1</sup>; B. Coasne<sup>2</sup>; M. Boero<sup>1</sup>; C. Massobrio<sup>1</sup>; 1. IPCMS / CNRS - University of Strasbourg, France; 2. Laboratoire Interdisciplinaire de Physique, 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<sub>2</sub> storage, ions batteries) and environment (water treatment). Recently, glassy nanoporous chalcogenides (chalcogels)

have been demonstrated to be efficient sorbents for remediation from gaseous and water waste media. From a computational point of view, producing glassy surface models capable of mimicking realistically the behavior of a chalcogel and its surface is mandatory in order to understand the structure and adsorption properties of such complex materials. In this work, first-principles and classical atomistic simulations are combined to study the properties of glassy chalcogenide surfaces. Several chemistries will be discussed. First-principles molecular dynamics is used to develop realistic models with special emphasis on their surface chemistry. A detailed account of the structure of the surface models is given in terms of topological features and chemical bonding properties (Wannier centers). By employing Grand Canonical Monte Carlo simulations we then show how the realistic details of the surface chemistry drastically affect the adsorption of various gases such as N<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub> and their mixtures.

2:40 PM

### (GOMD-S1-107-2016) Properties of Vapor Deposited CuZrAl Glasses from Molecular Dynamics Simulations

G. Bokas<sup>\*1</sup>; I. Szlufarska<sup>1</sup>; 1. University of Wisconsin-Madison, USA

We used molecular dynamics (MD) simulations to investigate structural properties of vapor-deposited CuZrAl metallic glasses (MGs). MGs were prepared by simulating physical vapor deposition. We found that vapor-deposited glasses have higher densities and significantly lower energies (by ~0.5 eV/atom) than glasses prepared by quenching CuZrAl from liquid. Deposition rate was found to play a critical role in the stability of the vapor-deposited MGs. The optimal substrate temperature that minimizes the energy of the MGs was predicted to be ~0.75 of the glass transition temperature T<sub>g</sub>. This value is in a reasonably good agreement with the experimental values of 0.8-0.85 T<sub>g</sub>. We compared the short and the medium range order of MGs to those of the quenched MGs. In vapor deposited MGs, both the total number of icosahedral clusters and of superclusters are higher than in the ordinary MGs. In summary, we demonstrated that it is possible to use MD simulations to create MGs that are significantly more stable than those prepared using traditional melt-quench MD simulations. Additionally, we discovered that deposited glasses have different structural and chemical order than the quenched structures. MGs created by simulated deposition have properties corresponding to glasses that have been prepared by quenching at cooling rates many orders of magnitude slower than those accessible to MD simulations.

3:00 PM

### (GOMD-S1-108-2016) On the role of Sm in solidification process of Al-Sm metallic glasses

L. Zhao<sup>\*1</sup>; G. Bokas<sup>1</sup>; I. Szlufarska<sup>1</sup>; 1. University of Wisconsin - Madison, USA

Insights into the structural evolution of metallic glass (MGs) during rapid solidification process are important for understanding of the glass forming ability (GFA) and mechanical properties of these materials. Here, we studied structural evolution during the rapid solidification of Al-Sm metallic glasses using molecular dynamics simulations. The icosahedral-ordering was monitored in the quenching process of Al-Sm systems with different Sm concentrations. During solidification the population of most types of Voronoi polyhedra was found to stay nearly constant, except for the icosahedral-like (ICO-like) clusters, whose population increases in the supercooled region. We found that at room temperature alloys with 5-15% Sm have the largest fraction of icosahedral-like clusters among all the concentrations we studied, which correlates with the highest atomic packing densities in Al-Sm MGs. Our simulations show that atoms with ICO-like structure exhibit much lower atomic mobility than other atoms in the supercooled temperature region, implying the highest stability and best GFA of Al-Sm alloys in the 5-15% Sm region. This range of compositions had been previously shown experimentally to exhibit the best GFA among Al-rich Al-Sm

\*Denotes Presenter

MGs. The approach used in this work can be applied to guide the design of new MGs with enhanced GFA.

### Session 5: Mechanical Properties of Glasses IV

Room: Wisconsin

Session Chair: Timothy Gross, Corning Incorporated

1:20 PM

#### (GOMD-S1-109-2016) Deformation mechanisms in silica glass under hydrostatic conditions and underneath an indentation imprint (Invited)

V. Keryvin<sup>1</sup>; J. Guin<sup>2</sup>; J. Sangleboeuf<sup>2</sup>; L. Charleux<sup>3</sup>; 1. University of South Brittany, France; 2. University of Rennes 1, France; 3. University of Savoie Mont-Blanc, France

Glasses are brittle materials and fail macroscopically in a purely elastic manner at room temperature. Yet, under constrained deformation loadings, glasses experience permanent deformation, without fracture. This is the case for the hydrostatic compression test, where, for pressures around 25 GPa, permanent volume changes up to 16 % for silica glass are developed. This is also the case underneath an imprint during nano-indentation tests or a scratching groove. In this presentation, the response under hydrostatic conditions is discussed including experiments, structure changes and constitutive modelling. In particular, the densification process is properly modelled thanks to recent in situ and ex situ experiments of hydrostatic compression. Then, the mechanical response during nano-indentation tests (load-displacement curves) as well as the residual imprints is studied in details. Constitutive modelling is employed to discuss these experimental results via finite element analyses (FEM). The roles of shear and shear flow are then discussed with respect to indentation results. An original chemical dissolution technique to probe densification at the nanometre scale will eventually be described. Its results will be compared to FEM simulations.

1:50 PM

#### (GOMD-S1-110-2016) Perfectly plastic flow in silica glass

G. Kermouche<sup>2</sup>; G. Guillonneau<sup>3</sup>; J. Michler<sup>4</sup>; J. Teisseire<sup>5</sup>; E. Barthel<sup>1\*</sup>; 1. CNRS/ESPCI, France; 2. EMSE, France; 3. ECL, France; 4. Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland; 5. SVI, France

We present novel in situ SEM observations of the uniaxial compression of amorphous silica micropillars and subsequent analysis through finite element simulations. Samples of decreasing sizes have been tested, and our results demonstrate that silica exhibits one of the highest ratios of shear yield stress to shear modulus of all materials, without measurable size effect. We have also measured that the yield stress over shear modulus ratio is significantly lower for normal glasses. Careful evaluation of the actual pillar section during compression was carried out. Thanks to this accurate calibration of the data, we prove that plastic flow in shear occurs without strain hardening, as anticipated from the absence of large scale defects in these materials. The consequences on the mechanisms relevant for hardness will be discussed. The resulting constraints imposed on the appropriate forms for constitutive models of amorphous silica will be examined. Generalization to normal glasses will be briefly discussed.

2:10 PM

#### (GOMD-S1-111-2016) Mapping between atomistic simulations and Eshelby inclusions in the shear deformation of amorphous Silicon

F. Boioli<sup>1\*</sup>; T. Albaret<sup>1</sup>; D. Rodney<sup>1</sup>; 1. ILM, University of Lyon 1, France

Localization of plastic deformation in shear bands leads to catastrophic failure in amorphous solids. Generally, it has been accepted that local irreversible rearrangements of small clusters of atoms, Shear Transformations (STs), are the elementary processes involved in the deformation of amorphous systems and several mesoscale

models based on STs have been proposed. Still the fundamental mechanisms underlying ST occurrence and shear band formation are not yet clear. In this work we investigate amorphous silicon by performing quasi-static shear simulations with Stillinger-Weber type potentials. First, the analysis of the shear simulations allows to identify local plastic rearrangements. By fitting their displacement field on collections of Eshelby spherical inclusions, we characterize their size and plastic strain. These two ingredients with a measure of the strain-dependent shear modulus suffice to reproduce the atomistic stress-strain curve. This result justifies the usual decomposition of plastic rearrangements into STs and provides atomic-scale parameters to characterize the STs needed to build mesoscale models. Second, by using the Nudged Elastic Band method, we calculate the energy barriers and the activation volumes involved in plastic rearrangements, thus accessing the strain-rate sensitivity of glass plasticity, another important parameter for mesoscale models.

2:30 PM

#### (GOMD-S1-112-2016) Nano-Ductility in Silicate Glasses is Driven by Topological Heterogeneity

B. Wang<sup>1</sup>; Y. Yu<sup>1</sup>; M. Wang<sup>1</sup>; J. C. Mauro<sup>2</sup>; M. Bauchy<sup>1</sup>; 1. University of California, Los Angeles, USA; 2. Corning Incorporated, USA

The existence of nanoscale ductility during the fracture of silicate glasses remains controversial. Here, based on molecular dynamics simulations coupled with topological constraint theory, we show that nano-ductility arises from the spatial heterogeneity of the atomic network's rigidity. Specifically, we report that localized floppy modes of deformation in under-constrained regions of the glass enable plastic deformations of the network, resulting in permanent change in bond configurations. Ultimately, these heterogeneous plastic events percolate, thereby resulting in a non-brittle mode of fracture. This suggests that nano-ductility is intrinsic to multi-component silicate glasses having nanoscale heterogeneities. Tuning the extent of heterogeneity would allow one to design tougher glasses from the atomic scale.

2:50 PM

#### (GOMD-S1-113-2016) Mechanoluminescence in a transparent glass composite (Invited)

Y. Gueguen<sup>1\*</sup>; M. Dubernet<sup>1</sup>; F. Céliari<sup>1</sup>; P. Houizot<sup>1</sup>; J. Sangleboeuf<sup>2</sup>; T. Rouxel<sup>1</sup>; 1. Institut de Physique de Rennes UMR UR1-CNRS 6251, France

Mechanoluminescence is the phenomenon of light emission during a mechanical loading. The phenomenon is known since a long time (in sugar, since the 17<sup>th</sup> century at least). Many materials have been developed to produce elasto-luminescence (light emission during pure elastic deformation). We have developed glass composites with elasto-luminescent particles, namely SrAl<sub>2</sub>O<sub>4</sub>:Eu,Dy crystal, in order to obtain "smart glasses", able to provide directly information on the stress they undergo, before they break. Because the light emission occurs during reversible deformation in this material, it allows for the development of load sensors: the light emission is reproducible and repeatable. Nevertheless, there is still a lack of efficient and simple model to establish the relationship between the stress applied on a material and the light it emits, especially for complex loading histories. We present here a model of mechanoluminescence. We highlight, through this model, that the intensity of the light emission is not connected to the current stress, but to the whole history of stress from the beginning of the loading. We also take into account the limited light emission in elasto-luminescent materials.

**Session 5: Mechanical Properties of Glasses V**

Room: Wisconsin

Session Chair: Yann Gueguen, Institut de Physique de Rennes UMR UR1-CNRS 6251

**3:40 PM****(GOMD-S1-114-2016) Crack nucleation criterion and its application to impact indentation in oxide glasses**J. Luo<sup>\*1</sup>; K. Vargheese<sup>1</sup>; A. Tandia<sup>1</sup>; G. Hu<sup>1</sup>; J. C. Mauro<sup>1</sup>; I. Corning Incorporated, USA

Molecular dynamics (MD) simulations are used to directly observe nucleation of median cracks in oxide glasses under indentation. Indenters with sharp angles can nucleate median cracks in samples with no pre-existing flaws, while indenters with larger indenter angles cannot. Increasing the tip radius increases the critical load for nucleation of the median crack. Based upon an independent set of simulations under homogeneous loading, the fracture criterion in the domain of the principal stresses is constructed. The fracture criterion, or "fracture locus", can quantitatively explain the observed effects of indenter angle and indenter tip radius on median crack nucleation. Our simulations suggest that beyond the maximum principal stress, plasticity and multi-axial stresses should also be considered for crack nucleation under indentation, even for brittle glassy systems.

**4:00 PM****(GOMD-S1-115-2016) Compositional Dependence of Indentation-Induced Residual Stresses of Sodium Aluminosilicate Glasses**K. Yoshida<sup>1</sup>; S. Yoshida<sup>\*1</sup>; A. Yamada<sup>1</sup>; J. Matsuoka<sup>1</sup>; A. Errapart<sup>5</sup>; V. Pukhkaya<sup>2</sup>; J. Teisseire<sup>2</sup>; E. Barthel<sup>3</sup>; C. R. Kurkjian<sup>4</sup>; 1. The University of Shiga Prefecture, Japan; 2. Surface du Verre et Interfaces - CNRS /Saint-Gobain, France; 3. Science and Engineering of Soft Matter, UPMC / CNRS / ESPCI PPMU UMR 7615, France; 4. Rutgers University, USA; 5. Trenz Electronic GmbH, Germany

Crack initiation of glass is affected by the stress state of the glass prior to fracture, but very few reports are now available on direct measurements of elastic and residual stresses of glass during and after contact loading. This is the reason why details of compositional variation of strength or brittleness of glass have not been clarified yet. In this study, residual stresses around conical (or axisymmetrical) indentations on sodium aluminosilicate ( $\text{Na}_2\text{O}-\text{Al}_2\text{O}_3-\text{SiO}_2$ , NAS) glasses were determined using a micro-photoelastic imaging system, and compositional variation of the residual stresses were evaluated. Birefringence data of indented glasses were converted into axisymmetrical stresses, assuming that elastic rules are applicable to this indentation-induced residual stresses in the elastic region outside the plastic zone. It is found that the size of plastic zone beneath the conical indent decreases with increasing  $\text{Al}_2\text{O}_3$ , or with decreasing the number of non-bridging oxygens, and that the residual stress at the interface between elastic and plastic regions increases with increasing  $\text{Al}_2\text{O}_3$  content in glass. This compositional change in residual stress will be discussed in connection with compositional variation of cracking behavior in NAS glass.

**4:20 PM****(GOMD-S1-116-2016) Mechanism and prediction of removal rate and surface roughness creation during optical polishing of glasses**T. I. Suratwala<sup>\*1</sup>; W. A. Steele<sup>1</sup>; M. D. Feit<sup>1</sup>; L. L. Wong<sup>1</sup>; N. Shen<sup>1</sup>; R. J. Dylla-Spears<sup>1</sup>; P. E. Miller<sup>1</sup>; R. P. Desjardin<sup>1</sup>; S. Elhadj<sup>1</sup>; I. Lawrence Livermore National Laboratory, USA

Glass optics with ultra-low roughness surfaces ( $<2 \text{ \AA}$  level rms) are strongly desired for high end optical applications. The complex microscopic interactions between slurry particles and the workpiece during optical polishing ultimately determine the resulting surface roughness and removal rate of the polished workpiece. In this study, a series of 100 mm diameter glass samples (fused silica,

phosphate, and borosilicate) were polished using various slurries on various polyurethane pads. Using an expanded Hertzian contact model, called the Ensemble Hertzian Multi-gap (EHMG) model, a platform has been developed to predict trends of both the resulting polished surface roughness and removal rate for a wide variety of polishing parameters. The mechanism of material removal for a given slurry particle is proposed to occur via nano-plastic deformation or via molecular removal by chemical reaction depending on the load per particle. The results show that the dominant factor controlling surface roughness is the particle size distribution followed by removal function of the glass and pad topology. Each of the key polishing parameters is shown to affect the material removal rate and roughness whose changes are dominated by very different microscopic interactions.

**4:40 PM****(GOMD-S1-117-2016) Void Structure and Mechanical Properties of Corona-Discharged Glasses**M. Ono<sup>\*1</sup>; K. Uraji<sup>1</sup>; T. Sekine<sup>1</sup>; T. Suzuki<sup>1</sup>; K. Ito<sup>2</sup>; M. Miyai<sup>3</sup>; M. Fujinami<sup>3</sup>; S. Ito<sup>1</sup>; 1. Asahi Glass Company, Japan; 2. National Institute of Advanced Industrial Science and Technology (AIST), Japan; 3. Chiba University, Japan

Corona-discharge treatment is known as a useful tool for surface modification of glasses, such as, nano-imprinting and selective etching, etc. Under corona-discharge electric field, alkali depletion surface layer forms in glass, and proton is introduced into the vacancy of alkali ion and hydroxyl group generates. To understand the structure of the alkali depletion layer in alkali-aluminosilicate glasses, we used the pulsed variable-energy positron beam to determine the size of void, which is open space of glass network, from the positron lifetime. Before the corona-discharge treatment, the observed void size was independent of the type of alkali ion and depended only on the alkali content. However, after the corona-discharge treatment, the size of void observed in the alkali depletion layer increased depending on the type and the content of alkali ions. The sizes of the voids in the depletion layer for potassium-containing glasses were about 0.54 nm in diameter and were larger than those (about 0.46 nm) for sodium-containing glasses. Using a Vikers nano-indenter, the mechanical behavior of the alkali depletion layer was investigated. The deformation and the recovery behaviors, respectively, during loading and unloading depended strongly on the size of voids in the layer. We will discuss the effect of the void structure on mechanical properties.

**5:00 PM****(GOMD-S1-118-2016) Effect of salt impurities on the chemical strengthening of float glass by ion-exchange**V. M. Sglavo<sup>\*1</sup>; H. Hassani<sup>1</sup>; 1. University of Trento, Italy

During the chemical strengthening of float glass by ion-exchange sodium atoms in the glass are substituted by potassium ions diffusing from the salt. An interesting aspect regards the poisoning/deactivation of the bath after each process and its enrichment in sodium or even additional impurities. In the present work, the effect of variable sodium concentration in the bath and of typical impurities present in commercial  $\text{KNO}_3$  on the performances of the strengthened float glass was analyzed. The ion-exchanged glass was analyzed from a mechanical and chemical point of view; the salt composition was studied in detail as well. The results point out that the residual stress decreases as a function of the sodium content within the bath; the same is for the potassium surface concentration potassium and the flexural strength. The presence of some specific impurities like Ca and  $\text{H}_2\text{O}$  also appear to be detrimental for the ion-exchange efficiency.

\*Denotes Presenter

5:20 PM

## (GOMD-S1-119-2016) Sequential Electric Field Assisted Ion Exchange: Engineered Stress Profile Glasses

A. Talimian<sup>\*1</sup>; V. M. Sglavo<sup>1</sup>; I. Università degli Studio di Trento, Italy

In the present work, engineered stress profile glasses were produced by sequentially subjecting borosilicate and soda lime silicate glass tubes to electric field assisted caesium-sodium and potassium-sodium ion exchange processes. Electric fields with intensities between 1000 to 4000 V/cm were applied to the tubes immersed in the molten salts. The current density was continuously monitored and controlled to avoid the formation of sparks surrounding the electrodes. The chemical concentration profiles beneath the glass surface were checked by energy dispersive X-ray spectroscopy. Higher intensities are required to send caesium into glass comparing with potassium. The resistivity of the glass was increased by introducing new alkali cation into the parent glasses. FTIR spectra show structural changes, know as cation induced relaxation of the network, might cause the higher resistivity instead of the mixed alkali effect. Desired stress profiles were produced by the optimisation of the parameters to get the designed chemical concentration profiles. Vickers' indentations and bending tests were employed to check the changes in strength, cracking threshold, shear cracking and densification under load. Samples with engineered stress profiles containing potassium and caesium layers showed multiple cracking and a bending strengths as high as one step electric field assisted ion exchanged glasses.

## Session 6: Chalcogenide Glasses I

Room: Senate A/B

Session Chair: Pierre Lucas, Univ of Arizona

1:20 PM

## (GOMD-S1-120-2016) Ga-Sb-S Chalcogenide Glasses and Their Applications in the Mid-infrared (Invited)

Z. Yang<sup>\*1</sup>; A. Yang<sup>1</sup>; M. Zhang<sup>1</sup>; J. Qiu<sup>1</sup>; L. Li<sup>1</sup>; Y. Wang<sup>1</sup>; B. Zhang<sup>1</sup>; D. Tang<sup>1</sup>; I. Jiangsu Normal University, China

Chalcogenide glasses have wide infrared (IR) transparent windows, high linear and nonlinear refractive indices, and low phonon energies, and therefore have received extensive studies in IR optics, nonlinear optics and IR lasers. In this study, a new chalcogenide glass system, Ga-Sb-S, was developed. The glasses have a wide transparent window of ~0.8-14 $\mu$ m, high linear refractive indices of ~2.62-2.70 (@10  $\mu$ m), high third-order nonlinear refractive indices of ~12.4 $\times 10^{-14}$  cm<sup>2</sup>/W (@ 1.55  $\mu$ m), low effective phonon energies of around 306cm<sup>-1</sup>, and large rare earth (RE) solubility. These properties make them promising materials for mid-infrared applications such as thermal imaging, nonlinear optics, and amplifiers or lasers. Surface crystallization was observed when the most thermally stable glass (e.g. Ga<sub>8</sub>Sb<sub>32</sub>S<sub>60</sub>) in the Ga-Sb-S system was drawn into fibers. A small amount of arsenic was added to improve the glass thermal stability against crystallization. Based on the optimized composition, RE doped fibers and step-index fibers were fabricated. Mid-IR emissions of the former and supercontinuum generation in the latter were investigated.

1:50 PM

## (GOMD-S1-121-2016) Statistics of Selenium Chain Length Distribution in Ge<sub>x</sub>Se<sub>100-x</sub> glassy alloys: Unique Insights from NMR spectroscopy

D. C. Kaseman<sup>\*1</sup>; S. Sen<sup>1</sup>; I. University of California Davis, USA

Chalcogenide glasses constitute an important class of materials with technological applications in areas ranging from infrared photonics and telecommunication to non-volatile phase change memory as well as in electrochemical devices as solid electrolytes and chemical sensors. An extensive understanding of the structure-property relationships is required in order to optimize the performance of these

glasses for the various applications. To this end, we have used a novel high-resolution, two-dimensional <sup>77</sup>Se nuclear magnetic resonance (NMR) spectroscopic technique to unambiguously identify and quantitate selenium chain environments in germanium selenide glasses. Subtle but systematic changes in NMR parameters are related to the effects of next-nearest neighbors in -Se-Se-Se- chain environments. Simulations of the experimental data indicate that the selenium chain length distribution follows closely the Flory-Schulz distribution originally developed for modeling chain length distribution in organic polymers. The implications of this important finding could be far reaching in understanding the physical nature of configurational entropy and its role in viscous flow and glass transition in these model chalcogenide glass-forming systems.

2:10 PM

## (GOMD-S1-122-2016) Relying on localized orbitals to understand structural features in chalcogenide glasses

A. Bouzid<sup>\*1</sup>; G. Ori<sup>1</sup>; M. Boero<sup>1</sup>; C. Massobrio<sup>1</sup>; I. Institut de physique et chimie des matériaux de Strasbourg, France

The structure of chalcogenide glasses has long been the object of intense debate, due to the delicate interplay between a predominant structural motif (as the tetrahedron for the GexSe(1-x) family) and the presence of composition dependent homopolar bonds and other structural defects. The question arises on the establishment of correlation between bonding properties and topological features, leading to a characterization of these glassy systems in terms of simple, and yet profound concepts, such as ionicity and covalency. In this contribution, we take advantage of a well recognized set of first-principles molecular dynamics results obtained on a large variety of chalcogenide glasses to demonstrate the delicate interplay existing between chemical composition and electronic structure properties. The key ingredient of such rationale is the use of the Wannier localized orbitals formalism. This formalism is capable of associating, to each set of degrees of freedom (and for a given theoretical framework), a "twin" system composed of virtual degrees of freedom (the Wannier centers) reflecting the localization of the valence electron densities. Analysis of the correlations between the atomic positions and the Wannier centers proved insightful to describe the bonding features of chalcogenide glasses.

2:30 PM

## (GOMD-S1-123-2016) Synthesis and Characterization of Cs<sup>+</sup> Ion Conducting Gallo-Germanium Selenide Glasses

A. Whale<sup>\*1</sup>; S. W. Martin<sup>1</sup>; I. Iowa State University, USA

The current glass system under study is xCsI + (1-x)[yGeSe<sub>2</sub>+(1-y)Ga<sub>2</sub>Se<sub>3</sub>]. Samples are synthesized using sealed quartz ampules in a rocking furnace for 24 hours then transferred to an annealer to reduce internal stresses. Since these glasses will primarily be used for Cs<sup>+</sup> ion conduction, they will be characterized using differential scanning calorimetry (DSC), Raman spectroscopy, and Fourier transform infrared spectroscopy (FTIR), with an emphasis on ionic conductivity. Results have shown higher conductivities in phase separated samples (crystallites <10%) than in either completely glassy or crystalline samples.

2:50 PM

## (GOMD-S1-124-2016) The Mixed Glass Former Effect in Glassy Solid State Electrolytes: The Physical Properties of the 0.5Na<sub>2</sub>S + 0.5[xSiS<sub>2</sub> + (1-x)PS<sub>5/2</sub>] glass system

D. Watson<sup>\*1</sup>; S. W. Martin<sup>1</sup>; I. Iowa State University, USA

The Mixed Glass Former Effect (MGFE) has been studied in the 0.5Na<sub>2</sub>S + 0.5[xSiS<sub>2</sub> + (1-x)PS<sub>5/2</sub>] glass system. When the modifier concentration is held constant, a nonlinear, non-additive trend in the physical properties is observed when the composition is varied from one binary glass end member to another. Extensive structural analysis has been done via <sup>29</sup>Si and <sup>31</sup>P MAS NMR, Raman and IR spectroscopies, which showed the propensity of the phosphorus



glass former to be the most modified in high and low concentration and silicon glass former to be the primary source of networking capability in the glass due to the presence of  $\text{Si}^2$  and  $\text{Si}^3$  units. The MGFE can be observed in the glass transition temperatures and densities as a function of composition. In this paper, these results will be discussed, showing how understanding of the network connectivity drawn from the glass transition temperatures and the packing fraction from densities can inform the overall structural model of the system.

## Session 6: Chalcogenide Glasses II

Room: Senate A/B

Session Chair: Pierre Lucas, Univ of Arizona

### 3:40 PM

#### (GOMD-S1-125-2016) Structure of binary Si-Se alloys: Results from one- and two-dimensional $^{29}\text{Si}$ and $^{77}\text{Se}$ NMR spectroscopy

M. A. Marple<sup>\*1</sup>; I. Hung<sup>2</sup>; Z. Gan<sup>2</sup>; S. Sen<sup>1</sup>; 1. University of California Davis, USA; 2. National High Magnetic Field Laboratory, USA

A wide range of inorganic glasses are characterized by predominantly corner-sharing tetrahedral networks, these include oxides such as  $\text{SiO}_2$  and  $\text{GeO}_2$ , halides such as  $\text{BeF}_2$  and  $\text{ZnCl}_2$  and chalcogenides such as  $\text{GeSe}_2$ . In contrast, amorphous  $\text{SiSe}_2$  is characterized by three different types of tetrahedral environments which are (i) entirely corner-sharing and (ii) singly and (iii) doubly edge-sharing. The relative fractions of these environments are known to be composition dependent in binary  $\text{Si}_x\text{Se}_{100-x}$  glasses, although their quantitative variation remains poorly constrained at best. Moreover, the degree of randomness in the connectivity between the Se-Se chain and the  $\text{SiSe}_4$  tetrahedral units in these glasses remains largely unknown to date. We have investigated the structural speciation and local site symmetry of  $\text{Si}_x\text{Se}_{100-x}$  glasses with Se contents ranging between 67 and 95 atom% using two-dimensional  $^{29}\text{Si}$  and  $^{77}\text{Se}$  MATPASS/CPMG NMR spectroscopy. The results provide important constraints on the compositional variation of Se and Si speciation and connectivity between the chain and tetrahedral units. The topological and entropic implications of this structural evolution and its connection with glass transition and fragility will be discussed.

### 4:00 PM

#### (GOMD-S1-126-2016) Thermophysical Properties of $\text{As}_x\text{Se}_{1-x}$ Glasses from $x=0.2$ to $0.5$

J. M. Lonergan<sup>\*1</sup>; C. Smith<sup>1</sup>; D. McClane<sup>1</sup>; K. Richardson<sup>1</sup>; 1. University of Central Florida, USA

The effect of varying the arsenic (As) to selenium (Se) ratio on the thermal properties of arsenic selenide glasses was studied. Glass transition temperature ( $T_g$ ), thermal conductivity ( $k$ ), and heat capacity ( $C_p$ ) were experimentally measured. Inflections in glass transition temperature ( $T_g$ ) and thermal conductivity ( $k$ ) were found at the structural coordination number ( $r$ ) of 2.4, whereas no discernible trend could be determined for heat capacity ( $C_p$ ). A maximum in total thermal conductivity of  $0.218 \text{ W/m}\cdot\text{K}$  was measured for the composition with 40 at% As. Gas kinetic theory was used to derive an expression for the photonic ( $k_p$ ) portion of thermal conductivity, which was calculated by measurements of absorption coefficient ( $\alpha$ ) and refractive index ( $n$ ). The maximum value for  $k_p$  was  $0.106 \text{ W/m}\cdot\text{K}$  for the glasses with 20 at% As and a minimum value of  $0.074 \text{ W/m}\cdot\text{K}$  was measured for the glasses with 50 at% As. These measurements indicate that no less than 40% of the thermal conductivity was due to photonic transport mechanisms. The fundamental thermal properties and transport mechanisms in arsenic selenide glass will be discussed.

## Session 7: Response of Glass to Extreme Conditions

Room: Madison

Session Chair: Randall Youngman, Corning Incorporated

### 1:20 PM

#### (GOMD-S1-127-2016) Elastic Deformations and Structural Metrics in Chain-Like Amorphous Polymers (Invited)

A. Bielawski<sup>1</sup>; E. Woeldgen<sup>1</sup>; J. Kieffer<sup>\*1</sup>; 1. University Of Michigan, USA

When subject to tensile stress, amorphous organic polymers can undergo extreme elongations, up to several times their original lengths, which is possible due to the ability of the material to undergo significant structural rearrangements. Such strain-induced rearrangements are typically associated with a reduction in the number of achievable structural configurations, i.e., a decrease in configurational entropy. A simple interpretation can be given based on the requirement for polymer chains to be more aligned under strain compared the zero-pressure configuration. In this respect organic polymers may provide a more sensitive model substance for the investigation of the amorphous state of matter. Here we report on an attempt to measure the isothermal and adiabatic elastic modulus of chain-like polymers concurrently, revealing the difference between the heat capacities at constant volume and constant pressure, which in turn provides information about the volume dependence of the system entropy. We discuss new insights to be gained using the results for poly-vinylidene fluoride, an electro-active polymer, which also exhibits strong anisotropy relative to the orientation of the dipole moment of the polymer chain.

### 1:50 PM

#### (GOMD-S1-128-2016) Control of stability and molecular orientation in organic glasses (Invited)

M. D. Ediger<sup>\*1</sup>; 1. University of Wisconsin-Madison, USA

We have used physical vapor deposition and the mobility of glassy surfaces to prepare what are likely the most kinetically stable glasses on the planet, in comparison to a liquid-cooled glass of the same composition. Our materials have the properties expected for "million-year-old" glasses, including high density, low enthalpy, high mechanical moduli, and low vapor uptake. We have discovered deposition conditions that combine high stability with substantial molecular orientation. We have used computer simulations to understand why some deposition conditions orient molecules vertically and others orient them horizontally. These developments present major opportunities to expand our understanding of amorphous packing and to design new classes of anisotropic solids for applications such as organic electronics.

### 2:20 PM

#### (GOMD-S1-129-2016) Annealing Effects in Sodium Silicate Glass around glass transition temperature and heterogeneous dynamics

Y. P. Vaills<sup>\*1</sup>; M. Naji<sup>2</sup>; 1. CEMHTI - CNRS, France; 2. Institute for Transuranium Elements, Germany

We evidenced the heterogeneous dynamics of the structural relaxation in a binary oxide glass. The in-situ Brillouin and Raman measurements depicted in this work evidence a novel and very promising way to follow the relaxation dynamics of glasses over various distances. The central result of our study is a direct experimental account of heterogeneous dynamics near the glass transition in a strong glass former sodium silicate at the intermediate range order: Two well distinct relaxation channels were identified, involving a slow and a fast process. At the short-range order, Raman spectroscopic measurements in  $(\text{Na}_2\text{O})_{0.27}(\text{SiO}_2)_{0.73}$  revealed a homogeneous relaxation near  $T_g$ . The fast relaxation time scale determined from BLS measurements is of the same order as relaxation dynamics corresponding to local rearrangements of  $\text{Q}_2$  species, while the slow relaxation dynamics occurs at the same time scale as the Si-O-Si bending vibration observed in silica around the glass transition.

2:40 PM

### (GOMD-S1-130-2016) Anomalies in Aging Behaviors of Supercooled Sodium Silicate Liquid under Pressure

D. Zhang<sup>1</sup>; B. Wang<sup>\*1</sup>; M. Bauchy<sup>1</sup>; 1. University of California, Los Angeles, USA

The aging behavior of supercooled sodium silicate liquid is studied with molecular dynamics simulations. A distinct pressure window is identified, within which the liquid shows minimal aging. This is found to be linked with anomalies in the transport properties, and coincides with a rigidity transition window analogue to the intermediate phase in composition-driven rigidity. Results show such a transition arises from the combination of thermally activated broken constraints and enhanced network connectivity under pressure, which contributes to the anomalies in the frequency and correlation of diffusion jumps.

3:00 PM

### (GOMD-S1-131-2016) Thermophysical Properties of Aerolevitated Glasses

I. Sorenson<sup>\*1</sup>; B. Bailey<sup>1</sup>; M. Welninski<sup>1</sup>; S. Feller<sup>1</sup>; M. Affatigato<sup>1</sup>; 1. Coe College, USA

We present ongoing analysis of the thermophysical properties of liquid alumina, calcium aluminate, and calcium silicate, specifically surface tension, viscosity, and density. Glasses were processed using an MDI aerodynamic levitation furnace using high purity reactants and reagents, with data collected high-speed camera and a pyrometer synced with LabView Rio<sup>®</sup>. To determine surface tension and viscosity, beads of molten glass were oscillated using a frequency generator and motions were later followed by Tracker software. A simple Fourier transform was applied to the motion data to determine the resonance frequency and thus calculate the surface tension. Oscillations were allowed to decay to determine the viscosity of the melt. Video frames of non-oscillated glass were analyzed using ImageJ<sup>®</sup> software to calculate radii and thus volume and density while the bead free-cooled. Calcium aluminate results were compared to those of Kargyl et. al. and Kumar et. al. under similar conditions. This research was supported by the National Science Foundation under grants DMR-MRI-0922924, DMR-RUI 1407404, and Coe College.

## Session 7: Characterization of Glass under Extreme Conditions I

Room: Madison

Session Chair: Yann Vaills, CNRS-CEMHTI

3:40 PM

### (GOMD-S1-132-2016) Raman scattering in extreme conditions of high temperature and irradiation (Invited)

P. Simon<sup>\*1</sup>; E. Fotso Gueutue<sup>1</sup>; A. Canizares<sup>1</sup>; M. Ammar<sup>1</sup>; F. Duval<sup>1</sup>; Y. P. Vaills<sup>1</sup>; N. Raimboux<sup>1</sup>; M. Dutreilh-Colas<sup>2</sup>; R. Mohun<sup>3</sup>; L. Desgranges<sup>3</sup>; C. Jegou<sup>4</sup>; 1. CNRS-CEMHTI, France; 2. CNRS—Univ. Limoges-SPCTS, France; 3. CEA/DEN/DEC, France; 4. CEA/DEN/DTCD, France

Raman scattering spectroscopy is well-known to be a powerful method for investigating matter under its various states, solid, liquid or gaseous. For high temperatures, the limitation comes from thermal emission of the sample and its environment, precluding recording of Raman data above about 700-1200°C depending on the laser wavelength and the sample properties (emissivity and Raman cross-section). Nevertheless, for higher temperatures, Raman scattering remains operational, owing to specific techniques such as UV excitation or time-resolved methods. In this talk, a detailed description of a time-resolved Raman setup will be given, with recent applications on some oxide materials: silicas with examples of structural relaxation monitoring around T<sub>g</sub>, and at higher temperatures, ceramics such as zirconia up to the vicinity of 2000°C, potentially accessing their molten state for some of them. In a second part,

another type of extreme environment will be reviewed: monitoring of damage under a particle beam, such as He<sup>2+</sup>, supplied by an accelerator facility. In situ Raman scattering allows accessing the irradiation-induced damage mechanisms and their kinetics. This will be illustrated by recent results on oxide ceramics of major interest in nuclear applications, such as uranium oxide and related compounds.

4:10 PM

### (GOMD-S1-133-2016) Temperature driven structural changes between oxide glasses and melts (Invited)

L. Cormier<sup>\*1</sup>; G. Lelong<sup>1</sup>; L. Hennet<sup>2</sup>; 1. UPMC - CNRS, France; 2. CNRS, UPR 3049, France

The temperature driven structural changes of oxide glasses and melts affect transport properties such as diffusion, conductivity and viscosity. Standard electrical furnaces can be used to probe these changes by using neutron/X-ray diffraction or, alternatively, aerodynamic levitation techniques with laser heating have been developed. Such techniques have also been implemented for NRXIS, also called X-ray Raman, which is a growing synchrotron spectroscopy that probes low energy absorption edges through the use of high-energy incident X-rays, allowing extreme environments. The structural changes between the glass and the melt are often subtle because they affect the medium range order, particularly in silicate glasses/melts. For borate glasses, a peculiar behavior is observed at short range order corresponding to a partial boron coordination change as temperature increases. We will present examples of diffraction and NRXIS experiments that highlight the great potentiality for in situ structural characterization at high temperatures in multicomponent oxide glasses/melts. These experimental data are usefully complemented by simulations (Reverse Monte Carlo, Molecular Dynamics, ab initio calculations) to provide structural models from data and deeper understanding of the structure.

4:40 PM

### (GOMD-S1-134-2016) Laser shock-induced spall and the intrinsic strength of glass

M. J. Davis<sup>\*1</sup>; 1. SCHOTT North America, Inc., USA

This study presents high strain-rate (~10<sup>7</sup> sec<sup>-1</sup>), spall-threshold results obtained via laser shock testing on three glasses of commercial significance (fused silica, soda-lime “float” glass, and a borosilicate). Whereas the measured spall thresholds (1-2 GPa, accounting for wave attenuation) agree reasonably well with conventional, flyer-plate shock wave experiments, they are 5-10 times lower than “intrinsic” strength values obtained from quasi-static tests. It is speculated that the rapid compress/decompress loading cycle associated with tensile waves arising from free-surface reflection was the cause. Attenuation effects associated with the ramp-wave inherent to glasses of this study was the likely basis for the difference in spall threshold between 2- and 3-mm thick glass samples. Long-pulse tests (185 nsec) with lower peak stresses were decidedly more damaging than those using short pulses (10 nsec) but with higher peak stresses. Finally, a surprisingly good correlation in stress-strain relations for fused silica between that obtained via quasi-static techniques and flyer-plate testing likely arises from a lack of irreversible processes and minimal heating during compression up to 9 GPa. While the presence of transverse stresses is unavoidable for flyer-plate tests, the low Poisson ratio of fused silica should minimize these stresses.

5:00 PM

### (GOMD-S1-135-2016) High Temperature Chalcogenide Glasses for Infrared Fiber Sensing in Advanced Small Modular Reactors

J. Roth<sup>\*1</sup>; S. W. Martin<sup>1</sup>; J. Ballato<sup>3</sup>; A. Qiao<sup>2</sup>; 1. Iowa State University, USA; 2. Pacific Northwest National Lab, USA; 3. Clemson University, USA

Non-oxide glasses have been of increasing importance in many fields. One unique interest is the use of chalcogenide based infrared fibers to probe the health of next generation nuclear reactors. If high temperature infrared fiber can be designed then new safety layers

can be added to these reactors by allowing technicians to probe the molecular fingerprint region of the spectrum to find trace amounts of unfavorable compounds inside the reactor. Unfortunately, current infrared sensing technology such as  $As_2Se_3$  fibers cannot be used as the cooling liquid for these new reactors melt at about the same temperature as the glass,  $360^\circ C$ . This study investigates families of ionic based glasses, such as the  $BaS + La_2S_3 + GeS_2$  system, to help create a more thermally stable infrared fiber that can be used continuously above  $600^\circ C$ . These sulfide based glasses prove to be a compromise between selenide and oxide glasses with their moderate glass transition temperatures and infrared transparency.

5:20 PM

**(GOMD-S1-136-2016) Assessment of gravelling impact phenomenon on helicopter glass windshields**

G. Langevin<sup>1</sup>; J. Sangleboeuf<sup>2</sup>; 1. University of Rennes 1, France; 2. Airbus Helicopters, France

Glasses can be subjected to various kinds of impacts on duty, which may alter their mechanical properties. In the specific case of helicopter windshields, this phenomenon is called gravelling: ground particles around the rotorcraft take off due to the local air flow and impact the windshields, creating characteristic patterns. The objectives of this work are to link: - the impact conditions (projectile-related as well as impacted material-related) to the damage topology, in order to be able to determine retrospectively what could have been the conditions leading to a given superficial damage; - the damage topology to the residual mechanical strength of the material. The aim here is to be able to predict future macroscopic alterations of the windshields, namely crack growth. An impact test protocol has been developed in order to reproduce gravelling damage in lab conditions, as well as finite elements models so as to reproduce the post-impact behavior of the glass and benchmark other potential windshield materials.

**Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications**

**Session 5: Glass-Ceramics and Optical Ceramics I**

Room: University C/D

Session Chair: HeeDong Lee, UES, Inc.

3:40 PM

**(GOMD-S3-031-2016) Challenges Towards Transparent Oxide Ceramics (Invited)**

H. Lee<sup>1</sup>; 1. UES, Inc., USA

The demands of high quality, transparent ceramics are urgent for various tactical and commercial applications such as lasers, LEDs, I.R. windows, etc. The transparent ceramics have many advantages over single crystals because of cost effectiveness and less technical restrictions for production. However, the production of optical quality, transparent ceramics appears to be a great challenge, and hinged on an availability of highly sinterable powder with high phase purity, as well as high chemical purity, along with advanced ceramic processing technologies. These fundamental technologies have been explored, and various transparent oxide ceramics including YAG,  $Y_2O_3$ ,  $Lu_2O_3$ , spinel, and ALON with a high optical quality were successfully demonstrated. The results, along with the technical challenges and issues, will be presented/discussed during presentation.

4:10 PM

**(GOMD-S3-032-2016) Toughening of Transparent Magnesium Aluminate Spinel by Dissolution/Precipitation of Alumina (Invited)**

A. Miller<sup>1</sup>; W. Miao<sup>2</sup>; I. Reimanis<sup>1</sup>; 1. Colorado School of Mines, USA; 2. Corning, Incorporated, USA

Magnesium aluminate spinel, a transparent ceramic for windows, domes, and armor applications, can be made harder and tougher via utilizing non-stoichiometric compositions. The present work examines the kinetics of precipitation and dissolution of alumina in spinel and the subsequent effect on mechanical and optical properties. Both dissolution and precipitation are controlled by the concentration of oxygen vacancies present in the spinel which is dependent on the temperature and partial pressure of oxygen. Systematic studies were performed with transparent spinel ( $MgO \ nAl_2O_3$ ) with  $n$  equal to either 1 or 2. Fracture toughness may be doubled with the appropriate heat treatment, but transmissivity is correspondingly sacrificed due to the microstructure modification. The potential to achieve an optimum combination of transmission and mechanical behavior is discussed.

4:40 PM

**(GOMD-S3-033-2016) Effect of Surface Roughness of Polycrystalline Ceramic Fiber on Scattering Loss**

H. Kim<sup>1</sup>; N. Usechak<sup>2</sup>; A. M. Urbas<sup>2</sup>; K. N. Shugart<sup>1</sup>; D. P. Brown<sup>1</sup>; B. Griffin<sup>1</sup>; R. S. Hay<sup>2</sup>; 1. AFRL & UES, USA; 2. Air Force Research Lab, USA

Transparent polycrystalline ceramics are attracting a lot of attention as laser gain media because of their superior thermal and optical properties over current glass-based gain media. In addition, fibers provide numerous advantages such as compactness, vibration-resistance, and reduced cooling requirements. Transparent polycrystalline ceramic fibers take advantages of both thermal and optical properties of ceramics and fibers. We have been developing polycrystalline yttrium aluminum garnet (YAG) fibers for optical applications. Recently it was found that surface roughness caused by grain boundary grooving in polycrystalline ceramic fiber dominates optical scattering. The surface roughness of the fiber was successfully reduced by polishing, while maintaining a circular cross section. The relationship between surface roughness and scattering loss of polycrystalline ceramic fibers will be discussed.

5:00 PM

**(GOMD-S3-034-2016) Study on Sintering of Calcium Fluoride Transparent Optical Materials**

V. Veerapandian<sup>1</sup>; Y. Li<sup>1</sup>; Y. Wu<sup>1</sup>; 1. Alfred University, USA

A study on the sintering of calcium fluoride ( $CaF_2$ ) transparent ceramics was performed to understand the densification mechanisms associated with different  $CaF_2$  powders.  $CaF_2$  nanopowders were synthesized by using a wet chemical precipitation route to compare with the commercial powders. The phase compositions and microstructural features of the powders and as-sintered ceramics were analysed and discussed to investigate the influences of different  $CaF_2$  powders on the sintering characteristics of  $CaF_2$  optical ceramics. Optical characterizations of as-sintered  $CaF_2$  transparent ceramics were conducted to achieve a better understanding on the correlations between the phases, microstructures and properties. In addition, the functions of sintering aids were investigated to understand their influences on the consolidation and properties of  $CaF_2$  optical ceramics.

Thursday, May 26, 2016

## Varshneya Frontiers of Glass Technology Lecture

Room: Madison

8:00 AM

### (GOMD-AW-005-2016) Chemically Strengthened Glasses and Glass-Ceramics (Invited)

M. Dejneka<sup>\*1</sup>; 1. Corning Incorporated, USA

Glass is scratch resistant, strong, and chemically durable, making it ideal for touch screens and covers for displays. Unfortunately, the strength of most glasses can be quickly degraded to less than 1% of its theoretical strength by handling due to the introduction of flaws which act as stress concentrators. We developed fusion formable glasses that can be ion exchanged to 800MPa compressive stress on the surface and achieve 50 microns depth of compression which better retain the strength of the pristine fusion surface after handling and use. We then discovered glasses with intrinsically superior damage resistance that withstood even greater loads before flaws could be introduced. These glasses have now been used to help protect more than 4.5 billion devices worldwide. Finally, we made the first fusion formable glass-ceramics and devised methods to pattern them without sacrificing strength.

## Symposium 1: Fundamentals of the Glassy State

### Session 2: Glass-Ceramics

Room: Capitol A

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

9:20 AM

### (GOMD-S1-137-2016) Glass ceramics as high temperature stable oxide thermoelectric materials (Invited)

M. Letz<sup>\*1</sup>; J. Lingner<sup>1</sup>; 1. SCHOTT AG, Germany

Semiconducting properties can be obtained in oxide glass ceramics which leads to the advantage of pore free materials with good stability to high temperature thermal cycling. In this way thermoelectric materials can be obtained which convert waste heat into electrical power and which are very stable in oxide atmosphere for temperatures up to 750 °C. As an example we present results of two glass ceramic systems. For an electron doped (n-doped) system we use a glass ceramic system which is in the field of crystallization of SrTiO<sub>3</sub> which is doped with Niobium and oxygen vacancies. For a hole doped (p-doped) system we investigate the Bi<sub>2</sub>Sr<sub>2</sub>Co<sub>2</sub>O<sub>x</sub> system. While the nanocrystalline structure of a glass ceramic gives low thermal conductivity together with large absolute values of the Seebeck coefficient, an improvement of the thermoelectric properties maximising the electric conductivity is the most challenging development target. The electronic conductivity  $\sigma$  is dominated by a percolating network of nano-grain crystals. In the present work we present material properties of different p- and n-doped glass ceramic and ceramic materials including thermal cycling in oxygen atmosphere up to 750 °C and show the performance of a test module with an electric power of 140 mW out of an area of 0.01 m<sup>2</sup> at a temperature of 700 °C on the high temperature site.

9:50 AM

### (GOMD-S1-138-2016) Strong and Tough Glass-ceramics for Emerging Markets (Invited)

Q. Fu<sup>\*1</sup>; G. Beall<sup>1</sup>; C. Smith<sup>1</sup>; R. Youngman<sup>1</sup>; B. Wheaton<sup>1</sup>; O. Gulbitten<sup>1</sup>; 1. Corning Incorporated, USA

Glass-ceramics have attracted significant interest in emerging markets such as consumer electronic products and biomedical devices. A combination of color, opacity, strength and toughness is

usually required for these new applications. Innovations in structural design at micro and macro levels, and compositional design in various glass-ceramic families, are critical to produce glass-ceramics that can meet these stringent requirements. At Corning Incorporated, advanced characterization tools like high-temperature X-ray diffraction (HTXRD), nuclear magnetic resonance (NMR) and automatic viscosity control (AVC) have been found important to the fundamental understanding of the crystallization mechanisms, microstructure control and near-net-shape ceramming of glass-ceramics. Meanwhile, compositional exploration has enabled the discoveries of novel transparent, colored, high toughness, and native-crack resistance glass-ceramics. All of these accomplishments have opened new avenues for the applications of glass-ceramics, suggesting a bright future for this material family.

10:20 AM

### (GOMD-S1-139-2016) Microstructural Evolution of Conductive WTi Phosphate Glass-Ceramics

B. Aitken<sup>\*1</sup>; L. Moore<sup>1</sup>; I. Dutta<sup>1</sup>; 1. Corning Incorporated, USA

WTi phosphate glass-ceramics were previously reported as displaying good electrical conductivity, with the latter enabled by a microstructure of apparently connected WO<sub>3-x</sub> crystallites. The electrical properties of these materials show a strong dependence on composition as well as ceram temperature and time. In order to correlate the property-process dependence with phase assemblage and microstructure, glass-ceramics from the WO<sub>3</sub>-TiP<sub>2</sub>O<sub>7</sub> join were studied by X-ray diffraction and electron microscopy. In addition, electrical and thermal conductivity, as well as Seebeck coefficient, were measured in order to evaluate the thermoelectric potential of these materials. Precursor glasses were made by melting batches comprised of WO<sub>3</sub>, TiO<sub>2</sub> and NH<sub>4</sub>H<sub>2</sub>PO<sub>4</sub> in silica crucibles. The latter were heat treated for 0.5-16 hr in N<sub>2</sub> with peak temperatures of 850-1050°C. When cerammed at lower temperature, these glass-ceramics contain internally-nucleated equant cubic WO<sub>3</sub> nanocrystals embedded in an amorphous Ti- and P-rich glassy matrix. Glass-ceramics made at higher top temperature are mostly crystalline, have higher electrical conductivity and are characterized by an intergrowth of prismatic ~1mm crystals of W<sub>7</sub>[PO<sub>4</sub>]<sub>2</sub>O<sub>17</sub> and two Ti phosphates. The greater conductivity and superior thermoelectric properties of the higher temperature materials are attributed in part to the conversion of WO<sub>3</sub> into a phosphorus tungsten bronze.

10:40 AM

### (GOMD-S1-140-2016) Synthesis of afterglow glass-ceramics with SrAl<sub>2</sub>O<sub>4</sub> from SrO-Al<sub>2</sub>O<sub>3</sub> supercooling melt

K. Shinozaki<sup>\*1</sup>; M. Kotaka<sup>1</sup>; T. Honma<sup>1</sup>; M. Affatigato<sup>2</sup>; T. Komatsu<sup>1</sup>; 1. Nagaoka University of Technology, Japan; 2. Coe College, USA

Eu<sup>2+</sup>, Dy<sup>3+</sup>-codoped SrAl<sub>2</sub>O<sub>4</sub>, well-known as a very bright long-lasting afterglow material, has been widely used for luminous paints in emergency lights, watches and so on. Usually, decay time of rare earth is us to ms order, on the other hand, Eu<sup>2+</sup> in SrAl<sub>2</sub>O<sub>4</sub> glows several hour. It has been pointed out that its long duration is caused by the existence of suitable charge traps in crystal, e.g., defects and incorporation of dopants. In this paper, we focused on the impact of synthesis paths on the afterglow. SrAl<sub>2</sub>O<sub>4</sub>; Eu<sup>2+</sup>, Dy<sup>3+</sup> glass-ceramics were synthesized via two different paths; (1) heat-treatments on precursor glasses in an electric furnace (conventional crystallization technique) and (2) crystallization of super-cooling melt during melt-cooling process, where the precursor glasses and supercooling melt were obtained using a gas levitation technique, which allows melting in non-contact process and inhibits nucleation in supercooling melts. Afterglow in the glass-ceramics was much affected from not only composition, but also synthesis paths, i.e., glass-ceramics synthesized through cooling process exhibits much longer duration time compared to heat-treated glasses and ceramics obtained by a solid-state reaction. We also investigated on the impact of addition of B<sub>2</sub>O<sub>3</sub> on the structure of crystal and the emission property.

11:00 AM

**(GOMD-S1-141-2016) Formation of  $\text{Li}_{1+x}\text{M}_x\text{Ge}_y\text{Ti}_{2-x-y}(\text{PO}_4)_3$  glasses with NZP stoichiometry and Li-ion conductivity of corresponding glass-ceramics**N. Lonnroth<sup>\*1</sup>; B. Aitken<sup>1</sup>; I. Corning Incorporated, USA

Lithium containing ceramics of NZP structure, such as LATP and LAGP have been extensively studied and are promising solid state electrolyte materials for Li-batteries due to their high Li-ion conductivity. Preparing the materials as a glass-ceramic eliminates time consuming ceramic process development, enables easy implementation of compositional changes and glass-forming melt can be readily cast into any desired shape. NZP glass ceramics with  $\text{Li}_{1+x}[\text{Cr}_x\text{Ge}_y\text{Ti}_{2-x-y}](\text{PO}_4)_3$  stoichiometry have been shown to be suitable electrolyte materials. There is a rather large glass formation range, they crystallize mainly or solely to the NZP phase and in particular in the  $\text{Li}_{1+x}\text{Cr}_x\text{Ge}_{0.9-x}\text{Ti}_{1.1}(\text{PO}_4)_3$  join conductivities up to  $3.2 \times 10^{-4} \text{ S/cm}$  have been measured. Here we study the effect of utilizing Nb instead of Cr on the glass and glass-ceramic formation. Glass batches were formulated to have compositions with the NZP stoichiometry. They were melted at  $1500^\circ\text{C}$  for 3h, formed into thin sheets by roller quenching on stainless steel and then cerammed at  $900^\circ\text{C}$  for 2h. The resultant glass-ceramics were analyzed by x-ray diffraction, calorimetry and impedance spectroscopy. The  $\text{Li}_{1+x}[\text{Nb}_x\text{Ge}_y\text{Ti}_{2-x-y}](\text{PO}_4)_3$  system is compared to the previously studied  $\text{Li}_{1+x}[\text{Cr}_x\text{Ge}_y\text{Ti}_{2-x-y}](\text{PO}_4)_3$  system and their differences are discussed.

11:20 AM

**(GOMD-S1-142-2016) In-situ Characterization of Conductive WTi Phosphate Glass-Ceramics**I. Dutta<sup>\*1</sup>; B. Wheaton<sup>1</sup>; L. Moore<sup>1</sup>; B. Aitken<sup>1</sup>; G. Moore<sup>1</sup>; I. Corning Incorporated, USA

Glass-ceramics are formed by the controlled crystallization of glass. The final material is multi-phase, consisting of crystalline components and residual glass. The crystalline phases typically impart some functionality, such as color, a desired thermal expansion or electrical property, that is different from that of the precursor glass. W-Ti-phosphate glass ceramics have previously been shown to be excellent electrical conductors. The conductivity of these materials has been attributed to an interconnected network of needle shaped  $\text{WO}_{3-x}$  crystallites. To better understand the origin of this conductivity and to control it, it is important to understand the nucleation and crystal growth processes of this system. In this study, several in situ techniques were used to characterize the temperature dependence of the phase assemblage, microstructure and atomic level structure of selected WTi phosphate glass-ceramics. In situ X-ray diffraction was used to understand the sequence of phase transformations. In-situ TEM up to  $1000^\circ\text{C}$  was used to visualize the evolution of the microstructure. In-situ Raman, up to  $1100^\circ\text{C}$ , was used to characterize atomic level structure and bonding during the nucleation and growth stages of this system, with the results demonstrating the relationship between phase constitution, microstructure and physical properties.

11:40 AM

**(GOMD-S1-143-2016) Silver Doped Lithium Disilicate Glass and Glass-Ceramics: Optical and Electrical Properties**S. Singh<sup>\*1</sup>; S. Kundu<sup>1</sup>; P. Mattos<sup>1</sup>; A. Rodrigues<sup>1</sup>; E. Dutra Zanotto<sup>1</sup>; I. Federal University of Sao Carlos, Brazil

Glass-ceramics are materials of great scientific and technological interest because different properties can be tailored for desired applications during the transformation from a glass to polycrystal. Nucleating agents are used to induce internal crystallization or to accelerate the crystallization process, and nanometals are one type of interesting, not widely explored nucleating agent. In this study, silver ( $\text{Ag}^0$ ) nanoparticles (NPs) were obtained in-situ in a silver-containing stoichiometric lithium disilicate (L2S) glass matrix

by reducing silver ions via heat treatment at  $580^\circ\text{C}$ . UV-visible spectroscopy of the  $\text{Ag}^0$ -L2S glass confirmed the characteristic surface plasmon resonance of  $\text{Ag}^0$  NPs upon heat treatment. XRD patterns demonstrated the gradual development of lithium disilicate crystals in L2S and  $\text{Ag}^0$ -L2S glasses after heat treatment. FTIR results demonstrated the splitting of the broad bands of L2S glass into sharp bands in  $\text{Ag}^0$ -L2S glass-ceramics. Impedance spectroscopy has shown a more significant decrease in the conductivity of  $\text{Ag}^0$ -L2S glass-ceramics in comparison with that of L2S, which is attributed to a pronounced crystallization process in the case of  $\text{Ag}^0$ -L2S. We assign the decrease in the ionic conductivity of glass-ceramics to the ion blocking effect produced by lithium disilicate crystals.

12:00 PM

**(GOMD-S1-144-2016) Influence of  $\text{Al}_2\text{O}_3$  and  $\text{B}_2\text{O}_3$  on sintering and crystallization of lithium silicate glass system**A. Gaddam<sup>\*1</sup>; J. M. Ferreira<sup>1</sup>; I. University of Aveiro, Portugal

This study reports the effect of  $\text{Al}_2\text{O}_3$  and  $\text{B}_2\text{O}_3$  added as dopants on the preparation of glass-ceramics (GCs) belonging to the lithium silicate glass system. Bulk glasses have been thoroughly characterized using various techniques such as Raman, UV-Vis, FTIR and MAS-NMR spectroscopies and the structural role of  $\text{Al}_2\text{O}_3$  and  $\text{B}_2\text{O}_3$  was identified in the glass network. The reasons for the crystallization of the metastable crystalline phase lithium metasilicate (LS) were discussed and the impact of the dopants on the thermodynamics and kinetics of crystallization was investigated. The addition of dopants was shown to modify the thermodynamic equilibrium of the system and this change is mainly entropy driven and also slowdown the kinetics of crystallization. The GCs were prepared by sintering route using glass powders. Differential thermal analysis and hot-stage microscopy were employed to investigate the glass forming ability, sintering and crystallization behaviour of the studied glasses. The crystalline phase assemblage was studied under non-isothermal heating conditions in the temperature range of  $800\text{--}900^\circ\text{C}$  in air. Well sintered and dense glass-ceramics were obtained after sintering of glass powders at  $850\text{--}900^\circ\text{C}$  for 1 h featuring crystalline phase assemblage dominated by lithium disilicate (LS<sub>2</sub>).

**Session 7: Modeling of Glass under Extreme Conditions**

Room: Madison

Session Chair: Benoit Ruffle, Montpellier University

9:20 AM

**(GOMD-S1-145-2016) Densified Silica Glass Remembers Its Compression Pathway (Invited)**L. Huang<sup>\*1</sup>; I. Rensselaer Polytechnic Institute, USA

Silica glass has been shown in numerous studies to possess significant capacity for permanent densification under pressure at different temperatures to form high density amorphous (HDA) silica. However, it is unknown to what extent the processes leading to irreversible densification of silica glass in cold-compression at room temperature and in hot-compression (e.g., near glass transition temperature) are common in nature. In this work, a hot-compression technique was used to quench silica glass from high temperature ( $1100^\circ\text{C}$ ) and high pressure (up to 8 GPa) conditions, which leads to density increase of  $\sim 25\%$  and Young's modulus increase of  $\sim 71\%$  relative to that of pristine silica glass at ambient conditions. Our experiments and molecular dynamics (MD) simulations provide solid evidences that the intermediate-range order of the hot-compressed HDA silica is distinct from that of the counterpart cold-compressed at room temperature. This explains the much higher thermal and mechanical stability of the former than the latter upon heating and compression as revealed in our *in-situ* Brillouin light scattering (BLS) experiments. Contrary to the common belief mainly based on previous investigations of hot-compressed and cold-compressed HDA silica at ambient conditions, our studies

<sup>\*</sup>Denotes Presenter

show that the structure and properties of HDA silica depend sensibly on the pathway of compression, not just on the resulting densification.

**9:50 AM**

**(GOMD-S1-146-2016) Time-resolved in situ tomographic imaging of phase transformations in silicates (Invited)**

E. Gouillart<sup>\*1</sup>; E. Boller<sup>3</sup>; E. Burov<sup>1</sup>; W. Woelffel<sup>1</sup>; D. Bouttes<sup>1</sup>;  
D. Vandembroucq<sup>2</sup>; M. Toplis<sup>4</sup>; 1. Joint Unit CNRS/Saint-Gobain, France;  
2. PMMH, ESPCI, France; 3. ESRF, France; 4. IRAP, France

Silicate melts and crystals can undergo rapid phase and microstructural transformations at high temperature, such as chemical reactions, phase separation, crystallization, etc. X-ray microtomography is a tool of choice to characterize their 3-D microstructure, and in situ 3-D imaging available in some synchrotron facilities is a unique way to witness from the inside turning points of such transformations. I will first describe the development of ultrafast tomography on the ID19 beamline of the ESRF, and mention some of the technical challenges that have been successfully overcome. 3-D imaging is now available with a time resolution that can be as good as one second, while keeping an excellent spatial resolution down to the micron. Moreover, dedicated set-ups are available, including furnaces operating in free or controlled atmosphere at temperatures as high as 1500°C. As a first application, we studied the evolution of phases during coarsening of phase-separated silicate liquids. In situ imaging brought to light the critical role of asymmetric viscosity for break-up and fragmentation of liquid bridges, resulting in a complex microstructure with a wide range of scales. I will also show how ultrafast imaging of soda-lime glass batch reactions resulted in new insights about the geometry of chemical reactions, and the origin of crystalline defects that are hard to dissolve in industrial glass melting.

**10:20 AM**

**(GOMD-S1-147-2016) Constitutive Modeling of Glass Using Molecular Dynamics**

V. Subramanian<sup>\*1</sup>; S. Goyal<sup>1</sup>; 1. Corning Incorporated, USA

Glass reacts to extreme stress by undergoing elastic and irreversible (plastic) deformation. Irreversible deformation can occur in glass via densification and isochoric shear flow. Such extreme stresses can occur during indentation and scratch of glass, which are commonly encountered during usage of cover glasses in mobile devices. Constitutive models incorporating the elastic and irreversible behavior of glass under extreme stress need to be available for modeling indentation and scratch of glasses. Several models have been proposed to date for silica that includes the irreversible deformation response. While these models may work well for a particular indentation setup it is not clear if they will predict the eventual fracture response accurately given that these models are not created using experimental data for the entire range of elastic and irreversible deformation for silica. Given the absence of shear testing data for glasses, molecular dynamics is used as a proxy for experiments to provide a complete description of combined densification and shear flow in silica.

**10:40 AM**

**(GOMD-S1-148-2016) Radiation-Induced Amorphization of Quartz: Insights from Rigidity Theory (Invited)**

B. Wang<sup>1</sup>; Y. Yu<sup>1</sup>; M. Wang<sup>1</sup>; M. Bauchy<sup>\*1</sup>; 1. University of California, Los Angeles, USA

As a typical aggregate used in concrete, understanding the structural and mechanical radiation-induced damage in quartz is of primary importance to ensure the integrity of the concrete used in nuclear plants. Here, molecular dynamics simulations are used to study such atomic-scale damage, and its consequence on macroscopic mechanical properties. This is achieved by direct simulations of high-energy ballistic impacts, inducing cascade collisions inside the atomic

network. Upon irradiation, a gradual amorphization of the quartz network is observed. The types of atomic defects that are formed are analyzed, with respect of the intensity and duration of the radiation. We find that over-coordinated silicon and oxygen species are far more prominent than oxygen vacancies (the so-called E' centers). The displacement energies are also calculated. In order to isolate the important atomic topology that affect macroscopic properties, while filtering out the less relevant structural details, the structure of irradiated samples is analyzed in the framework of topological constraint theory. We show that, upon irradiation, quartz undergo a rigid-to-flexible transition, which is correlated with structural signatures in the medium range order. This irradiation-induced rigidity transition is shown to feature strong analogies to usual composition-, temperature-, or pressure-driven rigidity transitions.

**11:10 AM**

**(GOMD-S1-149-2016) Pressure induced structural changes in Ca and Mg aluminosilicate glasses (MO/AL<sub>2</sub>O<sub>3</sub>≤1) recovered from 1-3 GPa: <sup>27</sup>Al MAS NMR studies**

S. Bista<sup>\*1</sup>; J. Stebbins<sup>1</sup>; 1. Stanford University, USA

Simple models of aluminosilicate glass structure suggest that non-bridging oxygen (NBO) decrease to zero as MO/Al<sub>2</sub>O<sub>3</sub> decreases to 1, although excess NBO are well known (few percent) in the Ca aluminosilicate at this composition. Previous studies of pressure effects on Al coordination have suggested that coordination increase is promoted by high NBO contents, especially in alkali aluminosilicate glasses. Very few previous studies have looked at Ca and Mg aluminosilicate with MO/Al<sub>2</sub>O<sub>3</sub><1 (peraluminous) and MO/Al<sub>2</sub>O<sub>3</sub>=1 (metaluminous) compositions. In this study, we have looked at several such compositions of Ca and Mg aluminosilicate glasses recovered from temperatures near to the glass transition at 1-3 GPa using <sup>27</sup>Al MAS NMR, and observed surprisingly rapid increases in Al coordination with pressure, with the most rapid increases recorded in the Mg system. Our study shows that the mechanism of the coordination increase is more complex than the simple consumption of NBO with increasing pressure, especially with high field strength modifier cations (Mg<sup>2+</sup>>Ca<sup>2+</sup>>Na<sup>+</sup>).

**11:30 AM**

**(GOMD-S1-150-2016) Influence of Network Topology on Ion-Exchange Strengthening of Glasses**

M. Wang<sup>\*1</sup>; Y. Yu<sup>1</sup>; B. Wang<sup>1</sup>; J. C. Mauro<sup>2</sup>; M. Bauchy<sup>1</sup>; 1. UCLA, USA;  
2. Corning Incorporated, USA

The brittleness of glasses seriously limits the range of their applications. To overcome this drawback, chemical strengthening through ion-exchange has emerged as the easiest and cheapest solution. However, the compressive stress induced by the replacement of small Na by larger K atoms typically remains much lower than its theoretical upper limit. Here, based on molecular dynamics simulations of different permanently densified sodium silicates (Na<sub>2</sub>O)<sub>30</sub>(SiO<sub>2</sub>)<sub>70</sub>, we investigate within the framework of rigidity theory the influence of the rigidity of the atomic network on the stress generated by ion-exchange. We report that, upon ion-exchange, a window of cooling pressure of 8-16 GPa, corresponding to the isostatic regime of the glass network, features the largest compressive stress, which reaches its theoretical limit. This demonstrates that finely tuning the rigidity of glass networks can enhance the effect of ion-exchange and, thereby, could lead to the design of stronger glasses.

## **Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications**

### **Session 3: Optical Materials for Components and Devices I**

Room: Wisconsin

Session Chair: Pierre Lucas, Univ of Arizona

**9:20 AM**

#### **(GOMD-S3-035-2016) Hydrothermal Synthesis and Characterization of 2D Nanomaterials for Optical Applications (Invited)**

S. Whipkey<sup>1</sup>; Y. Liu<sup>1</sup>; Y. Wu<sup>\*1</sup>; 1. Alfred University, USA

2-dimensional (2D) nanomaterials have been of much research interest due to their unique nanoscale structure and properties. Hydrothermal synthesis is one way to effectively produce these thin nanostructure materials, which are ideal for further processing into transparent 2D materials for applications such as laser host materials and optical displays. Hydrothermal synthesis of a variety of rare-earth doped nanomaterials with intended applications in optoelectronics applications has been investigated. A focus has been put on producing particles with thin, 2D morphologies, as these are ideal for further sintering into transparent ceramics. The optical and luminescent properties of the resulting materials has been analyzed and compared to similar materials created via alternate methods to determine potential benefits or detriments the hydrothermal method may have over others. Control of the morphology and chemical compositions of the resulting nanomaterials is critical to understanding the potential for tailoring these materials for future optical applications.

**9:50 AM**

#### **(GOMD-S3-036-2016) High Anneal Point Rare Earth Aluminosilicates for Display Applications**

M. Dejneka<sup>\*1</sup>; C. L. Chapman<sup>1</sup>; 1. Corning Incorporated, USA

High performance liquid crystal and OLED (organic light emitting) displays require high processing temperatures to fabricate high mobility thin film transistors. Most glasses warp and compact when heated near 700°C where crystalline Si transistors are grown on the glass substrates. Furthermore the ideal glass should have a low liquidus temperature for glass stability and to enable precision drawn sheet with flat pristine surfaces. Glasses with higher anneal points and sufficient liquidus temperatures were made by mixing rare earth oxides with alkaline earth aluminosilicates and optimizing the composition to obtain glasses with anneal points up to 840°C, good compaction performance, increased modulus, and better melting behavior than their rare earth free counterparts.

**10:10 AM**

#### **(GOMD-S3-037-2016) Development of Germano-Gallate Glasses and Optical Fibers for Near- and Mid-Infrared Applications**

T. Skopak<sup>\*1</sup>; Y. Ledemi<sup>2</sup>; S. Morency<sup>2</sup>; M. Dussauze<sup>1</sup>; T. Cardinal<sup>1</sup>; E. Fargin<sup>1</sup>; Y. Messaddeq<sup>2</sup>; 1. Université de Bordeaux, France; 2. Université Laval, Canada

Optical applications in the 3-5  $\mu\text{m}$  region, as molecular sensing, require adapted glass compositions with extended infrared transmission. Even though multiple exotic glasses like fluoride or chalcogenide glasses exhibit attractive properties (as low phonon energy or high refractive index), their processing remains a major issue. On the other hand, little attention has been devoted to gallium oxide based glasses, which may constitute excellent candidates for near- and mid-infrared optical applications. Glasses from the  $\text{Ga}_2\text{O}_3$ - $\text{GeO}_2$ - $\text{BaO}$ - $\text{K}_2\text{O}$  system could offer wider transparency in the long wavelength range (from 250 nm to 6  $\mu\text{m}$ ) as compared to classical

oxide glasses. Several compositions were studied. Structural investigations have been conducted using Raman spectroscopy. Thermal analysis was performed by DSC while transmission windows and refractive index were characterized. The best glass composition,  $28\text{Ga}_2\text{O}_3$ - $37\text{GeO}_2$ - $23\text{BaO}$ - $12\text{K}_2\text{O}$  in mol.%, was selected to be drawn into a fiber using several techniques (glass preform drawing, Powder in tube and Rod in tube) in order to find the more suitable one. The results obtained from each approach are compared and discussed. Finally, step-index optical fibers (core made of the selected composition and cladding of silica glass) were successfully produced by using the Powder in tube method.

**10:30 AM**

#### **(GOMD-S3-038-2016) Sol-Gel $\text{TiO}_2$ glass thin films for flexible cytocompatible photonics**

L. Li<sup>\*1</sup>; P. Zhang<sup>2</sup>; H. Lin<sup>3</sup>; S. Geiger<sup>1</sup>; A. Zerdoum<sup>1</sup>; Y. Liu<sup>1</sup>; N. Xiao<sup>1</sup>; O. Ogbuu<sup>1</sup>; Q. Du<sup>3</sup>; X. Jia<sup>1</sup>; J. Hu<sup>3</sup>; 1. University of Delaware, USA; 2. Tianjin University, China; 3. Massachusetts Institute of Technology, USA

Flexible integrated photonics is a new technology that has only started to burgeon in the past few years, which enables a wide cross-section of emerging applications ranging from flexible optical interconnects to conformal sensors on biological tissues.  $\text{TiO}_2$ , a typically biocompatible material, works as a good candidate for the fabrication of biocompatible and flexible integrated photonics. Using a sol-gel method, we deposited amorphous  $\text{TiO}_2$  films at a low temperature ( $< 250^\circ\text{C}$ ), which exhibited a low optical loss of 3 dB/cm. Structural and optical properties of the films were characterized by FT-IR, UV-vis, Refractometry, etc. Further, we fabricated and tested  $\text{TiO}_2$  optical waveguides and resonators monolithically integrated on flexible polymer substrates, and resonator quality factors as high as 20,000 were measured. Despite the inherent mechanical rigidity of the  $\text{TiO}_2$  material, we experimentally demonstrated repeated folding of the devices down to  $< 0.3$  mm radius without degrading their optical performance by using the developed multi-neutral-axis mechanical design. Finally, we showed through in-vitro tests that the  $\text{TiO}_2$  devices are non-cytotoxic. These results indicate that sol-gel  $\text{TiO}_2$  can serve as a promising material platform for novel biophotonic devices.

**10:50 AM**

#### **(GOMD-S3-039-2016) Role of metallic nanoparticles on the optical properties and luminescence intensities of rare earth doped tungsten phosphate glasses**

M. Dousti<sup>\*1</sup>; G. Poirier<sup>2</sup>; A. de Camargo<sup>1</sup>; 1. Universidade de São Paulo, Brazil, Brazil; 2. Instituto de Ciências e Tecnologia, Universidade Federal de Alfenas, Brazil

Recently, glasses have attracted great attention due to their superior mechanical, structural, thermal and optical properties, i.e., high rare earth (RE) solubility and thermal stability. The emission wavelengths of RE ions cover a wide spectral region. However, the limited emission cross-section of RE doped glasses needs to be improved. Hence, several approaches have been proposed such as energy transfer from a second type of RE ions, a transition metal ion, or noble metals in the form of ions, nanocrystals and nanoparticles. Since the very early report on 1985 on the enhancement of the luminescence intensity of  $\text{Eu}^{3+}$  ions by small silver particles in borate glasses, the influence of the type, morphology and distribution of metal clusters and nanoparticles on RE ion emission has been studied extensively, aiming at an understanding of the nature of the interactions between the ions and the metals. In this work, we briefly review the state of the art on this subject and present recent progress in our laboratory on the effect of silver nanoparticles on the emissive behavior of a new RE doped ( $\text{Er}^{3+}$ ,  $\text{Tb}^{3+}$ ,  $\text{Eu}^{3+}$ ) tungsten-phosphate glass. Probable mechanisms to enhance the near-infrared emission of  $\text{Er}^{3+}$  ions or the luminescence quenching of  $\text{Eu}^{3+}$  ions will be discussed.

\*Denotes Presenter

11:10 AM

**(GOMD-S3-040-2016) Micro-poling of a borosilicate glass employing laser-induced samarium absorption**

A. Lepicard<sup>\*1</sup>; T. Cardinal<sup>2</sup>; F. Adamietz<sup>2</sup>; V. Rodriguez<sup>2</sup>; K. Richardson<sup>3</sup>; M. Dussauze<sup>1</sup>; 1. University of Bordeaux, France; 2. ICMCB-CNRS, France; 3. University of Central Florida, USA

In integrated photonics, nanotechnology, lab-on-a-chip and other photonic applications, there is a strong need to locally control glass surface properties enabling a “smart substrate”. Recently, we have showed the ability to change the surface reactivity of a glass substrate using thermal poling. Thermal poling involves application of a DC electric field to a glass substrate heated below its  $T_g$ . Following treatment, the glass exhibits a locally modified structure associated with a strong static electric field, resulting in an enhanced reactivity towards atmospheric water. In this talk, a new approach to thermal poling is presented. As the sample is subjected to the electric field, a 1064 nm cw laser is shined through a transparent electrode and focused on a Sm-doped glass. Samarium absorbs at this wavelength and produces heat. The poled glass is characterized using micro-Second Harmonic Generation ( $\mu$ -SHG), electron microprobe and Atomic Force Microscopy. The irradiated area presented a strong SHG response, a large depletion of sodium in its center, a change in topography and surface potential. The samarium absorption process locally provides enough energy for the cations to gain mobility. They migrate under the applied electric field. Thermal poling is hence controlled on a spatially defined scale, which gives possibilities to spatially control nonlinear optical properties and surface reactivity.

11:30 AM

**(GOMD-S3-041-2016) Substitution effect of ZnO on structure and properties in ZnO-SnO-P<sub>2</sub>O<sub>5</sub> glasses**

A. Saitoh<sup>\*1</sup>; Y. Hashida<sup>1</sup>; G. Tricot<sup>2</sup>; P. Freudenberger<sup>3</sup>; L. Ma<sup>3</sup>; R. Brow<sup>3</sup>; H. Takebe<sup>1</sup>; 1. Ehime University, Japan; 2. Université de Lille 1, France; 3. Missouri University of Science and Technology, USA

Composition dependences of thermal and optical properties (including the zero photoelastic response) and structure of ZnO-SnO-P<sub>2</sub>O<sub>5</sub> glasses are studied. These effects are seen in the pyrophosphate composition ( $x\text{ZnO}-(67-x)\text{SnO}-33\text{P}_2\text{O}_5$ ) for the density, glass transition temperature, thermal expansion coefficient, viscosity, refractive index, and photoelastic constant properties. The effect on those properties caused by phosphate network modification is revealed by <sup>31</sup>P MAS-NMR, micro-Raman spectroscopies, and High Performance Liquid Chromatography technique. The compositional parameter of O/P ratio reveals the changes from correlation structure of  $\text{Sn}^{2+}-\text{Q}^1(\text{P}_2\text{O}_7^{4-})$  to  $\text{Sn}^{2+}-\text{Q}^0(\text{PO}_4^{3-})$  and/or  $\text{Zn}^{2+}-\text{Q}^0(\text{Q}^n$ : where n is the number of phosphate tetrahedral bonded to a given  $\text{PO}_4$  tetrahedron). The changes in thermal and optical properties can be divided into two regions between (I) low and (II) high ZnO concentrations. Particularly, the ternary composition glass with close to zero photoelastic constant stands on the boundary regarding change of tendency with above properties.

**Session 5: Glass-Ceramics and Optical Ceramics II**

Room: University C/D

Session Chair: Yiquan Wu, Alfred University

9:20 AM

**(GOMD-S3-042-2016) Advanced Optical Materials for Next Generation EO/IR Sensors (Invited)**

C. R. Baleine<sup>\*1</sup>; A. Kirk<sup>1</sup>; S. Aiken<sup>1</sup>; C. Bungay<sup>1</sup>; S. Tuenge<sup>1</sup>; K. Richardson<sup>2</sup>; C. Smith<sup>2</sup>; L. Siskin<sup>2</sup>; T. Mayer<sup>3</sup>; A. Swisher<sup>3</sup>; M. Kang<sup>3</sup>; A. Pogrebniyakov<sup>3</sup>; C. G. Pantano<sup>3</sup>; 1. Lockheed Martin, USA; 2. University of Central Florida, USA; 3. Pennsylvania State University, USA

Next generation Electro-Optical / Infrared (EO/IR) sensors require novel optical materials that serve specified optical functions and possess attributes which can be tailored to accommodate specific

optical design, manufacturing or component/device integration constraints. Gradient-index (GRIN) coatings and lenses can provide significant performance enhancement and/or reduce size, weight, and power (SWaP). The effective refractive index of the GRIN components is engineered to create the desired refractive index profiles allowing optimization of the optical performance over conventional homogeneous infrared (IR) materials. Anti-reflective (AR) GRIN coatings have been designed and fabricated which show significant performance enhancement over current state of practice wide field of views (W-FOV) AR coatings. Bulk GRIN materials with broadband optical transmission have also been developed.

9:50 AM

**(GOMD-S3-043-2016) Thin film doped garnet materials and devices for monolithic on-chip optical isolation (Invited)**

X. Sun<sup>2</sup>; Q. Du<sup>1</sup>; T. Goto<sup>3</sup>; M. Onbasli<sup>1</sup>; J. Hu<sup>\*1</sup>; C. Ross<sup>1</sup>; 1. Massachusetts Institute of Technology, USA; 2. Harbin Institute of Technology, China; 3. Toyohashi University of Technology, Japan

Optical isolators, i.e. one-way optical valves that allow only uni-directional propagation of light, are an important class of photonic devices essential for stabilizing laser operation and eliminating cross-talk between different components within an optical circuit. Conventional isolators rely on magneto-optical Faraday rotation in bulky, single-crystal garnets to realize isolation. Nevertheless, the large footprint and high cost of these isolators are not compatible with on-chip integration. To resolve the challenge, we have demonstrated monolithic integration of polycrystalline Ce or Bi substituted yttrium iron garnet (YIG) thin films on a silicon platform combining pulsed laser deposition followed by rapid thermal annealing. The technique utilizes an undoped garnet seed layer to facilitate crystallization of the doped layer forming the YIG phase. We will discuss efforts made to reduce thermal budget, simplify growth protocols as well as improve magneto-optical characteristics of the material. Using the deposited garnet thin films, monolithic nonreciprocal optical isolators with a high magneto-optical figure-of-merit were demonstrated showing a high extinction ratio of 19.5 dB and an insertion loss of 7.4 dB [Nat. Photonics 5, 758 (2011) & ACS Photonics 2, 856 (2015)]. Prospects of further enhancing the isolator performance leveraging innovative photonic designs will also be discussed.

10:20 AM

**(GOMD-S3-044-2016) The Effects of Composition on the Refractive Index Change for GeSe<sub>2</sub>-As<sub>2</sub>Se<sub>3</sub>-PbSe Glass Ceramics**

L. Siskin<sup>\*1</sup>; C. Smith<sup>1</sup>; A. Buff<sup>2</sup>; B. Gleason<sup>2</sup>; K. Richardson<sup>1</sup>; 1. University of Central Florida, USA; 2. Clemson University, USA

Chalcogenide glass ceramics hold great potential for improving existing optical systems by decreasing the cost of crystalline elements while improving the thermo-mechanical properties of infrared-transparent glasses. Another potential advantage is the ability to create GRIN elements by selectively crystallizing the material to different degrees at different locations. One hurdle that needs to be overcome with this process is the ability to maintain optical transparency while crystallizing a large enough volume fraction of glass in order to create a useful amount of refractive index change ( $\Delta n \sim 0.01 - 0.1$ ). In this study the refractive index, thermo-optic behavior and short-wave transmission edge of base, nucleated, and nucleated with subsequent growth glass ceramics for the  $(\text{GeSe}_2-2\text{As}_2\text{Se}_3)_{(1-x)}-(\text{PbSe})_x$  were characterized. Correlation on the effect of crystalline phase on overall optical performance will be discussed.



10:40 AM

**(GOMD-S3-045-2016) Preparation of MgAl<sub>2</sub>O<sub>4</sub> Transparent Ceramic Mixed with phosphor by spark plasma sintering following by HIP sintering**Q. Huang<sup>\*1</sup>; Q. Deng<sup>1</sup>; B. Han<sup>1</sup>; 1. Ningbo Institute of Material Technology and Engineering, Chinese Academy of Sciences, China

Transparent MgAl<sub>2</sub>O<sub>4</sub> ceramic mixed with phosphor commercial or homemade was prepared by spark plasma sintering (SPS) following by HIP sintering. The influence of the sintering temperature, holding time and pressure on the transparent MgAl<sub>2</sub>O<sub>4</sub> ceramic was studied. Because of the uniform distribution of the phosphor in transparent ceramic, this method avoids the precipitation of phosphor in resin and improves the uniformity of the light. Owing to higher thermal conductivity and excellent mechanical performance, it can be used to package LED. SEM and other analysis methods were applied to study phase composition and microstructure of the ceramics. The yellow light emission was observed from the ceramic under the excitement of blue-ray. The electro-optical parameters of the LED packaged with ceramic were tested.

11:00 AM

**(GOMD-S3-046-2016) Conversion of ceramics into single crystals: grain boundary kinetics, impurity effects and space charge enhancement**Y. Liu<sup>\*1</sup>; Y. Wu<sup>1</sup>; 1. Alfred University, USA

Transforming polycrystalline ceramics into single crystals has been regarded as a promising alternative method for producing laser materials. However, the effects of both intrinsic and extrinsic mechanisms on the conversion process still remain controversial from an experimental perspective. We herein have chosen both an oxide material (Al<sub>2</sub>O<sub>3</sub>) and a non-oxide material (Sr<sub>3</sub>(PO<sub>4</sub>)<sub>3</sub>F) as test subjects. A single crystal seed was first bonded to the polycrystalline matrix of a ceramic material, which was subjected to isothermal annealing to initiate solid-state conversion. Grain boundary motion and growth was investigated and compared to the motion of the single-polycrystal interface. Dopant impurities and sintering additives were observed to significantly affect grain boundary kinetics, as well as the overall conversion rate. The effect of space charge, induced by an externally applied electric field, was also examined in the context of its effect on the conversion process. AC impedance spectroscopy was employed to investigate the characteristics of the space charge, which was correlated with reduced grain boundary energies.

11:20 AM

**(GOMD-S3-047-2016) Spectral and laser properties of Yb:LuAG transparent ceramics fabricated by tape-casting method**Y. Cao<sup>\*1</sup>; C. Ma<sup>1</sup>; 1. Renmin University of China, China

Yb-doped LuAG laser ceramics with different Yb<sup>3+</sup>-doping concentrations were successfully fabricated by non-aqueous tape-casting method and vacuum sintering technology. TG-DTA curves of green body, XRD patterns and SEM morphologies of the ceramics were presented. The optical in-line transmittance of the Yb-doped LuAG ceramics was about 83% at 1030 nm. The fluorescence lifetime of annealed and un-annealed ceramic samples was compared. From the spectroscopic properties, it can be seen that the ceramics had a large emission cross-section of  $2.9 \times 10^4$  cm<sup>2</sup> with a FWHM of about 7.2 nm at 1030 nm. Under one hundred percent population inversion, the maximum gain coefficient was estimated to be 12.4 cm<sup>-1</sup> at 1030 nm. With a fiber-coupled diode laser as pump source, CW laser at 1030 nm was demonstrated and the maximum output power of 338.9 mW was achieved with a slope efficiency of 19%. A tuning range from 1028 nm to 1036 nm was obtained.

**Symposium 4: Glass Technology and Cross-Cutting Topics****Session 2: Liquid Synthesis and Sol-gel-derived Materials I**

Room: Capitol B

Session Chair: John Kieffer, University Of Michigan

9:20 AM

**(GOMD-S4-051-2016) Building a Better Environment by Doing Things Purely (Invited)**M. A. Anderson<sup>\*1</sup>; 1. UW Madison (Retired Prof.), USA

Our program is concerned with the production and use of micro and nanoporous materials for a variety of environmentally friendly applications. This talk will be divided into the material science of building nanoporous oxide materials and to their practical applications. The first part of the talk will be devoted to the sol-gel chemistry of producing nanoparticulate oxides and thin-films composed of these oxides. In this first part of the talk, I will discuss the various physical chemical steps in the sol-gel process: sol-preparation, coating, gelation, drying and final firing of the materials. This is basically colloid chemistry and as well ceramic engineering. Some interesting optical and physical properties of nanoparticles and their aggregates will also be described. The second portion of the talk will touch on a variety of technologies that we are currently pursuing with particular attention to the use of these materials in ultracapacitors, cathode coatings in batteries, corrosion control, photocatalysis and photo-electrocatalysis, sensors, water treatment, and even concrete. These are very different applications but all use our nanoporous oxide materials!

9:50 AM

**(GOMD-S4-052-2016) Tuning the Bandgap of Nanoporous Glasses**M. Sundararajan<sup>\*1</sup>; G. Chen<sup>1</sup>; 1. Ohio University, USA

Efficiency of photocatalysts greatly depends on their electronic structure such as bandgap, but very few photocatalysts have their optical bandgap covering the whole visible region of sun light, leading to poor efficiency of solar energy conversion. There are a few ways to modify the bandgap of photocatalysts and most of those rely on changing chemical compositions of the materials. In this study, we demonstrate a physical method to modify the optical bandgap of amorphous nanoporous photocatalysts by manipulating their residual stresses. We synthesize mesoporous (TiO<sub>2</sub>)<sub>x</sub>·(SiO<sub>2</sub>)<sub>1-x</sub> glasses through a sol-gel method and study the relation between the stress manipulation and optical bandgap tuning. Our results show that the bandgap of nanoporous glasses can be controlled using this physical method. The mechanism behind this novel method will be explained.

10:10 AM

**(GOMD-S4-053-2016) Effect of Metal Nanoparticles on Melting Gels**L. C. Klein<sup>\*1</sup>; S. Kallontzi<sup>1</sup>; L. Fabris<sup>1</sup>; A. Jitianu<sup>2</sup>; 1. Rutgers University, USA; 2. Lehman College, CUNY, USA

Hybrid gels prepared using substituted alkoxysilanes show the behavior of gelling and softening and are called "melting gels." Ultimately, they become crosslinked and consolidated, as the temperature is increased. While the gel is softened, it can be poured onto substrates to make thick coatings, which can be imprinted to give surface texture. However, a heat treatment is needed to produce a hard and durable hybrid glass. Generally, the heat treatment is carried out for 24 hours at about 150°C. With the addition of metal nanoparticles, it is possible to shorten the time substantially, without changing the transparency or electrical insulating properties. Metal nanoparticles that are effective include Cu, Ag and Au.

\*Denotes Presenter

Cu nanoparticles of about 70 nm size were able to reduce the consolidation time from 24 hours to 1 hour. The catalytic effect of these metals is being investigated.

**10:30 AM**

**(GOMD-S4-054-2016) Solid-state electrolytes based on organically modified sol-gel derived silica networks**

W. Wang<sup>\*1</sup>; J. Kieffer<sup>1</sup>; 1. University of Michigan, USA

We developed a novel two-step synthesis method that allows us to functionalize the pore walls of a sol-gel derived silica network with organic polymer in order to create highly conductive pathways in this hybrid material. In the first step, a percolating 3D silica network is created via sol-gel synthesis, using APTES and TEOS as silica precursor. In the next step, the pore fluid in the wet gel is replaced by poly(ethylene oxide) solution with dissociated lithium ions. The active sites on silica react with the functionalized polymer and anchor the polymer chains inside the network. IR spectroscopy, Raman and Brillouin light scattering and impedance spectroscopy are used to identify the structural and chemical origins that underlie the performance of these hybrid electrolytes. Accordingly, a larger weight fraction of ion conducting polymer can be embedded into pores using two-step synthesis compared to a one-pot method. This greatly enhances the ionic conductivity without sacrificing mechanical stability because a continuous silica backbone is ensured. A room temperature ionic conductivity in excess of  $10^{-5}$  S/cm can be reached. In this presentation we provide a cumulative account of a systematic materials design effort, in which we sequentially implemented several important design aspects so as to identify their respective importance and influence on the materials performance characteristics.

**10:50 AM**

**(GOMD-S4-055-2016) Branching and Fractal Structure in Ceramic Aggregates (Invited)**

G. Beaucage<sup>\*1</sup>; 1. University of Cincinnati, USA

Ceramic aggregates are often described in terms of their mass fractal dimension. However, for a given mass fractal dimension may structures exist that vary in terms of branch content. Variability of branch content has largely been ignored in the literature, though it can effect the mechanical and transport properties of aggregates quite dramatically. This presentation will discuss methods for quantification of branch structure in ceramic aggregates using small angle x-ray scattering.

## Symposium 1: Fundamentals of the Glassy State

### **Session 7: Characterization of Glass under Extreme Conditions II**

Room: Madison

Session Chair: Patrick Simon, CNRS-CEMHTI

**1:20 PM**

**(GOMD-S1-151-2016) NMR Studies of Permanent Compression in Oxide Glasses (Invited)**

R. Youngman<sup>\*1</sup>; M. N. Svenson<sup>2</sup>; J. C. Mauro<sup>1</sup>; M. M. Smedskjaer<sup>2</sup>; 1. Corning Incorporated, USA; 2. Aalborg University, Denmark

Pressure-induced structural rearrangement in oxide glasses is manifested by modification of both short- and intermediate-range structures, including changes to the local coordination numbers of network forming cations and alteration of the modifier environment. NMR spectroscopy is an especially useful tool for examining these changes in network structure, especially for boron-containing glasses, which are particularly sensitive to permanent compression. Here we describe studies based on hot isostatic compression

of several different borate and borosilicate glasses, where changes in short-range structure following both compression and thermal annealing (relaxation) treatments have been examined using solid-state NMR. Changes in boron coordination, arrangement of these polyhedra into various superstructural groups, as well as the impact of compression and annealing on the local geometry of the network modifying sodium atoms, will be discussed. Such changes in network structure aid in understanding the pressure-induced properties of these glasses, such as density, elastic moduli, hardness and crack resistance.

**1:50 PM**

**(GOMD-S1-152-2016) Static vs dynamic compressibility of vitreous silica under pressure**

C. Weigel<sup>1</sup>; B. Coasne<sup>3</sup>; A. Polian<sup>2</sup>; M. Foret<sup>1</sup>; R. Vacher<sup>1</sup>; B. Ruffle<sup>\*1</sup>; 1. Montpellier University, France; 2. Université P. et M. Curie, France; 3. Joseph Fourier University, France

The talk will discuss the elastic properties of vitreous silica submitted to high pressures in a diamond anvil cell. A particular emphasis will be given to the observed difference between static and dynamic compressibility. We show for example that the compressibility of a silica sample immersed in helium or neon fluid is much smaller than expected from its elastic properties measured by Brillouin light scattering. It results from gas atom penetration into the interstitial free volume of the glass network. This adsorption-induced expansion can be described by a generalized poromechanical model. We also address the case of silica pressurized under argon.

**2:10 PM**

**(GOMD-S1-153-2016) In-situ high pressure study of amorphous Ta<sub>2</sub>O<sub>5</sub> by Raman and Brillouin spectroscopies**

V. Martinez<sup>\*1</sup>; C. Elodie<sup>1</sup>; G. Massimo<sup>2</sup>; M. Christine<sup>1</sup>; V. Dolique<sup>2</sup>; G. Cagnoli<sup>2</sup>; A. Mermet<sup>1</sup>; 1. ILM, France; 2. LMA, France

Albert Einstein predicted the existence of gravitational waves in 1918 and the detection of these could be a test of the General relativity Theory. The gravitational wave detectors (GWD) are giant laser interferometers whose sensitivity is limited by the thermal noise from the amorphous coating of the mirrors made of alternate thin amorphous layers of SiO<sub>2</sub> and TiO<sub>2</sub>-doped Ta<sub>2</sub>O<sub>5</sub> deposited by Ion Beam Sputtering. This study is focused on amorphous Ta<sub>2</sub>O<sub>5</sub> films which structure is little known. Indeed, up to now, Ta<sub>2</sub>O<sub>5</sub> has not garnered much attention because it is not a bulk glass former. Raman and Brillouin spectroscopies were performed to characterize the film structure at short and mid-range order and the elastic properties. The structural evolution as a function of annealing will be discussed. In order to clarify the glass structure, in-situ Raman and Brillouin spectroscopies during high pressure experiments by a diamond anvil cell have been performed. The structural and mechanical properties as a function of pressure evolution from these experiments will be discussed. The drastic structural modifications observed at around 5 GPa will be exposed.

**2:30 PM**

**(GOMD-S1-154-2016) Characterization of boron-aluminum substitution in lanthanum boroaluminosilicate glasses by Brillouin and NMR spectroscopy**

A. Mabrouk<sup>\*1</sup>; N. Pellerin<sup>1</sup>; Y. P. Vaills<sup>1</sup>; 1. University d'orleans, France

Fission products and minor actinides are nuclear wastes which are highly active and present long half-time. Their storage requires vitreous matrices extremely stable having excellent long-term performances. The boro-alumino-silicate glass matrices have largely proved their stability and their interest for the new generation of the nuclear glass [1] and lanthanides are commonly used to simulate the minor actinides in simplified matrices. This work aims to study the influence of the boron-aluminum substitution in the vitreous system SiO<sub>2</sub> – Al<sub>2</sub>O<sub>3</sub> – B<sub>2</sub>O<sub>3</sub> – Na<sub>2</sub>O – La<sub>2</sub>O<sub>3</sub> in the peraluminous domain, that means, a defect of charge compensators compared to aluminum

$Al^{3+}$  present in the glass network. These glasses are investigated by Brillouin scattering which can probe the structure from microscopic to macroscopic scale [2], and by NMR spectroscopy ( $^{29}Si$ ,  $^{27}Al$ ,  $^{23}Na$  and  $^{11}B$ ) offering structural description on the network and environments change with Al-B substitution. In addition, XRD, DSC and TEM are employed to characterize this vitreous system. The phase separation is observed with boron addition above 7.5 % mol. In the homogeneous region, the introduction of boron tends to increase the measured Brillouin frequency and decreases the glass transition temperature.

### **Symposium 3: Optical and Electronic Materials and Devices - Fundamentals and Applications**

#### **Session 3: Optical Materials for Components and Devices II**

Room: Wisconsin

Session Chair: Juejun Hu, Massachusetts Institute of Technology

##### **1:20 PM**

#### **(GOMD-S3-048-2016) Chalcogenide Glass-Based Sensors for Molecular Detection (Invited)**

P. Lucas<sup>\*1</sup>; G. Coleman<sup>1</sup>; S. Jiang<sup>2</sup>; B. Bureau<sup>3</sup>; 1. University of Arizona, USA; 2. Advalue Photonics, USA; 3. University of Rennes, France

Chalcogenide glasses offer a unique combination of wide transparency in the mid-infrared and superior glass-forming ability. This enables the design of complex optical components for the collection of vibrational signals in the 2-16 micron range. The superior rheological properties of chalcogenide glasses permits drawing of fibers or molding of complex structures such as micro-structured surfaces or resonators; while the wide compositional landscape allows tuning of the physical properties such as optical cut-off and chemical stability. Here we review the benefits and limitations of compositional engineering of chalcogenide glasses for the design of optical sensors and present various approaches for the sensitive and selective detection of molecular signals in the infrared.

##### **1:50 PM**

#### **(GOMD-S3-049-2016) Mid-Infrared Methane Gas Sensing using Chalcogenide Glass on Silicon Platform**

Z. Han<sup>\*1</sup>; P. Lin<sup>3</sup>; L. C. Kimerling<sup>1</sup>; A. Agarwal<sup>1</sup>; D. T. Tan<sup>2</sup>; 1. MIT, USA; 2. Singapore University of Technology and Design, Singapore; 3. Texas A&M University, USA

Several gases have their absorption fingerprint in the mid-infrared (MIR) range, which allow us to distinguish and measure their concentrations. In this work, we demonstrate methane gas sensing using a MIR microphotonic waveguide-based evanescent device on a Chalcogenide glass (ChG)-on-silicon platform. Thermal evaporation and lift-off techniques are applied to fabricate an integrated waveguide on a silicon dioxide substrate. Spiral waveguide designs (from 6 to 12 mm lengths) are used to increase interaction with methane. A tunable pulsed MIR laser guides light within our sensor device located within a microfluidic methane gas flow channel. Our data shows that efficient coupling is accomplished with a normal adiabatic taper. An absorption spectrum with a peak at 3.3  $\mu m$  is detected with a MIR InSb camera, which aligns closely with the reference methane gas absorption from NIST.

##### **2:10 PM**

#### **(GOMD-S3-050-2016) Development of micro-components for infrared integrated optics applications based upon Ge-Se-Te films (Invited)**

C. Vigreux<sup>1</sup>; A. Pradel<sup>\*1</sup>; 1. universit  de Montpellier, France

Development of micro-components for IR integrated optic devices requires the elaboration of IR waveguides. Amorphous chalcogenide films from the Ge-Se-Te system are well suited to such development. Depending upon the aimed application, films with different Se content in the films can be used. In the talk, we will present the development of two different types of waveguides: optical structures, such as straight or S-bend waveguides, spirals, Y-junction or Mach-Zehnder interferometer for further development as environmental sensors were prepared by stacking and further etching of the films with compositions lying in the Se-rich (> 60 at. %) region and Ge content of about 25 at. %. When a high transmission region up to 20 microns was required for the development of a modal filter to be a part of a spatial interferometer the use of pure Ge-Te films has been mandatory.

##### **2:40 PM**

#### **(GOMD-S3-051-2016) Electro spraying of chalcogenide glass films to direct print gradient refractive index coating**

S. Novak<sup>\*1</sup>; C. Li<sup>1</sup>; P. Lin<sup>3</sup>; C. Lumdee<sup>1</sup>; W. Deng<sup>4</sup>; P. G. Kik<sup>1</sup>; J. Hu<sup>2</sup>; A. Agarwal<sup>2</sup>; K. Richardson<sup>1</sup>; 1. University of Central Florida, USA; 2. Massachusetts Institute of Technology, USA; 3. Texas A&M University, USA; 4. Virginia Tech, USA

Chalcogenide glasses (ChGs) are well-known for their optical properties, making them ideal candidates for emerging applications of mid-infrared microphotonic devices, such as lab-on-a-chip chemical sensors, which currently demand additional flexibility in processing and materials available to realize new device designs. This work has evaluated electro spray as an alternative method of chalcogenide glass film deposition, due to the unique advantages of electro spray over traditional ChG film deposition techniques such as spin-coating and thermal evaporation. In particular, electro spray allows localized depositions, allowing the possibility of 2-D and 3-D printing. In this work, knowledge of processing protocols was exploited to fabricate multi-layer films from two different glass compositions to yield an effective refractive index gradient (GRIN). Such a film could theoretically be utilized to create an array of microresonators with a wide variation in resonances due to the variation in refractive index. Optical properties of importance to device applications were defined, including surface roughness, refractive index profile, and infrared transmission. The use of a serpentine path of the spray over the substrate was also demonstrated to obtain uniform thickness, blanket films, and demonstrates process compatibility with roll-to-roll processing.

##### **3:00 PM**

#### **(GOMD-S3-052-2016) Influence of light flux and photon energy on photostructural evolution in thermally deposited As-S thin films**

J. R. Oelgoetz<sup>\*1</sup>; J. Allen<sup>1</sup>; C. Thomas<sup>1</sup>; L. R. Nichols<sup>1</sup>; J. Buzek<sup>2</sup>; M. Vlcek<sup>2</sup>; R. Golovchak<sup>1</sup>; H. Jain<sup>3</sup>; A. Kovalskiy<sup>1</sup>; 1. Austin Peay State University, USA; 2. University of Pardubice, Czech Republic; 3. Lehigh University, USA

Thermally deposited chalcogenide glass thin films (ChGF) exhibit photo-induced effects under irradiation. The mechanism of these transformations is quite complex and includes photostructural relaxation, bond switching and defect formation processes both on the surface and inside of ChGF. The efficiency of light-induced structural changes in ChGF strongly depends on the wavelength of incident light and connectivity of glass backbone. The goal of this work is to relate kinetics of photoinduced shift of optical absorption edge with the evolution of photostructural transformations of different As-S compositions. In-situ Raman microscopy is used to control the relative change in intensities of appropriate bands

under irradiation with light of different energies and fluxes. This method utilizes confocal microscope to be able to measure Raman spectra in micron-size areas and depth profiling, allowing the analysis of several hundred nm thick thin films directly on the substrate. Optimized irradiation conditions, which minimize structural instability in ChGF are determined for different compositions. Models of photoinduced structural evolution for different irradiation conditions are presented. The Raman microscopy data are compared with photoinduced structural transformations on the surface of the film obtained by high-resolution X-ray photoelectron spectroscopy.

### Session 5: Glass-Ceramics and Optical Ceramics III

Room: University C/D

Session Chair: Woohong (Rick) Kim, Naval Research Laboratory

#### 1:20 PM

##### (GOMD-S3-053-2016) Transparent Ceramics for Laser Materials (Invited)

W. Kim<sup>\*1</sup>; C. Baker<sup>1</sup>; G. Villalobos<sup>1</sup>; J. Frantz<sup>1</sup>; B. Shaw<sup>1</sup>; S. Bowman<sup>1</sup>; L. Busse<sup>1</sup>; S. Bayya<sup>1</sup>; M. Hunt<sup>1</sup>; B. Sadowski<sup>2</sup>; I. Aggarwal<sup>2</sup>; J. Sanghera<sup>1</sup>; 1. Naval Research Laboratory, USA; 2. Sotera Defense Solutions, USA

High energy laser (HEL) systems typically require an efficient, high power, and compact laser gain media that is protected from harsh environments with rugged transparent windows as the output aperture of the system. The presence of trace amounts of transition metals or impurities in window or gain media will result in catastrophic failure of the system due to localized heat generated by absorption of the high power laser. We have developed various optical ceramic materials for ideal exit window apertures and laser gain media to satisfy the strict requirements needed for HEL applications. These successes are mainly due to our novel material synthesis and purification methods combined with unique and well-established sintering technologies developed in our laboratory. Here, we review various powder synthesis and purification methods as well as post-process techniques to provide an efficient route to obtain low optical loss ceramics that are desirable for scaling to high power lasers. We also demonstrate a draw of small diameter single crystal fibers suitable for high power fiber lasers using these high quality ceramics as seed materials. Finally, we present results for antireflective surface structures (ARSS) fabricated directly onto the surface of various substrates including transparent ceramics, single crystals, and glasses. Very low reflection losses and high laser damage thresholds have been demonstrated for these optics with ARSS.

#### 1:50 PM

##### (GOMD-S3-054-2016) Fabrication of Re:YAG transparent ceramics for laser application (Invited)

X. Chen<sup>1</sup>; T. Lu<sup>2</sup>; Y. Wu<sup>\*1</sup>; J. Qi<sup>2</sup>; 1. Alfred University, USA; 2. Sichuan University, China

Transparent YAG ceramics have become an attractive alternative material for high-power, high efficiency solid-state lasers due to their favorable characteristics, including the ability to accommodate high concentrations of dopants, increased design freedom, easy manufacture, low cost, and significantly superior optical and thermal properties. Due to the sophisticated fabrication techniques and advanced equipment required to process transparent ceramics, in addition to the fact that the materials are still not completely understood, there are still some problems to be solved in the fabrication, property characterization, and application of transparent laser ceramics. We have performed both theoretical and experimental research concerning the sources of optical loss in transparent laser ceramics, including pores, grain boundaries, color centers, etc. In pursuit of this research, we have solved some of the key scientific problems in the laser ceramic field. We have determined and illustrated the diffusion routes of two sintering aids (e.g., Si<sup>4+</sup> and Mg<sup>2+</sup>) in the YAG structure using theoretical calculations, and have

subsequently revealed the mechanism and role of sintering aids in the sintering process.

#### 2:20 PM

##### (GOMD-S3-055-2016) Fabrication of high-quality magneto-optical TAG transparent ceramics (Invited)

S. Zhou<sup>\*1</sup>; Y. Tang<sup>1</sup>; X. Yi<sup>1</sup>; D. Hao<sup>1</sup>; S. Zhang<sup>1</sup>; 1. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, China

Terbium aluminum garnet Tb<sub>3</sub>Al<sub>5</sub>O<sub>12</sub> (TAG) single crystal is an excellent magneto-optical material with good transmittance in the 500-1500nm region, high thermal conductivity, and higher Verdet constant than the most commonly used terbium gallium garnet Tb<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> (TGG) single crystal. However, it is extremely difficult to grow TAG single crystal from the melt because of its incongruent melting nature. TAG transparent ceramics not only remain the excellent magneto-optical property of TAG crystal, but also can realize large size growth. In this work, (Tb<sub>1-x</sub>R<sub>x</sub>)<sub>3</sub>Al<sub>5</sub>O<sub>12</sub> (R=Ce, Si, Ti) transparent ceramics were synthesized by solid state reaction and vacuum sintering. Effect of additions on TAG transparent ceramic was characterized by XRD, SEM, transmittance spectra and the performance measurements. The Verdet constant of the Ce<sup>3+</sup> doped TAG transparent ceramic measured at 632.8nm was -199.55 rad.T<sup>-1</sup>.m<sup>-1</sup>, which was larger than that of the pure TAG transparent ceramic (-172.8 rad.T<sup>-1</sup>.m<sup>-1</sup>), Si:TAG (-173.4 rad.T<sup>-1</sup>.m<sup>-1</sup>) and Ti:TAG (-184.2 rad.T<sup>-1</sup>.m<sup>-1</sup>). The Ti-doping has an obvious effect on controlling average grain size, homogenizing grain size, and eliminating pores, and therefore Ti:TAG has the highest transmittance (81% in the region of 550nm-1500nm).

#### 2:50 PM

##### (GOMD-S3-056-2016) Synthesis and Characterization of Calcium Lanthanum Sulfide using a Wet Chemistry Route

Y. Li<sup>\*1</sup>; Y. Wu<sup>1</sup>; 1. Alfred University, USA

Calcium lanthanum sulfide (CaLa<sub>2</sub>S<sub>4</sub>) has been extensively studied as a promising candidate for advanced infrared optical ceramics. In the present research, we report a successful synthesis of CaLa<sub>2</sub>S<sub>4</sub> via a wet chemistry method followed by thermal decomposition. The CaLa<sub>2</sub>S<sub>4</sub> precursors were first prepared by a facile ethanol-based wet chemistry route. The CaLa<sub>2</sub>S<sub>4</sub> precursors were subsequently thermally decomposed in argon at high temperature, producing CaLa<sub>2</sub>S<sub>4</sub>. The phase composition and morphology of the processed powders were confirmed and observed by X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM), respectively, to investigate the influence of different stoichiometries. Surface area and pore size analyses of the powders were conducted by applying Brunauer-Emmett-Teller (BET) and Barrett-Joyner-Halenda (BJH) methods, respectively. Spectroscopic characterization was performed to correlate the optical properties of the synthesized materials with the characteristics of the CaLa<sub>2</sub>S<sub>4</sub> powders.

#### 3:10 PM

##### (GOMD-S3-057-2016) Computed radiography at keV and MeV energies using glass-ceramic imaging plates

R. L. Leonard<sup>1</sup>; A. Evans<sup>\*1</sup>; A. Moses<sup>2</sup>; L. Arrowood<sup>2</sup>; A. Lubinsky<sup>3</sup>; J. Johnson<sup>1</sup>; 1. University of Tennessee Space Institute, USA; 2. Consolidated Nuclear Security, LLC, USA; 3. SUNY Stony Brook, USA

High energy x-rays are advantageous in certain radiography applications for nondestructive testing (NDT), where a large penetration depth is desired. Glass-ceramic imaging plates for computed radiography (CR) with high transparency at the stimulating laser wavelength, may have a relatively thick cross-section for more efficient absorption of the high energy x-rays, with very little reduction in spatial resolution. The authors discuss their most recent findings using fluorochlorozirconate-based glass-ceramic imaging plates for CR at x-ray energies up to 9 MeV. Representative radiographs, as well as results for modulation transfer frequency, determined from edge phantom images, will be presented.

## Symposium 4: Glass Technology and Cross-Cutting Topics

### Session 2: Liquid Synthesis and Sol-gel-derived Materials II

Room: Capitol B

Session Chair: Gregory Beaucage, University of Cincinnati

1:20 PM

#### (GOMD-S4-056-2016) Sol-gel derived Yb:YAG ceramics for high-power thin disk lasers (Invited)

R. M. Almeida<sup>\*1</sup>; 1. Instituto Superior Técnico, ULisbon, Portugal

The thin disk laser concept enables good thermal management and high beam quality in diode pumped high power lasers having an Yb-doped YAG single crystal as the active material. Sol-gel processing is a possible alternative technique to prepare a similar but polycrystalline active material at a lower cost. The present work describes the preparation of YAG ( $Y_3Al_2O_{12}$ )-matrix polycrystalline ceramics, doped with a wide range of Yb concentrations (from 0 to 100 at%Yb), by a spin-coating sol-gel method using a combination of acetate and alkoxide precursors. The samples with different Yb concentrations were first characterized by X-ray diffraction to ensure that the cubic YAG phase was obtained, which was confirmed by Spectroscopic Ellipsometry in terms of its refractive index. Structural characterization was also done by means of infrared (FTIR) and Raman spectrometries, in order to follow the continuous replacement of  $Y^{3+}$  by  $Yb^{3+}$  in the YAG structure. Finally, photoluminescence (PL) characterization was carried out by exciting the  $Yb^{3+}$  ions with a 967 nm laser diode, together with measurement of the  $Yb^{3+}$  excited state lifetimes. Using Er co-doping to provide an internal standard, the absolute intensities of the PL peaks of  $Yb^{3+}$  were compared and the optimum Yb concentration for maximum PL efficiency was determined based on a figure of merit defined as: (PL peak cross section)  $\times$  (PL lifetime).

1:50 PM

#### (GOMD-S4-057-2016) Collidal Silica Coatings for Textile Protection

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The goal of this research is to rapidly deposit thermal protection coatings onto polymer fibers. This is achieved by mixing colloidal silica and dilute aqueous  $CaCl_2$ , and dragging the fibers through the sol. The focus is on polymer filaments, such as polyethylene terephthalate (PET), polyamide, and Nylon 6.12. Pretreating the filaments in a detergent solution improves the uniformity of the coatings. Slow drying in water saturated air reduces the tendency to crack. Generally, the coatings increase the filament diameter by about 10% and increase the weight by 5%. The coated fibers retain their flexibility. They are visually crack-free and shiny, and the surfaces are hydrophobic. Tape tests indicate good adhesion after drying. The coatings are designed to increase the heat resistance of the polymers and to extend their lifetime in char tests.

2:10 PM

#### (GOMD-S4-058-2016) Boria Effects on High Temperature Silicon Carbide Oxidation: Comparison of Sol-Gel Derived and Thermally Grown Borosilicate Glass Films

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Ceramic matrix composite (CMC) components will be introduced into civilian aircraft engines next year. Composites comprised of silicon carbide (SiC) fibers coated with a boron nitride (BN) layer embedded in a SiC matrix will oxidize into thermally grown borosilicate glass if exposed to the high temperature combustion environment. Excessive oxidation will lead to CMC degradation, but little is known about the thermally grown borosilicate glass composition or structure. The goal of this work is to compare

well-characterized sol-gel derived borosilicate glass films to thermally grown borosilicates formed in high temperature oxidation studies conducted between 800 – 1300°C. Sol-gel derived borosilicate glass coatings of defined boria concentration and less than 1  $\mu m$  thickness were applied onto SiC substrates to understand the effects of boria on SiC oxidation. Additionally, free-standing glasses were cast and both films and glasses were extensively characterized for composition, bonding, and phase by elemental quantification, vibrational spectroscopy, and x-ray analysis techniques. Finally, boron-containing SiC substrates were oxidized and characterized by similar techniques. Oxygen transport through sol-gel derived and thermally grown borosilicate glasses will be compared.

2:30 PM

#### (GOMD-S4-059-2016) Sol-Gel Synthesis and Characterization of Annealed Pyrolytic Graphite/Sodium Borosilicate Glass Composites

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Sodium borosilicate (NBS) glass composites with up to 40wt% of annealed pyrolytic graphite (APG) have been fabricated through a sol-gel process. A sol-gel process was chosen, as the aqueous precursors afforded the opportunity to first establish a dispersion of APG in solution via ultrasonication and subsequently form a network around the dispersion. APG was dispersed in a precursor solution to yield a composite with a glass matrix of 80wt%  $SiO_2$ , 15wt%  $B_2O_3$ , and 5wt%  $Na_2O$ . A variety of gels with increasing weight percentages of APG were produced with subsequent heat treatments to facilitate gelation, condensation, drying, and aging. Gels were then hot pressed under vacuum to yield fully dense, homogeneous glass. Density and CTE values, X-Ray diffraction patterns, and FT-IR spectra for both unloaded and APG-loaded sol-gel derived NBS glass have been consistent with those of its traditional melt-quenched counterpart. Sol-gel-derived NBS with 25wt% APG was found to have an in-plane thermal conductivity of  $25 \pm 1 W/mK$ , and the APG-loaded samples hold promise for enhanced electrical conductivity, as the high aspect ratio of APG encourages the formation of percolating networks within the glass matrix.

2:50 PM

#### (GOMD-S4-060-2016) Free Carbon embedded in Silicon Oxycarbide Glass: an Analysis of Experimental and Computational <sup>29</sup>Si NMR Data

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We analyze experimental <sup>29</sup>Si NMR spectra of amorphous silicon oxycarbide (SiCO) materials synthesized via the sol-gel or polymer route and annealed at 1000-1100°C. The samples vary in composition, but can be described as stoichiometric (SiC-SiO<sub>2</sub>) glass matrix into which “free” graphite-like carbon is dispersed. NMR data shows characteristic broad peaks corresponding to mixed  $\{Si\}C_xO_{(4-x)}$  tetrahedra in the glass matrix. While the dominant  $\{Si\}O_4$  peak is located around -108 ppm, careful analysis and fitting of the high field chemical shifts indicate a residual signal between -130 and -150 ppm. The integrated intensity of the residual peak correlates linearly to the amount of “free” carbon in the SiCO glass. Based on a relation between NMR shift and Si-O-Si bond angle distribution, we relate the residual peak to wide Si-O-Si angles (average  $>160^\circ$ ) surrounding Si nuclei. Similar signals are found in zeolites for Si atoms at internal surfaces. While “free” carbon promotes an open porous structure of SiCO materials, we find no evidence of bonding between “free” carbon and SiCO glass. DFT GIPAW calculations indicate a substantial shift of the  $\{Si\}CO_3$  peak if bonding between Si and  $sp^2$ -like C exists. From the absence of such a signal we conclude that the “free” carbon phase in SiCO is embedded into the glass matrix inside voids or cages without substantial bonding to the glass.

\*Denotes Presenter

# Author Index

\* Denotes Presenter

<b>A</b>	
Aaldenberg, E.*	56
Abu Jeib, H.	42, 58
Adam, J.	24
Adamietz, F.	42, 84
Adhikari, P.	65
Adhikari, P.*	65
Affatigato, M.	39, 42, 44, 78, 80
Agarwal, A.	87
Aggarwal, I.	88
Agnello, G.*	32
Ahmadzadeh, M.	40
Aiken, S.	84
Aitken, B.	81
Aitken, B.*	80
Akgun, U.	41
Akola, J.*	73
Al Sayoud, A.	45
Alam, T. M.*	53
Albaret, T.	74
Alderman, O. L.	63
Alderman, O. L.*	64
Ali, S.*	67
Allan, D. C.	52
Allen, J.	87
Almeida, R. M.*	89
Ambrosone, A.	23
Ammar, M.	78
Anderson, M. A.*	85
Angeli, F.	50
Arrowood, L.	88
Asaduzzaman, A.	70
Asmussen, M.	33
<b>B</b>	
Backhouse, D. J.	37
Bado, P.*	30
Bai, J.	33
Bai, J.*	37
Bailey, B.	78
Baker, B.	44
Baker, C.	88
Baker, S.	57
Baker, S. P.*	57
Bakowska, E.	60
Balabajew, M.	45
Baldi, G.	36
Baleine, C. R.*	84
Ballato, J.	23, 41, 78
Ballato, J.*	23
Baltisberger, J.	53
Banerjee, J.	64
Baral, K.*	65
Barlow, S. T.	26
Barney, E.	33, 39
Barthel, E.	75
Barthel, E.*	74
Bauchy, M.	39, 42, 60, 66, 68, 74, 78, 82
Bauchy, M.*	55, 82
Bayya, S.	88
Beall, G.	80
Beasley, M.	63
Beaucage, G.*	86
Behrens, H.	52
Bellouard, Y.*	24
Bénard-Rocherullé, P.	48
Benmore, C. J.	63, 64
Beresna, M.	30
Besser, M.	37
Bhattacharai, B.	39
Bhattacharai, B.*	58
Bichara, C.	73
Bielawski, A.	77
Bingham, P. A.	33
Birnie, D. P.*	50
Bista, S.*	82
Biswas, P.	40, 59
Biswas, P.*	58
Bitzek, E.	54
Blanchet, T.	56
Bliss, M.	28
Boechler, N.	36
Boero, M.	48, 55, 73, 76
Boero, M.*	64
Boetti, N.	23, 24
Bohach, G.	42
Boioli, F.*	74
Bokas, G.	73
Bokas, G.*	73
Boller, E.	82
Bonham, C. C.	28
Boolchand, P.	72
Bormuth, A.	54
Bouttes, D.	82
Bouzid, A.	55
Bouzid, A.*	59, 76
Bowman, S.	88
Brauer, D. S.*	29
Brilland, L.	24
Brito, A.	22
Brow, R.	33, 37, 47, 56, 84
Brown, D. P.	79
Brückner, R.	29
Bruener, P.	31
Brun, M.	24
Bryce, D.	69
Buff, A.	84
Bungay, C.	84
Bureau, B.	43, 87
Burov, E.	26, 82
Burov, E.*	63
Busse, L.	88
Buzek, J.	87
<b>C</b>	
Cagnoli, G.	71, 86
Caillaud, C.	24
Calas, G.	50
Calas, G.*	72
Calvert, P.*	61
Camuri Crovace, M.	39
Canfield, N. L.	28
Canizares, A.	78
Cao, Y.*	85
Capobianco, N.	72
Cardinal, T.	83, 84
Carras, M.	24
Cassar, D. R.	69
Cassar, D. R.*	52
Cavillon, M.*	23
Ceci-Ginistrelli, E.	23, 24
Célaríé, F.	74
Celik, H.	29
Cerkauskaite, A.	30
Chabinyk, M. L.	64
Chapman, C. L.	83
Chapman, C. L.*	32
Charleux, L.	74
Chass, G.*	47
Chbeir, R.	72
Chen, G.	39, 42, 85
Chen, G.*	58
Chen, S.	29, 31
Chen, W.*	46
Chen, X.	88
Chen, Y.	37, 70
Chen, Y.*	38
Cheng, J. Y.*	38
Chenu, S.	48
Chevreur, P.*	33
Chin, A.	89
Ching, W.	65
Ching, W.*	67
Chokshi, T.	30
Chopinot, M.	26
Christine, M.	71, 86
Chua, Y.	63
Cicconi, M.	72
Ciccotti, M.*	62
Cleri, F.	55
Coasne, B.	73, 86
Coleman, G.	36, 87
Collin, M.	50
Conrad, R.	25, 48, 66
Conrad, R.*	26
Copenhaver, K. E.*	89
Corkhill, C. L.*	26, 37
Cormack, A.	32
Cormier, L.	72
Cormier, L.*	78
Coulet, V.	73
Crawford, C. L.	34
Crawford, C. L.*	34
Crego, A.	39
Criscenti, L.*	46
Crum, J. V.	60
Cuello, G.	73
Curtis, B.*	49
Cushman, C. V.	31
Czaja, A.	72
<b>D</b>	
Dalal, S. S.	71
Damart, T.*	54
Darnell, L. P.	28
Dasmahapatra, A.	65
Dasmahapatra, A.*	55
Davies, J. R.	28
Davis, M. J.*	78
Day, D. E.	30, 44
Day, D. E.*	22
de Camargo, A.	54, 83
de Ligny, D.*	72
de Oliveira, M.*	54
Dejneka, M.*	80, 83
DeLamielleure, M.	32
Delaye, J.	65
Deloule, E.	33
Deng, Q.	85
Deng, W.	87
Desgranges, L.	78
Deshkar, A.	69
DesJardin, R. P.	75
Dettmann, M.	41
Deubener, J.*	35, 52
Deymier, P.	36, 45
Dharmawardhana, C. C.	65
Diaz Cuenca, A.	29
Dierolf, V.	25
Dixon, D.*	27
Dolekcekic, E.*	29
Dolique, V.	71, 86
Dong, G.*	25

Dongol, R. .... 41  
 Dongol, R.\* ..... 56  
 Dousti, M.\* ..... 83  
 Doyle, W. F.\* ..... 61  
 Drabold, D. .... 39, 40, 58, 59  
 Drabold, D.\* ..... 58  
 Dragic, P. .... 23  
 Drevinskas, R. .... 30  
 Drossel, B. .... 54  
 Du, J. .... 42, 59, 60  
 Du, J.\* ..... 46  
 Du, Q. .... 83, 84  
 Dubernet, M. .... 74  
 Ducasse, T. .... 50  
 Dugan, M. .... 30  
 Dumitrica, T. .... 55  
 Duran, C. A.\* ..... 32  
 Dussauze, M. .... 42, 83, 84  
 Dutra Zanotto, E. .... 39, 52, 69, 81  
 Dutra Zanotto, E.\* ..... 35  
 Dutreilh-Colas, M. .... 78  
 Dutta, I. .... 80  
 Dutta, I.\* ..... 81  
 Duval, F. .... 78  
 Dylla-Spears, R. J. .... 75

E

Ebert, W.\* ..... 34  
 Eckert, H. .... 54  
 Eckert, H.\* ..... 44  
 Edem, M.\* ..... 47  
 Ediger, M. D. .... 40, 41, 63, 64, 70, 71  
 Ediger, M. D.\* ..... 51, 77  
 Edwards, A. .... 45  
 Elhadj, S. .... 75  
 Elia, A. .... 34  
 Elisberg, B. .... 45  
 Elodie, C. .... 71, 86  
 Enz, P. A. .... 38  
 Errapart, A. .... 75  
 Eskelsen, J. R. .... 60  
 Evans, A.\* ..... 88  
 Ewsuk, K. .... 45, 46, 53

F

Fabes, B.\* ..... 51  
 Fabris, L. .... 85  
 Falk, M. .... 30  
 Fang, H. .... 70  
 Fargin, E. .... 83  
 Fedotova, I. .... 36  
 Feit, M. D. .... 75  
 Feller, S. .... 39, 42, 44, 78  
 Fernandes, R. G.\* ..... 40  
 Ferrand, K. .... 34  
 Ferraris, M. .... 36  
 Ferre, S. .... 24  
 Ferreira, E. B. .... 40  
 Ferreira, E. B.\* ..... 35  
 Ferreira, J. M. .... 81  
 Ferreira, J. M.\* ..... 22  
 Fett, T. .... 56  
 Fischer, C. .... 27  
 Fisher, A. J. .... 26  
 Flores-Ruiz, H. .... 73  
 Florian, P. .... 53  
 Foret, M. .... 86  
 Foret, M.\* ..... 69  
 Fotso Gueutue, E. .... 78  
 Fragoso, T. D. .... 52  
 Francis, C. .... 42  
 Frantz, J. .... 88  
 Freudenberger, P. .... 84

Freudenberger, P.\* ..... 47  
 Fu, Q.\* ..... 80  
 Fujinami, M. .... 75  
 Fukunishi, T. .... 67

G

Gaddam, A.\* ..... 81  
 Gaerke, D. A.\* ..... 26  
 Galois, L. .... 72  
 Galois, L.\* ..... 50  
 Gan, Z. .... 77  
 Ganguly, J. .... 70  
 Ganisetti, V.\* ..... 54  
 Gao, P. .... 32  
 Garg, K. .... 40  
 Gasnier, E. .... 27  
 Geiger, S. .... 83  
 George, J.\* ..... 27  
 Geske, J. .... 54  
 Giboire, I.\* ..... 27  
 Gilles, C. .... 24  
 Gin, S. .... 50  
 Gin, S.\* ..... 50  
 Gleason, B. .... 84  
 Goel, A. .... 38, 40  
 Goel, A.\* ..... 69  
 Golovchak, R. .... 30, 43, 87  
 Gomez, J. .... 64  
 Gonçalves, T. .... 54  
 Gong, Y.\* ..... 32, 41, 50  
 Goto, T. .... 84  
 Gouillart, E. .... 63  
 Gouillart, E.\* ..... 26, 82  
 Goyal, S. .... 82  
 Grandinetti, P. .... 53  
 Greasley, S. L. .... 29  
 Greaves, N. .... 46, 47  
 Grehl, T. .... 31  
 Griffin, B. .... 79  
 Griscom, D. L.\* ..... 22  
 Gross, T. M.\* ..... 57  
 Gueguen, Y.\* ..... 74  
 Guillonéau, G. .... 74  
 Guimarães dos Santos, G.\* ..... 39  
 Guin, J. .... 74  
 Gujral, A. .... 41  
 Gujral, A.\* ..... 64  
 Gulbiten, O. .... 80  
 Gulbiten, O.\* ..... 45  
 Guo, W. .... 36  
 Guo, X. .... 31, 45, 62  
 Gupta, P.\* ..... 45, 69

H

Hakanson, K. .... 42  
 Hamilton, J. .... 32, 60  
 Hammann, B. A. .... 53  
 Han, B. .... 85  
 Han, Z.\* ..... 87  
 Hand, R. J. .... 37  
 Hannon, A. C. .... 33  
 Hannon, A. C.\* ..... 64  
 Hao, D. .... 43, 88  
 Harms, J. .... 30  
 Harrison, M. T.\* ..... 27  
 Hashida, Y. .... 84  
 Hassani, H. .... 75  
 Hauke, B.\* ..... 39  
 Hawkins, T. .... 23  
 Hay, R. S. .... 79  
 Hayashi, K. .... 58  
 He, L. .... 52  
 Heald, S. .... 64

Hehlen, B. .... 65, 69  
 Heilmaier, M. .... 67  
 Hennes, L. .... 78  
 Henritzi, P. .... 54  
 Hernandez-Rueda, J. .... 24  
 Herrig, V. .... 41  
 Higo, Y. .... 66  
 Hodge, T. L.\* ..... 43  
 Hoffmann, M. .... 56  
 Holbrook, C.\* ..... 72  
 Honma, T. .... 57, 80  
 Hopf, J. .... 60  
 Hou, J. .... 31  
 Houizot, P. .... 74  
 Hoyt, M. R.\* ..... 38  
 Hrma, P. .... 27  
 Hsu, J. .... 33, 37  
 Hsu, J.\* ..... 33  
 Hu, G. .... 35, 75  
 Hu, J. .... 83, 87  
 Hu, J.\* ..... 84  
 Huang, C. .... 41, 64  
 Huang, L. .... 35, 47  
 Huang, L.\* ..... 81  
 Huang, Q.\* ..... 85  
 Hubert, M.\* ..... 26, 33  
 Hughes, K. .... 31  
 Humble, G. .... 30  
 Humble, G.\* ..... 44  
 Hunault, M. .... 72  
 Hung, I. .... 77  
 Hunt, M. .... 88  
 Hupa, L. .... 29  
 Hyatt, N. C. .... 26, 37  
 Hynek, D.\* ..... 42

I

Icenhower, J. P.\* ..... 49  
 Ikeda, H. .... 47  
 Ingram, D. .... 58  
 Inoue, H. .... 66  
 Inoue, H.\* ..... 46  
 Ionescu, E.\* ..... 67  
 Ishikawa, T. .... 66  
 Ispas, S. .... 74  
 Ispas, S.\* ..... 65  
 Ito, K. .... 75  
 Ito, S. .... 75

J

Jacobsohn, L. .... 41  
 Jaffe, M.\* ..... 61  
 Jain, H. .... 25, 43, 45, 87  
 Jain, H.\* ..... 30  
 Jamison, R. .... 45  
 Janicek, P. .... 24  
 Jantzen, C. M. .... 34  
 Jantzen, C. M.\* ..... 34  
 Jean, J. .... 67  
 Jegou, C. .... 78  
 Jerden, J. .... 34  
 Jia, X. .... 83  
 Jiang, J. .... 64  
 Jiang, S. .... 87  
 Jiang, S.\* ..... 24  
 Jin, T.\* ..... 28  
 Jin, Y. .... 31  
 Jitianu, A. .... 85  
 Johnson, J. .... 88  
 Johnson, K. E.\* ..... 40  
 Johnson, M. .... 73  
 Johnson, N. D. .... 71  
 Johnson, N.\* ..... 57

\*Denotes Presenter

# Author Index

Jollivet, P. ....	50
Jones, J. ....	28, 29
Jones, J.* ....	22
Jones, M. ....	23
Ju, Q. ....	28
Jumpertz, L. ....	24

## K

Kallontzi, S. ....	85
Kamitsos, E. I. ....	72
Kang, M. ....	84
Kaseman, D. C.* ....	76
Kaur, G. ....	40
Kaur, N.* ....	40
Kazansky, P. G. ....	30
Keizer, S. ....	42
Kermouche, G. ....	74
Keryvin, V.* ....	74
Khanolkar, A. ....	36
Kieffer, J. ....	86
Kieffer, J.* ....	70, 77
Kielty, M. W.* ....	41
Kik, P. G. ....	87
Kilymis, D. A. ....	65
Kim, B. ....	32
Kim, C. ....	33, 37
Kim, C.* ....	33
Kim, D. ....	27, 28
Kim, D.* ....	28
Kim, H.* ....	41, 79
Kim, J.* ....	32
Kim, S. H. ....	64, 71
Kim, S. H.* ....	31
Kim, W.* ....	88
Kimerling, L. C. ....	87
King, E. A.* ....	52
Kirk, A. ....	84
Klameth, F. ....	54
Kleebe, H. ....	67
Klein, L. C.* ....	61, 85, 89
Klotz, J. ....	60
Kmiec, S. ....	42
Kob, W. ....	47
Kob, W.* ....	44
Kobera, L. ....	69
Komatsu, T. ....	57, 80
Kopatz, J. ....	31
Kordesch, M. ....	58
Kotaka, M. ....	80
Kovalskiy, A. ....	87
Kowal, T. ....	30
Kramer, D.* ....	31
Kramer, M. ....	37
Krol, D.* ....	24
Kroll, P. ....	55, 65
Kroll, P.* ....	65, 89
Kruger, A. A. ....	27, 28
Krüger, S. ....	35
Kuang, Y. ....	59
Kucera, C. ....	23
Kumar, A. ....	60
Kumar, V. ....	40
Kundu, S. ....	81
Kuo, P.* ....	42
Kurkjian, C. R. ....	75

## L

LaComb, M. M.* ....	53
LaCourse, W. ....	32
Lakshmikantha, S.* ....	38
Lamberson, L. ....	57
Lampin, E.* ....	55
Langevin, G.* ....	79

Laplace, A. ....	33
Lebullenger, R. ....	48
Ledemi, Y. ....	83
Lee, H.* ....	79
Lee, S. ....	41
Lee, S.* ....	69
Lelong, G. ....	72, 78
Lemmens, K.* ....	34
Leonard, D. N. ....	60
Leonard, R. L. ....	88
Lepicard, A.* ....	42, 84
Lepry, W. C.* ....	28
Letz, M.* ....	80
Li, A. ....	60
Li, A.* ....	31
Li, C. ....	87
Li, L. ....	76
Li, L.* ....	51, 83
Li, N.* ....	65
Li, S. ....	55
Li, Y. ....	79
Li, Y.* ....	39, 88
Lin, H. ....	83
Lin, P. ....	87
Linford, M. R.* ....	31
Lingner, J. ....	80
Liu, J. ....	60
Liu, S. ....	34
Liu, Y. ....	83
Liu, Y.* ....	39, 85
Liu, Z. ....	52
Locker, S. T.* ....	25
Loneragan, J. M.* ....	77
Lonnroth, N.* ....	81
Lopez Iscoa, P. ....	36
Lotarev, S. ....	30
Lousteau, J. ....	23
Lousteau, J.* ....	24
Louzada Neto, F. ....	52
Love, C. ....	44
Lu, T. ....	88
Lu, X.* ....	42, 60
Lubinsky, A. ....	88
Lucas, P.* ....	36, 45, 87
Lukins, C. D. ....	27
Luksic, S. A.* ....	27
Lumdee, C. ....	87
Lunt, B. M. ....	31
Luo, J. ....	35, 71
Luo, J.* ....	64, 75
Luther-Davies, B. ....	36

## M

Ma, C. ....	85
Ma, L. ....	84
Mabrouk, A.* ....	86
Mack, M. ....	32
Magon, C. ....	54
Major, G. I. ....	31
Maldonis, J.* ....	37
Manley, R. ....	32
Marcial, J. ....	40, 69
Marple, M. A.* ....	77
Marques, A. C. ....	22
Martin, S. W. ....	38, 42, 49, 76, 78
Martin, S. W.* ....	48
Martinez, V.* ....	71, 86
Massera, J. ....	23, 36, 43
Massera, J.* ....	29
Massimo, G. ....	71, 86
Massobrio, C. ....	48, 55, 73, 76
Masuno, A. ....	46, 66
Masuno, A.* ....	66

Mathew, R. ....	47
Matsuoka, J. ....	67, 75
Matthewson, J. ....	38
Mattos, P. ....	81
Mauro, J. C. ....	39, 45, 52, 74, 75, 82, 86
Mauro, J. C.* ....	35, 62
Maw, Z. ....	66
Mayer, T. ....	84
McAnany, S.* ....	25
McClane, D. ....	77
McCloy, J. ....	34, 49, 69
McCloy, J.* ....	40, 62
McDonald, L.* ....	44
McFarland, B.* ....	89
McLaren, C.* ....	45
Mellott, N. ....	32, 41, 50
Mermet, A. ....	71, 86
Messaddeq, Y. ....	83
Miao, W. ....	79
Michler, J. ....	74
Micoulaut, M. ....	71
Micoulaut, M.* ....	68, 70, 73
Milanese, D. ....	24
Milanese, D.* ....	23, 36
Miller, A.* ....	79
Miller, P. E. ....	75
Mishra, A.* ....	23, 43
Misture, S. T. ....	32
Miyai, M. ....	75
Mohun, R. ....	78
Möncke, D.* ....	47, 72
Montorsi, M. ....	48
Montouillout, V. ....	27
Moore, G. ....	81
Moore, L. ....	80, 81
Morency, S. ....	83
Morin, E. I.* ....	53
Moses, A. ....	88
Müller, R. ....	52
Murakami, K. ....	67
Muralidharan, K. ....	45
Muralidharan, K.* ....	46, 70
Murphy, K. ....	60

## N

Nadler, J. ....	89
Naji, M. ....	77
Nakane, S. ....	47
Narayanan, M.* ....	39
Narisawa, M. ....	67
Naruphontjirakul, P.* ....	29
Nascimento, M. L. ....	52
Nazhat, S. N. ....	28
Neeway, J. ....	42, 49, 60
Neeway, J.* ....	33
Neill, L. M. ....	49
Neill, L. M.* ....	37, 50
Neill, O. K. ....	37
Neuefeind, J.* ....	63
Newman, R. ....	70
Ni, Y. ....	55
Nichols, L. R. ....	87
Nichols, L. R.* ....	44
Niessen, V. ....	25
Nimmo, J. P. ....	65, 89
Nishiyama, N.* ....	66
Nolan, D. ....	25
Norris, E. G.* ....	28
Novajra, G. ....	23
Novak, S.* ....	87

## O

O'Hara, K. A. ....	64
--------------------	----



Obata, A. ....	28	Reiser, J.* .....	49	Shen, Y.* .....	69
Oelgoetz, J. R. ....	44	Ren, H. ....	36	Sheth, N.* .....	71
Oelgoetz, J. R.* .....	87	Ribes, M. ....	48	Shi, Y. ....	35
Ogbuu, O. ....	83	Rice, D. M. ....	53	Shih, Y.* .....	63
Ohishi, Y.* .....	23	Rice, J. A.* .....	49	Shimotsuma, Y.* .....	30
Okhrimchuk, A. ....	30	Richardson, K. ....	42, 77, 84, 87	Shinozaki, K.* .....	57, 80
Olhero, S. H. ....	22	Riedel, R. ....	67	Shneidman, V. A.* .....	35
Onbasli, M. ....	84	Rimsza, J. M.* .....	59	Shpotyuk, Y. ....	43
Ono, M.* .....	75	Rino, J. P.* .....	46	Shugart, K. N. ....	79
Opila, E. ....	70, 89	Risbud, S. H. ....	40	Sibirkin, A. ....	36
Ori, G. ....	55, 76	Rizzi, G. ....	56	Sidebottom, D. ....	38
Ori, G.* .....	48, 73	Rocherullé, J. ....	23	Sidebottom, D.* .....	53
<b>P</b>					
Palla, P. ....	55	Rocherullé, J.* .....	48	Sigaev, V. ....	30
Pandey, A.* .....	40, 59	Rodney, D. ....	54, 74	Silva, B. C. ....	22
Pantano, C. G. ....	31, 49, 50, 64, 71, 84	Rodrigues, A. ....	81	Simon, P.* .....	78
Parise, J. B. ....	64	Rodrigues, A. M. ....	52	Singh, S.* .....	81
Parruzot, B. ....	49, 50	Rodriguez, V. ....	42, 84	Sisken, L. ....	84
Patel, A.* .....	30	Roling, B. ....	45	Sisken, L.* .....	84
Pellerin, N. ....	27, 86	Romero-Sanchez, L. ....	29	Siwei, L. ....	29
Perepezko, J. H. ....	38, 69	Ronchetto, E.* .....	56	Skinner, L. ....	63
Perepezko, J. H.* .....	69	Rosales Sosa, G. A.* .....	66	Skopak, T.* .....	83
Perret, A. ....	79	Rösner, H. ....	63	Smedskjaer, M. M. ....	57, 62, 86
Peterlechner, M. ....	63	Ross, C. ....	84	Smektala, F. ....	43
Peterson, I.* .....	32	Rossington, K. ....	26	Smith, C. ....	77, 80, 84
Petit, L. ....	36	Roth, J.* .....	78	Smith, N. J. ....	31
Pföss, B. S.* .....	48	Rouxel, T. ....	74	Smith, N. J.* .....	60
Philipps, K.* .....	66	Rouxel, T.* .....	57, 68	Soraru, G.* .....	67
Piarristeguy, A. ....	73	Ruan, S. ....	37	Sorenson, I.* .....	78
Pierce, E. M.* .....	60	Ruan, S.* .....	40	Southern, S. ....	69
Pierre, A. C.* .....	61	Rufflé, B. ....	69	Srivastava, D.* .....	53
Pignatelli, I. ....	60	Ruffle, B.* .....	86	Stabler, C. ....	67
Piovesan, V. ....	27	Runge, K. ....	46	Stebbins, J. ....	53, 82
Pizani, P. S. ....	54	Ryan, J. ....	33, 42, 49, 60	Stebbins, J.* .....	68
Pogrebnyakov, A. ....	84	Ryan, J.* .....	71	Steele, C. J. ....	27
Poirier, G. ....	83	Rygel, J.* .....	26	Steele, W. A. ....	75
Poletti, F. ....	24	<b>S</b>			
Polian, A. ....	69, 86	Sadowski, B. ....	88	Steltsova, E. ....	32
Ponomarev, I. ....	65	Said, A. ....	30	Stennett, M. C. ....	26
Ponomarev, I.* .....	65	Saitoh, A. ....	47	Stevensson, B. ....	47
Poologasundarampillai, G. ....	28	Saitoh, A.* .....	84	Strong, K. T.* .....	45
Poologasundarampillai, G.* .....	28	Saleh, M. ....	40	Sturgell, B. ....	31
Porter, A. E. ....	29	Salvo, M. ....	36	Subramanian, V.* .....	82
Powell, C. ....	70	Sanghera, J. ....	88	Sun, X. ....	84
Powell, C. T. ....	38	Sangleboeuf, J. ....	74, 79	Sun, Y. ....	40
Powell, C. T.* .....	70	Sant, G. ....	55, 60	Sundaram, S. K. ....	25, 41, 56
Pradel, A. ....	73	Savytsky, D.* .....	25	Sundararajan, M. ....	58
Pradel, A.* .....	48, 87	Schaut, R. ....	35, 60	Sundararajan, M.* .....	42, 85
Prange, A.* .....	25	Schaut, R.* .....	68	Sundararaman, S.* .....	47
Prasai, K. ....	58	Scherer, G. W.* .....	51	Suratwala, T. I.* .....	61, 75
Prasai, K.* .....	39, 59	Schick, C. ....	63	Suzuki, T. ....	23, 75
Priven, A.* .....	62	Schmidt, V.* .....	63	Svenson, M. N. ....	86
Provino, L. ....	24	Schnare, D. ....	32	Swisher, A. ....	84
Pugliese, D. ....	23, 24	Schreiber, D. ....	60, 71	Szabo, J. ....	33, 37
Pukhkaya, V. ....	75	Schroers, J. ....	52	Szlufarska, I. ....	73
<b>Q</b>					
Qi, J. ....	88	Schropp, R. E.* .....	59	<b>T</b>	
Qi, S. ....	36	Schweiger, M. J. ....	27, 28	Takebe, H. ....	47, 84
Qian, Q. ....	43	Schweizer, K.* .....	52	Talimian, A.* .....	76
Qiao, A. ....	78	Seaman, J. H. ....	56	Tamalonis, A. ....	64
Qiu, J. ....	25, 43, 76	Seaman, J. H.* .....	56	Tan, D. T. ....	87
<b>R</b>					
Raimboux, N. ....	78	Sekine, T. ....	75	Tandia, A. ....	56, 75
Raiturcar, N. ....	89	Sementa, L. ....	48	Tandia, A.* .....	54
Ranasinghe, K. S. ....	44	Sen, S. ....	76, 77	Tang, D. ....	36, 76
Ranasinghe, K. S.* .....	30	Sen, S.* .....	68	Tang, G.* .....	43
Raty, J. ....	71	Sendelbach, S. ....	64	Tang, Y. ....	88
Rehman, M. ....	40	Seward, T. P.* .....	50	Tang, Y.* .....	43
Reimanis, I. ....	79	Sglavo, V. M. ....	76	Tanguy, A. ....	54
Reiser, J. ....	37	Sglavo, V. M.* .....	75	Tao, G. ....	36
		Shadle, D. ....	42	Tarantino, G. ....	39
		Shashikala, H. ....	38, 39	Teerakapibal, R.* .....	41
		Shaw, B. ....	88	Teisseire, J. ....	74, 75
		Shen, N. ....	75	Thomas, C. ....	87
		Shen, Y. ....	69	Thomas, C.* .....	43
				Tietje, S. ....	68



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55 Cs 132.9054 Cesium	56 Ba 137.327 Barium	57 La 138.90547 Lanthanum	58 Ce 140.116 Cerium	59 Pr 140.90765 Praseodymium	60 Nd 144.242 Neodymium	61 Pm 144.9128 Promethium	62 Sm 150.36 Samarium	63 Eu 151.964 Europium	64 Gd 157.25 Gadolinium	65 Tb 158.92535 Terbium	66 Dy 162.5 Dysprosium	67 Ho 164.93032 Holmium	68 Er 167.259 Erbium	69 Tm 168.93421 Thulium	70 Yb 173.054 Ytterbium	71 Lu 174.967 Lutetium	
87 Fr 223 Francium	88 Ra 226 Radium	89 Ac 227 Actinium	90 Th 232.03756 Thorium	91 Pa 231.03688 Protactinium	92 U 238.02891 Uranium	93 Np 237 Neptunium	94 Pu 244 Plutonium	95 Am 243 Americium	96 Cm 247 Curium	97 Bk 247 Berkelium	98 Cf 251 Californium	99 Es 252 Einsteinium	100 Fm 257 Fermium	101 Md 258 Mendelevium	102 No 259 Nobelium	103 Lr 260 Lawrencium	

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