11th International Conference
on Bulk Metallic Glasses
(BMG XI)

PROGRAM and ABSTRACTS BOOKLET

June 5-9, 2016
Washington University in St. Louis, MO USA
BMG XI Organizing Committees

Organizing Co-Chairs:
Prof. K. F. Kelton - Washington University in St. Louis (USA)
Prof. K. M. Flores - Washington University in St. Louis (USA)
Prof. T. G. Nieh - University of Tennessee (USA)

International Advisory Committee:
Prof. Mingwei Chen - Tohoku University (Japan)
Prof. Jinn Chu - National Taiwan University of Science and Technology (Taiwan)
Prof. Jürgen Eckert - ESI Leoben (Austria)
Prof. Takeshi Egami - University of Tennessee / ORNL (USA)
Prof. A. L. Greer - University of Cambridge (UK)
Prof. A. Inoue - Josai International University (Japan) & Tianjin University (China)
Prof. W. L. Johnson - California Institute of Technology (USA)
Prof. C. T. Liu - City University of Hong Kong (Hong Kong, China)
Prof. Do Hyang Kim - Yonsei University (Korea)
Prof. Yi Li - Shenyang National Laboratory (China)
Prof. Jörg Löffler - ETH Zurich (Switzerland)
Prof. Evan Ma - Johns Hopkins University (USA)
Prof. T. G. Nieh - University of Tennessee (USA)
Prof. Jan Schroers - Yale University (USA)
Prof. Gang Wang - Shanghai University (China)
Prof. Wei-Hua Wang - Institute of Physics, CAS (China)

US Advisory Committee:
Prof. Michael Atzmon - University of Michigan
Prof. Marios Demetriou - California Institute of Technology
Prof. John Lewandowski - Case Western Reserve University
Prof. Mo Li - Georgia Institute of Technology
Dr. Dan Miracle - Air Force Research Laboratory
Prof. Yang Zhang - University of Illinois at Urbana-Champaign
# Schedule Overview

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<thead>
<tr>
<th>Sunday June 5</th>
<th>Monday June 6</th>
<th>Tuesday June 7</th>
<th>Wednesday June 8</th>
<th>Thursday June 9</th>
</tr>
</thead>
<tbody>
<tr>
<td>AM 1</td>
<td>Keynote and Plenary Session (Whitaker 100)</td>
<td>Glass Design I (Whitaker 100)</td>
<td>Mechanical Behavior I: Deformation</td>
<td>Structure I (Whitaker 100)</td>
</tr>
<tr>
<td>AM 2</td>
<td>Lunch and Group Photo (Lopata Gallery/Brookings Steps)</td>
<td>Lunch and &quot;Glass Design&quot; Roundtable (Lopata 101)</td>
<td>Lunch and &quot;Testing Standards&quot; Roundtable (Lopata 101)</td>
<td>Box Lunch and Excursion to Cahokia Mounds</td>
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<tr>
<td>Noon</td>
<td>Dynamics I (Whitaker 100)</td>
<td>Glass Design II (Whitaker 100)</td>
<td>Mechanical Behavior II: Composites (Brauer 12)</td>
<td>Structure II (Whitaker 100)</td>
</tr>
<tr>
<td>PM 1</td>
<td>Applications I: Metallic Glass Nanostructures (Brauer 12)</td>
<td>Mechanical Behavior III: Deformation and Structure (Brauer 12)</td>
<td>Mechanical Behavior IV: Shear Banding and Fracture (Brauer 12)</td>
<td>Mechanical Behavior V: Plasticity</td>
</tr>
<tr>
<td>PM 2</td>
<td>Registration (Whitaker Hall)</td>
<td>Stability and Relaxation (Whitaker 100)</td>
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*The 11th International Conference on Bulk Metallic Glasses June 5-9, 2016
Washington University in St. Louis, MO USA*
### BMG XI Schedule

<table>
<thead>
<tr>
<th>Date</th>
<th>Location/Chair</th>
<th>Time</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sunday, June 5th</td>
<td></td>
<td>2:00-5:00 PM</td>
<td>Conference Registration - Sheraton Clayton Plaza Hotel, Thomas Eliot House, Whitaker Hall Lobby</td>
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<tr>
<td></td>
<td></td>
<td>5:30-8:00PM</td>
<td>Welcome Reception. 6:00PM Chancellor Mark Wrighton</td>
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<tr>
<td>Monday, June 6th</td>
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<tr>
<td>Monday, June 6th</td>
<td>Whitaker Hall, Room 100,</td>
<td>9:00 AM</td>
<td>Opening Remarks, Kenneth Kelton</td>
</tr>
<tr>
<td>Opening Session</td>
<td>Chair Kenneth Kelton</td>
<td>9:15 AM</td>
<td>Elasticity in Metallic Glasses, Liquids, and Crystals (Keynote)</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>William L. Johnson</td>
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<td>10:20 AM</td>
<td>Coffee Break</td>
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<tr>
<td></td>
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<td>10:20 AM</td>
<td>Attractiveness and Usefulness of Multicomponent Metastable Alloys (Keynote)</td>
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<tr>
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<td>11:05 AM</td>
<td>Link Between Slow Glassy Dynamics and Crystallization Through Local Structural Ordering (Plenary)</td>
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<tr>
<td></td>
<td></td>
<td>11:40 AM</td>
<td>Topological Excitations in Liquids and Glasses (Plenary)</td>
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<td></td>
<td>T. Egami</td>
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<tr>
<td>Time</td>
<td>Location</td>
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<tr>
<td>12:15 - 1:30 PM</td>
<td>Lopata Hall Gallery</td>
<td>Lunch in Lopata Hall Gallery</td>
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<tr>
<td>1:30 PM</td>
<td>Brookings Hall Steps</td>
<td>Group Photo on Brookings Hall Steps</td>
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<tr>
<td>2:10 PM</td>
<td>Whitaker Hall, Room 100, Chair Hajime Tanaka</td>
<td>Quasi-Elastic Neutron Scattering and Machine Learning Studies of the Arrhenius Crossover Phenomenon and Its Correlation with the Kinetic Fragility in Glass-Forming Metallic Liquids (Invited)</td>
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<tr>
<td></td>
<td><strong>Yang Zhang</strong></td>
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<tr>
<td></td>
<td></td>
<td>Department of Nuclear, Plasma, and Radiological Engineering, Department of Materials Science and Engineering, Program of Computational Science and Engineering, University of Illinois at Urbana-Champaign</td>
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<tr>
<td>2:35 PM</td>
<td></td>
<td>A one Parameter fit for Glassy Dynamics as a Corollary of the Liquid to Solid Transition (Invited)</td>
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<tr>
<td></td>
<td><strong>Zohar Nussinov</strong>, Kenneth F. Kelton, and Nicholas B. Weingartner</td>
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<td></td>
<td></td>
<td>Department of Physics, Washington University, St. Louis, MO 63130, U.S.A.</td>
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<tr>
<td>3:00 PM</td>
<td></td>
<td>Five-fold Symmetry as Indicator of Dynamic Arrest in Metallic Glass-forming Liquids</td>
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<tr>
<td></td>
<td><strong>Maozhi Li</strong>, Yuanchao Hu, Fuxiang Li, Haiyang Bai and Weihua Wang</td>
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<td></td>
<td></td>
<td>Department of Physics, Renmin University of China, Beijing 100872, China</td>
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<tr>
<td>3:15 PM</td>
<td></td>
<td>Structural Relaxation Time in Supercooled Pt$<em>{57.5}$Cu$</em>{14.7}$Ni$<em>{5.3}$P$</em>{22.5}$ Nanowires determined through Electron Correlation Microscopy</td>
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<td></td>
<td><strong>Pei Zhang</strong>, Ze Liu, Jan Schroers, Paul M. Voyles</td>
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<td></td>
<td>Department of Materials Science and Engineering, University of Wisconsin, Madison, WI, USA.</td>
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<tr>
<td>3:30-3:50 PM</td>
<td>Whitaker Hall Lobby</td>
<td>Coffee Break</td>
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<tr>
<td>Time</td>
<td>Session Details</td>
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<tr>
<td>3:50 PM</td>
<td>The Role of Atomic Interactions on Thermodynamics and Fragility of Simulated Metallic Glasses (Invited)</td>
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<td></td>
<td>James R. Morris, Alex Arrico, Takeshi Egami</td>
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<tr>
<td></td>
<td>¹Oak Ridge National Laboratory, Oak Ridge, TN 37831,</td>
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<td></td>
<td>²University of Tennessee, Knoxville, TN 37996</td>
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<tr>
<td>4:15 PM</td>
<td>A Locally-Preferred Structure Characterizes Dynamical Regimes of a Supercooled Liquid</td>
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<td></td>
<td>Ryan Soklaski, Vy Tran, Zohar Nussinov, K.F. Kelton and Li Yang</td>
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<tr>
<td></td>
<td>Department of Physics and Institute of Materials Science and Engineering, Washington University in St. Louis, St. Louis, MO 63130, USA,</td>
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<tr>
<td>4:30 PM</td>
<td>Predicting the Diffusion Kinetics and Atomic Mechanism of Metallic Glass at Experimental Timescale</td>
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<td></td>
<td>Yun-Jiang Wang, Shigenobu Ogata, and L. H. Dai</td>
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<td></td>
<td>State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China</td>
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<tr>
<td>4:45 PM</td>
<td>Correlations Between Structure Orders and Dynamics in Cu-Zr Metallic Glasses</td>
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<td>Ames Laboratory-USDOE, Iowa State University, Ames, Iowa 50011, USA</td>
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<tr>
<td>5:00 PM</td>
<td>Structure Evolution of Cu-Zr-Ti Metallic Glasses</td>
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<td></td>
<td>Anupriya Agrawal, Rohan Mishra, Katharine M. Flores, Wolfgang Windl</td>
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<td>¹Washington University in St. Louis, St. Louis, MO 63130</td>
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<td>²The Ohio State University, Columbus, OH 63210</td>
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<tr>
<td>6:00-9:00 PM</td>
<td>Edison Family Courtyard BBQ &amp; Blues Dinner</td>
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<td>2:10 PM</td>
<td>Nanoporous Gold from Au Based Amorphous Alloys: Mechanisms of Dealloying and Applications (Invited)</td>
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<td>Time</td>
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<td>Presenter</td>
<td>Institution</td>
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<tr>
<td>2:35 PM</td>
<td>Guided Evolution of Bulk Metallic Glass Nanostructures (Invited)</td>
<td>André D. Taylor</td>
<td>Yale University</td>
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<tr>
<td>3:00 PM</td>
<td>Designing Catalytic Amorphous Metals – Energy Conversion to Environmental Remediation</td>
<td>Sundeep Mukherjee</td>
<td>Department of Materials Science and Engineering, University of North Texas</td>
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<tr>
<td>3:15 PM</td>
<td>Bio-inspired Functional Surfaces from Metallic Glasses</td>
<td>Molla Hasan, Golden Kumar</td>
<td>Department of Mechanical Engineering, Texas Tech University, Lubbock, TX 79409, United States</td>
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<tr>
<td>3:30-3:50 PM</td>
<td>Coffee Break</td>
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<tr>
<td>3:50 PM</td>
<td>Shaping Metallic Glasses by Electromagnetic Pulsing (Invited)</td>
<td>Georg Kaltenboeck, Marios D. Demetriou, Scott Roberts and William L. Johnson</td>
<td>California Institute of Technology, Pasadena, CA 91125, Glassimetal Technology, Pasadena, CA 91107,</td>
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<tr>
<td>4:15 PM</td>
<td>Determining the Influence of Processing on Bulk Metallic Glass Properties (Invited)</td>
<td>Jörg F. Löffler</td>
<td>Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland</td>
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<tr>
<td>4:40 PM</td>
<td>Crystallization and Mechanical Properties of Laser Rapid Prototyping Zr-based Bulk Amorphous/Nanocrystalline Composites</td>
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<td>4:55 PM</td>
<td>3D Metallic Glass Cellular Structures</td>
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<td></td>
<td>Department of Engineering Mechanics, School of Civil Engineering, Wuhan University, Wuhan, China,</td>
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<td>Edison Family Courtyard</td>
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<tr>
<td>6:00-9:00 PM</td>
<td>BBQ &amp; Blues Dinner</td>
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**Tuesday, June 7th**

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<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>9:00 AM</td>
<td>Identifying Bulk Metallic Glass Compositions Through Combinatorial Strategies (Plenary)</td>
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<td></td>
<td>Jan Schroers, Yanhui Liu, Yanglin Li</td>
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<tr>
<td></td>
<td>Mechanical Engineering and Materials Science Department, Yale University, 15 Prospect St, New Haven, Ct 06520, USA</td>
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<tr>
<td>9:35 AM</td>
<td>Accelerating the Design of Functional Glasses through Modeling (Plenary)</td>
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<td>John C. Mauro, Adama Tandia, K. Deenamma Vargheese, Yihong Z. Mauro, and Morten M. Smedskjaer</td>
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<td>Science and Technology Division, Corning Incorporated, Corning, USA</td>
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<td>10:10 AM</td>
<td>High Pressure Induced Formation of Bulk Ultrastable Metallic Glass and Rejuvenation (Plenary)</td>
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<td>R. J. Xue, Chao Wang, Ping Wen, Xiao Hui Yu, Hai Yang Bai, Wei Hua Wang</td>
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<td>Institute of Physics, Chinese Academy of Sciences, Beijing 100190, People’s Republic of China</td>
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<td>10:45-11:05 AM</td>
<td>Coffee Break</td>
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<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker(s)</th>
<th>Affiliation</th>
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<tbody>
<tr>
<td>11:05 AM</td>
<td>Alloying Different Nanogranular Metallic Glasses (Invited)</td>
<td>Na Chen, Hongxia Zhang and Kefu Yao</td>
<td>School of Materials Science and Engineering, Tsinghua University, Beijing 100084, P.R. China</td>
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<tr>
<td>11:45 AM</td>
<td>Laser Deposition as a High-throughput Tool for Discovering New Bulk Metallic Glass Alloys</td>
<td>Peter Tsai, Katharine M. Flores</td>
<td>Washington University, Institute of Materials Science &amp; Engineering</td>
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<tr>
<td>12:00 PM</td>
<td>Molecular Dynamics Simulation of Metallic Glass Formation</td>
<td>David Riegner, Logan Ward, Katharine Flores and Wolfgang Windl</td>
<td>The Ohio State University</td>
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<tr>
<td>12:15-2:10 PM</td>
<td>Lunch Roundtable Discussion: Glass Design</td>
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<tr>
<td>2:40 PM</td>
<td>Theoretical Insight into Rejuvenation in Metallic Glasses</td>
<td>B. S. Shang, P. F. Guan, and W. H. Wang</td>
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<tr>
<td>Time</td>
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<tr>
<td>2:55 PM</td>
<td>Alloy Design in Platinum Based Bulk Metallic Glass, from Stabilizing the Liquid Phase to Fine-tuning the Glass Transition and Crystallization Temperature.</td>
<td>Hamed Kazemi, Cyrill Cattin and Ludger Weber</td>
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<tr>
<td>3:10 PM</td>
<td>New Bulk Phase-separated Zr-based Metallic Glasses Containing a High Population Density of Glassy Nanospheres</td>
<td>Jie He, Zhongyuan Wang, Ivan Kaban, Jiuzhou Zhao, Do Hyang Kim, Jürgen Eckert and A. Lindsay Greer</td>
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<tr>
<td>3:25 PM</td>
<td>New Toxic Element Free Metallic Glass for Biomedical Applications</td>
<td>Oriane Baulin, Damien Fabrègue, Hidemi Kato, Aléthéa Liens, Takeshi Wada, Jean-Marc Pelletier</td>
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**Whitaker Hall Lobby**

**Tuesday, June 7th Concurrent Session A**

**Stability & Relaxation**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Description</th>
<th>Speaker(s)</th>
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<tbody>
<tr>
<td>3:40-4:00 PM</td>
<td>Coffee Break</td>
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<tr>
<td>4:00 PM</td>
<td>Separation of Time Scales of the Frozen-in Relaxation Processes in a Metallic Glass at Deep Supercooling (Invited)</td>
<td>Isabella Gallino</td>
</tr>
<tr>
<td>4:25 PM</td>
<td>In-situ Neutron Diffraction study of Crystallization Pathways in Zr-Cu-Al Bulk Metallic Glasses with Gradually Enhanced Glass-forming Abilities</td>
<td>Si Lan, Xiaoya Wei, Jie Zhou, Xuelian Wu, Zhaoping Lu, Mikhail Feygenson, Jörg Neuefeind, Xun-Li Wang</td>
</tr>
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1Department of Physics and Materials Science, City University of Hong Kong, Hong Kong, P. R. China, 2Herbert Gleiter
<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
<th>Speaker(s)</th>
<th>Location</th>
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<tbody>
<tr>
<td>4:40 PM</td>
<td>Devitrification of Metallic Glass Alloys and Synthesis of Nanostructures</td>
<td>Y. Shen, J.H. Perepezko</td>
<td>University of Wisconsin-Madison, Department of Materials Science and Engineering, 1509 University Ave., Madison, WI 53706, USA</td>
</tr>
<tr>
<td>4:55 PM</td>
<td>Processing Dependent Phase Selection in Al$<em>{90}$Sm$</em>{10}$ Amorphous Alloys</td>
<td>Fanqiang Meng, Wenjie Wang, Matthew F. Besser, Matthew J. Kramer and Ryan T. Ott</td>
<td>Ames Laboratory, US Department of Energy, Iowa State University, Ames, IA 50011, USA</td>
</tr>
<tr>
<td>Brauer Hall Lobby 6:00-8:00 PM</td>
<td>Poster Session &amp; Reception</td>
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<tr>
<td>Tuesday, June 7th Concurrent Session B Mechanical Behavior I: Deformation &amp; Structure</td>
<td>Brauer Hall, Room 12, Chair Jan Schroers 11:05 AM</td>
<td>Universal Fast Secondary Relaxation and Plasticity Initiation in Metallic Glasses (Invited)</td>
<td>Center for advanced structural materials, Department of mechanical and biomedical engineering, City University of Hong Kong, Kowloon, Hong Kong, China</td>
</tr>
<tr>
<td>11:30 AM</td>
<td>Effect of Thermal Cycling on Shear Transformation Zone Spectra in a Metallic Glass</td>
<td>T. J. Lei, Y. Sun, A. L. Greer and M. Atzmon</td>
<td>Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan 48109, USA</td>
</tr>
<tr>
<td>11:45 AM</td>
<td>Structural Heterogeneity Induced Plasticity in Metallic Glasses</td>
<td>Yanfei Gao</td>
<td>Department of Materials Science and Engineering, University of Tennessee</td>
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<td>Materials Science and Technology Division, Oak Ridge National Laboratory</td>
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<tr>
<td>Time</td>
<td>Session</td>
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<tr>
<td>12:00 PM</td>
<td>Correlating the Failure Behavior of Metallic Glasses at Different Temperatures with their Structural Evolution</td>
<td>Lopata Hall Gallery &amp; Lopata Hall Room 101</td>
<td>Lunch Roundtable Discussion: Glass Design</td>
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<tr>
<td>12:15-2:10 PM</td>
<td>Lunch Roundtable Discussion: Glass Design</td>
<td>Lopata Hall Gallery &amp; Lopata Hall Room 101</td>
<td>Lunch Roundtable Discussion: Glass Design</td>
</tr>
<tr>
<td>Tuesday, June 7th Concurrent Session B Mechanical Behavior II: Composites</td>
<td>Effects of Changes in Test Temperature on Tension Behavior and Toughness of BMG Composites (Invited)</td>
<td>Brauer Hall, Room 12, Chair Yong Yang</td>
<td>Effects of Changes in Test Temperature on Tension Behavior and Toughness of BMG Composites (Invited)</td>
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<tr>
<td>2:25 PM</td>
<td>Property Manipulation of TRIP Bulk Metallic Glass Composites (Invited)</td>
<td>Brauer Hall, Room 12, Chair Yong Yang</td>
<td>Property Manipulation of TRIP Bulk Metallic Glass Composites (Invited)</td>
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<tr>
<td>2:50 PM</td>
<td>Influence of Microstructure on Deformation Behavior in BMGMCs</td>
<td>Brauer Hall, Room 12, Chair Yong Yang</td>
<td>Influence of Microstructure on Deformation Behavior in BMGMCs</td>
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<tr>
<td>3:15 PM</td>
<td>Coffee Break</td>
<td>Whitaker Hall Lobby</td>
<td>Coffee Break</td>
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<tr>
<td>Tuesday, June 7th Concurrent Session B Mechanical Behavior III:</td>
<td>Insights on Shear Bands in BMGMCs from FFT-based Continuum Modeling</td>
<td>Brauer Hall, Room 12, Chair Katharine Flores</td>
<td>Insights on Shear Bands in BMGMCs from FFT-based Continuum Modeling</td>
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<td>Time</td>
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<tr>
<td>4:20 PM</td>
<td>Fe-based Bulk Metallic Glasses: Brittle or Ductile?</td>
<td>Emmanuelle Marquis, Wolfgang Windl and Stephen Niezgoda</td>
<td>The Ohio State University</td>
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<td>4:35 PM</td>
<td>Nonlinearity and Anisotropy of Elastic Moduli during Compression of the BMG</td>
<td>Shengfeng Guo</td>
<td>Faculty of Materials and Energy, Southwest University, Chongqing 400715, China</td>
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<tr>
<td>4:50 PM</td>
<td>Investigation on the Intrinsic Mechanical Properties of Nanosized Metallic Glasses via Particle Compression</td>
<td>S. Y. Kim, J. W. Kim, K. Nakayama and E. S. Park</td>
<td>Research Institute of Advanced Materials, Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Republic of Korea</td>
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<tr>
<td>5:05 PM</td>
<td>How the Voronoi Diagram of 3D Spheres Can be used for the Accurate and Efficient Analysis of Geometry and Topology of Metallic Glasses?</td>
<td>Deok-Soo Kim, Joonghyun Ryu, Youngsong Cho, Mokwon Lee, Jehyun Cha, and Chanyoung Song</td>
<td>Seoul, Korea</td>
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<td>6:00-8:00 PM</td>
<td>Poster Session &amp; Reception</td>
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**Wednesday, June 8th**

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<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker(s)</th>
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<tbody>
<tr>
<td>9:00 AM</td>
<td>Extending the Range of the Glassy State in Metals (Plenary)</td>
<td>A. L. Greer</td>
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Whitaker Hall, Room 100,
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<th>Speaker(s)</th>
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<tr>
<td>Wednesday,</td>
<td>Plenary Session</td>
<td>Whitaker Hall Lobby</td>
<td>Cynthia</td>
<td>Mingwei Chen</td>
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<tr>
<td>June 8th</td>
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<td>Volkert</td>
<td>Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan</td>
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<tr>
<td>9:35 AM</td>
<td>Spatial Heterogeneity of Metallic Glasses (Plenary)</td>
<td></td>
<td></td>
<td>W. H. Liu, C. T. Liu, B. A. Sun, and Herbert Gleiter</td>
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<tr>
<td>10:10 AM</td>
<td>Structural Features and Mechanical Behavior of a Nanoglass with and</td>
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<td>Center for Advanced Structural Materials, Department of Mechanical and</td>
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<td></td>
<td>without Cryogenic Treatment (Plenary)</td>
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<td>Biomedical Engineering, College of Science and Engineering, City</td>
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<td>University of Hong Kong, Hong Kong</td>
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<td>10:45-11:05 AM</td>
<td>Coffee Break</td>
<td>Whitaker Hall Lobby</td>
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<tr>
<td>Wednesday,</td>
<td>Concurrent Session A</td>
<td>Whitaker Hall, Room 100</td>
<td>Mo Li</td>
<td>Jason J. Maldonis, Pei Zhang, and Paul M. Voyles</td>
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<tr>
<td>June 8th</td>
<td>Structure II</td>
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<td>Materials Science and Engineering, University of Wisconsin-Madison</td>
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<tr>
<td>11:05 AM</td>
<td>Structure of Metallic Glasses from Fluctuation Electron Microscopy</td>
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<td>Mikhail I. Mendelev</td>
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<td></td>
<td>and Computational Structure Refinement (Invited)</td>
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<td></td>
<td>Division of Materials Sciences and Engineering, Ames Laboratory, Ames, IA 50011</td>
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<td>Mesoscale Metallic Glass Deformation Simulation Incorporating Medium</td>
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<td>Range Order From Fluctuation Electron Microscopy</td>
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<td>11:30 AM</td>
<td>Development of Interatomic Potentials Appropriate for Metallic</td>
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<td>Jinwoo Hwang, Pengyang Zhao, Soohyun Im, and Yunzhi Wang</td>
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<td>Glasses (Invited)</td>
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<td></td>
<td>Department of Materials Science and Engineering, The Ohio State University, Columbus, OH 43212</td>
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<td>12:10-2:15 PM</td>
<td>Lunch Roundtable Discussion: Testing Standards</td>
<td>Lopata Hall Gallery &amp;</td>
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<td>2:15 PM</td>
<td>The Structural Pathway of Metallic Liquids to Vitrification (Invited)</td>
<td>Whitaker Hall, Room 100</td>
<td>K. Georgarakis, A.R. Yavari</td>
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<td>†WPI-AIMR, Tohoku University,</td>
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<td>Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, TN</td>
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<tr>
<td>2:55 PM</td>
<td>Unveiling the Distinct Features of Inherent Heterogeneity in Metallic Glass</td>
<td>Whitaker Hall, Room 100</td>
<td>Yuan-Chao Hu, Peng-Fei Guan, Mao-Zhi Li, Chain-Tsuan Liu, Yong Yang, Hai-Yang Bai and Wei-Hua Wang</td>
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<td>†Institute of Physics, Chinese Academy of Sciences, Beijing 100190 China</td>
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<td>‡Department of Mechanical and Biomedical Engineering, City University of Hong Kong,</td>
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<td>3:10 PM</td>
<td>Crystal Gene: Common motifs Transcending Crystals, Glasses, and Liquids</td>
<td>Whitaker Hall, Room 100</td>
<td>Feng Zhang, Yang Sun, Zhuo Ye, Yue Zhang, Xiaowei Fang, Zejun Ding, Cai-Zhuang Wang, Mikhail I. Mendelev, Ryan T. Ott, Matthew J. Kramer, Kai-Ming Ho</td>
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<td>Ames Laboratory, US Department of Energy, Ames, Iowa 50011, USA</td>
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<tr>
<td>3:25 PM</td>
<td>Formation of Monatomic Metallic Glasses through Ultrafast Liquid Quenching (Invited)</td>
<td>Whitaker Hall, Room 100</td>
<td>Scott X. Mao</td>
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<td>Department of Mechanical and Materials Science, University of Pittsburgh, Pittsburgh, PA 15261, USA</td>
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<td>6:45-9:45 PM</td>
<td>Conference Banquet at Kemoll's Restaurant</td>
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<tr>
<td>11:05 AM</td>
<td>Thin Film Metallic Glasses: Novel Coating Materials for Advanced Applications (Invited)</td>
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<td>Chia-chi Yu, Cheng-Min Lee, Chia-Lin Li, Yusuke Tanatsugu, Chia-Hao Chang, <strong>Jinn P. Chu</strong></td>
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<td></td>
<td>Department of Materials Science and Engineering National Taiwan University of Science and Technology, Taipei 10607, Taiwan</td>
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<td>11:30 AM</td>
<td>Corrosion Resistant Amorphous Coatings for Deep-sea Applications</td>
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<td><strong>Cheng Zhang</strong>, Zhi Wei Zhang, Wei Wang and Lin Liu</td>
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<td>School of Materials Science and Engineering, Huazhong University of Science and Technology, Wuhan, Hubei, P.R. China</td>
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<td>Lunch Roundtable Discussion: Testing Standards</td>
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<td><strong>Jan Schroers</strong>, Yale University &amp; <strong>Nick Hutchinson</strong>, Materion Brush Inc.</td>
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<td>2:15 PM</td>
<td>Universal Slip Statistics: from Nanopillars to Earthquakes (Invited)</td>
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<td></td>
<td>Dept. of Physics, University of Illinois at Urbana Champaign, 1110 West Green Street, Urbana, IL 61801</td>
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<td>2:40 PM</td>
<td>Cavitation and Internal Stresses during Shear-Banding of Metallic Glasses</td>
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<td>Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign</td>
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<td>2:55 PM</td>
<td>Engineering High Fracture Toughness into Bulk Metallic Glasses</td>
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<td><strong>J. J. Kruzic</strong>, B.S. Li, S.H. Xi, H. Shakur Shahabi, S. Scudino, J.</td>
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<td>Materials Science, School of Mechanical, Industrial, and Manufacturing</td>
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<td>Engineering, Oregon State University, Corvallis, OR, 97330</td>
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<td>3:10 PM</td>
<td>Nature of Crack-tip Plastic Zone in Metallic Glasses</td>
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<td><strong>Yan Chen</strong> and Lanhong Dai</td>
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<td>State Key laboratory of Nonlinear Mechanics, Institute of Mechanics,</td>
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<td>Chinese Academy of Sciences, Beijing 100190, People’s Republic of China</td>
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<td>Conference Banquet at Kemoll’s Restaurant</td>
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### Thursday, June 9th

**Thursday, June 9th Plenary Session**

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<th>Time</th>
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<tr>
<td>9:00 AM</td>
<td>Tailoring Structural Inhomogeneity in Metallic Glasses to Enable</td>
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<td>Tensile Ductility at Room Temperature (Plenary)</td>
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<td><strong>E. Ma</strong></td>
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<td></td>
<td>Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, MD 21218, USA</td>
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<tr>
<td>9:35 AM</td>
<td>Early Plasticity in Metallic Glasses (Plenary)</td>
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<td><strong>C.A. Volkert</strong>, D. Tönnies, K. Samwer and R. Maass</td>
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<td></td>
<td>Institute of Materials Physics, University of Göttingen</td>
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<tr>
<td>10:45-11:05 AM</td>
<td>Coffee Break</td>
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**Thursday, June 9th Concurrent Session A**

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<tr>
<td>10:30 AM</td>
<td>Structural Crossover in a Supercooled Metallic Liquid and the Link to</td>
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<td>a Liquid-to-liquid Phase Transition (Invited)</td>
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<td><strong>S. Lan, M. Blodgett, K.F. Kelton, J. L. Ma, J. Fan, and X.-L. Wang</strong></td>
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<td>Department of Physics and Material Science, City University of Hong</td>
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<td>Kong 83 Tat Chee Ave., Kowloon, Hong Kong</td>
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<tr>
<td>10:55 AM</td>
<td>Liquid-Liquid Phase Transition in Metallic Glasses during Ultrafast Heating</td>
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<td></td>
<td>Stefan Kuechemann, Konrad Samwer</td>
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<tr>
<td>11:10 AM</td>
<td>Thermodynamic Connection to the Structural Variation of Zr-Al-Co Glass Forming Alloys</td>
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<tr>
<td>11:50 AM</td>
<td>Closing Session</td>
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<tr>
<td>12:20 PM - 5:00 PM</td>
<td>Lunch &amp; Excursion to Cahokia Mounds</td>
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<td>Thursday, June 9th Concurrent Session B</td>
<td>Mechanical Behavior V: Plasticity</td>
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<tr>
<td>10:30 AM</td>
<td>Theoretical Strength of Amorphous Solids (Invited)</td>
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<tr>
<td>10:55 AM</td>
<td>Deformation Behaviour of Metallic Glasses Without Shear Banding at Room Temperature</td>
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<td>11:10 AM</td>
<td>Thermal Activation in Metallic Glass by Creep Deformation and Stress Relaxation</td>
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<td>Time</td>
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<tr>
<td>11:25 AM</td>
<td>Tensile Ductility of Bulk Metallic Glasses Processed by High-Pressure Torsion</td>
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<td>Soo-Hyun Joo, Hidemi Kato and <strong>Hyoung Seop Kim</strong></td>
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<td></td>
<td>Department of Materials Science and Engineering, Pohang University of Science and Technology, Pohang 790-784, South Korea</td>
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<td>Whitaker Hall, Room 100</td>
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</table>
Keynote Speakers

Monday, June 6, 2016
Elasticity in Metallic Glasses, Liquids, and Crystals

William L. Johnson

138-78 Keck Laboratory, Calif. Inst. of Tech., Pasadena, CA 91125

*wlj@caltech.edu

The temperature dependence of the elastic constants and thermal expansion behavior of metallic glasses and the corresponding crystallized solids are well described by the classical Debye-Gruneisen (DG) theory of anharmonicity and lattice vibrations. Above the glass transition, the undercooled liquid exhibits both vibrational as well as configurational excitations; the temperature dependence of the high frequency elastic constants reflects distinct contributions from both types of excitation. Ultrasonic measurements are used to probe elastic response in the megahertz and gigahertz range for metallic glasses, crystallized samples, and the corresponding liquids. The theory of potential energy landscapes provides a natural framework to analyze such ultrasonic data and separate the configurational and vibrational contributions to elasticity. Based on this approach, a unified picture of elasticity for all three states is developed that provides new insights into the thermodynamics and kinetics of melting as well as the origin of the glass transition itself.
Attractiveness and Usefulness of Multicomponent Metastable Alloys

A. Inoue\textsuperscript{1,2,3,*}, F.L. Kong\textsuperscript{2}, S.L. Zhu\textsuperscript{1} and F. Al-Marzouki\textsuperscript{3}

\textsuperscript{1}School of Materials Science and Engineering, Tianjin University, Tianjin, China, \textsuperscript{2}International Institute of Green Materials, Josai International University, Togane 283-8555, Japan, \textsuperscript{3}Department of Physics, King Abdulaziz University, Jeddah 22254, Saudi Arabia

*Corresponding author: inoue@jiu.ac.cn

For the last several decades, we have been developing nonequilibrium metallic engineering materials including bulk glassy alloys, bulk nanocrystalline alloys and bulk nanocomposite materials in various alloy systems by effective combination of appropriate multicomponent alloy designs, unique preparation techniques and optimum preparation conditions. The multicomponent metastable metallic alloys have been extended in extremely wide alloy groups of simple metal-, early transition metal-, late transition metal- and lanthanide metal-based alloys which can be categorized as multicomponent type alloys. The multiplication of alloy components gives additional novel opportunities to develop new engineering metallic materials with useful functional properties, resulting in a new material science field as multicomponent metastable alloy science and technology. Among these multicomponent metastable metallic materials developed in our group to date, Fe-, Zr-, Ti-, Ni-, Pd-, Cu- and Al-based multicomponent alloys have been used as practical materials by utilizing their useful engineering characteristics which can be obtained only in specially designed metastable structure states, in conjunction with unique simple production techniques and processes resulting from multicomponent alloy liquids with low melting temperatures. More recently, the extension of the multicomponent alloy science has also caused the materials science and engineering fields of high-entropy type alloys and pseudo high entropy (high-order multicomponent) type alloys in glassy, amorphous and nanocrystalline states which can exhibit different properties in comparison with bulk glassy alloys. In addition, the multiplication of alloy components has caused new mixed metastable phase structures in Fe- and Fe-Co-based alloys with different alloy compositions as compared with conventional amorphous and glassy alloys as well as the modifications of structure and fundamental properties through the controls of alloy compositions and the preparation conditions. Thus, the multicomponent alloy design is also expected to enable the syntheses of new type of metastable alloys with functional properties caused by the formation of unique mixed structures. This paper aims to present the attractiveness and usefulness of multicomponent metastable metallic alloys through the introduction of some recent results on the formation and properties of Fe-, Al-, Cu- and Ti-based multicomponent metastable alloys obtained mainly for the last three years by our group.
Plenary Speakers

Monday, June 6, 2016
Link Between Slow Glassy Dynamics and Crystallization Through Local Structural Ordering

Hajime Tanaka* and John Russo

Institute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan

*Corresponding author: tanaka@iis.u-tokyo.ac.jp

When a liquid is cooled below the melting point, it is either crystallized or vitrified depending upon the cooling rate. However, it is not clear what physical factors control the ease of crystallization, or the glass-forming ability. This problem is particularly important in metallic glasses. For hard disks and spheres, we systematically control the size polydispersity, which can be regarded as the strength of frustration effects on crystallization. We revealed that crystal-like bond orientational order grows in both size and lifetime when approaching the glass transition point [1,2]. Our study suggests an intriguing scenario that the strength of frustration controls both the glass-forming ability and the fragility of liquid. Under strong frustration on crystallization, a direct link between glassy structural order and the rotational symmetry of the crystal may be lost. Even in such a case, however, slow dynamics may still be associated with low local free-energy configurations. We report a correlation between structural order and slow mobility in some glass-forming systems, suggesting a link between static growing length and the diverging relaxation time. Furthermore, we revealed that such structural order also plays a crucial role in crystal nucleation and polymorph selection [3]: Crystallization is a process of the enhancement of spatial coherence of crystal-like bond orientational order and 'not' driven by translational order at least in the nucleation stage. The ageing of glasses and non-linear rheology of glass-forming liquids may also be understood on the basis of local structural ordering.

Topological Excitations in Liquids and Glasses

T. Egami¹,²*

¹Joint Institute for Neutron Sciences, Department of Materials Science and Engineering, Department of Physics and Astronomy, University of Tennessee, Knoxville, TN, USA
²Oak Ridge National Laboratory, Oak Ridge, TN, USA

*Corresponding author: egami@utk.edu

Topological excitations, excitations in the topology of atomic connectivity (anankeons), are the elementary excitations in high-temperature liquid, and they determine its dynamic and thermal properties. In the supercooled state the anankeon excitations slow down, and they become more collective, and are observed as the beta-relaxation. They persist even below the glass transition, and at low temperatures they become the quantum-mechanical tunneling states. At high temperatures they can be directly observed by inelastic x-ray or neutron scattering, while in the glassy state their profiles can be detected by x-ray or neutron diffraction under stress and in colloids under shear flow. We discuss how understanding the nature of anankeons lead to more universal view of the dynamics and mechanical properties of the liquid and glassy state in general, regardless of the dimension, softness, fragility and chemistry.
Concurrent Session A
Dynamics I

Monday, June 6, 2016
Quasi-Elastic Neutron Scattering and Machine Learning Studies of the Arrhenius Crossover Phenomenon and Its Correlation with the Kinetic Fragility in Glass-Forming Metallic Liquids

Yang Zhang¹,*

¹Department of Nuclear, Plasma, and Radiological Engineering, Department of Materials Science and Engineering, Program of Computational Science and Engineering, University of Illinois at Urbana-Champaign

*Corresponding author: zhyang@illinois.edu

Most metallic glasses are produced by quenching high-temperature metallic liquids sufficiently fast that the timescale for structural relaxation becomes very long. Therefore, an in-depth understanding of the relaxational dynamics of the metallic liquids and its connection to the kinetic fragility is important to unveil the atomic origin of the glass-forming abilities. We performed Quasi-Elastic Neutron Scattering (QENS) measurements of the mean effective diffusion coefficient of glass-forming metallic liquids in the generalized hydrodynamic regime. We observed a universal Arrhenius crossover from high-temperature Arrhenius to low-temperature super-Arrhenius behavior at approximately reduced Arrhenius crossover temperature $\theta_A = T_A/T_g \sim 2T_g$. By comparing with many other molecular and network liquids, we found a distinct correlation between the reduced Arrhenius crossover temperature $\theta_A$ and the kinetic fragility index $m$. Intriguingly, the high-temperature activation barrier $E_\infty$ is universally found to be $\sim 11 k_B T_g$ for metallic and molecular liquids. Furthermore, we used machine learning algorithms to analyze the simulated atomic trajectory and found the onset of enhanced dynamical clustering/heterogeneity below $\theta_A$, which marks the crossover from uncorrelated dynamics to landscape-influenced correlated dynamics. These observations provide a way to estimate the low-temperature glassy characteristics ($T_g$ and $m$) from high-temperature liquid quantities ($E_\infty$ and $\theta_A$) [1-5].

A one Parameter fit for Glassy Dynamics as a Corollary of the Liquid to Solid Transition

Zohar Nussinov, Kenneth F. Kelton, and Nicholas B. Weingartner

1Department of Physics, Washington University, St. Louis, MO 63130, U.S.A.

This talk consists of two inter-related (theoretical and experimental) components. (1) We apply thermodynamic considerations to suggest that the only energy density at which the eigenstates of a clean many body atomic system undergo a non-analytic change is that of the melting (or freezing) transition. We invoke this to analyze the evolution of a liquid upon supercooling. Expanding the state of a supercooled liquid in the complete eigenbasis of the many-body Hamiltonian, only the higher energy liquid-type eigenstates contribute significantly to measurable hydrodynamic relaxations (e.g., those probed by viscosity) while static thermodynamic observables become weighted averages over both solid- and liquid-type eigenstates. Consequently, when extrapolated to low temperatures, hydrodynamic relaxation times of deeply supercooled liquids (i.e., glasses) may seem to diverge at nearly the same temperature at which the extrapolated entropy of the supercooled liquid becomes that of the solid. In this framework, the increasingly sluggish (and spatially heterogeneous) dynamics in supercooled liquids as their temperature is lowered stems from the existence of the single non-analytic change of the eigenstates of the clean many-body Hamiltonian at the equilibrium melting transition present in low energy solid-type eigenstates. We derive a single (possibly computable) dimensionless parameter fit to the viscosity, report on an associated universal collapse of the viscosity of all glass formers. Following these considerations, (2) we then contrast this theory with experimental data and indeed find that this predicted collapse appears over 16 decades of relaxation times for metallic, organic, and silicate systems. We discuss other experimental ramifications of the theory.
Five-fold Symmetry as Indicator of Dynamic Arrest in Metallic Glass-forming Liquids

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With sufficient high cooling rates, a variety of liquids, including metallic melts, will cross a glass transition temperature and solidify into glass accompanying a dramatic increase of the shear viscosity in approximate 17 orders of magnitude. Due to the intricate atomic structure and dynamic behaviors of liquid, it is yet difficult to capture the underlying structural mechanism responsible for the dramatic slowing down during glass transition, which impedes deep understanding of the formation and nature of glasses. Here, we report that a universal structural indicator, the average degree of five-fold local symmetry, can well describe the slowdown dynamics during glass transition. A straightforward relationship between structural parameter and viscosity (or $\alpha$-relaxation time) is deduced, which establishes an explicit relation between the dramatic dynamic arrest and the underlying structural evolution. This finding would be helpful in understanding the long-standing challenges of glass transition mechanism in the structural perspective\cite{1}.

Structural Relaxation Time in Supercooled Pt\textsubscript{57.5}Cu\textsubscript{14.7}Ni\textsubscript{5.3}P\textsubscript{22.5} Nanowires determined through Electron Correlation Microscopy

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Electron Correlation Microscopy (ECM) is a new way to measure the structural relaxation time of liquids with nanometer-scale spatial resolution using coherent electron scattering. We have applied ECM with a 3.5-nm probe to Pt\textsubscript{57.5}Cu\textsubscript{14.7}Ni\textsubscript{5.3}P\textsubscript{22.5} glassy nanowire in a field-emission scanning transmission electron microscope to investigate the supercooled liquid region. The time autocorrelation function $g_2(t)$ was calculated from a time series of electron nanodiffraction patterns and fit to the Kohlrausch-Williams-Watt function to obtain the structural relaxation time $\tau$ and stretching exponent $\beta$. The measured $\tau$ and $\beta$ continuously decreases when heating from the glassy state to higher temperatures in the supercooled liquid. We also show that for ECM experiments, the length of time series must be at least $30\tau$ to obtain a well-converged $g_2(t)$ and the time per frame must be less than $0.1\tau$ to obtain sufficient sampling. Preliminary results also suggest that atoms near the nanowire surfaces relax faster than in the bulk.
The Role of Atomic Interactions on Thermodynamics and Fragility of Simulated Metallic Glasses

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This talk will discuss the role of interatomic interactions on the fragility of simulated metallic glasses, and the challenges with comparing with experimental results. Bulk metallic glasses are typically “fragile” liquids, with a viscosity that rises rapidly as the temperature approaches the glass transition. We present two new approaches for examining fragility: one based upon seminal work by Kauzmann [1]; and one based upon the development of structural order, based on recent experimental evidence [2]. We use two different CuZr potentials, and demonstrate that both predict “strong” behavior in the undercooled liquid, in contrast to experiments. The results suggest that the strong/fragile behavior is directly related to the development of chemical short-range order and dynamics in the liquid.

Research supported by the U.S. Department of Energy, BES-MSED.

A Locally-Prefe\-rred Structure Characterizes Dynamical Regimes of a Supercooled Liquid

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Recent experimental results suggest that metallic liquids universally exhibit a high-temperature dynamical crossover, which is correlated with the glass transition temperature (\(T_g\)). We demonstrate, using classical molecular dynamics results for Cu\(_{64}\)Zr\(_{36}\), that this temperature, \(T_A \approx 2 \times T_g\), is linked with cooperative atomic rearrangements that produce domains of connected icosahedra. Supercooling to a new characteristic temperature, \(T_D\), is shown to produce higher-order cooperative rearrangements amongst connected icosahedra, which manifests as the formation of large Zr-rich connected domains that possess macroscopic proportions of the liquid’s icosahedra. This coincides with the decoupling of atomic diffusivities, large-scale domain fluctuations, and the onset of glassy dynamics in the liquid. These extensive domains then abruptly stabilize above \(T_g\) and eventually percolate before the glass is formed. All characteristic temperatures (\(T_A\), \(T_D\) and \(T_g\)) are thus connected by successive manifestations of the structural cooperativity that begins at \(T_A\).

2. Ryan Soklaski, Vy Tran, Zohar Nussinov, Zachary Markow, KF Kelton, and Li Yang, accepted by the Philosophical Magazine.
Predicting the Diffusion Kinetics and Atomic Mechanism of Metallic Glass at Experimental Timescale

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The long-range atomic diffusion is related to various dynamic processes of metallic glasses. But it is an infrequent event at ambient temperature that is inaccessible to the normal molecular dynamics timescale, which excludes a direct atomic-scale observation of the diffusion mechanism in the glassy state. Here the diffusion kinetics and its mechanism of a CuZr glass is explored with the well-tempered metadynamics, which enables simulations of diffusion at experimentally relevant timescale. Metadynamics clarifies a long-standing proposed string-like collective diffusion mechanism involving simultaneous activation of multiple atoms before glass transition. The conclusion is further supported by the significant activation entropy, \((12 \pm 5)k_B\), and large activation volume, \((7.7 \pm 3.8)\ \text{Å}^3\), which all agree quantitatively with the experimental measurements and indications. The study provides experimental timescale insights into diffusion mechanisms and kinetics of metallic glass without sacrificing atomic details.
Correlations Between Structure Orders and Dynamics in Cu-Zr Metallic Glasses

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The atomic structures of metallic glasses (MGs) are very sensitive to the cooling rates. Most molecular dynamics (MD) simulations suffer from the ultrahigh cooling rates on the order of \(10^{10-13}\) K/s, where the employed models are hardly given enough time to relax. In this work, an extended sub-\(T_g\) annealing up to \(1.8\) \(\mu\)s was applied to a \(\text{Cu}_{64.5}\text{Zr}_{35.5}\) MG in order to reduce the effect of the high cooling rate used in MD simulations. The effective cooling rate can reach \(2.8\times10^7\) K/s, which is about two orders of magnitude lower than the ones used in conventional MD simulations. The icosahedral short-range order and the Bergman-type medium range order (BMRO) formed around Cu atoms are significantly enhanced after the annealing. Using the newly developed cluster-alignment methods, we revealed that the dominant short range orders around Zr atoms are Z15 and Z16 clusters. Interestingly, the Zr-centered short range order also forms a network, which has been largely ignored in most of the previous studies. The spatial correlation between the Cu-centered icosahedra network and Zr-centered network is analyzed. The spatial distribution and temperature dependence of these networks are found to be closely related with the dynamics slow-down in \(\text{Cu}_{64.5}\text{Zr}_{35.5}\) MG. Finally, the relaxation process is found to be accompanied by a significant chemical short range ordering due to the large negative heat of mixing between Cu and Zr.
Structure Evolution of Cu-Zr-Ti Metallic Glasses

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Studying the evolution of melt structure of metallic glasses as we approach their glass transition temperature is essential to understand glass formation. We have used molecular dynamics simulations to characterize the changes in the structure and dynamics of Cu50Zr50-xTx (0 < x < 50) alloys. We have studied the structure and dynamics of amorphous phase obtained from simulated quenching of melts and contrasted them with their evolution on heating and melting the crystalline phase. In this talk, we will focus on changes in short and medium range order and diffusivity as a function of composition and temperature to highlight the differences in behavior of the amorphous glasses from their crystalline form.
Concurrent Session B
Applications I: Metallic Glass Nanostructures
Monday, June 6, 2016
Nanoporous Gold from Au Based Amorphous Alloys: Mechanisms of Dealloying and Applications.


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Among a large variety of applications, amorphous alloys can be regarded as precursors for the production of nanoporous metals, materials composed by ligaments and pores with size of tens or hundreds of nanometers. Nanoporous metals can be produced by dealloying, a process in which the less noble elements in an alloy are chemically or electrochemically dissolved into an electrolyte leaving on the surface the noble element. The interest for nanoporous gold (NPG) is increasing due to the relatively simple synthesis techniques and its structural, morphological and chemical flexibility. NPG can be modified with functional groups allowing a broad range of possible applications such as catalysis, electrocatalysis, electronics, and optics.

In this work, the production of NPG via dealloying of Au-based amorphous precursors is outlined, showing how the final morphology can be tailored by controlling processing parameters and alloy composition. Moreover, the functionalisation of NPG will be addressed describing a variety of possible applications.
Guided Evolution of Bulk Metallic Glass Nanostructures

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Bulk metallic glasses (BMGs) possess many of the desired characteristics of electrocatalysts. They exist in a wide range of compositions and can be thermoplastically formed into complex geometries over length scales ranging from 10 nm to a few centimeters [1, 2]. In this study we will show how free standing Pt$_{42.5}$Cu$_{27}$Ni$_{9.5}$P$_{21}$ BMG nanowires can be modified with additional elements for specific needs [3]. We demonstrate that dealloying the Pt$_{42.5}$Cu$_{27}$Ni$_{9.5}$P$_{21}$ BMG produces a high surface area nanoporous structure with extreme durability. Remarkably 86% of the electrochemical active surface area (ECSA) after 3000 cycles is retained in comparison to Pt/C ETEK, which loses ca. 100% of its ECSA after 1500 cycles. We will also show that Ru can be readily deposited onto the surface using either galvanic displacement or underpotential deposition, for enhanced methanol electrooxidation activity. Using this “tool-box” of methods allows for the fabrication of active surfaces containing elements that are outside of the glass formability regime.

Designing Catalytic Amorphous Metals – Energy Conversion to Environmental Remediation

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Materials for catalytic applications require large electrochemical surface area together with desirable chemistry. Accelerated development of low-cost electro-catalysts necessitates efficient synthesis of hierarchical structures with morphologies that provide high dispersion and effective utilization of the active species. Metallic-glasses are attractive for energy conversion and environmental remediation due to their unique combination of desirable properties and processing ability. They can be synthesized in a wide range of compositions that are not available in crystalline form, which allows continuous control of their electronic and catalytic properties. We have demonstrated that by starting with a homogeneous and isotropic material, the chemistry and morphology can be tuned to obtain hierarchical nanostructures with high catalytic activity. In addition, metallic glasses were found to be very effective in environmental remediation. We have demonstrated rapid dissociation of toxic organic chemicals by metallic glasses, where the amorphous structure and bi-functional mechanism from transition metals play critical roles.
Bio-inspired Functional Surfaces from Metallic Glasses

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Mimicking bio-inspired topography in synthetic materials has resulted in remarkable properties such as superhydrophobicity, drag-reduction, anti-reflection, and dryadhesion. Surprisingly, the target materials for bioinspired technologies have been mostly polymers due to their processing advantages. Here, we show that bio-inspired functionalities can also be enabled in metallic materials such as metallic glasses by suitable surface texturing. Intrinsically hydrophilic metallic glasses can be rendered hydrophobic when the surfaces are hierarchically patterned using thermoplastic embossing. The shiny metallic surfaces can be changed into optically absorptive by mimicking the topography of moth’s eye. Here, we present the effects of systematic variation in surface texture and chemistry on wetting and optical behavior of metallic glasses. These studies allow decoupling of topographic and chemical effects on tribological properties.
Concurrent Session B
Manufacturing
Monday, June 6, 2016
Shaping Metallic Glasses by Electromagnetic Pulsing

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While metallic glasses are generally known for their attractive mechanical properties, perhaps their most promising attribute is their potential for “thermoplastic” processing. By virtue of being glasses, they can be softened to viscous liquid states above the glass transition where viscoplastic shaping can be performed in a manner similar to processing conventional thermoplastics. Owing to unique electrical resistivities, metallic glasses can be rapidly and uniformly heated when electrical energy is dissipated in them [1]. Combining ohmic dissipation with the classic concept of a Lorentz force generated on a current-carrying conductor exposed to a magnetic field creates a powerful platform to process metallic glasses. Here, we show that electromagnetic coupling of electric current and a magnetic field can thermoplastically shape a metallic glass without conventional heating sources or applied mechanical forces [2]. This electromagnetic forming approach lays the groundwork for a versatile, time and energy efficient manufacturing platform for ultra-strong metals.

Determining the Influence of Processing on Bulk Metallic Glass Properties

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Bulk metallic glass (BMG) forming is generally carried out via rapid cooling of the melt to bypass the “nose” of the time-temperature-transformation diagram for crystallization. However, detailed information on how the (certainly not constant) cooling rate affects melt flow behavior during casting is lacking.

In this talk, I present ways of monitoring such casting processes via high-speed thermography and illustrate how different processing routes (including those in hydrogen-containing atmosphere [1]) generate modified glass-forming ability and mechanical properties. Here I also present recent results using high-speed thermography to describe BMG deformation on the microscopic scale [2], and illustrate how fast differential scanning calorimetry at heating and cooling rates of several $10^4$ K/s can be used to understand the thermophysical properties of undercooled liquids in more detail [3]. This understanding can in turn be used to optimize casting processes of BMG-forming liquids and thus to improve processing-property relationships in BMGs.

Crystallization and Mechanical Properties of Laser Rapid Prototyping Zr-based Bulk Amorphous/Nanocrystalline Composites

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The fabrication of bulk metallic glasses (BMGs) with large cross sections has remained an alchemist’s dream because of the limited glass-forming ability (GFA) of these materials. The small molten pool deposition characteristic with point by point in laser rapid prototyping (LRP) makes this technology be able to be used to prepare BMGs without the limitation of critical cooling rate and critical casting diameter. In present work, deformation mechanisms related to the improvement of strength and ductility were investigated by focusing on how nanocrystallines/ductile dendrites affected the initiation and propagation of deformation bands, shear bands or twins. The improved tensile elongation and strain hardening behavior was explained by the homogeneous distribution of dendrites large enough to form deformation bands or twins and nanocrystallines act as an effect resistance to suppress shear sliding of the amorphous matrix. Based on the present model and experiment results, LRP may be a promising way to fabricate high-performance BMG composites without size and shape limit.
3D Metallic Glass Cellular Structures

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3D Metallic glass structures (3DMGs) are fabricated through thermoplastic forming (TPF)-based patterning of MG sheets combined with a parallel joining technique [1]. To demonstrate this capability and benchmark 3DMGs, we have fabricated honeycomb-like MG architectures covering a wide range of relative densities. 3DMGs exhibit high elasticity of up to 40% loading strain, high elastic energy storability, and high energy absorption which is superior compared to those made from other materials such as conventional metals and ceramics, based on our theoretical analysis. The combination of MG properties and introduced versatile fabrication method suggest the possibility of developing a wide range of 3DMGs with excellent performance for specific applications.

Plenary Session

Tuesday, June 7, 2016
Identifying Bulk Metallic Glass Compositions Through Combinatorial Strategies

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The multicomponent nature of bulk metallic glasses imposes a challenge for their discovery process. Rough estimations suggest that only a minute fraction of potential compositional space for bulk metallic glass formers has been explored thus far.

Here we introduce combinatorial strategies to fabricate libraries comprising of ~1000 different compositions. We use magnetron co-sputtering from three elemental targets that are oriented to create compositional gradients. The resulting composition library is explored for promising compositions. We use a massively parallel characterization method to determine the solidification temperatures, which we correlate with glass forming ability. Also in a massively parallel fashion, we determine the thermoplastic forming ability, which reflects in addition to the glass forming ability, the BMG’s ability for plastic-like processing. Both methods are effective in navigating through the vast composition space towards glass forming compositions. We will introduce novel methods to quantify glass forming ability and related properties. The vast amounts of data are stored, managed, and shared through an online web site, which will be introduced.
Accelerating the Design of Functional Glasses through Modeling

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Functional glasses play a critical role in current and developing technologies. These materials have traditionally been designed empirically through trial-and-error experimentation. However, here we report recent advancements in the design of new glass compositions starting at the atomic level, which have become possible through an unprecedented level of understanding of glass physics and chemistry. For example, new damage-resistant glasses have been developed using models that predict both manufacturing-related attributes (e.g., viscosity, liquidus temperature, and refractory compatibility), as well as the relevant end-use properties of the glass (e.g., elastic moduli, compressive stress, and damage resistance). We demonstrate how this approach can be used to accelerate the design of new industrial glasses for use in various applications. Through a combination of models at different scales, from atomistic through empirical modeling, it is now possible to decode the “glassy genome” and efficiently design optimized glass compositions for production at an industrial scale.
High Pressure Induced Formation of

Bulk Ultrastable Metallic Glass and Rejuvenation

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Owing to the nonequilibrium and metastable nature, glasses are accompanied by relaxations all the time, which deteriorate their properties and hinder their applications. Although extensive efforts have been devoted to search for ultrastable glass, only the 2D film deposited ultrastable glasses can be fabricated so far. We report the formation of an ultrastable Pd-based metallic glass (MG) with bulk size of ~3 mm in diameter under high pressure (HP). The bulk ultrastable MG shows remarkably enhanced thermal and kinetic stability with substantially increased glass transition temperature $T_g$, crystallization temperature $T_x$, density and mechanical properties. This result demonstrates that the high pressure is a unique and effective method to produce bulk MGs with high thermal and kinetic stability and excellent properties. We also show that rejuvenation can be achieved and preserved in bulk MGs by using high pressure annealing, which is a controllable method to continuously alter the energy states of MGs. Contrary to the conventional annealing at ambient pressure, the proposed rejuvenation under HP can be enhanced by the increase of annealing temperature. Using double aberration corrected scanning transmission electron microscopy, it is revealed that the unique rejuvenation, which is attributed to coupling effect of high pressure and high temperature, originates from the structural heterogeneity that contains “negative flow units” with a higher atomic packing density compared to that of the elastic matrix of MGs. The results may assist in the understanding of the microstructural origin of the rejuvenation in MGs.
Concurrent Session A
Glass Design I
Tuesday, June 7, 2016
Alloying Different Nanogranular Metallic Glasses

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Emerging as a new type of non-crystalline solids, nanogranular metallic glasses (NGMGs) can be defined as single- or multi-phase glassy solids having granular nanostructure with a granule size of a few nanometers, typically less than 100 nm. Owing to the combination of their glassy nature and nanostructure, they show very unique properties. Using the technique we developed, we synthesized different metal-based NGMGs in a variety of glass-forming alloy systems to obtain specific functionalities. Furthermore, these individual NGMGs can be nanoalloyed together to form non-crystalline solid solutions – NGMG alloys. Based upon this bottom-up approach, immiscible FeSc and CuSc NGMGs are intermixed at the nanoscale [1]. The produced NGMG alloys show tunable ferromagnetic, electric and mechanical properties. Our experimental testing of these NGMG alloys provides a novel material design concept to create new structures for modifying the properties.

Using Machine Learning to Design New Bulk Metallic Glass Alloys

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Owing to their low computational cost and flexibility, machine-learning-based techniques have proven to be powerful design tools for using existing data to predict new materials. In this work, we will discuss the application of machine learning to the prediction of several properties of metallic glasses, including glass-forming ability and supercooled liquid range. Each model was created by employing machine learning algorithms to automatically discover how characteristics of a material, such as the mean atomic radius, relate to each property. We will demonstrate that machine learning models can extrapolate to yet-unstudied alloy systems, and are fast enough to quickly identify promising alloys out of millions of candidates. Finally, we will discuss how these models can be used to discover alloys with large critical casting thicknesses and supercooled liquid ranges.
Laser Deposition as a High-throughput Tool for Discovering New Bulk Metallic Glass Alloys

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In designing bulk metallic glass alloys, arguably the most important attribute is the inherent glass forming ability (GFA) of an alloy. Unfortunately, while various empirical rules, structural models, and predictive parameters have been proposed as guidelines for identifying good glass formers, none of the guidelines are truly predictive \textit{a priori}. In this work we used laser deposition to fabricate continuously graded composition libraries within the Cu-Zr-(Ti) and Ni-Nb systems. Within a library, regions of glass formation were rapidly identified by observing the ultra-smooth surface topography of vitrified material. By varying processing parameters, the optimum glass formers in an alloy system could be accurately deduced. Instrumented nanoindentation was also performed to quickly assess the interrelationships between chemical composition, GFA, and important mechanical properties. Our results not only demonstrate a novel combinatorial approach for discovering alloys but also introduces a high-throughput methodology to observe property trends that may further our understanding of GFA and the origins of mechanical toughness in BMGs.
Molecular Dynamics Simulation of Metallic Glass Formation

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Using molecular dynamics (MD) simulations, thermodynamic and structural properties of undercooled CuZr and AlLa liquids were recorded as they approached the glass transition. Our results indicate that glass forming occurs when the system undergoes a subtle or gradual transition from liquid to glass, with crystallization being the most extreme possible path. We quantify the severity of the glass transition in terms of atomic coordination, and group traits consistent to the experimental glass formers. Liquids that remain relatively unchanged, or rearrange prior to undercooling, can be separated from those that undergo widespread, drastic, coordination changes. Additional analysis reveals that these characteristics are obtained by comparing only the starting liquid and final glass configuration, and may be independent of the transition path itself, eliminating the bulk of the computational expense. Most importantly, these results can accurately filter glass formers for both systems by combining experimental and simulation data.
Concurrent Session A
Glass Design II
Tuesday, June 7, 2016
Correlation of Glass Formability with Volume and Structure Evolution in Supercooled Metallic Liquids


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Studies of the thermodynamic properties (volume, specific heat) of metallic glasses with high melting temperatures are very limited. Here, we report results from measurements of the volume evolution with temperature for fifteen equilibrium and supercooled liquids that form bulk metallic glasses with critical casting thickness \( t_c \) ranging from 3 to 16 mm. The liquids were processed in a containerless environment, using the technique of electrostatic levitation. Considering \( t_c \) as a practical measure of glass formability, an inverse correlation is found between glass formability and the changes in volume between the liquidus and glass transition temperatures; larger changes were observed for the poorer glass formers and smaller for the better ones. Using published data, a similar correlation was demonstrated between \( t_c \) and structural changes in the supercooled liquids. However, in contrary to a widely-held belief, the changes in these properties do not correlate as well with the fragility of the liquids.
Theoretical Insight into Rejuvenation in Metallic Glasses

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Cryogenic thermal cycling (CTC) could induce either rejuvenation or aging effect into metallic glasses, but the physic origin for those two contradictory consequences is still unclear. Based on systematic computational simulations, it is found that the relationship between holding time in CTC and intrinsic critical time of experimental sample at upper cycling temperature is the key for determining the influence of CTC. Furthermore, the mechanism of CTC induced rejuvenation can be come down to the activation of localized soft modulus zones companying with volume dilation. Unlike high temperature annealing, the alpha-relaxation during CTC is achieved intermittently by the local rearrangements of small part of atoms at the temperature far below the glass transition temperature (Tg) [1].

Alloy design in platinum based bulk metallic glass, from stabilizing the liquid phase to fine-tuning the glass transition and crystallization temperature.

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Hard (>550HV) BMGs exhibiting strong glass forming ability (GFA, dc>5mm) have been developed in the Pt-Si-B system. Series of alloys with general formula of Pt₄₉.₉₅ (Si-B-MD)₃₃.₄ (Cu-REM) ¹₆.₆₅ (where MD and REM stand for metalloid and rare-earth metal, respectively) were made to evaluate the evolution of glass transition (Tg), crystallization (Tx) and melting temperature (Tm). Replacing Si by Ge was found to significantly increase the width of the supercooled liquid region, caused by the destabilization of the formation of α-Pt. The glassy state gave a high-energy X-ray diffraction pattern corresponding to a new orthorhombic nanocrystalline structure with 2nm crystallite size yet exhibited a glass transition and a crystallization peak. Furthermore minor addition of scandium was found to increase Tx by up to 20°C. The improvement of GFA by addition of REM was also explained by inhibiting the formation of primary phases from the liquid phase upon solidification.
New Bulk Phase-separated Zr-based Metallic Glasses Containing a High Population Density of Glassy Nanospheres

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Bulk metallic glasses (BMGs) with a phase-separated structure have recently been reported in several alloy systems [1,2]. The occurrence of phase separation and thus induced structure are mainly determined by the thermodynamic properties of the liquid solution of the corresponding alloy composition. Here, we designed new phase-separated Zr-based BMGs utilizing Cu/Fe immiscibility [3]. The Zr-based BMGs contains 2–5 nm diameter glassy spheres with a population density and volume fraction of ~5.2×10²⁴ m⁻³ and ~49.3%, respectively. The Zr-based BMGs dependent on alloy compositions exhibit remarkable plasticity at room temperature. It was found that the nanospheres inside the shear band dissolve through mechanical mixing driven by the sharp strain localization there, while those nearby in the matrix coarsen by Ostwald ripening due to the increased atomic mobility. This work presents direct visual evidences for deformation-related effects, in particular increased atomic mobility, in the region around shear bands [4].

New Toxic Element Free Metallic Glass for Biomedical Applications

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Metallic glasses exhibit improved properties compared to pure metals, high strength and low Young Modulus, especially Mg-based glasses. This last feature is interesting for application as bone void filler to prevent bone osteolysis due to stress shielding. Most part of the glasses for biomedical applications contain toxic elements such Be or Ni to improve the ductility. In this work a new metallic glass was elaborated, Mg85Ca8Au7. From a first observation, the sample exhibits some ductility. The super-cooled liquid region was evaluated to be equal to 25.9 °C. The resistance to crystallization and thermal stability were investigated with different experimental methods. At 120°C, no crystallization was detected after 30 minutes, which is a crucial advantage for the process of sterilization in medicine. Mechanical properties has been investigated by hardness and nanoindentation. The results are promising and now the effect of small addition of others elements is investigated to increase Delta T.
Concurrent Session A
Stability & Relaxation
Tuesday, June 7, 2016
Separation of Time Scales of the Frozen-in Relaxation Processes in a Metallic Glass at Deep Supercooling

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Annealing of a glass below the glass transition temperature leads to structural changes, termed relaxation or aging, as the glassy state approaches equilibrium. At deep supercooling the time scales for the diffusion of small and medium sized atoms is expected to decouple from the internal relaxation time of the entire matrix, which is governed by the motion of the large size atoms. Recently, we have probed the separation of equilibration time scales by aging the Au$_{49}$Cu$_{26.9}$Si$_{16.3}$Ag$_{5.5}$Pd$_{2.3}$ bulk metallic glass composition at low temperatures [1]. Multiple plateaus in the enthalpy relaxation and enthalpy recovery were observed using DSC and Flash-DSC. The aging mechanism was also studied on the microscopic level by measuring the time scales on which this system rearranges its internal structure, using XPCS. The system ages by visiting distinct stationary regimes interconnected by intermittent dynamics, similar to fast-motion popping events, typical of stick-slip dynamics.

In-situ Neutron Diffraction study of Crystallization Pathways in Zr-Cu-Al Bulk Metallic Glasses with Gradually Enhanced Glass-forming Abilities

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Crystallization kinetics of Zr-Cu-Al BMGs, i.e. Zr₅₆Cu₃₆Al₈, Zr₅₄Cu₃₈Al₈, Zr₄₈Cu₄₅Al₇, Zr₄₆Cu₄₉Al₆, and Zr₄₆Cu₄₆Al₈, with gradually enhanced glass-forming abilities (GFA), were studied using time-resolved neutron diffraction [1, 2]. According to the property of their crystalline products and thermo-physical behaviors, these BMGs can be divided into two types: Cu₁₀Zr₇-type and Zr₂Cu-type. For Zr₂Cu-type BMG, i.e. Zr₅₆Cu₃₆Al₈ and Zr₅₄Cu₃₈Al₈, there is just one crystallization peak, and neutron diffraction patterns show highly-ordered crystalline phase after devitrification, corresponding to an ordinary pathway of continuous nucleation and growth. For Cu₁₀Zr₇-type BMGs, i.e. Zr₄₅Cu₄₉Al₆ and Zr₄₆Cu₄₆Al₈, two crystallization peaks were observed. The poorly-ordered devitrified Cu₁₀Zr₇-type alloys, with better GFA, corresponds to a unique crystallization pathway of site-saturated nucleation and slow growth. Zr₄₈Cu₄₅Al₇ BMG behaves the mixing-type crystallization behavior, which has two crystalline products: Zr₂Cu-type and Cu₁₀Zr₇-type products. These results suggest that the unique crystallization pathway for Cu₁₀Zr₇-type BMGs would be a distinctive feature of alloys with excellent GFA.

11. The neutron scattering measurements with time resolution ~ 1 min were carried out using NOMAD at the Spallation Neutron Source (SNS), Oak Ridge National Laboratory (ORNL).
Devitrification of Metallic Glass Alloys and Synthesis of Nanostructures

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While the nanocrystalline state is often viewed as 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, primary crystallization of amorphous Al alloys can yield nanocrystals with sizes of 10-20 nm and densities of 10^21 - 10^22 m^-3. 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 and guidance to promote BMG synthesis as well as challenges for the fundamental understanding of the reaction mechanisms.
Processing Dependent Phase Selection in Al\textsubscript{90}Sm\textsubscript{10} Amorphous Alloys

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Phase selection during devitrification of Al-Sm amorphous sputtered thin films (STF) and melt-spun ribbons (MSR) has been studied by time-resolved wide-angle and small-angle X-ray scattering WAXS/SAXS. Amorphous structures in both STF and MSR exhibit very similar structural order at room temperature, however during low temperature annealing, the amorphous STF separates into Al-rich and Sm-rich amorphous phases followed by formation of FCC-Al and Al\textsubscript{20}Sm\textsubscript{5} phases\cite{1}, while MSR transforms polymorphically to a metastable big cubic Al\textsubscript{60}Sm\textsubscript{10} phase. In both cases, the initial devitrifying transition occurs throughout the entire sample, after which the resulting crystalline phases follow different pathways. Following high temperature annealing, both pathways converge toward FCC-Al and Al\textsubscript{4}Sm phases. The different devitrification behaviors are believed to be due to the chemical/topological short-range ordering atomic arrangement formed during the synthesis processing. The corresponding changes in the atomic- and nano-scale structure that occur during the phase selection as measured by the WAXS/SAXS experiments are discussed.

Concurrent Session B
Mechanical Behavior I Deformation and Structure

Tuesday, June 7, 2016
Universal Fast Secondary Relaxation and Plasticity Initiation in Metallic Glasses

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It has long been recognized that the relaxation spectrum of glassy solids is intrinsically connected to their disordered structural features and deformation behaviors. However, such connections still remain elusive for metallic glasses. In the past, only a primary relaxation peak corresponding to glass transition was found on their relaxation spectra; only recently was one additional secondary relaxation peak identified merely on a limited number of metallic glasses. However, through the extensive study of a variety of metallic glasses over a wide range of temperatures, here we provide the compelling evidence for the existence of a fast secondary relaxation process common to different types of metallic glasses. Compared to the previous findings of the slow relaxation process, the activation energy of the fast relaxation process is affected by thermal treatment but generally insensitive to the chemical composition of metallic glasses. Furthermore, it can be demonstrated that the initiation of plasticity in metallic glasses is strongly affected by the fast relaxation process. By “resonating” with the fast relaxation process, plasticity can be obtained even in the metallic glass which otherwise shows an extremely brittle behavior in conventional mechanical tests.
Effect of Thermal Cycling on Shear Transformation Zone Spectra in a Metallic Glass

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We have recently reported on quasi-static anelastic relaxation measurements in amorphous Al₈₆.₈Ni₃.₇Y₉.₅. Direct spectrum analysis yielded relaxation-time spectra with distinct peaks, corresponding to a quantized hierarchy of shear transformation zones (STZs).[¹] Similar results were also obtained from published dynamic relaxation data.[²] Recently, Ketov et al. showed that thermal cycling of amorphous La₅₅Ni₂₀Al₂₅ enhanced its compressive plasticity.[³] The purpose of the present work is to further explain the effect of the thermal cycling by determining the STZ properties for the same alloy. Quasi-static anelastic relaxation measurements were performed with and without thermal cycling, over a wide range of time constants, using mandrel bending and nanoindenter cantilever measurements. Details of the corresponding STZ spectra and properties will be presented. These will also be compared with results obtained for alloys that exhibit less-pronounced beta relaxations than La₅₅Ni₂₀Al₂₅.

Structural Heterogeneity Induced Plasticity in Metallic Glasses

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Deformation processes in metallic glasses are known to be inhomogeneous in space and jerky in time, but there is a lack of in situ, nondestructive evaluation of such processes on appropriate spatiotemporal scales. It has also been demonstrated that the fracture toughness decreases sharply for bulk metallic glasses transitioning from as-cast to annealed states. First, we have utilized a nanomechanical testing method to measure the stresses for the onset of plasticity, and developed a stochastic statistical model to characterize the structural heterogeneity (including defect density and strength) inside the metallic glasses. The synergy between experimental and theoretical works found that, with increasing the structural relaxation, the defect density drops by two orders of magnitude, and correspondingly the fracture of metallic glasses changes from a significantly plastic (metal-like) mode to an extremely brittle one (fragile glass). Second, an unmixing method from signal processing is employed to identify the localized heat sources inside the bulk from the measured thermographs on the surface. From a linear instability analysis, the evolution of this heterogeneous process proves the coupled structural/thermal softening mechanisms.
Correlating the Failure Behavior of Metallic Glasses at Different Temperatures with their Structural Evolution

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The lack of detailed understanding of correlations between structure and mechanical behavior of metallic glasses (MGs) under a variety of environmental conditions (in particular, temperature) is a significant stumbling block in exploiting MGs in structural applications [1]. This deficiency may be traced to the inherent difficulties associated with extracting atomic level structural information from experiments, and the inability of earlier molecular dynamics (MD) simulations to reproduce experimental observations over a wide temperature range. Here, by careful construction of our atomistic models of two MGs, we essentially reproduce the major deformation modes from localized shear banding (SB) to homogeneous plastic flow merely by changing the temperature within a unified simulation framework. This enables us to find that different failure modes exhibit distinctively different evolution pathways in the atomistic structure of MGs. Since our simulations show the same trend for both systems, our findings might be generic for a wide range of MGs.

Concurrent Session B
Mechanical Behavior II: Composites
Tuesday, June 7, 2016
Effects of Changes in Test Temperature on Tension Behavior and Toughness of BMG Composites

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Tensile and toughness behavior of a Zr-based bulk metallic glass matrix composite (BMGMC) containing a bcc crystalline phase were examined over temperatures from 77K (-196°C) to 653K (380°C). The composite exhibited some tensile plasticity at all test temperatures and unique flow and fracture behavior at elevated temperatures. In the toughness tests conducted at low temperatures, the notch toughness of the BMGMC exceeded that of fatigue-precracked samples; but at room temperature and above, the trend was mixed and depended on temperature and displacement rate. These various observations are rationalized based on the changes to the flow and fracture behavior of both the glass and the crystalline phases over this temperature range. At low temperatures, the crystalline phase is sensitive to defects and changes in stress state, and can undergo a ductile-to-brittle transition. At higher temperatures, both constituents possess lower strength and are less sensitive to defects, enabling more significant crack-tip blunting in the fatigue-precracked samples. EBSD results provide insight into active deformation mechanisms in the bcc phases, and measurements of dendrite shape as a function of macroscopic strain state in the tension experiments provide insight into load sharing behavior in the composite.
Property Manipulation of TRIP Bulk Metallic Glass Composites

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To overcome the limitation concerning catastrophic failure of bulk metallic glasses (BMGs), the concept of developing heterogeneous microstructure with in-situ formed secondary phases has been used. In the present study, we newly developed a novel TRIP (transformation-induced plasticity) Ti-based BMG composite with super-elastic secondary phase. The super-elastic secondary phase is quite unique and effective for designing highly tough BMG composite with TRIP behavior through its outstanding energy absorbing property. Because properties of super-elastic secondary phase highly depend on martensitic transformation temperature (MTT) due to compositional variations, we systematically investigated the correlations among MTT, various properties and content of additional elements in secondary superelastic TiCuNiSiSn alloys and related BMG composites. Finally, we offer a novel methodology for property optimization of TRIP BMG composites. Indeed, the TRIP BMG composites open up a new direction for developing extremely sustainable as well as controllable BMGCs in service.
Influence of Microstructure on Deformation Behavior in BMGMCs

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Bulk metallic glass-matrix composites (BMGMCs) consisting of an amorphous matrix and a homogenous distribution of tough crystalline dendrites formed in situ offer a promising solution to the low fracture toughness and brittleness of pure bulk metallic glasses. Recent studies have shown that the coarseness of the microstructure can be controlled at constant volume fraction through semi-solid processing technology. This work addresses the disconnect between the morphology and size of the precipitated dendritic reinforcement and the overall mechanical behavior of the composite. Synthetic 3D microstructures were produced using images of real BMGMCs, and then subjected to uniaxial tension, compression, and shear deformation simulations. We’ve implemented the elastic-viscoplastic formulation of the fast Fourier transform (FFT) based approach for simulating microstructural deformation in two-phase heterogeneous materials. We analyze the overall composite mechanical performance and study the underlying deformation behavior at the microstructural level to help explain the macroscopic trends.
Concurrent Session B
Mechanical Behavior III: Deformation and Structure

Tuesday, June 7, 2016
Insights on Shear Banding in BMGMCs from FFT-based Continuum Modeling

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In bulk metallic glass-matrix composites (BMGMCs), the nature of shear bands and their interaction with the crystalline phase reinforcement play an important role in the overall mechanical behavior of the composite. However, the rapid timescales involved with their formation has posed a hindrance for experimentalists in studying the precise way in which they initiate and propagate in the amorphous matrix, and furthermore terminate at an adjacent interface. These phenomena will be examined here with fast Fourier transform (FFT) based continuum modeling, which makes it possible to simulate deformation in two-phase heterogeneous systems at higher spatial and temporal resolutions than that offered by traditional finite element methods given the same computational resources. We conduct a thorough analysis of the stress and strain evolution during shear banding in both phases of Zr-Ti-based composites and compare our results with characterization work on deformed microstructures obtained from experimental BMGMC tensile test specimens.
Fe-based Bulk Metallic Glasses: Brittle or Ductile?

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Fe-based bulk metallic glasses (BMGs) typically exhibit ultrahigh strength but a poor ductility at room temperature. To overcome the negligible plasticity we have developed a series of Fe-based BMGs from structural [1] and compositional [2] design rules. I will describe our efforts in the development of Fe-based BMG composite reinforced with ductile α-Fe dendrites and monolithic Fe-based BMGs which exhibit a super large compressive plasticity. Such a discovery is guided by understanding a composition-strength-ductility map, in which most of Fe-based BMGs are classified into three types: FeC-based, FeB-based, and FeP-based. Among these, the FeP-based BMGs often possess a lower glass transition temperature, a lower shear modulus, and a higher Poisson's ratio, resulting in a lower shear flow barrier and a higher plasticity. Our findings will provide a new insight into how to prevent the brittle failure and develop the high performance of Fe-based BMGs.
Nonlinearity and Anisotropy of Elastic Moduli during Compression of the BMG

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Stress-strain relationship in bulk metallic glasses is linear up to the elastic limit. It suggests simple Hook behavior. However, in situ X-ray diffraction studies during deformation indicated that there was a significant structural contribution due to local anelastic-like relaxation. We investigated structural response during elastic deformation and also preformed ultrasound measurement during compression of the BMG. The high energy X-ray diffraction studies were carried out and local atomic strains were obtained using the anisotropic pair distribution function method. Acoustic waves were propagated along and perpendicular to the compressive load axis. The longitudinal and transverse velocities were determined using pulse-echo technique at frequency of 30 MHz at each compressive load. We determined Lamé coefficients up to the 4-th order. Acoustic measurements revealed, in agreement with the structural studies, nonlinearity and anisotropic behavior of the elastic moduli. The work was supported by the U.S. DOE, DE-AC05-00OR-22725.
Investigation on the Intrinsic Mechanical Properties of Nanosized Metallic Glasses via Particle Compression

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Although metallic glasses (MGs) exhibit remarkable mechanical properties such as high yield strength and high elastic limit far above those of crystalline counterparts, the brittleness with highly localized shear deformation restricts their use as structural materials. Therefore, controlling shear localization remains as a major task, and studies on the deformation of small volume MGs via nanopillar test have attracted considerable attention with chances of understanding shear localization. However, pillar fabrication using focused ion beam leaves tapered and irradiated surfaces which complicate deformation behaviors. To exclude these extrinsic effects, we performed in-situ compression tests of MG nanoparticles prepared by gas atomization with careful viscosity control, and investigated the intrinsic mechanical properties. Moreover, we confirmed the validity of particle compression method for the evaluation of mechanical properties by comparison with nanoindentation and nanocompression results. The results could provide effective guidelines for evaluating nanomechanical properties and understanding the fundamentals of MG deformation.
How the Voronoi Diagram of 3D Spheres Can be used for the Accurate and Efficient Analysis of Geometry and Topology of Metallic Glasses?

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Efforts for a structure model of metallic glasses explaining both short- and medium-range orders remains unsuccessful [1]. Geometry of atomic arrangements is frequently a basis for understanding the properties of metallic glasses. Examples: Radial distribution function, free volume, etc. However, many geometric features are not easy to calculate, particularly for possibly intersecting polysized atoms and computation was frequently conducted using Monte Carlo or grid enumeration which resulted in approximation and sometimes in contradiction among similar studies. Seemingly correct analytic methods such as the ordinary Voronoi diagram of atomic centers [2, 3] and Laguerre tessellation also frequently produce approximation. We introduce Voronoi diagram of spheres [4] and its derivative constructs [5] as a new tool kit which guarantees mathematical correctness and efficiency for atomic arrangement [6, 7] and show how geometric questions in metallic glass communities can be conveniently handled: E.g., Volume/area of model, voids/tunnels with volume/area, neighborhood reasoning, etc.

Plenary Session

Wednesday, June 8, 2016
Extending the Range of the Glassy State in Metals

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It has become clear that metallic glasses are ideally suited for exploration of the effects of deformation on the structure and properties of glasses. It is expected that plastic deformation can change the structure and properties, but is more surprising that there can be very significant effects even well within the (nominally) elastic regime. In this talk we explore the ranges of energy that can be achieved in the metallic glassy state, from very high (‘rejuvenated’) to very low (‘relaxed’ and even ‘ultrastable’). We also explore the extent to which directionality (anisotropy) can be induced in metallic glasses. In each case, we examine the potential applications of the properties that can be induced.

Our recent and pending publications on these topics include:

Spatial Heterogeneity of Metallic Glasses

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Distinct structural and chemical heterogeneities of metallic glasses have recently been extensively reported in the literature. These spatial heterogeneities, suggested by simulations and experiments, have been considered as “microstructure” to qualitatively explain various properties of metallic glasses. Nevertheless, the nature of the spatial heterogeneity in the disordered materials has not been well understood, which is limited by the technical challenges in experimentally characterizing the structure and dynamics of the nano-scale “microstructure”. In this talk, I will introduce our recent work on experimental characterization of the spatial heterogeneity of metallic glasses by amplitude-modulation atomic force microscopy and angstrom beam electron diffraction. Evident variation in phase-lag distribution unveils the viscoelastic origin of the nano-scale spatial heterogeneity. Importantly, the evolution of spatial heterogeneity intrinsically correlates with sub-Tg beta-relaxation. The characteristic relaxation time and activation energy of heterogeneity evolution are in accord with those of excess enthalpy release by beta-relaxation.
Structural Features and Mechanical Behavior of a Nanoglass with and without Cryogenic Treatment

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Nanoglasses constitute a new group of amorphous materials, which are produced by extremely high cooling rates. In this study, the nanoglass of Sc$_{75}$Fe$_{25}$ produced by cold pressing of alloy powder is characterized by high rate nanoscale indentation tests at ambient temperature. Our results reveal that the nanoglass contains a distinctly higher level of loosely packed regions embedded in the tightly bonded matrix, as compared with regular metallic glasses. It is surprisingly to find out that such structure in the nanoglass is featured with a high structural instability, and that deep cryogenic treatments will result in a ~50 % reduction in its elastic modulus. Furthermore, such modulus reduction will be recovered gradually by extensive aging treatments at room temperature. In comparison, a Zr-based metallic glass shows a hardening effect rather than softening after the same cryogenic treatment. The structure evolution in these materials will be discussed.

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Concurrent Session A
Structure I
Wednesday, June 8, 2016
Structure of Metallic Glasses from Fluctuation Electron Microscopy and Computational Structure Refinement

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We have used fluctuation electron microscopy and hybrid Reverse Monte Carlo structural refinement to investigate the atomic structure of several classes of metallic glass, focusing on their nanometer-scale medium-range order (MRO). In both metal-metal (Zr-Cu-Al, Al-Sm) and metal-metalloid (Pd-Si) metallic glasses, we find a mix of two MRO structure types. One type has approximate four- and six-fold rotational symmetry, so we call it “crystal-like”. The other has less rotational symmetry at medium-range. In metal-metal glasses, the short-range order (SRO) is approximately icosahedral, but not in Pd-Si. We have developed a computed reciprocal space method to connect structural features in computer models to features in the FEM data, and a real-space point-matching approach to supplement Voronoi polyhedron indices for analysis of SRO. The point-matching results are amenable to machine learning, which enables automatic clustering methods to identify prototypical structures. The MRO structures we find are connected to glass-forming ability and crystallization across alloys systems.
Development of Interatomic Potentials Appropriate for Metallic Glasses

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Ab initio calculations provide the most physically sound way to describe interatomic interaction. However, ab initio molecular dynamics (AIMD) itself cannot provide reliable data for the structure and other properties of metallic glasses because of the absence of the long range order and slow kinetics in these systems. Therefore, classical molecular dynamics (CMD) simulation should be performed. However, the results of the CMD simulations strongly depend on the quality of the employed semi-empirical potentials. In this presentation, utilizing the AIMD liquid structure and phase transformation data in the potential development procedure will be discussed. Next, it will be shown how CMD simulations can be used to obtain reliable initial glass models for the AIMD simulations. Finally, a method to obtain structure factors from small AIMD models will be presented. Applications of all these methods will be illustrated by presenting semi-empirical potentials for Ni-Zr and Al-Sm alloys.
Mesoscale Metallic Glass Deformation Simulation Incorporating Medium Range Order From Fluctuation Electron Microscopy

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We present a new mesoscale deformation model of metallic glasses (MGs) that incorporates nanoscale medium range ordering (MRO) information from fluctuation electron microscopy (FEM). Mesoscale simulation involving diverse STZ types can provide useful insights into shear banding and overall deformation of MGs [1]. We demonstrate that more realistic deformation can be simulated by incorporating the experimentally measured MRO information using FEM directly into the heterogeneously randomized STZ environment in our model. Our method assumes that each MRO type, which resides at the same length scale of STZ, will have a different set of parameters that characterize the STZ events [2]. For example, increasing the volume fraction of crystal-like MRO [3] in the model can lower the yield stress and homogenize shear band distribution, which can lead to higher ductility. The change in the ductility can be quantified using extreme value statistics analysis [1], and compared to the experimentally measured ductility.

Concurrent Session A
Structure II
Wednesday, June 8, 2016
The Structural Pathway of Metallic Liquids to Vitrification

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A glassy metal forms when a metallic liquid is cooled rapidly enough so that crystallization is avoided upon solidification. However, the way the atomic structure of the liquid transforms to the glassy structure is not well understood. The acquisition of structural information in the supercooled liquid regime, between the melting $T_m$ and the glass transition temperature $T_g$, is most often hindered by crystallization. Advances in containerless solidification and synchrotron radiation techniques offer new possibilities for observing in-situ the structural evolution of rapidly cooled metallic liquids. Recent results indicate a rapid increase of the local order in the short and medium range (SRO and MRO) as the supercooled liquid approaches the glass transition temperature $T_g$, below which the structure is considered as “frozen”. The undercooled liquid enters into a different structural configuration below the melting temperature $T_m$, indicating the existence of three non-crystalline regimes in the liquid’s pathway to vitrification. The structural evolution below the melting temperature deviates from that of the liquid pointing to a liquid-(supercooled) liquid transition. The structural rearrangements in the supercooled liquid are found to be correlated with a rapid increase in viscosity and with the fragility of metallic liquids. The evolution of the atomic structure of metallic liquids during vitrification may shed light on glass formation and on the structural origins of the sluggish long-range order kinetics that suppress nucleation and growth of crystalline phases [1].


\* The work is dedicated to the memory of Professor Alain Reza Yavari.
Scattering Studies of Metallic Liquids Using the Neutron ElectroStatic Levitator (NESL) at the Spallation Neutron Source (SNS)

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There is great interest in understanding the relationship between chemical and topological structure [1-4], dynamics [5], bulk properties [6,7], and glass-forming ability (GFA) in metallic alloys. Of particular interest is the influence of the local structure and dynamics in the equilibrium and supercooled liquid states on GFA. Experimental studies, however, are limited by difficulties in accessing these high-temperature states given the high reactivity of metallic alloys with crucibles and the surrounding atmosphere. The Neutron Electrostatic Levitator (NESL) [8], recently commissioned for use at the Spallation Neutron Source (SNS), combines a containerless sample environment with elastic, quasielastic, and inelastic neutron scattering capabilities for studying both chemical short- and medium-range order and local atomic dynamics. The results of recent experiments studying both chemical ordering [9] and local excitations in glass-forming metallic liquids will be presented, and plans for future work will be discussed.

Unveiling the Distinct Features of Inherent Heterogeneity in Metallic Glass

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Heterogeneity is commonly believed to be intrinsic to metallic glasses. Nevertheless, how to distinguish and characterize the heterogeneity in atomic level is still debated. Based on extensive molecular dynamics simulations that combine isoconfigurational ensemble and atomic pinning methods, we directly reveal that metallic glass contains flow units and an elastic matrix which can be well distinguished by their distinctive atomic-level responsiveness and mechanical performance. The microscopic features of the flow units, such as the shape, spatial distribution dimensionality, and correlation length, are characterized from atomic position analyses. Furthermore, the correlation between the flow units and the landscape of energy state, free volume, atomic-level stress, and especially the local bond orientation order parameter is discussed [1].

Crystal Gene: Common motifs Transcending Crystals, Glasses, and Liquids

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We establish through typical metallic systems Cu-Zr and Al-Sm the concept of “crystal gene”, that is, structural order in the short-to-medium range order that transcends crystals, liquids, and glasses. With such a connection between crystalline and amorphous phases, a mature toolset for treating crystals can be used to assist the identification of complicated structural order in amorphous systems, which is a fundamental difficulty in physics and materials science. In addition, as demonstrated in the example of the Al₉₀Sm₁₀ system, the crystal gene persists from liquid to crystalline phases during the crystallization processes observed in experiments. Therefore, the identification and quantification of the crystal gene bring new insight into the atomistic transformation mechanism from the amorphous to various metastable crystalline phases, which can ultimately lead to a better understanding of phase selection in metallic alloys.
Formation of Monatomic Metallic Glasses through Ultrafast Liquid Quenching

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It has long been conjectured that any metallic liquid can be vitrified into a glassy state provided that the cooling rate is sufficiently high. Experimentally, however, vitrification of single-element metallic liquids is notoriously difficult. True laboratory demonstration of the formation of monatomic metallic glass (MG) has been lacking. Herein we report an experimental approach to vitrify monatomic metallic liquids by achieving an unprecedented high liquid quenching rate of $10^{14}$ K/s. Under such a high cooling rate, melts of pure refractory body-centered cubic (bcc) metals, such as liquid tantalum and vanadium, are, for the first time, successfully vitrified to form MGs suitable for property interrogations. With in situ transmission electron microscopy observation, we investigated the formation condition and the thermal stability of the as-obtained monatomic MGs [1]. The availability of monatomic MGs being the simplest glass formers offers unique possibilities to study the structure and property relationships of glasses. Our technique also exhibits great control over the reversible vitrification-crystallization processes, suggesting its potential in micro-electro-mechanical applications. The ultra-high cooling rate, approaching the highest liquid quenching rate attainable in the experiment, makes it possible to explore the fast kinetics and structural behavior of supercooled metallic liquids within the nano- to pico-second regimes. Results of single elemental FCC and HCP metallic liquids through this ultrafast liquid quenching will also be presented.

Concurrent Session B
Applications II: Metallic Glass Coatings
Wednesday, June 8, 2016
Thin Film Metallic Glasses: Novel Coating Materials for Advanced Applications

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Thin film metallic glasses (TFMGs) possess exceptional mechanical properties adopted from its bulk form such as high strength, large elastic limits, and excellent corrosion and wear resistances due to its amorphous nature. TFMGs have been reported to improve substrate mechanical properties [1, 2] owing to its high strength and toughness. In addition, TFMGs are free from grain-boundary and thus can be applied as diffusion barrier in electronic applications [3] which may improve the efficacy of devices. TFMGs are also potentially useful for the biomedical applications, including the property enhancements of medical tools [4] and the suppression of biological cell attachments. Therefore, TFMGs appear to be promising structural and multifunctional coating materials. In this presentation, many potential applications along with their excellent properties based on versatile TFMGs are described.

Key words: thin film metallic glasses, substrate mechanical property, electronic application, biomedical application

Corrosion Resistant Amorphous Coatings for Deep-sea Applications

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In deep sea environment, hydrostatic pressure has been proved to deteriorate corrosion resistance for most metallic materials. To resolve this problem, corrosion resistant coatings is required. This study is concerned to evaluate corrosion performance of a Fe-based amorphous coating in a high hydrostatic pressure of 80 atm, compared to commercial 316L stainless steel (SS) alloy. In-situ high pressure electrochemical investigations reveal that pitting resistance was increased at 80 atm for amorphous coating while decreased for SS alloy. Pitting nucleation and growth behaviors were studied by pitting incubation technique, which indicates different pressure-dependent behaviors for the two alloys. Nanoscale passive films were analyzed by XPS and TEM/EELS. Effect of pressure on composition, cross-sectional structure, film thickness and nano-mechanical properties of the passive films formed on the two materials will be discussed. The findings may pave the way for exploring amorphous coatings as a robust corrosion resistant coating for deep-sea applications.
Concurrent Session B
Mechanical Behavior IV: Shear Banding & Fracture

Wednesday, June 8, 2016
Universal Slip Statistics: from Nanopillars to Earthquakes

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The deformation of many solid materials is not continuous, but discrete and jerky, with intermittent slips, similar to earthquakes. A simple model predicts that the statistical distributions of the slips should be universal, i.e. the same for many different materials, spanning a wide range of scales, from nanometer-sized pillars to earthquake faults that are a hundred kilometers long. We show a comparison of the model predictions to recent experiments on nanocrystals, bulk metallic glasses, rocks, granular materials, and earthquakes and find good agreement with the model predictions. Tools from the theory of phase transition, such as the renormalization group are used to explain the wide applicability of the simple model. The study provides intuition and a unified framework to understand fundamental properties of shear-induced deformation of solids. It also provides many new predictions for future experiments [1-3]. The results can be used for materials testing, evaluation, and hazard prevention.

Cavition and Internal Stresses during Shear-Banding of Metallic Glasses

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Bulk metallic glasses deform inhomogeneously at low homologous temperatures via shear-banding. Whilst the dynamics of shear-bands has been summarized by our previous studies [1], little is known about structure inside and around a shear-band. In this talk we demonstrate that shear bands can have long range stress fields, which reach local stress values as high as the yield stress of the material. By measuring nanomechanical properties along an isolated shear band, the indirect signature of long range and strongly position dependent internal stresses along the shear band are revealed. The strongest internal stresses are located near cavities on the shear-band plane, where cavity end-points exhibit stress patterns that are reminiscent of mixed mode crack-tip stress fields [2, 3]. The findings are discussed in terms of a shear-band-to-crack transition and internal stress development during shear-band dynamics in a bulk metallic glass.

Engineering High Fracture Toughness into Bulk Metallic Glasses

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While notched toughness values for bulk metallic glasses (BMGs) tend to be consistently high, large variability has been reported in pre-cracked mode I fracture toughness. For example, some studies have reported a large discrepancy between the notched and pre-cracked toughness values while others have found them to be quite similar. To confuse matters further, both behaviors have even been observed in a single study. Assuming such differences are related to the internal structure and associated deformability of the BMG, it should be possible to induce high toughness behavior by creating favorable metallic glass structures. The effects of two mechanical treatment methods, imprinting and cold rolling, on fracture toughness will be presented. In the first case, imprinting a Zr52.5Ti5Cu18Ni14.5Al10 (at.%) BMG was shown to 1) ductilize pre-cracked bending beams, 2) significantly reduce the observed scatter in the fracture toughness, and 3) achieve high toughness behavior typical of notched samples. In the second case, cold rolling a Zr63.78Cu14.72Ni10Al10Nb1.5 BMG was found to significantly increase the fracture toughness. Overall, these results suggest that mechanical treatments can induce favorable glass structures that promote high pre-cracked toughness in BMGs and drastically reduce the discrepancy between the notched and pre-cracked behavior.
Nature of Crack-tip Plastic Zone in Metallic Glasses

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The fracture of metallic glasses (MGs) can be induced by shear banding or by cavitation [1-2]. Plastic zone in front of a crack tip, which is greatly involved with localized shear band, cavitation and the resultant fracture morphology, is a key clue to unveil the secrets of the intrinsic ductility and fracture. However, the characteristics of plastic zone, i.e., stress and strain distributions, size and shape, have not been clearly unraveled for MGs so far. To solve this problem, an analytical solution of the plastic zone for mode I crack under plane strain condition is derived [3]. Two length scales of the plastic zone are revealed to control shear flow instability and cavitation. The critical values of the mode I stress intensity factor and the plastic zone size at crack initiation are obtained based on free volume evolution dynamics. The ductile-to-brittle transition in MGs is revealed to be attributed to a shape change of the critical plastic zone.

Plenary Session

Thursday, June 9, 2016
Tailoring Structural Inhomogeneity in Metallic Glasses to Enable Tensile Ductility at Room Temperature

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Metallic glasses boast high strength, but their low ductility has been a major concern. Taking a structural perspective and citing selected examples, in this talk we advocate purposely enhanced structural inhomogeneities, in an otherwise compositionally uniform and single-phase amorphous alloy, to promote distributed plastic flow. Four current tactics (the “4R’s”) to improve deformability are highlighted, from the standpoint of structural, and consequentially mechanical, heterogeneities that can be tailored in the monolithic glassy state. Highly rejuvenated glass structures, coupled with constraints on the shear banding instability, lead to tensile ductility and necking, which is unusual for glasses at room temperature. Possibilities of strain hardening and strain rate hardening that are needed to stabilize uniform elongation are discussed. Innovative design and processing of amorphous alloys, with internal structures tuned to facilitate flow, offer new possibilities in pushing the envelope of ductility accessible to these high-strength materials.
Early Plasticity in Metallic Glasses

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Plastic deformation of metallic glasses at technically relevant temperatures is mediated by the operation of localized shear bands. Understanding the emergence of shear bands from smaller deformation entities, such as shear transformation zones, has become a topic of intense research in the past years, with the goal of ultimately mediating the brittle behavior the shear bands cause. However, since shear transformation zones as well as shear bands may operate at time and length scales that are barely accessible experimentally, systematic studies must often be performed to gain indirect insight.

We present several small-scale mechanical studies on metallic glasses which have been designed to test our understanding of the emergence of shear bands [1-3]. We vary specimen size [1,2], strain rate [2], acquisition rate, and stress state in microcompression or spherical nanoindentation studies, and by analyzing the mechanical response and the distributions of strain bursts, infer certain limits on the inherent behavior of emerging shear bands and the cooperativity of the shear transformation zones.

Concurrent Session A
Structure III
Thursday, June 9, 2016
Structural Crossover in a Supercooled Metallic Liquid and the Link to a Liquid-to-liquid Phase Transition

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Time-resolved synchrotron measurements were carried out to capture the structure evolution of an electrostatically levitated metallic-glass-forming liquid during free cooling. The experimental data show a crossover in the liquid structure at ~1000 K, about 115 K below the melting temperature and 150 K above the crystallization temperature. The structure change is characterized by a dramatic growth in the extended-range order below the crossover temperature. Molecular dynamics simulation has identified that the growth of the extended-range order was due to increased correlation between solute atoms. These results provide structural evidence for a liquid-to-liquid-phase-transition in the supercooled metallic liquid.
Liquid-Liquid Phase Transition in Metallic Glasses during Ultrafast Heating

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Upon cooling a glass forming supercooled liquid exhibits a remarkable change of the shear viscosity in a relatively small temperature interval. Motivated by a decoupling of the translational diffusion from shear viscosity, there is an active debate about liquid-liquid phase transition during cooling in the supercooled liquid of metallic glass formers.

In our measurements we investigated the thermodynamic and structural properties in the supercooled liquid of metallic glasses during heating. We used a capacitor discharge to heat up metallic glasses with rates of \(10^6\) K/s in order to avoid crystallization \([1]\). Combining the discharge with a novel chopper technique \([2]\), we show that the peak position of the first peak of the structure factor exhibits a significant drop close to the melting temperature of the crystal. At the same temperature the specific heat capacity exhibits a maximum \([3]\). We discuss the results in the light of a liquid-liquid phase transition.

\[1\] W. L. Johnson et al., Science 332, 828 (2011)
Thermodynamic Connection to the Structural Variation of Zr-Al-Co Glass Forming Alloys

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Free surface condition of metallic melts can be achieved with containerless high-temperature/high-vacuum electrostatic levitation (ESL) technique, which could minimize heterogeneous nucleation size and wide undercooled liquid region easily. In the present study, we experimentally measured thermophysical properties such as time-temperature profile, specific volume, interfacial free energy and TTT diagram in Zr-Al-Co alloy system which has different glass-forming ability (GFA) by a slight composition modification using ESL technique. In addition, we analyzed structural changes of the alloy system with synchrotron X-ray scattering to understand the influence of compositional change on atomic level local ordering evolution. Furthermore, we try to characterize the variation in structural signature and thermophysical properties in liquid state according to GFA. These results will demonstrate how to predict thermophysical properties originated from atomic cluster connection change of metallic melts according to GFA and show vitrification mechanism of glass-forming alloys more precisely.
Concurrent Session B
Mechanical Behavior III: Plasticity
Thursday, June 9, 2016
Theoretical Strength of Amorphous Solids

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Metallic glass represents not only a new class of structural and functional materials but also a simplest model system for studying mechanical properties of the disordered or amorphous solids. One of the fundamental questions is the theoretical strength, or the maximum shear stress that the amorphous solid could bear. In crystalline materials, this question was addressed by Frenkel in a simple saw-tooth model; he predicted that the maximum (shear) stress of a close-packed crystal is approximately \( G/2\pi \), where \( G \) is the shear modulus of the solid. The theoretical strength plays a key role in discovering crystal defects, dislocations. In amorphous solids, predicting the theoretical stress turns out to be a formidable task, due largely to the disordered atomic structure.

In this talk, I shall go through two routes in searching for theoretical strength in metallic glasses. One is the finite deformation theory and the other a random potential model. The theoretical strength obtained from the two independent and different theoretical models is found, roughly about \( G/10 \). The close resemblance between the values in crystalline and amorphous solids indicates the insignificance of the underlying atomic structures in theoretical strength. However, by comparing with existing experimental data of the strength in metallic glasses, we could see the significance. One outcome of the prediction of the possible defects in the two different types of solids: In crystals, dislocation is the main culprit for degradation of the theoretical strength while in metallic glasses it is the less coordinated fluctuation of stress and strain, or local deformation that contributes to the yielding of the amorphous solids.
Deformation Behaviour of Metallic Glasses Without Shear Banding at Room Temperature

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Plastic deformation of large-sized metallic glasses (MGs) is highly localized into shear band under uniaxial stress. Associated with this, the deformation behaviour of metallic glasses is characterized with 2% elastic limit and very little plastic strain and they usually failure in a catastrophic manner at room temperature. It is also believed that MG sample only deforms elastically in the rest of sample volume without shear band. On the other hand, deformation of MG is homogeneous via viscous flow at high temperatures near or above the glass transition and low strain rates. Thus if the shear banding can be suppressed, the deformation behaviour of metallic glasses would be expected to be quite different at room temperature. In our talk, we will summarise our recent findings in the difference in the mechanical behaviour of metallic glasses when without shear banding. The mechanism for such a difference will also be discussed.
Thermal Activation in Metallic Glass by Creep Deformation and Stress Relaxation

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The creep and stress relaxation experiments at high temperatures were performed to investigate flow behavior and viscous nature of as-cast Zr₆₅Cu₁₈Ni₇Al₁₀ metallic glass. The creep activation volume and the activation energy are 0.12 nm³ and ~3 eV, respectively. The values are less than other Zr-based metallic glasses, owing to the under glass transition temperature $T_g$ test temperatures. It is noted that there is lower degree of disorder in Zr₆₅Cu₁₈Ni₇Al₁₀ metallic glass. The activation volume of the creep is 3-4 times higher than that of stress relaxation; it is related to much less atomics in the stress relaxation process compared with creep. It could be mainly caused by the different organizational behaviors. The rather larger non-dimensional parameter $\beta_{KWW}$ (0.93) value suggests that there are much more homogeneity near $T_g$. As an example, a referenced publication is shown below [1].

Tensile Ductility of Bulk Metallic Glasses Processed by High-Pressure Torsion

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Over the past decade, several methods have been proposed to increase the ductility of BMGs. Through appropriate composition selection, several bulk metallic glasses (BMGs) have been found to exhibit reasonably good plasticity. Moreover, pre-testing of deformation processes can delay catastrophic failure. The results showing increased ductility have been obtained from compression tests. However, significantly increased tensile ductility through pre-treatment has not yet been reported. Recently, high-pressure torsion (HPT) has been developed in order to produce bulk nano/ultrafine structured metallic materials with grain sizes from 20 to 200 nm. Because of its ability to impose extremely high strains compared to other severe plastic deformation (SPD) processes, there have been several studies on HPT-processed BMGs (HPT-BMGs) and amorphous ribbons, as well as polycrystalline materials. Nevertheless, mechanical property changes due to altered microstructures in HPT-BMGs are not clearly understood. In this report, we present clear tensile ductility in a Zr-based BMG via a HPT process. Enhanced tensile ductility and work-hardening behavior after the HPT process were investigated, focusing on the microstructure, particularly the changed free volume, which affects deformation mechanisms (i.e., initiation, propagation, and obstruction of shear bands). Our results provide insights into the basic functions of hydrostatic pressure and shear strain in the microstructure and mechanical properties of HPT-processed BMGs.
Posters

Tuesday, June 7, 2016
Interplay between Thermophysical Properties and Glass Transition in Pd-based Fragile Glass Formers

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An exceptional high glass-forming ability (GFA) was reported in Pd-Cu-Ni-P quaternary alloy system which shows the slow kinetics in liquid state[1]. Furthermore, slight modification as well as fluxing treatment enhanced the GFA, which is possible to compare the compositional dependence on GFA in Pd-Cu-Ni-P alloy system. In the present study, we experimentally measured thermophysical properties such as specific volume, viscosity, and surface tension in Pd-Cu-Ni-P alloys which have different GFA by a slight composition change, using a containerless high-temperature/high-vacuum electrostatic levitation technique. Pd-based alloy system shows more fragile properties than Zr-based BMGs in the supercooled liquid region near glass transition temperature[2], even though it shows the best GFA reported so far. These results were compared with the results obtained from an earlier study of the Pd-Cu-Ni-P alloy system and typical BMG formers in order to provide a clear picture on the crucial conditions for sluggish kinetics which impedes the crystallization.

On the Fragility of Mg$_{65}$Cu$_{25}$Gd$_{10}$ Bulk Metallic Glass

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Fragility is a key concept to understand the behavior of glass forming liquids. Fragility index, $m$ of Mg$_{65}$Cu$_{25}$Gd$_{10}$ bulk metallic glass is evaluated by using Vogel-Fulcher-Tamman (VFT) fit and Lasock’s plot. In addition to the above methods, Moynihan and Augis & Bennett methods are also utilized to determine the fragility index, $m$. The fragility index $m$ is 42 at the heating rate 5K/min. Bulk metallic glasses typically have the fragility parameter values range from 20 to 70 and, hence, can be classified in the intermediate strong glasses category according to the Angell’s[1] classification scheme. This indicates the bulk metallic glass Mg$_{65}$Cu$_{25}$Gd$_{10}$ behaves more like an intermediate strong glass. The authors also draw the attention to the relationship among fragility index $m$, glass forming ability (GFA) and heating rate. Ikeda et al[2] relation between $T_{g0}/T_g$ and fragility index $m$ is also checked.

The Distributed Eigenstate Hypothesis of Glass Formation

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Despite decades of intense focus and research, a comprehensive understanding of the physical mechanism underpinning the formation of glasses and the glass transition has remained elusive. No universally accepted theory of the glass transition, which is applicable to all types of supercooled liquids, has been found. To that end, we have formulated the Distributed Eigenstate Hypothesis (DEH) of glass formation. The DEH leads to a unique functional form for the viscosity of supercooled liquids. This functional form contains only a single fitting parameter, and has been demonstrated to be applicable to supercooled liquids across all fragilities, bonding types, and classifications. Furthermore, scaling of the viscosity data of real liquids by the single parameter of the DEH form, leads to a universal collapse of the data over sixteen orders of magnitude.
Local Structural Mechanism for Frozen-in Dynamics in Metallic Glasses

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Glass transition usually occurs in a narrow temperature range, but the related dynamics changes in physical and mechanical properties over a few orders of magnitude. Up to date, there is still no consensus on what the general percolation entity is and how the entity responses to the sudden slow-down dynamics during glass transition. In this work, we demonstrate that the one-dimension local translation symmetry (LTS) ordering is a universal structural motif associated with the glass transition for various metallic glasses. The quantitative evolution of LTS ordering with temperature indicates that a percolating LTS network forms to serve as the “backbone” of the rigid glass solid when the temperature approaches the freezing point, resulting in the frozen-in dynamics accompanying the glass transition. The percolation transition occurred via pinning different LTS networks together, which only needs to introduce a small amount of “joint” atoms in-between them and therefore results in a low energy release.
Medium-Range Structure of Zr-Cu-Al Bulk Metallic Glasses from Structure Optimization Based on Fluctuation Microscopy

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Zr₅₀Cu₃₅Al₁₅ metallic glass, a relatively poor glass former, is compared to a better glass former, Zr₅₀Cu₄₅Al₅ [1], across three annealing states. Hybrid reverse Monte Carlo structure simulations combine experimental data from fluctuation electron microscopy (FEM) with an empirical potential to generate realistic atomic structures of these glasses. The structure is constrained by the FEM data on the medium-range order scale and by the empirical potential on the short-range order scale, leading to atomic models with structural features that are not seen in models quenched using molecular dynamics. The resulting models are analyzed using Voronoi tessellation as well as a new Fourier masking and back-transform technique designed to identify and isolate medium-range order features. We show that the glass-forming ability of Zr₅₀Cu₃₅Al₁₅ is poorer than Zr₅₀Cu₄₅Al₅ due to higher stability of crystal-like short- and medium-range order structures.

Thermal Structural Evolution of Zr-based Metallic Glasses Investigated by in-situ High Energy X-ray Diffraction

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In this work, the continuous structural evolutions of Zr65Cu17Ni8Al10 and Zr80Pt20 metallic glass samples were studied by in-situ high energy X-ray diffraction. Samples were sealed in vacuumed capillaries and heated from room temperature up to 1300 K. Diffraction patterns were collected and then the structure functions and pair distribution functions were obtained. Glass transition and nano-crystallization were observed in the Zr65Cu17Ni8Al10 sample during the heating and the corresponding structures were analyzed. The extrapolated structure function changes smoothly from the supercooled region to the liquid state. In the Zr80Pt20 sample, a transition is observed at 430 °C resulting in nano-crystalline phase. Another phase transition is observed at higher temperature, which is stable up to 1300 K. Combining some molecular dynamics (MD) simulation results, the different thermal structural evolutions are tentatively explained by the different topological and chemical effects of the atomic pairs in the two kinds of metallic glasses.
In-situ X-ray Diffraction Studies of Bulk Metallic Glasses with Varying Effective Temperature

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The low plasticity of bulk metallic glasses (BMGs) at room temperature has limited their wide spread applications. The thermal history of the BMGs was found to be one of the important factors that heavily influence the plasticity of the BMGs. Recently, the effective temperature, $T_f$, was proposed to characterize the disordered structure of the BMGs inherited from liquids or the effect of thermal annealing and rejuvenation. The relations of $T_f$ with some mechanical properties, such as fracture toughness, were investigated. In this work, the structures of Zr44Ti11Cu10Ni10Be25 and Pd43Cu27Ni10P20 BMGs with different effective temperatures were studied through high-energy x-ray diffraction during deformation in the elastic regime. Obtained isotropic and anisotropic pair distribution functions show the effect of $T_f$ on these BMGs’ structures. In particular, we examine relation of the local non-affine deformation to the fracture toughness and the effective temperature.

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On the Prediction Glass Formability: Whether Molecular Dynamics Simulation Superior than Empirical-geometrical Approaches

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The metallic glasses are new families of engineering materials which exhibit extraordinary physical and mechanical properties, like bio-compatibility, high corrosion resistance, low elastic modulus and high failure strength. However, the practical manufacturing of these kind of materials is remained still a great challenge as high cooling rate is commonly required to produce them, in particular in bulk form. When their sizes in all dimensions are larger than a few millimeters, they are commonly called the bulk metallic glasses (BMGs). For a fixed cooling rate, there is a critical diameter such that samples with smaller diameter than this critical threshold result in BMGs. This size is commonly attributed to the glass formability of the corresponding alloying system.

An interesting question is this regard is to predict the glass formability of a metallic system, or to find systems with good glass formability; without performing expensive experimental studies. Furthermore, recent studies showed that metallic systems exhibit different glass formability as their chemical composition change. Therefore, another interesting question is to find the best glass former composition(s) for a specific alloying system. There are several geometrical based approaches, e.g. Egami’s works, to qualitatively predict the glass formability of metallic systems, in particular for binary ones. However, these approaches are not universal and there are several instances for the failure of these approaches.

In the present work, it is shown that how the molecular dynamics (MD) simulation helps us to predict the glass formability of metallic system, and best glass former compositions. In particular, we present the success of MD simulation for systems that exhibit significantly different glass formability (according to the available experimental data), while their geometrical characteristics are almost the same. Finally we present some sufficient conditions to predict whether a system is a good metallic glass formers.
An Indicator for Evaluating the Stability of Newtonian Viscous Flow in Various Metallic Glass Systems

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Viscous flow has been recognized as one of the most beneficial properties of metallic glasses, as it gives superior thermoplastic forming ability for near-net shape forming process. Recently, the phenomenon is becoming increasingly important as it contributes to the plastic deformation not only in supercooled liquid region (SCLR) but also in lower temperature region. Although deformation mechanism at lower temperature has been separated from the behavior in SCLR in the form of inhomogeneous flow, it takes place through stress induced viscous flow with vein patterns. Therefore, investigation of viscous flow is essential to get a perspective on the general deformation behavior of metallic glasses.

Meanwhile, viscous flow can be divided into two regions, Newtonian and non-Newtonian, regarding the stability of flow. In this research, we will systematically discuss the relationship between several factors and the stability of Newtonian viscous flow, and propose a governing indicator for the stability.
Structure and Dynamics in Metallic Liquids


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It is widely held that there must be a connection between liquid dynamics and structure. Recently, based on high-energy synchrotron x-ray scattering studies and viscosity measurements of containerlessly processed supercooled liquids, we demonstrated this, showing a direct link between the structural evolution in the liquid and kinetic fragility. Here, new results that strengthen this connection are presented. An onset of shortrange ordering in the liquid is observed near the temperature at which shear flow becomes cooperative, TA, corresponding to the onset of a super-Arrhenius viscosity. The nature of the atomic potential should underlie both structure and dynamics. Supporting this, we present the results of an analysis of the experimentally determined pair distribution functions that demonstrates a correlation between fragility and the steepness of the repulsive portion of the potential.
Microstructural Fluctuations at Equilibrium and under an Elastic Field of Cu-Zr Metallic Glass by Molecular Dynamics simulations

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We present MD simulations results on a Metallic model Glass (Cu-Zr) referring to the microstructural re-arrangements taking place at room temperature at equilibrium and under strain. It came out that approximately 1.5% of the system’s atoms perform short distance displacements, of the order of an Angstrom, that appear to be correlated with the collective motion of 2 or 3 neighboring atoms. Although most of these atomic movements are reversible, a small fraction of the neighboring atoms do not return at their original sites, thus altering locally the microstructure. These fluctuating atoms are not homogeneously distributed in the system, which under this perspective appears non-homogeneous, exhibiting high and low mobility regions. Under strain, these movements increase in number and distance, while the high mobility regions are formed from larger number of particles that participate in such displacements. Several quantities relevant to atomic motion processes were evaluated and compared with available data.
Size-dependent Deformation Behavior Variation of Metallic Glass Nanoparticles

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In nanosized crystalline materials, “smaller is stronger” phenomenon is observed due to dislocation starvation mechanism induced by the reduction of sample sizes down to the scale of individual deformation units. Likewise, nanosized metallic glasses (MGs) are expected to exhibit abnormal mechanical properties and there have been numerous studies on the size-dependent strength and the deformation mode of small volume MGs using nanopillars fabricated by focused ion beam (FIB) milling method. However, conflicting results have been reported regarding the size dependency of deformation behaviors, and limitations of FIB as a sample preparation method were pointed out. To settle a complicated problem, we fabricated MG nanoparticles with diameters ranging from tens to hundreds of nanometers through the selective dissolution of phase-separating metallic glasses and investigated deformation behaviors distinguishable from common shear banding via in-situ compression tests of MG nanoparticles. These results could provide deeper understanding of the size-dependency of MG deformation behaviors.
Effects of Mechanical Heterogeneities in Bulk Metallic Glasses and Composites across Varying Length Scales

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Heterogeneities in metallic glasses have distinct implications for the tensile ductility and plastic deformation mechanisms in the glasses and their composites. In this work, nanoindentation modulus mapping is used to detect mechanical heterogeneities in a bulk metallic glass (BMG) and BMG-crystalline composites. The Zr-based BMG, produced through both arc melting and laser processing, revealed heterogeneities on the order of 100s of nanometers. These heterogeneities are not observed in STEM analysis, indicating that they are structural, not chemical, in nature. In the Ti-based composites, which exhibit a wide range of macroscale mechanical behaviors despite only slightly varying nominal compositions, heterogeneities are observed in the glass phase on a similar scale. Furthermore, on the micron length scale where the glass and crystalline phases themselves are heterogeneities, a range of modulus mismatches between the two phases is also observed. This hierarchy of heterogeneities is significant for understanding the deformation behavior of these materials.
Plastic Deformation Behavior of Fe-Co-B-Si-Nb-Cr Bulk Metallic Glasses Under Nanoindentation

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In this work, we investigate the effect of Cr addition on thermal properties and indentation behavior of Fe52Co20-xB20Si4Nb4Crₓ alloys with x = 0, 1, 3 and 5 at.%, respectively. Among all studied alloys, the Fe52Co17B20Si4Nb4Cr3 bulk metallic glass (BMG) exhibits the highest thermal stability with large supercooled liquid region of 40 K and the pronounced plastic deformation features which is serrated flow (pop-in event) and significant pile-up of materials around indents. This demonstrates that the appropriate addition of Cr in Fe-based BMG can induce the internal atomic structure modulation and promote the mechanical softening, which are discussed in terms of free volume concept.
Flaw Tolerance of Metallic Glasses

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The flaw tolerance of bulk metallic glasses (BMGs) is evaluated using a thermoplastic synthesis approach. We found that flaw tolerance quantified by the notch toughness decreases apparently with decreasing radius until a critical value. Below this critical value, measured notch toughness is independent of its radius, revealing a flaw tolerance behavior of BMGs. We explain such flaw tolerance by a critical strain or stress controlled fracture where the critical radius is defined by a critical plastic zone originating from the BMGs’ inherent crack tip blunting capability. This zone defines a characteristic distance over which stable shear banding plastic process develops prior to fracture instability. The specific characteristic distance and crack blunting capability vary widely among BMGs, which rationalizes the vast variety in their fracture behavior and suggest specific flaw tolerance. Our finding is encouraging for BMGs’ structural applications since flaws smaller than the critical value are increasingly difficult to avoid but are “indistinguishable” in their influence to fracture toughness.
Effect of Fictive Temperature on Fracture Toughness of Metallic Glasses

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We manipulate the fictive temperature, $T_f$, the temperature where the liquid falls out of equilibrium, with thermal annealing and recently developed non-affine thermal strain, or thermal cycling technique. Whereas thermal annealing is used to reduce $T_f$, thermal cycling allows us to increase $T_f$. Fracture toughness, using our novel fabrication method, which allows for precise and highly reproducible measurements, is used to quantify the effect of the various $T_f$s. We found that the effect on fracture toughness by varying $T_f$s is specific to the metallic glasses and can vary dramatically. This finding suggests a “mechanical fragility” which is specific to a metallic glass.
Tensile Plasticity of Zr-based Bulk Amorphous Alloys under Electric Pulse Current

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The tensile deformation behavior of a Zr55Cu30Al10Ni5 BMG under a pulse current with various parameters was studied. The result showed that the tensile strength and elongation is closely to the current density and pulse width. The samples exhibited a significantly enhanced plastic deformation with an elongation of 15%~20% and necking phenomenon was observed. The range of measured deformation temperature was between about 280℃ and 350℃, which was far lower than the glass-transition temperature 410℃ (Tg) of the Zr55Cu30Al10Ni5 BMG. All the stress-strain curves showed an inhomogeneous deformation under a pulse current with different parameters. X-ray diffractometer analysis showed that the deformed samples still kept an amorphous structure. The region of the sample closed to the fracture contained more free volume. Electroplastic Effect has been identified to exist in the plastic deformation of BMGs in the present study.
Fatigue Property Improvements by Thin Film Metallic Glass

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Thin film metallic glasses (TFMGs) with unique physical and mechanical properties have been widely investigated in recent years. They have attracted industrial interests as well as for the potential applications with their superior mechanical properties. 200-nm-thick Zr-based TFMGs with 10 nm titanium adhesion layer were coated on various substrates. Effects of TFMGs films on the four-point fatigue property improvements of magnesium alloys, Ti-6Al-4V[1], 316L stainless steel[2], Ni-based alloy substrates[3] were investigated. The fatigue life improved more than 17 times on stainless steel and Ti-6V-4V. It is demonstrated that TFMG films with high strength retarded the cracks propagated during fatigue cycles, resulting in increased fatigue life. The especially significant improvements from TFMGs were largely attributed to improved ductility, flexibility and increased adhesion strength from the titanium adhesion layer.

High Strain Rate Induced Ductile to Brittle Transition of a Zr-based Bulk Metallic Glass

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Recently, within the framework of the cooperative shear model, the volume of shear transformation zone (STZ) which mainly depended on temperature, free volume and strain rate has been put forward to be an indicator of DBT of BMGs. The former two (temperature and free volume) affecting DBT have been confirmed by uniaxial tension experiments, while the later one (strain rate) has been rarely shed light on. In the present work, quasi-static and dynamic tensile tests for a Zr-based bulk metallic glass were conducted at room temperature. A significant ductile to brittle transition (DBT) behavior was identified based on the change of macroscopic fracture mode from shear fracture to normal tensile fracture and microscopic fracture feature from micron-scaled vein patterns to nano-scaled dimples with increasing strain rate. The effect of strain rate on the DBT behavior is revealed by the critical value of shear transformation zone volume within the framework of the cooperative shear model.
Loading Force Dependent Plastic Dynamics Transition of Chaotic and Self–organized Critical States in Ni$_{62}$Nb$_{38}$ Metallic Glass

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The shear-branching process during nanoscratch is investigated for Ni$_{62}$Nb$_{38}$ metallic glass at room temperature. Detrended fluctuation analysis is introduced to explore the influence of loading force on temporal scaling behavior and shear-branching process. The Hurst exponent $\epsilon$ (0.5, 1) is associated with a positive and persistent process during the shear-branching process, when loading force ranges from 500$\mu$N to 2000$\mu$N. Hurst exponent reflects 1000$\mu$N is the turning point of loading force at room temperature. When loading force is higher or lower than 1000$\mu$N, the inhomogeneous shear-branching process is gradually becoming dominant, which is further certified by the dynamic model.
Partial Crystallization in Platinum-based Bulk Metallic Glasses

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New platinum-based BMGs, exhibiting platinum mass fractions above 0.85, critical casting diameters around 5 mm, supercooled liquid regions in the range of 50°C, and Vickers hardness values above 550 HV₀.₅, are studied with regard to the effect of partial crystallization on thermophysical and mechanical properties. With the degree of crystallization both the glass transition and the crystallization temperature increase, while the stability of the supercooled liquid decreases, thus indicating a compositional change within the remaining non-crystalline phase. Back-scattered electron microscopy, high-energy X-ray diffraction, and nanoscale secondary ion mass spectrometry are used to analyse both the crystalline and the non-crystalline phase. The thermal annealing induced formation of a nano-crystalline hexagonal phase renders the alloy harder, with partially crystalline glasses exhibiting Vickers hardness values in excess of 700 HV₀.₅, yet also more brittle. In an attempt to combine maximal surface hardness with bulk ductility, local crystallization by laser annealing is examined.
Gradual Martensitic Transformation of B2 phase on TiCu-based Bulk Metallic Glass Composite during Deformation

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In this study, we investigate the progress of stress-induced martensitic transformation depending on the stress state on TiCu-based bulk metallic glass composite via systematical TEM analysis. On the stage of elastic deformation, the martensitic transformation from B2 to B19` phase occurred from interface between B2 particle and amorphous matrix with ~50 nm region. Just after yielding, the martensitic transformed region was extended toward B2 particle with distance of ~130 nm from the interface. Moreover, the deformation twinning of B19` phase in martensitic transformed region was also observed. When 1% plastic deformation occurred, the martensitic transformed region reached up to ~600 nm. Based on these results, it is believed that the high level of stress is concentrated around the interface due to the elastic mismatch of B2 and amorphous phases. As a result, structural gradient morphology originated from phase transition was formed into the B2 particle during early stage of deformation.
Investigations on the Damage Mechanisms in Aluminum based Metal Matrix Composites with Metallic Glass Particle Reinforcement

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The reinforcement of a soft matrix material with hard particles is an established strategy to develop materials with tailored properties. Using new metallic glasses with high crystallization temperatures, i.e. in the system NiNbX (X=Sn, Ta), for composite production by liquid metal infiltration is a novel approach. However, designing of composite components needs comprehensive knowledge regarding material properties and damage mechanisms.

In this contribution, the particles were produced by grinding of melt-spun ribbons. Therefore, the particle shape is a plate-like resulting in notch-effects on the edges in the surrounding matrix [1]. Former results showed that the particles are situated in a layered alignment within the composite [2]. Potential influence of these circumstances is investigated in this contribution by means of in-situ characterization of the composite under compression. Scanning electron microscopy during the test allows for detecting micro crack initiation and observing the damage evolution under quasi-static loading conditions.

Meso-mechanical Constitutive Model of Bulk Metallic Glass Matrix Composites

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The deformation behaviors of the metallic glass matrix and the toughening phase were described by the extended free volume model and the unified visco-plastic model, respectively. The algorithmic tangent operators of the two models were derived. Then based on the extended Mori-Tanaka(M-T) method, a new meso-mechanical constitutive model was proposed to predict the response of metallic glass matrix composites. The stress-strain response of the in-situ dendrite phase metallic glass matrix composites and the different kinds of the ex-situ particle phase metallic glass matrix composites were predicted by the proposed model. Numerical predictions are compared with experimental results. It is shown that the meso-mechanical constitutive model can describe both hardening and softening behaviors of bulk metallic glass matrix composites under monotonic loading, and the simulation results agreed with experimental data well for both in-situ phase and ex-situ phase reinforced metallic glass matrix composites.
Vertically Aligned Metallic Glass Nanowire Arrays Free of Capillary Coalescence

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Arrays of metallic glasses (BMGs) nanorods have promising applications in fuel cell, surface coating and nanoimprint. Here, we demonstrate the fabrication of high aspect-ratio (>20) BMG nanorods by mechanically holding the nanorods via polymer depositing. Uncured polydimethylsiloxane (PDMS) solution is poured onto nanoimprinted BMG sample after the removing the nanoporous template. PDMS is then thermally cured and subsequently removed by mechanically peeling off. Solution substitution and supercritical carbon dioxide (CO\textsubscript{2}) drying have also been carried out for comparison purpose. Experimental results demonstrated that polymers can effectively prevent the occurrence of tip clustering induced by capillary force, indicating this is an efficient, scalable and simple approach to prepare vertically aligned high aspect ratio BMG nanorods free of capillary coalescence.
On Thermoplastic Forming of a New Platinum based Bulk Metallic Glass

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Thermoplastic forming is used to produce near net shape workpieces of relatively complex geometry out of a new platinum-based bulk metallic glass with moderate glass forming ability. The alloy exhibits a platinum mass fraction above 0.85, Vickers hardness above 550 HV₀.₅, and a supercooled liquid region in the range of 50K. It’s critical casting diameter is around 5 mm, which is lower than the smallest dimension of the workpieces to be produced. Atomization and copper mould casting are used to produce feedstock material of varying geometry and size. The effect of key processing parameters (i.e., processing temperature, forming pressure, and geometrical aspects of both mould and feedstock) on the microstructure of the workpieces is studied in detail, and particular attention is given to material uniformity and interfacial cohesion.
Electronic Properties of Cu-Zr Amorphous Alloys

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Amorphous Cu-Zr alloys have been widely studied from the point of view of their topology since a full understanding of the structural processes is paramount to exploit their properties. The simplicity of their composition has allowed plenty of theoretical and experimental papers; however, the electronic properties have been disregarded.

In this work we present a study of the electronic properties of amorphous CuₓZrₓ⁻¹₀₀ alloys (x = 20, 36, 50, 64, 80), whose generation process is described elsewhere [1]. We report partial and total electronic densities of states. Our results show that Zr plays a paramount role because as its content increases, the number of states at the Fermi level increases mainly influenced by the Zr d orbitals, but with contributions from Cu and Zr p orbitals as well. This result is very interesting in terms of understanding the possible electronic mechanisms that generate superconductivity in amorphous Cu-Zr alloys [2].

Valence Band Study of Metallic Glasses – Explaining the Trend in Electronic and Magnetic Properties

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Metallic glasses are very attractive as high-performance soft-magnetic materials due to their homogeneous and isotropic structure down to the atomic scale. However, fundamental scientific understanding is lacking for spin-exchange interactions between metal and metalloid atoms, which typically constitute a metallic glass. Using an integrated experimental and ab-initio molecular dynamics approach, we have demonstrated the interaction mechanism between transition metals and metalloids for Co(x)Fe(1-x) amorphous alloys. Valence band studies were carried out using Ultraviolet Photoemission Spectroscopy (UPS) to explain the trend in electronic and magnetic properties for several metallic glass systems.
Complex Metallic Glass Articles Made by Thermoplastic Forming

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Metallic glasses (MGs) possess superlative mechanical properties, which have attracted interest in producing MG articles. To realize such products, thermoplastic forming (TPF) of MGs has shown promise as a robust and scalable technology for the processing of MGs. TPF also offer a means for producing parts of complex geometries, especially on the miniature scale. However, as the demand for more elaborate designs increases, TPF technology must keep up. We present novel TPF methods and processing protocols for the formation of complex articles made from metallic glass, including some specific examples. We design these processing protocols by combining nucleation and growth theories with tailored flow stresses.
Combinatorial Development of Antibacterial Zr-Cu-Al-Ag Metallic Glasses

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Metallic alloys are normally composed of multiple constituent elements in order to achieve integration of a plurality of properties required in technological applications. However, conventional alloy development by sequential trial-and-error approach requires completely unrelated strategies to optimize compositions out of a vast phase space, making alloy development time consuming and labor intensive. Utilizing a typical metallic glass forming alloy system Zr-Cu-Al-Ag as an example, we demonstrate how glass formation and antibacterial activity, two unrelated properties, can be simultaneously characterized and the optimal composition can be efficiently identified employing combinatorial approach.
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