Stored charge density showed the increasing trend with the increasing percent content of HAp in the composites. Bovine serum albumin protein adsorption on the positively-poled surfaces was maximum after 6-hour. BSA release from the positively-poled surfaces was performed for up to 48-hour at 7.4 pH. A decreasing trend in percent release of BSA was observed with the increasing charge density. The presentation will discuss processing and characterization of BCPs and BSA adsorption and release behavior from them.

4:40 PM
Magnetic Nanoparticle Interactions with Hydroxyapatite: *Otto Wilson*[1]; Meron Haimanot[1]; [1]Catholic University of America

Enhanced functionality can be imparted to biomaterial implants at the macroscale, microscale, or nanoscale level and can involve a multitude of features related to bioactivity. These factors work together to orchestrate cell function, overall tissue healing, and promote seamless integration of the biomaterial implant into the neighboring tissue. Magnetic nanoparticles (MNPs) were adsorbed onto nanophase hydroxyapatite (HAp) particles to develop magnetically active hydroxyapatite. MNP modified HAp particles were characterized via electrophoretic mobility, particle size ananlysis, and electron microscopy. The MNPs rapidly adsorbed onto the surface of the HAp via heterocoagulation based interactions. MNP surface modification of HAp imparts magnetic behavior and allows the HAp to be translated in solution via magnetic fields. Applications for this novel HAp in hard tissue engineering will be presented with a focus on mechanically stimulated scaffolds for enhanced cell activity.

5:00 PM
Solid-Binding Peptide-Based Antibacterial Implants: *Hilal Yazici*[1]; Mary Rood[1]; Brandon Wilson[1]; Mustafa Gungormus[1]; Candan Tamerler[1]; Mehmet Sarikaya[1]; [1]University of Washington

Implant-associated infections are a primary cause of early implant failures. Prescribed oral antibiotics are not always effective because of the inability to reach the infection site and an increase in bacterial resistance. A novel class of peptides, the antimicrobial peptides (AMPs), is useful mainly because of the difficulty for microorganisms to develop resistance towards them. In the present study, we use a novel bi-functional peptide based approach that exhibits both titanium-binding (TiBP1) antimicrobial (AMP) properties for implant surface functionalization. The efficiency of TiBP1-AMP bi-functional was evaluated both in solution by analyzing bacterial growth using optical density measurement and on the functionalized titanium surface with fluorescence microscopy, scanning electron microscopy analysis at various time points. For example, Streptococcus mutans adhesion was reduced on the TiBP1-AMP peptide-based functionalized substrate compared to controls. The approach may be a candidate for the prevention of implant infections. This research is supported by GEMSEC at UW.

5:20 PM
Development of Anti-Microbial Silver Coating on Stainless Steel: *Paul DeVasConCellos*[1]; Susmita Bose[1]; Amit Bandyopadhyay[1]; Lewis Zirkle[2]; [1]BRC, Washington State University; [2]Surgical Implant Generation Network (SIGN)

Silver has been utilized for many years as an antimicrobial agent. With an increasing amount of antibiotic-resistant bacteria, silver-coatings and treatments are again being noticed as an effective way to prevent infection. In situations where cost effectiveness is necessary, the use of silver coatings on medical implants could be a valuable addition to help prevent infections. This is especially crucial when surgeries are performed in environments where sanitation is not ensured as well as environments in North American Hospitals. This research presents methods and feasibility of silver coatings on stainless steel (SS) which is a practical material for low cost implants. There are many parameters that can be adjusted for each method to apply silver coatings. In an effort to optimize antimicrobial effectiveness and keep human cell-toxicity to a minimum, we have experimented with various coating parameters and observed their effects on the utility of silver coating on SIGN SS-implants.

Bulk Metallic Glasses VII: Simulation and Modeling

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee
Program Organizers: Peter Liaw, The University of Tennessee; Hahn Choo, The University of Tennessee; Yanfei Gao, The University of Tennessee; Gongyao Wang, University of Tennessee

Wednesday PM Room: 213
February 17, 2010 Location: Washington State Convention Center

Session Chairs: Christopher Schuh, MIT; John Lewandowski, Case Western Reserve University

2:00 PM Invited
Influence of Condensed Bond Enthalpy on Metallic Glass Stability: *Dan Miracle*[1]; Garth Wilks[2]; Amanda Dahlman[3]; [1]AF Research Laboratory; [2]General Dynamics, Inc.; [3]SOCHE

While empirical guidelines suggest that the enthalpy of mixing influences glass stability, previous work has failed to show a correlation. This work seeks to establish a connection between nearest neighbor bond energy and glass-forming ability through evaluation of interatomic bond enthalpies. An approach to determine bond enthalpies from available thermodynamic data will be briefly described and resulting bond enthalpies will be presented. The number and type of atom bonds that are present in a metallic glass structure are estimated as a function of metallic glass constitution using the efficient cluster packing structural model. By combining these two analyses, we estimate the enthalpy associated with glass formation, and explore correlations with experimental measurements of glass-forming ability.

2:20 PM
Model Experiments to Mimic Fracture Surface Features in Metallic Glasses: *Lisa Deibler*[1]; John Lewandowski[1]; [1]Case Western Reserve University

The purpose of this study is to examine how changes in viscosity, specimen geometry, and degree and type of inhomogeneity affect the fracture surface observations on a model of metallic glass fracture. Experiments were conducted on tensile samples of various geometries constructed to contain liquids of different viscosity that were tested at three temperatures. The influence of mixtures, layers, and dispersions of two different viscosity materials on the fracture surface features was also investigated. The observed fracture surfaces of these viscous materials were quantitatively examined to provide a comparison with surface features found in several metallic glasses.

2:30 PM Invited
Modeling the Mechanical Behavior of Metallic Glasses Using STZ Dynamics: Eric Homer[1]; *Christopher Schuh*[1]; [1]MIT

Recent advancements in a meso-scale model for the mechanical behavior of metallic glasses have allowed a single modeling technique to bridge the disparate timescales associated with different modes of deformation in a metallic glass, a task which has proven difficult using other modeling approaches. A discussion of the modeling technique, which is based on the shear transformation zone, and its application using finite element analysis and the Kinetic Monte Carlo algorithm are presented. Recent analyses of simulations performed with this technique elucidate the conditions under which spatial and temporal correlations between shear transformation zones lead to different modes of observed macroscopic deformation. These correlation analyses provide some of the first insights into the localized microscopic processes that lead to inhomogeneous deformation analogous to nascent shear banding. Details regarding the extension of the modeling technique to three-dimensional systems and complex loading conditions are discussed.

2:50 PM
Continuum Model for Bulk Metallic Glass Composites: *Fadi Abdeljawad*[1]; Mikko Haataja[1]; [1]Princeton University

Recent experimental work has suggested that the problem of catastrophic failure by shear band propagation in Bulk Metallic Glasses (BMGs) can be solved by forming composites with a two-phase microstructure consisting of the glassy BMG matrix phase and a non-percolating, soft crystalline phase. In this talk, we present a continuum model of plastic deformation in two-dimensional BMG composites. The elastic energy density is a periodic nonlinear function of

the strains, while the structural heterogeneity of the glassy phase is accounted for by defining a quenched, spatially varying random variable that corresponds to the maximum local strain needed to cause a slip event. Simulations of BMGs with various sizes of crystalline domains under simple shear loading show that deformation patterns and mechanical strength are affected by the area fraction and spatial distribution of the crystalline domains, implying a size effect in the strength of BMG composites.

3:00 PM Invited
Deformation and Failure of Glasses at Nanoscale: *Ju Li*[1]; Erik Bitzek[1]; [1]University of Pennsylvania

Recent experiments on nanoscale amorphous materials have suggested interesting ductility - size scale dependencies (PNAS 104, 11155; PRB 77, 155419). Such size effect may shed light on the connection between plastic deformation and underlying spatio-temporal hierarchies of structural flow defects, the smallest of which is a single shear transformation zone (STZ) ~1nm^3. A mesoscale computational model (on the same level as discrete dislocation dynamics for crystalline materials) is constructed, which utilizes detailed statistical information about shear transformations, damage accumulations and damage repairs from atomistic simulations. Adjacency to surfaces/interfaces and the loading constraints could have strong effect on the apparent ductility of nanoscale glasses.

3:20 PM
Numerical Deformation Simulations on Bulk Metallic Glasses Using First-Principles Methods: *Lizhi Ouyang*[1]; Despina Louca[2]; Gongyao Wang[3]; Yoshihito Yokoyama[4]; Peter Liaw[3]; [1]Tennessee State University; [2]University of Virginia; [3]University of Tennessee; [4]Tohoku University

It was found recently that the cyclic fatigue loading causes the local structure changes in Zr-Cu-Al bulk metallic glasses (BMG). To reveal their atomistic origins, we performed numerical fatigue tests on Zr50Cu40Al10 and Zr60Cu30Al10 (in atomic percent) using first-principles methods. Large periodic models with 600 atoms are constructed for the two metallic glasses using the quenching and annealing technique. The local strain distributions of the deformed models generated by the numerical fatigue loadings are analyzed to identify irreversible structural changes and potential shear-band nucleation sites. The structure evolutions of the two BMGs under numerical cyclic loading are examined and the changes in their pair distribution functions are compared with the experimental results.

3:30 PM Break

3:40 PM Invited
Simulating Poisson Ratio Effects on Shear Banding Behavior in Metallic Glasses: *James Morris*[1]; Takeshi Egami[2]; [1]Oak Ridge National Laboratory; [2]University of Tennessee

Shear banding occurs commonly during deformation of bulk metallic glasses, often leading to failure. Understanding and controlling this phenomenon is important to improving the properties of metallic glasses. Several studies have suggested that an increased Poisson ratio is correlated with improved mechanical properties; for example, the fracture energy can change by three orders of magnitude as the Poisson ratio changes from 0.3 to 0.4 [J. J. Lewandowski et al., Phil. Mag. Letters 85, 77-87 (2005)]. To understand this behavior, we have begun molecular dynamic simulations of glasses under simple shear, using a model with a tunable Poisson ratio. The inhomogeneous shearing behavior is examined as a function of Poisson ratio, temperature, and strain rate. These results are compared with a phenomenological model which predicts the coexistence of two states with distinct viscosities.

This research was sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy.

4:00 PM
Reverse Monte Carlo Simulation of Medium-Range Atomic Order in Bulk Metallic Glass Incorporating Fluctuation Electron Microscopy: *Jinwoo Hwang*[1]; Paul Voyles[1]; [1]University of Wisconsin Madison

We have investigated medium-range order in Zr-based BMGs using fluctuation electron microscopy (FEM) and Reverse Monte Carlo (RMC) simulation. Initial RMC simulations incorporating FEM and electron diffraction reduced density function (RDF) data showed that including FEM data in RMC more uniquely confines the short to medium-range atomic structure compared to RDF data alone, and that the FEM signal is likely to arise from nanometer-scale planar order in the structure. However, the MRO in the model was anisotropic due to limitations in the simulation and experiment. Improved FEM data obtained using highly-coherent, variable probe-size nanodiffraction in an aberration-corrected STEM will be presented, as will the results of more isotropic FEM RMC simulations which incorporate approximate chemical information in the form of EAM empirical potentials.

4:10 PM
Reliability of Methods of Computer Simulation of Structure of Amorphous Alloys: *Mikhail Mendelev*[1]; Mattew Kramer[1]; [1]Ames Laboratory

There are several computer simulation methods to generate atomic models of glasses. We analyzed advantages and disadvantages of these methods. We took a model created by the MD simulation with a semi-empirical potential as a target system and explored how its structure can be reproduced using different simulation techniques. First, we explored effect of the cooling rate and found that if the cooling rate is ~ 10^13 K/s the system has no time to adjust its structure to the change in temperature/density. It was also found that a small model size used in ab initio MD simulations can affect the final structure. Finally we used the target PPCFs to explore a possibility to create the atomic models from diffraction data using the RMC method. We created models with the PPCFs which almost coincided with the target ones but the structure of these models was different from the target structure.

4:20 PM Invited
Connecting Atomic Structure and Plastic Deformation in Zr-Based Bulk Metallic Glasses: *Paul Voyles*[1]; Jinwoo Hwang[1]; Jonathan Puthoff[1]; Don Stone[1]; [1]University of Wisconsin, Madison

We have recently used broadband nanoindentation creep to measure the volume of shear transformation zones (STZs) in three Zr-Cu-Al alloys in the context of the Johnson-Samwer cooperative shear model of plastic deformation. The STZs occupy 100-300 atomic volumes, which corresponds to spheres 1.5 to 2 nm in diameter. We use fluctuation electron microscopy (FEM) to measure structure at this length scale, which is difficult to access from more conventional techniques. Reverse Monte Carlo simulations incorporating FEM data show that consistency with FEM requires nanoscale regions with pseudo-planar order in the model and constrains the partial pair distribution functions. Higher-quality, variable probe-size FEM data from a new aberration-corrected STEM and hybrid reverse Monte Carlo simulations incorporating EAM potentials for Zr-Cu-Al will be presented.

4:40 PM
Computational Studies on Free Volume and Plastic Flow in Metallic Glasses: *Joshua Askin*[1]; Ashwini Bharathula[1]; Wolfgang Windl[1]; Katharine Flores[1]; [1]The Ohio State University

Positron annihilation spectroscopy studies reveal a trimodal lifetime distribution corresponding to 3 distinct defect volume ranges in bulk metallic glass structures which evolve in a regular manner with plastic deformation. These volumetrically distinct defects are hypothesized to be inherent interstitial holes, flow defects and nano-scale voids. To test this hypothesis, we developed an electron density model based on radial averaging of ab-initio charge density,[1] which we use to visualize evolution of "free/excess" volume or lower density regions during MD annealing and deformation. Rather than using different cooling rates to control density, a series of voids are injected into the glass structure under constant volume conditions. Under constant-volume annealing, the void redistributes amongst other defects. Under constant-volume shear, strain localization only occurs above a critical void size, indicating a requisite combination of applied shear and available excess volume. References[1] Metallurgical and Materials Transactions A, 39A 2008 1779-1785.

4:50 PM
Structure and Anelastic Relaxation in Metallic Glasses: *Garth Wilks*[1]; Daniel Miracle[1]; Amanda Dahlman[1]; [1]Air Force Research Laboratory

Variation in the constitution of several metallic glass ribbons are used to probe their deformation activation energy spectra via anelastic bend stress relaxation. The specific effects of vacancy and anti-site defects predicted by the Efficient Cluster Packing model are used to rationalize deviations in spectra between material conditions, particularly the effects that the energy, type, and concentration of such defects contribute to local free volume dilatation and their ability to act as sites for unit shear process nucleation.

5:00 PM

Avalanches, Size-Effects, and Critical Behavior in Shared Model Metallic Glasses: K. Michael Salerno[1]; *Craig Maloney*[2]; Mark Robbins[1]; [1]Johns Hopkins; [2]Carnegie Mellon University / Civil & Environmental Engineering

We perform computer simulations of sheared binary Lennard-Jones glasses in 2D at zero temperature and in the limit of small strain rate. The strain energy is released in discrete bursts with a Gutenberg-Richter size distribution. The plastic strain is organized into lines of slip which accumulate during avalanches over a system-size dependent characteristic strain scale deltagamma_c. deltagamma_c should give rise to interplay between indentation rate and system size which may be observable in micro-pillar indentation experiments on metallic glasses. Furthermore, we show that the spatial organization of the plastic deformation has a novel kind of fractal geometry, with orientation-dependent scaling exponents. These results further suggest that micro-pillar indentation experiments performed on bulk-metallic glass samples should exhibit a kind of self-organized critical behavior similar to that observed in crystalline samples [1]. [1] Dimiduk, DM , et al. Science 312 (5777). 1188-1190 (2006).

5:10 PM Invited

Stress and Temperature Induced Phase Transformation in Zr-Based Metallic Glass via Molecular Dynamics Simulation: *Yunche Wang*[1]; Chun-Yi Wu[1]; Jinn Chu[2]; Yanfei Gao[3]; Peter Liaw[3]; [1]National Cheng Kung University; [2]National Taiwan University of Science and Technology; [3]The University of Tennessee

Transformation between crystalline and amorphous phases in the Zr47Cu31Al13Ni9 metallic glass is studied with the molecular dynamics (MD) simulation to understand atomic stress and strain distributions under uniaxial stress and various heat treatments. In this paper, a molecular model of the Zr-based metallic glass is obtained by sputter MD simulation. Then, a portion of the as-deposited film is used as initial structures for uniaxial tension/compression tests and heat treatment. The discontinuity in volume change upon heating is observed around the Tg of the metallic glass, and corresponding microstructures are studied. It is found that the uniaxial compression of the glass has superior plasticity than that of its tensile behavior. Atomic stress and strain calculations reveal atomic constitutive relationships to facilitate identification of microstructural changes.

5:30 PM

Directional Deformation Memory and Orthogonal Bauschinger Effect in Metallic Glasses: *Erik Bitzek*[1]; David Rodney[2]; Ju Li[1]; [1]University of Pennsylvania; [2]Institut Polytechnique de Grenoble

In crystalline materials the Bauschinger effect whereby plastic deformation in one direction leads to a different deformation behavior upon re-straining in the opposite direction is well known. In bulk metallic glasses (BMGs) however, no such effect has been reported. Furthermore, as the free-volume model of plastic deformation is inherently isotropic, the accumulation of damage is usually believed to be directionally independent, as long as no shear bands are formed. Here we present results of MD simulations on BMGs which show a directional dependence of the deformation memory: when strained along one axis and then unloaded, the samples show a different deformation behavior depending on whether they are strained again in the same direction, or orthogonal to the initial loading direction. The simulations are compared with recent experiments, and the origin of the orthogonal Bauschinger effect is discussed in terms of the directional properties of the shear transformation zones.

5:40 PM

Atomistic Simulations to Estimate Plasticity of Cu-Zr Bulk Metallic Glasses: *Kyung-Han Kang*[1]; Byeong-Joo Lee[1]; [1]POSTECH

Understanding the origin of and thus improving the plasticity is one of the hot issues in the bulk metallic glass (BMG) society. Many reports suggest that plasticity of BMGs may be correlated with several properties such as free volume, short range ordered structure, the ratio of shear modulus to bulk modulus, Poisson's ratio, atomic displacement and viscosity. In this study, a special attention was focused on the evaluation of the correlation between the above mentioned properties and plasticity in the Cu-Zr binary BMGs, by comparing the experimentally reported composition dependence with that of various properties obtained from atomistic calculations based on a modified embedded-atom method (MEAM) interatomic potential. It was found that the free volume and the distribution of short range ordered structures have a relatively clear correlation with plasticity. The correlation between the plasticity and other individual properties will also be presented.

Carbon Management and Carbon Dioxide Reduction: Session I

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS Extraction and Processing Division, TMS: Energy Committee

Program Organizers: Subodh Das, Phinix LLC; Brajendra Mishra, Colorado School of Mines; Neale Neelameggham, US Magnesium LLC

Wednesday PM Room: 310
February 17, 2010 Location: Washington State Convention Center

Session Chair: Subodh Das, Phinix , LLC

2:00 PM

Upcoming Carbon Management Legislations: Impacts and Opportunities for the Global Aluminum Industry: *Adam Gesing*[1]; Subodh Das[1]; [1]Phinix, LLC

The European Union is planning to include the aluminum industry in its carbon management system in 2013. Additionally, if and when enacted, "The American Clean Energy and Security Act" of 2009 will also force U.S. industries to comply with much debated "carbon cap and trade" system. The Waxman and Markey legislation – along with the Environmental Protection Agency mandate under the Clean Air Act – will specifically include US aluminum industry with CO2 equivalent sources of more than 25,000 tons per year. This paper will review the carbon management system as it now operates and how it is likely to be applied to the European and American aluminium industry.

2:30 PM

Cost-Effective Gas Stream Component Analysis Techniques and Strategies for Carbon Capture Systems from Oxy-Fuel Combustion (An Overview): *John Clark*[1]; Danylo Oryshchyn[1]; Thomas Ochs[1]; Steve Gerdemann[1]; Cathy Summers[1]; [1]National Energy Technology Lab

Limited analysis of combustion gas streams where carbon capture is not of interest is done mainly to ascertain operation parameters. Stringent regulations on acid gases and particulates promote careful flue gas analysis. Unregulated components are typically not analyzed.Typically not more than four points (two in the boiler and one each in the flue and the stack) are sampled. A successful oxy-fuel process with carbon capture and compression is anticipated to require a many as 12 sample points with analysis for water, nitrogen, oxygen, argon, NOx, SOx, and carbon monoxide. Carbon dioxide captured for beverages produces a high value product and the cost associated with analysis is warranted. However, carbon capture for disposal must keep all costs to a minimum. This paper will compare alternative approaches for cost-effective sampling and analysis of the carbon dioxide product streams from oxy-fuel combustion, through all stages of production through compression and pipeline/vessel delivery.

3:00 PM

Strategic Approaches for CO2 Reduction Rate from Fossil Fuel Use in Steel Industry: *Malti Goel*[1]; [1]INSA

Technology advancements in fossil fuel based energy generation are currently being aimed at minimization of CO2 emissions. To attain energy security, India must accelerate the pace of economic development, while achieving reduction in CO2 emissions per unit of energy. It would need access to advanced coal utilization technologies to be demonstrated on indigenous coal characteristics. Of specific importance would be: improvement in coal quality, increasing efficiency of fossil fuel use, and suitability of other CO2 sequestration technologies for reducing CO2 footprints. There is need to address related risks and financial burden through adoption of policies and regulations including the issue of open access in energy research. In this paper, seven important areas of strategic plan that need to be pursued for managing CO2 emissions in energy sector are discussed. A case study from steel industry is presented.