SYMPOSIUM Z

Amorphous and Nanocrystalline Metals for Structural Applications

November 28 - December 1, 2005

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* Invited paper

SESSION Z1: Deformation and Fracture of Nanostructured Metals I
Monday Morning, November 28, 2005
Constitution A (Sheraton)

8:15 AM *Z1.1
Life of a dislocation in a nanocrystalline grain.

Helena Van Swygenhoven, Paul Scherrer Institution, Villigen PSI, Switzerland.

Molecular dynamics simulations of nanocrystalline fcc metals have demonstrated the ability of grain boundaries to emit and absorb dislocations in the absence of dislocation sources within the grains. Even when considering possible artefacts inherent to the simulation method such as the associated high stress/short times and the quality of the empirical potential description (Nat. Mat. 3 (2004) 399), synergies between simulations and experiment are extremely useful. Here, the atomistic details of the mechanism responsible for nucleation, propagation and absorption in terms of grain boundary structures, local hydrostatic/shear stresses and local crystalline order are provided. The results are then discussed in terms of experimental measurements of activation volume in nanocrystalline metals. The dislocation activity observed in simulations, suggest that in terms of X-ray diffraction there would be no permanent dislocation network build up during deformation and therefore no footprint of the deformation mechanism. A new type of in-situ experiment at the Swiss Light Source (Science 304 (2004) 273), where the peak shift and peak broadening is followed during tensile deformation, validates the predictions from simulations. Results for electrodeposited nanocrystalline Ni demonstrates a reversible peak broadening during plastic deformation at room temperature. However at lower temperatures the broadening is not reversible anymore, suggesting that the propagation of dislocations is hindered. These results are discussed in terms of theatomistic simulations.

8:45 AM Z1.2
Nano-Crystalline Tantalum with Ultra-High Hardness of 16 GPa.

Bing Yang[1], Ming Zhang[2], Michael K. Miller[1] and T. G. Nieh[2,1]; [1]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [2]Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee.

Nano-crystalline Tantalum film with grain size of ∼30 nm was prepared by sputtering coating on a silicon substrate. The micro-structure, grain size, and chemical composition of the Ta films were verified by subsequent TEM and atomic probing studies. The hardness of the Ta film was measured by nano-indentation technique with a hysitron tribo-indenter at various indentation depths and loading rates. The average hardness of the Ta film is 16 GPa, which corresponds to a yielding strength of approximately 5 GPa. The present study demonstrated that, with higher stacking fault energy and fewer defects, nano-crystalline bcc metals with strength close to the theoretical strength of ideal crystals can be obtained.

9:00 AM *Z1.3
Hardness and Strain Rate Sensitivity of Cu over a Wide Grain Size Range.

Lei Lu, Ji Chen and Ke Lu; Shenyang National Laboratory for Materials Science, Institute of Metal Research, CAS, Shenyang, China.

The nature of the deformation mechanism operating in nanocrystalline materials is still not clearly understood. One of the crucial issues in debate is whether or not the plastic deformation is dominated by grain boundary (GB) activities (such as GB sliding and GB diffusional creep) when grain sizes are small enough. The transition in plastic deformation mechanism from lattice dislocation activities to GB dominated process may be manifested by a deviation from the classical Hall-Petch relation when grain sizes are extremely small, or alternatively by a much enhanced strain rate sensitivity (>0.5). However, these behaviors have not yet been observed experimentally so far, at least in pure metal systems. The present work reports a systematic investigation on hardness (H) and strain rate sensitivity (m) of Cu polycrystalline samples over a wide grain size (d) range from 23 mm down to 10 nm. Measurement results using nanoindentation technique revealed that hardness still follows the empirical Hall-Petch relationship even when d is as small as 10 nm. Measured m values increase with a decreasing d. When d=10 nm, m= 0.06, one order of magnitude higher than that in the coarse-grained Cu. A steep drop in the activation volume for flow stress (V*) is seen as d is reduced from macro scale to the submicrometer regime, and it decreases slightly for d <100 nm, reaching 8b3 at d=10 nm. A transition grain size around 100 nm was noticed in the m∼d and V*∼d correlations, which may correspond to a change in plastic deformation mechanism. But GB dominated plastic deformation process has not been detected in the Cu specimens even for d∼10 nm.

9:30 AM Z1.4
Evidence of plastic deformation in the grain boundaries of nanostructured materials.

Xun-Li Wang[1,2], Alexandru D. Stoica[1], Jon Almer[3] and C. T. Liu[2]; [1]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [2]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [3]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois.

In polycrystalline materials made of micron sized grains, it is generally accepted that the deformation is dominated by the dislocation process. However, this deformation mechanism is expected to change when the grain size is reduced to ∼30 nm or below. Molecular dynamics simulations suggest that at small grain size, the deformation mechanism is dominated by the grain-boundary activities. However, due to the lack of quality samples, there is little experimental evidence to prove one way or the other. To answer this question, we have conducted an in-situ synchrotron study of nanostructured Ni (obtained by eletrodeposition) under uni-axial tensile deformation. Through the measurement of inter- and intra-granular strains, we are able to observe the grain-orientation-dependent load partition during deformation. Using these data, we show that the plastic deformation in nanostructured Ni is mainly limited to the grain-boundary zone. This research was supported by Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy under Contract DE-AC05-00OR22725 with UT-Battelle, LLC. Use of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-Eng-38.

SESSION Z2: Deformation and Fracture of Amorphous Metals I
Monday Morning, November 28, 2005
Constitution A (Sheraton)

10:15 AM *Z2.1
Metallic Glasses for Structural Applications.

A. Lindsay Greer, Dept. of Materials Science & Metallurgy, University of Cambridge, Cambridge, United Kingdom.

The mechanical properties of metallic glasses are now receiving much attention, and their potential as structural materials is assessed. A wide-ranging comparison is made with conventional engineering materials, although the comparison is complicated by the distinctive plastic flow in metallic glasses. For structural applications, the comparatively high cost of metallic glasses restricts their use to high value-added products, where performance, aesthetics or simple novelty are important. Also, with their small process-zone size, typically < 1 mm, even bulk metallic glasses are best applied in comparatively small components. For niche applications, however, metallic glasses have some outstanding properties, including: high strength, approaching the theoretical limit; uniquely high capacity for elastic energy storage per unit volume or mass; low damping; and in some cases very high toughness. Such properties, combined with an ability to be deposited as thin films, makes metallic glasses attractive for many MEMS applications, some of which are already on the market.

10:45 AM *Z2.2
Newtonian and Non-Newtonian Flow in Glasses.

Ricardo B. Schwarz and Douglass J. Safarik; MST-8, Los Alamos National Laboratory, Los Alamos, New Mexico.

We investigated Newtonian and non-Newtonian flow in bulk metallic glasses by compressing cube-shape specimens that have a central hole. The hole localized the deformation along well-defined shear planes, which enabled us to plastically deform the same volume of glass along different glide directions. We found that the glass has a memory of its previous plastic deformation, but this memory is largely independent of the previous glide direction. The transition from Newtonian to non-Newtonian flow is abrupt and occurs at a Deborah number, De $=\tau^* d\gamma/dt = 0.5$, where $d\gamma/dt$ is the plastic shear strain rate and τ is the relaxation time for the annihilation of the flow defects. This value of De is consistent with that observed at the onset of flow instabilities in Newtonian liquids, which occurs at De ≈ 1.

11:15 AM *Z2.3
A Recipe for Ductilization of Metallic Glasses via Generation of Optimum Sized Nanocrystals.

Alain Reza Yavari[1,2], Khalil Hajlaoui[1], Alain LeMoulec[1], Beatrice Doinneau[1], Gavin Vaughan[2] and Ake Kvick[2]; [1]Euronano, LTPCM-CNRS, Institut National Polytechnique de Grenoble, St-Martin-d'Heres, France; [2]European Synchrotron Radiation Facilities (ESRF), Grenoble, France.

Unlike conventional crystalline alloys, in which dislocation-mediated plastic flow is associated with strain hardening and macroscopic ductility, metallic glasses show strain softening and abrupt failure associated with shear localization. However, it is known that certain structural properties such as high Poisson ratio and high free-volume content make a metallic glass more ductile. Here we report on an easy to use method for obtaining ductile BMG-based composites containing dispersions of nanocrystals. The nanocrystals must have dimensions inferior to the elementary shear band thickness and the nanocrystal generation process must be such that free volume is retained from above the glass transition Tg. Evidence of ductilization is obtained both by in-situ tensile deformation in a TEM showing shear delocalization and crack blunting as well as by conventional deformation in compression.

11:45 AM Z2.4

Free Volume - Toughness Connections in Bulk Metallic Glasses. Upadrasta Ramamurty, Rejin Raghavan and Palla Murali; Department of Metallurgy, Indian Institute of Science, Bangalore, KA, India.

We have investigated the connections between the free volume and impact toughness in the Zr-based bulk metallic glass, Vitreloy-1, by examining the toughness variations with structural relaxation as well as testing temperature. Results show a marked reduction in toughness with relaxation time, which is well correlated with the free volume reduction. Examination of the impact toughness variation of the as-cast glass within the temperature range of 123-423 K indicates a ductile-to-brittle transition (DBT) at around 150 K, implying that the inhomogeneous plasticity mediated by shear bands becomes inoperative below a critical temperature resulting in brittle fracture. Samples that were brittle at room temperature exhibit a marked brittle-to-ductile transition at elevated temperature (423 K), suggesting that the minimum amount of free volume required for extensive plasticity (and hence high toughness) in metallic glasses is strongly dependent on the temperature. Micromechanical reasons for these transitions will be discussed in detail in this presentation.

SESSION Z3: Structure of Nanocrystalline Metals
Monday Afternoon, November 28, 2005
Constitution A (Sheraton)

1:30 PM Z3.1

Grain Boundary Segregation in Nanocrystalline Ni-W Alloys: an Atom Probe Tomography Study. Andrew J. Detor[1], Michael K. Miller[2] and Christopher A. Schuh[1]; [1]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; [2]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

The three-dimensional atom probe can directly map the position of specific alloying elements in a material, at near atomic-level resolution. For nanocrystalline alloys, the distribution of solute atoms is strongly affected by the large density of grain boundaries present. This solute distribution has been characterized in electrodeposited nanocrystalline Ni-W, with grain sizes ranging from 2 to 20 nm. Subtle segregation of W atoms to the grain boundaries has been found in concentration profiles and composition distribution analysis. These atom probe results are in contrast to previous studies of other nanocrystalline alloy systems, where significant segregation was observed. However, these observations are in line with recent experiments, computer simulations, and thermodynamic modeling in the Ni-W system and have important implications for the thermodynamic stability of these nanocrystalline structures. Research at the SHaRE User Facility was sponsored by the Division of Materials Sciences and Engineering, U. S. Department of Energy, under Contract DE-AC05-00OR22725 with UT-Battelle, LLC.

1:45 PM *Z3.2

Formation Mechanism of Five-fold Deformation Twins in Nanocrystalline fcc Metals. Yuntian T. Zhu, Materials Science & Technology Division, Los Alamos National Lab, Los Alamos, New Mexico.

Five-fold deformation twins (DTs) have been recently observed in nanocrystalline face-centered-cubic (fcc) metals and alloys synthesized by severe plastic deformation techniques. However, numerous molecular dynamics (MD) simulations in the literature have not observed five-fold DTs in nanocrystalline fcc metals. The discrepancy between experimental observations and MD simulations has raised an issue on their formation mechanism and conditions. Here we propose a partial dislocation-twin boundary interaction mechanism that provides a clear path for the formation of five-fold DTs. The mechanism requires an orientation change of applied stresses, which explains why MD simulations under a constant load orientation do not produce five-fold DTs. Another condition is that the grain size needs to be smaller than a critical size so that twinning is favored over dislocation slip as a deformation mechanism. Each proposed twinning step is corroborated with high-resolution TEM observations.

2:15 PM Z3.3

TEM and Auger Analysis of the Grain Boundary Chemistry in Nanocrystalline Al Thin Films. B. G. Mendis, D. S. Gianola and K. J. Hemker; Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland.

Refined grain sizes that naturally occur in many MEMS/ NEMS structures offer important technological benefits related to an enhancement of the strength of the material. Considerable effort has been directed at understanding the fundamental deformation mechanisms responsible for the increased strength in these materials. Recent results, however, indicate that microstructural instabilities in the form of grain growth take place during tensile loading of nanocrystalline sputter deposited Al thin films, thereby reducing its strength and enabling the film to undergo extended plastic deformation. A possible explanation for this observation of stress-assisted grain growth is that the grain boundaries are originally pinned by impurity elements but able to break free as a result of stress-coupled grain boundary motion. High resolution TEM lattice images of the grain boundary structure clearly preclude the presence of an Al2O3 intergranular layer. Electron Energy Loss Spectroscopy (EELS) was employed in an attempt to detect the presence of impurities (specifically oxygen) in the grain boundaries of nanocrystalline Al thin films similar to those used in the tensile experiments. Near edge fine structure of the Al L2,3 EELS ionization edge has confirmed that the local atomic bonding at the grain boundary is more closely related to what would be expected for pure Al than for Al2O3. Preliminary EELS results do suggest an increase in oxygen at the grain boundary of a few atomic percent, but experimental artifacts such as the presence of a surface, native oxide and possible grain boundary grooving effects will also be discussed. The TEM results will also be compared and contrasted with Auger measurements and used to shed light on the possibility of grain boundary pinning in this material.

SESSION Z4: Structure of Amorphous Metals
Monday Afternoon, November 28, 2005
Constitution A (Sheraton)

3:30 PM *Z4.1

An Atomic Structural Model for Metallic Glasses. Daniel B. Miracle, Materials and Manufacturing Directorate, Air Force Research Laboratory, Dayton, Ohio.

A structural model is described for metallic glasses based on a new sphere packing scheme- the dense packing of solute-centered atomic clusters. This model combines random positioning of solvent atoms with atomic order of solutes over distances up to ~1 nm. This model shows that metallic glasses contain no more than three topologically distinct solute species and that these solutes possess specific radius ratios relative to solvent atoms. Model validation is achieved by quantitative comparisons between experimental measurements and model predictions in a wide range of metallic glasses. Predictions include solvent-solute partial coordination numbers, the nature and extent of medium-range solute ordering and metallic glass topologies (relative sizes and concentrations of constituent atoms). Good agreement is achieved in each of these areas. In particular, this model predicts compositions for a broad range of metallic glasses. This model provides specific guidance for the exploration of new bulk metallic glasses and may provide new insights into other metallic glass studies. The new scheme introduced here for the efficient filling of space in extended systems of unequal spheres may have relevance to problems in other fields.

4:00 PM Z4.2

Atomic Packing in Amorphous Alloys: Generalization to Binary Metallic Glass Systems. Howard Sheng, Weikun Luo and En Ma; Johns Hopkins University, Baltimore, Maryland.

The atomic arrangements and local (short to medium range) structures in amorphous alloys are of fundamental interest but remain unresolved at present. The efficient packing of atoms is thought to play a major role in enhancing glass-forming ability. This issue has been under constant discussion for several decades, and is brought to attention once again in recent structural models for metallic glasses. We have recently resolved the atomic-level structure for several representative binary metallic glasses. In this talk, we will discuss the MD and ab initio calculations and comparisons with experimentally obtained partial pair distribution functions. Our focus is on the short to medium range topological as well as chemical ordering. The systems studied cover a range of atomic size ratios and hence different local packing "units" (such as icosahedra, trigonal prisms, etc.). The evolution as a function of undercooling will be discussed as well.

Comparisons are made with existing and simplifying structural models. We summarize the general trends in solute-centered packing schemes and short-range ordering, as well as in "cluster" packing that leads to medium-range order. This work was supported by the US-DoE.

4:15 PM Z4.3
Aluminum-like medium-range order measured in $Al_{92}Sm_8$ explored by fluctuation electron microscopy.
William G. Stratton, Joe Hamann, John H. Perepezko and Paul M. Voyles; Materials Science and Engineering, University of Wisconsin - Madison, Madison, Wisconsin.

We have used fluctuation electron microscopy (FEM) to measure the type and characteristic size of nanoscale structural order in high Al-content amorphous alloys. FEM is a quantitative electron microscopy technique that studies the statistics of the diffracted intensities from multiple nanoscale volumes of a sample to characterize nanoscale structural order. High Al-content alloys devitrify by primary crystallization to a high density ($> 10^{20}$ m^{-3}) of pure Al nanocrystals. TEM-based variable coherence FEM on amorphous $Al_{92}Sm_8$ has shown that primary crystallization is correlated with aluminum-like nanoscale structural order [1]. Those measurements were most sensitive to order near a 1.6 nm length scale, with only limited response to smaller or larger ordered regions. STEM-based variable resolution FEM enables us to systematically probe length scales from 0.5 to 3 nm, better revealing the length scale of the intrinsic structural order of the material. The support of the NSF under contract DMR 02-05858 (W. G. S. and P. M. V.) and the ARO under contract DAAD 19-02-1-0245 (J. H. and J. H. P.) are greatfully acknowledged. [1] W. G. Stratton, et al., App. Phys. Lett., 86 (2005) 141910

4:30 PM Z4.4
Structural and Thermal Properties of Simulated Cu- and Zr-based Metallic Glasses. M. J. Lambert, K. M. Flores and W. Windl; The Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio.

We performed Molecular Dynamics (MD) simulations of a series of known Cu-Zr, Cu-Zr-Al, and Zr-Cu-Ni-Ti-Al glasses using Embedded Atom Method (EAM) potentials. Using room-temperature MD simulations, we found that all ordered Cu-Zr intermetallics found on the phase diagram are stable, with all theoretical lattice parameters within two percent of their experimental equivalent. This gave us confidence in the predictive power of the employed potentials. Using a novel annealing technique that allows us to simulate even extremely slow quench rates, we then produced glassy structures of different alloy compositions at varying quench rates and examined their nearest-neighbor coordination. Radial distribution functions (RDF's) of the modeled systems exhibit excellent agreement with experimental data, suggesting that the predicted atomic structure should have realistic features similar to real materials. Additional simulations of the glass transition temperatures compare favorably with experimental results. Comparing the detailed features and changes in the nearest-neighbor order and the simulated glass transition temperatures with available experimental critical cooling rate data, we establish a set of criteria to predict the effect of alloy composition on glass forming ability.

4:45 PM Z4.5
NMR Study of Dynamics in Metallic Supercooled Liquids and Glasses. Lilong Li and Yue Wu; Department of Physics and Astronomy and Curriculum in Applied and Materials Sciences, University of North Carolina at Chapel Hill, Chapel Hill, North Carolina.

Using high temperature nuclear magnetic resonance (NMR), we studied dynamics in metallic supercooled liquids and glasses, probing both the rattling processes (β relaxation) and slow process (α relaxation) using various approaches. The study of the fast processes reveals that the amplitude of the vibrational types of motion follows linear temperature dependence above certain temperature T_c ($T_c > T_g$, T_g being the glass transition temperature) and drops dramatically below T_c. Below T_g, the temperature dependence of the amplitude of such motion is linear again. This observation agrees with the prediction of mode coupling theory (MCT). For the slow process, we used various NMR techniques to cover a broad range of time scale to study the dynamics. We see that our results on the motion of ^{31}P in $Pd_{43}Ni_{10}Cu_{27}P_{20}$ differ from the tracer diffusion results of heavy elements obtained by other group. Light elements and heavy elements exhibit the same temperature dependence for the α relaxation time scale at high temperatures, but from T_c, they starts to differ; at T_g, qualitative changes are observed for the motion of ^{31}P but none for heavy elements in tracer diffusion studies. We explain the results with a combination of MCT and decoupled modes.

SESSION Z5: Poster Session: Processing, Structure, and Structure Evolution
Monday Evening, November 28, 2005
8:00 PM
Exhibition Hall D (Hynes)

Z5.1
Abstract Withdrawn

Z5.2
Abstract Withdrawn

Z5.3
Influence of the Zr-Content on the Oxidation of Cu-Zr based Bulk Metallic Glasses and Nanocrystalline Alloys. Uwe Koster and Monika Meuris; Dept. Biochem. & Chem. Eng., University of Dortmund, Dortmund, Germany.

Cu-Zr based bulk metallic glasses are of increasing interest in particular due to their excellent mechanical properties, e.g. high elastic limit and strength. The Cu-rich Cu60Zr30Ti10 and the Zr-rich Zr69.5Cu12Ni11Al7.5 glass are examples of such glasses which combine good glass forming ability with excellent mechanical properties making them a material of choice for a variety of applications. Any application of such glasses, however, requires adequate thermal stability, i.e. resistance against crystallization and oxidation. The aim of this paper is a detailed investigation on the oxidation reactions of Cu-Zr based metallic glasses and nanocrystalline alloys of similar compositon by thermogravimetry and cross sectional scanning and transmission electron microscopy in order to reveal the influence of the Zr-content and the microstructure on the proceeding oxidation reactions. Oxidation of these metallic glasses was observed to proceed quite differently depending on the Zr-content. Oxidation in the Zr-rich Zr69.5Cu12Ni11Al7.5 seems to be controlled by oxygen diffusion through a homogeneous scale towards the ZrO2/glass interface. In the Cu-rich Cu60Zr30Ti10 metallic glass, on the other hand, a layered scale structure was found to develop with an assembly of Cu-oxide needles at the outer surface; during ongoing oxidation thicker oxide scales lose contact to the remaining metallic glass and start to peel off due to developing stresses and formation of voids at the interface. These results will be compared with the oxidation behaviour of binary Cu-Zr metallic glasses as well as nanocrystalline alloys of similar composition. Finally, strategies for designing bulk metallic glasses with excellent mechanical properties and improved oxidation resistance and first results will be discussed.

Z5.4
Systematic Study of the Devitrification Process of $Zr_{52.5}Cu_{17.9}$ $Ni_{14.6}Al_{10}Ti_5$ Bulk Metallic Glass. Ling Yang[1,2], X.-L. Wang[2,3], A. D. Stoica[2], C. T. Liu[3], J. Almer[4], Z. P. Lu[3], W. D. Porter[3] and D. Shi[1]; [1]Chemical and Materials Engineering, University of Cincinnati, Cincinnati, Ohio; [2]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [3]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [4]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois.

In order to study the detailed crystallization mechanisms during the devitrification of bulk metallic glass, we have carried out a systematic study of $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ (BAM11). The experiments included in-situ synchrotron scattering by detecting wide angle and small angle spectrum simultaneously during isochronal and isothermal annealing, DSC under the same conditions, TEM, and atomic probe analysis. The in-situ data clearly demonstrate that crystallization happens in two stages, corresponding to the two successive exothermal peaks on DSC traces. The first stage, where the major amorphous peaks sharpened appreciably, is consistent with the growth of icosahedral short-range order. The second stage is the nucleation of the tetragonal Zr2Ni phase. Small angle scattering showed an increase of the intensity before the start of the crystallization, but the interference peak appeared after the crystallization happened. Combined, these data reveal details of atomic ordering mechanisms during devitrification. This research was sponsored by Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy under Contract DE-AC05-00OR22725 with UT-Battelle, LLC. Use of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, under Contract No. W-31-109-Eng-38. Part of this work was sponsored by the U.S. Department of Energy (USDOE), Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Transportation Technologies, as part of the High Temperature Materials Laboratory User Program, under contract number DE-AC05-00OR22725 with UT-Battelle, LLC.

Z5.5

Pair Distribution Function Study on As-cast, Structurally Relaxed and Crystallized Zr55Cu35Al10 Bulk Metallic Glasses. Cang Fan[1], H. Choo[1], S. J. L. Billinge[2], A. S. Masadeh[2], T. Proffen[3], W. Dmowski[1], T. W. Wilson[1], L. J. Kecskes[4], P. K. Liaw[1] and T. Egami[1]; [1]Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee; [2]Dept. of Physics and Astronomy, Michigan State University, East Lansing, Michigan; [3]LANSCE, Los Alamos National Laboratory, Los Alamos, New Mexico; [4]US Army Research Laboratory, Aberdeen Proving Ground, Maryland.

In the past, nanocrystal-containing bulk metallic glass composites (nano-BMGCs) with enhanced strength and plasticity have been synthesized either by casting or by a heat-induced crystallization of nanocrystal-forming amorphous alloys [1,2]. In the case of heat-induced nanocrystallization, the structural relaxation of the amorphous alloys occurs first. It has been reported in Fe-, Co-, or Ni-based amorphous alloys that such structural relaxation results in brittleness [3]. However, we found that in certain Zr-based BMGs the plastic strain to failure increases further after such structural relaxation. Reasons for the increased plasticity remain uncertain. To understand this behavior further, we investigated changes in the local atomic structure (short-range to medium-range order) on as-cast, structurally relaxed, partially crystallized, and fully crystallized structures by neutron and synchrotron x-ray, scattering measurements on the Zr55Cu35Al10 BMGs. The neutron and synchrotron x-ray scattering results were studied by pair distribution function analyses. In addition, high-resolution transmission electron microscopy was performed to investigate the as-cast and crystallized structures to complement the neutron-scattering structural studies. This work is supported by the NSF International Materials Institutes Program (IMI) under DMR-0231320 with Dr. C. Huber as the Program Director. [1] C. Fan, and A. Inoue, Appl. Phys. Lett. 75, 3644 (1999). [2] C. Fan, C. Li, A. Inoue, and V. Haas, Phys. Rev. B, 61, 3761 (2000). [3] H.S. Chen, Mater Sci Eng, 26, 79 (1976).

Z5.6

Thermodynamic Limits of Crystallization and the Prediction of Glass Formation Tendency. X. Y. Yao, R. Napolitano, Cai-Zhuang Wang, M. J. Kramer and K. M. Ho; Ames Laboratory - US DOE, Iowa State University, Ames, Iowa.

The minimum degree of undercooling which is thermodynamically necessary for the diffusionless transformation of a liquid alloy to a solid solution, for a given alloy composition, is expressed by the T0 curve in the phase diagram. T0 curves play an important role in the rapid quenching of liquid alloys and would be very useful for understanding the glass-forming tendency of the alloys. However, only a very few quantitative estimates of T0 curves have so far been reported. We have calculated the T0 curves for some selected binary systems using the CALPHAD (CALculation of PHAse Diagrams) method and with some parameters generated by ab initio calculations. Results have been obtained for the following five simple eutectic binary alloys: Al-Ge, Ag-Ge, Au-Ge, Al-Si and Au-Si .We found that a common and interesting feature is that the valleys of the T0 curves are far away from the corresponding eutectic points. We have also performed the calculations for several Al-RE binary alloys and compare the results with reported observations of glass formation. The results show that the glass forming composition of the Al-RE alloys is strongly correlated with the valley of the T0 curves in the phase diagram.

Z5.7

Time scales for relaxation and crystallization of the Zr58.5Cu15.6Ni12.8Al10.3Nb2.8 bulk metallic glass forming alloy. Isabella Gallino, Minalben Shah and Ralf Busch; Mechanical Engineering, Oregon State University, Corvallis, Oregon.

A new experimental method was developed to study the isothermal enthalpy relaxation kinetics below the glass transition region of bulk metallic glass forming alloys using differential scanning calorimetry. The method was applied to the Zr58.5Cu15.6Ni12.8Al10.3Nb2.8 alloy and the results reveal that the enthalpy relaxes in an Arrhenius-like fashion. The activation energy obtained from the Arrhenius fit is comparable to the activation energy required for the diffusion of the medium size atoms. This suggests that solid-state diffusion is the governing mechanism for the enthalpy relaxation process. The stretching exponents for the relaxation are close to unity, which indicates that this alloy is a rather strong glass former. This is confirmed by Vogel Fulcher Tammann (VFT) fits of the heating rate dependence of the glass transition. The kinetics of isothermal crystallization is also studied by constructing the time temperature transformation (TTT) diagram.

Z5.8

Oxidation and Crystallization of the Refractory Alloy Glass Nb35Ni60Sn5. Isabella Gallino[1], Ralf Busch[1], Lioba Jastrow[2], Haein Choi-Yim[3] and Uwe Koester[2]; [1]Department of Mechanical Engineering, Oregon State University, Corvallis, Oregon; [2]Department of Biochemical & Chemical Engineering, University of Dortmund, D-44221 Dortmund, Germany; [3]W. M. Keck Laboratory of Engineering Materials, California Institute of Technology, Pasadena, California.

The newly discovered Ni-Nb-Sn glass [1] is considered a promising refractory material due to its high glass transition temperature (Tg > 881K). An adequate oxidation resistance at high temperatures is therefore necessary. In this paper, for the first time, the oxidation behavior of the Nb35Ni60Sn5 refractory alloy glass has been studied in dry air in the temperature range of about 800-850K. Isothermal thermogravimetric analyses reveal paralinear oxidation kinetics with similar oxidation rates that Zr-based glasses experience 200K below [2]. X-ray diffraction and cross-sectional electron microscopy allows phase identification in the scales and revealing their formation mechanism. The oxide scale resulting from oxidation at 800K consists of an outer layer of Ni oxide and a continuous inner layer of Nb oxide. This sequence of different oxide layers is repeated during longer oxidation or oxidation at higher temperatures. The depletion of Nb in the alloy underneath the scale seems to induce the crystallization of Ni-rich intermetallics such as NbNi3 and the ternary intermetallic NbNi2Sn. Thermodynamics and kinetic aspects of the interaction between oxidation and crystallization will be discussed. [1] H. Choi-Yim, D.H. Xu, and W.L. Johnson: Appl. Phys. Lett. Vol. 82 (2003), p. 1030 [2] U. Koester and Triwikantoro: Mater. Sci. Forum Vol. 360-363 (2001), p. 29

Z5.9

Electromagnetic Levitation Processing of Ca- and Mg-Based Metallic Glass-Forming Alloys. Edward Robert Arata and Jorg F. Loffler; Department of Materials, Laboratory of Metal Physics and Technology, ETH Zurich, Zurich, Switzerland.

Alloys based on Ca and Mg prepared by traditional methods such as arc melting, induction heating in a silver boat, or resistive heating in a graphite or boron nitride crucible generally suffer from massive evaporation, inefficient heating, and contamination. To deal with these problems, we have built an induction system to melt samples by electromagnetic levitation. Ca- and Mg-based samples (density $\sim$ 2.5 g/cm3) were successfully produced in volumes up to two cubic centimeters with minimal evaporation losses. Heating and mixing were achieved very quickly with the high-frequency field, minimizing the time in which evaporation could occur. Once fully homogenized, the alloys were allowed to drop out of the levitation coil directly into a copper mold connected to a suction casting system, making possible a one-step process from pure elements to the cast sample. Samples produced using this method were then analyzed in detail and processed centrifugally to identify low-lying eutectics. The results we present demonstrate the applicability of an electromagnetic levitation system to Bulk Metallic Glass processing, which, specifically, facilitates the alloying of low-melting materials, homogeneous mixing of the melt, and the combination of melting and casting in a one-step process.

Z5.10

Analysis of the Samples of Fe-Cu-Nb-Si-B Amorphous Alloys Obtained by Dynamic Compacting Method. Grigory Aleksandrovich Potemkin, Victor A. Golubev, Ludmila V. Zueva, Andrey V. Strikanov and Aleksey V. Sten'gach; RFNC-VNIIEF, Sarov, Russian Federation.

The Dynamic Compacting (DC) method is promising method to produce considerable-size nonporous wares. The phenomenon is based on the impact of shock wave on the initial powders of amorphous alloys. Every time when the shock wave propagates through the bulk of substance then the temperature rises substantially. Therefore there is a need of study of the DC's effect on the structure and properties of the amorphous alloys. The results of the thermal analysis (in particular, Differential Scanning Calorimetry) of the samples of the soft magnetic alloys are presented in the report. These results concern with amorphous alloys of 5BDSR, GM414, 10NSR trademarks before DC and after DC, respectively. It is shown there is single low-temperature endothermic peak (near 300C) and there are several high temperature exothermic peaks (near 540C, 650C, and 700C). The first peak is related to glass-transition, the following peaks are related to formation of nano-crystalline phases. It was proved by XRD analysis data. The optimal regimes of the thermal processing of final wares were chosen on the base of thermal- and XRD-analysis. The study of the effects of these regimes on the properties (magnetic conductivity, specific losses etc.) of the circular magnetic conductors was executed. In particular, thermal- as well as thermo-magnetic processing of magnetic conductors based on 5BDSR amorphous alloy (after DC) essentially improves their magnetic properties. For example, magnetic conductivity μ increases approximately by factor

17 with respect to the magnitude before DC.

Z5.11

Phase Separation in Liquid and Amorphous Ni-Nb-Y Alloys. Norbert Mattern, Uta Kuehn, Annett Gebert and Ludwig Schultz; IFW Dresden, Dresden, Germany.

Phase-separated amorphous alloys can be prepared in the Ni-Nb-Y system by rapid quenching from the melt. The microstructure formed consists of amorphous Nb-enriched and Y-enriched regions with a size distribution from micrometer dimension down to several nanometers. Calculation of the ternary phase diagram were performed by the CALPHAD method. The miscibility gap in the solid and liquid state of the binary Nb-Y system extends into the ternary Ni-Nb-Y melt as a consequence of the positive mixing enthalpy between Nb and Y. Experimental investigations confirm the decomposition of the melt. Microstructure and thermal properties of the phase separated amorphous alloys will be discusses.The two-phase amorphous Ni-Nb-Y alloys crystallize in a first step by the primary precipitation of the cubic Ni2Y phase from the Y-rich amorphous phase. At higher temperature the remaining Nb-rich amorphous phase crystallizes mainly into Ni7Nb6.

Z5.12

Abstract Withdrawn

Z5.13

Glass-Forming Ability and Mechanical Properties of a New Zr-Based Metallic Glass. Jun Shen, Harbin Institute of Technology, Harbin, China.

In this presentation, we demonstrate the systematic study on a newly developed Zr51Cu20.7Ni12Al16.3 bulk metallic glass (BMG) in terms of glass-forming ability (GFA), thermodynamic behavior and mechanical property. Analysis via X-ray diffraction, scanning electron microscopy and transmission electron microscopy indicates that the well-crystallized 10-mm alloy consists of complicated primary crystalline phases, namely, NiZr2, Al1.7Ni0.3Zr, one rhombohedral phase (composition close to Zr6Cu10Ni9Al4O5) and one monoclinic phase (composition close to Zr57Cu25Ni7Al11). However, with minor yttrium addition, the as-cast 10 mm sample shows a fully amorphous structure, indicating that the GFA has been largely enhanced. The new alloy exhibits a very high compressive strength which is the highest among all reported Zr-based BMGs

Z5.14

Metallic Glass Formation in the Hf$_2$Cu-Cu$_{10}$Hf$_7$-HfNi Alloy System. Robert Harvey Woodman[1] and Laszlo J. Kecskes[2]; [1]Dynamic Science, Inc., Army Research Laboratory, APG, Maryland; [2]Ordnance Materials Branch, Army Research Laboratory, APG, Maryland.

We report the development of a bulk-metallic-glass-forming alloy, Hf$_{44.5}$Ti$_5$Cu$_{27}$Ni$_{13.5}$Al$_{10}$. Faced with a need for a metallic glass with glass-forming ability similar to Zr$_{57}$Nb$_5$Cu$_{15.4}$Ni$_{12.6}$Al$_{10}$, but with a density of 11.0 kg/m^3 or greater, we first examined Hf-substituted versions of known Zr-based alloys. The results led us to examine the equilibrium phase relationships of the major components - Hf, Cu, and Ni. We eventually focused on the compatibility triangle Hf$_2$Cu-Cu$_{10}$Hf$_7$-HfNi. Alloying with Nb, Ti, Al, and Sn produced alloys of variable glass-forming ability, with the best to date being Hf$_{44.5}$Ti$_5$Cu$_{27}$Ni$_{13.5}$Al$_{10}$. We examine the effect of the alloying elements on the equilibrium phase assemblage, and discuss the implications for the development of glass-forming alloys.

Z5.15

Dynamical Heterogeneity in Glass Al from Molecular Dynamics Simulations. M. I. Mendelev, J. Schmalian, K. M. Ho and Cai-Zhuang Wang; Ames Laboratory - US DOE, Iowa State University, Ames, Iowa.

We performed molecular dynamics simulations to study the liquid and glass states of Al using a frequently employed embedded-atom potential (i.e., Ercolessi-Adams (EA)-potential). Below 800K we find that the characteristic time scales of the relaxation become considerably larger compared to the high temperature liquid (which exists as a concurrent phase, depending on the initial values of the simulation, down to 600K). While the pair distribution function of the glassy and the liquid states display only minor differences, the dynamics of both states is vastly different. In the glassy state, particles diffuse on long time scales with a diffusion constant more than an order of magnitude smaller than in the liquid state. Even more interesting is that the diffusion in the glassy regime resembles much more the vacancy diffusion of crystalline solids than ordinary Brownian motion with only short term memory. Analyzing the spatial correlation of the most mobile particles, we find a considerable spatial correlation of such mobile objects. In addition we were able to demonstrate that there is a strong correlation between the local particle density and the mobility of particles. These results demonstrate that dynamical heterogeneity in glasses is directly related to local structural properties (e.g., density) and that the slow diffusion in a highly viscous, glassy fluid is very similar in character to vacancy diffusion in crystalline solid and fundamentally different from Markovian diffusion in liquids.

Z5.16

Biocompatibility of Zr-based metallic glasses. Stefano Buzzi[1], Kaifeng Jin[1], Samuele G. P. Tosatti[2], Isabel Gerber[3], Peter J. Uggowitzer[1] and Jorg F. Loffler[1]; [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Zurich, Switzerland; [2]Biomedical Interfaces Team, Laboratory for Surface Science and Technology, ETH Zurich, Zurich, Switzerland; [3]Institute of Cell Biology, ETH Zurich, Zurich, Switzerland.

Metallic glasses are promising materials for medical devices because of their high strength and elasticity. As a first step in the evaluation of their biocompatibility, cytotoxicity tests were performed on different Zr-based metallic glasses. The two alloys with the best results, Zr-Ti-Cu-Ni-Al (VIT 106a) and the recently developed nickel-free alloy Zr-Cu-Fe-Al [1], were then systematically investigated with a particular focus on the influence of surface modification. Three surface treatments were applied (electropolishing, bathing in diluted nitric acid, oxygen plasma) and the surfaces were analyzed by photoelectron spectroscopy (XPS). Cytotoxicity was tested by measuring the viability and metabolic activity of mouse fibroblasts. The results show that the surface consists almost exclusively of zirconium oxide, which yields good biocompatibility in both alloys. This biocompatibility is additionally improved by passivation in nitric acid, because of stabilization of the oxide layer. Following this surface treatment the results are comparable to those for the negative cytotoxic control (polystyrene). [1] K. Jin, J. F. Loffler, Appl. Phys. Lett. 86 (24), 241909 (2005) 1-3

Z5.17

Influence of Decomposition on Glass-Forming Ability and Magnetic Properties in Fe-Based Metallic Glasses. Giovanni Mastrogiacomo, Jurg Kradolfer and Jorg F. Loffler; Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Wolfgang-Pauli-Str. 10, CH-8093 Zurich, Switzerland.

The glass-forming ability of Fe-based metallic glasses is strongly correlated with the amount of metalloids they contain. Structural models suggest that about 20 at.% metalloids should be present to achieve a good glass-former. However, the addition of non-ferromagnetic elements causes magnetic and mechanical properties to deteriorate. Therefore we developed several Fe-based metallic glasses without metalloids starting from a Fe-Cr-Co system, where the b.c.c α phase has the tendency to decompose. This destabilization of the solid state may cause a reduction in the liquidus temperature, which enhances glass formation via a reduction of the gap between the liquidus temperature and the glass transition temperature. The key points in the development of metalloid-free Fe-based metallic glasses were the addition of zirconium and an increase in the Co/Fe ratio. Alloying of zirconium suppresses the formation of the high-temperature γ phase and destabilizes the solid state, according to the instability criterion suggested by Hume-Rothery where low solubility is achieved for alloying elements with atomic size ratios differing by more than 15%. In addition, an increase in the Co/Fe ratio enlarges the miscibility gap, which causes a decrease in the liquidus temperature. X-ray measurements and differential scanning calorimetry confirm the glassy state of these metalloid-free Fe-based metallic glasses, and the metallic glass with the highest Fe and Co fraction reveals the presence of plasticity. Further, magnetization measurements show a saturation magnetization of up to 1.1 T plus an inverted hysteresis, which can be attributed to the decomposing tendency of the Fe-Cr-Co system.

Z5.18

Formation of bulk Fe-Co-B-Si-Nb glassy alloys by flux melting and water quenching. Teruo Bitoh[1], Akihiro Makino[2], Akihisa Inoue[2] and Lindsay Greer[3]; [1]Department of Machine Intelligence and Systems Engineering, Akita Prefectural University, Yurihonjo, Japan; [2]Institute for Materials Research, Tohoku University, Sendai, Japan; [3]Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, United Kingdom.

It is well known that the main competition to prepare glassy alloys is attributed to oxides and other inclusion in the molten metal which act as heterogeneous nucleation sites for crystallization. An approach to eliminate the inclusions is to heat and cool the molten metal while it is immersed in molten oxide flux [1, 2]. The formation of the large bulk Fe-Co-B-Si-Nb glassy alloy specimens by flux melting and water quenching has been investigated. The $[(\mathrm{Fe}_{0.5}\mathrm{Co}_{0.5})_{0.75}\mathrm{B}_{0.20}\mathrm{Si}_{0.05}]_{96}\mathrm{Nb}_4$ alloy, which exhibit super-high fracture strength of 4210 MPa in a glassy state [3], was selected. The glassy cylindrical specimens with diameter up to 5 mm have been prepared by the copper mold casting [3]. The mother alloy was prepared by arc-melting the mixture of pure Fe, Co and Nb metals, and pure B and Si crystals. Small pieces of the mother alloy and dehydrated B_2O_3 (just enough to immerse the whole specimen) were put together in a dry, cleaned fused silica tube. The B_2O_3 and the specimen were melted under Ar flow by a torch, held in the molten state for 2-3 minutes, and then cooled to a temperature (approximately 800 K) where B_2O_3 was still molten. This thermal cycle was repeated several times, and finally the system was quenched in water. The structure of the specimens was examined by X-ray diffractometry (XRD). The bulk specimens with the very smooth surface and with good metallic luster have been obtained. The XRD profile taken from the cross section of the specimen with 5.7 mm in diameter (and approximately 9 mm in length) consists only of a halo and no appreciable Bragg line is observed. Therefore, the large bulk glassy specimen has been synthesized by the B_2O_3 flux melting and water quenching, though the cooling rate (approximately 100 K/s) is lower than that of the copper mold casting. To our knowledge, this specimen is the thickest of any ferrous glassy alloys formed until now. The B_2O_3 flux melting causes the increase in the supercooled liquid region ($\Delta T_x = T_x - T_g$, where T_g is the glass transition temperature) before crystallization through the increase in the onset of crystallization (T_x), as already reported for the glassy Pd-Cu-Ni-P alloy [2]. This indicates that the flux melting is effective for the retardation of crystallization through the suppression of heterogeneous nucleation. [1] H. W. Kui, A. L. Greer and D. Turnbull, Appl. Phys. Lett. 45 (1984) 615. [2] A. Inoue, N. Nishiyama and H. Kimura, Mater. Trans., JIM 38 (1997) 179. [3] A. Inoue, B. L. Shen and C. T. Chang, Acta. Mater. 52 (2004) 4093.

Z5.19

Dynamic Compacting of Powders of Some Amorphous Alloys. Victor Golubev, Andrey V. Strikanov, Vladimir G. Bugrov, Grigory A. Potemkin and Valery B. Kudel'kin; Russian Federal Nuclear Center, All-Russian Research Institute of Experimental Physics, Sarov, Russian Federation.

At present amorphous metallic alloys have the broad expansion in various fields of science & engineering as a result of their unique properties. In particular, soft magnetic amorphous alloys are extensively used in electrical engineering. However the production of considerable-size nonporous wares based on the powders (or tapes) of these alloys is heavy problem owing to high hardness of the particles. Therefore shock wave's compacting or Dynamic Compacting (DC) method is promising one to produce the wares on the base of powders of amorphous alloys because it can provides high strength and near zero porosity of the wares. The experimental D-U diagrams of soft magnetic amorphous alloys were obtained to realize this method of compacting. The calculations of the amplitude and duration of shock wave were carried out. The several versions of explosive devices using shock plane wave generator to produce circular magnetic conductors were developed and were tested. These magnetic conductors are based on amorphous alloys of 5BDSR, GM414, 10NSR trademarks (Fe with Cu, Nb, Si, B additives). XRD analysis proved that amorphous state of the alloys remains the same up to 20 GPa shock wave's pressures. The mechanical, structural, electrical and magnetic properties both initial amorphous alloys and compacted one were obtained and compared as a result of the implemented works. It was stated that DC leads to increase of magnetic conductivity by factor ~15 with respect to initial amorphous alloys powder. Besides the specific losses decrease in ~4 times.

Z5.20

Abstract Withdrawn

Z5.21

Development of Bulk Aluminum Glass Using a Wedge-Casting Method. Wynn S. Sanders, Jenifer S. Warner, John V. Lloyd and Daniel B. Miracle; Air Force Research Laboratory, Wright-Patterson AFB, Ohio.

Amorphous metals (metallic glasses) have undergone intense development in recent years. Many new bulk metallic glasses have been developed, yielding breakthroughs in Zr-, Pd-, and La-based systems that can be cast several centimeters thick. Unfortunately, these breakthroughs have not aided the development of Al-based glasses, which have been acknowledged by the amorphous metals community to be one of the most difficult-to-obtain bulk metallic glass forming systems. Typically, Al-based glasses can only be produced in a melt-spun ribbon. However, this technique makes it difficult to quantify the relative merit of different alloy compositions. To overcome this problem, a new wedge-cast technique has been developed for the exploration of metallic glasses. By directly comparing the maximum thickness obtained, the relative glass-forming ability of different systems is easily compared. This has enabled the discovery of a ternary aluminum-rich glass with a maximum thickness of 0.95 mm, which is nearly twice as thick as the previously reported best Al-glass forming system, Al-Gd-Ni. Development of this alloy is ongoing and its critical cast thickness is expected to increase further with the addition of quaternary alloying elements. A comprehensive evaluation of quaternary additions to the Al-La-Ni system is being undertaken to achieve the goal of developing an al-based metallic glass with a critical thickness exceeding 1 mm. The results obtained in this study will be reported and discussed.

Z5.22

Nanocrystallization Induced by Reactive Nitrogen Sputtering. Mukul Gupta and Rachana Gupta; Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institute, Villigen, AG, Switzerland.

Thin films of pure Fe and NiFe alloy were deposited using an $Ar+N_2$ mixture. The nitrogen partial pressure, during sputtering process was varied in the range of $0 \leq R_{N_2} \leq 100\%$, keeping the total gas flow at constant. It was found that nitrogen atoms gradually occupy interstitial sites in bcc Fe and fcc NiFe and restrict the long range ordering causing nanocrystallization at lower nitrogen partial pressure. When nitrogen partial pressure exceeds beyond a certain value both Fe and NiFe become amorphous. Further increase in nitrogen partial pressure results in formation of nitrides of Fe and NiFe and at still higher nitrogen partial pressure the nitrides themselves become nanocrystalline or amorphous. A mechanism inducing nanocrystallization and amorphization in Fe and NiFe due to reactive nitrogen sputtering is discussed in this work.

Z5.23

Fabrication of High Density Refractory Metal/Metallic Glass Nano-Composites. Min Ha Lee[1] and Daniel J. Sordelet[1,2]; [1]Materials and Engineering Physics Program, Ames Laboratory (USDOE), Ames, Iowa; [2]Materials Science and Engineering, Iowa State University, Ames, Iowa.

Bulk metallic glasses (BMGs) exhibit favorable properties including high yield strength, relatively low elastic modulus, high elastic strain limit and nearly-perfect elastic behavior at room temperature. Despite the list of desirable characteristics, BMG undergoes catastrophic failure at room temperature due to shear localization when subjected to a compressive mechanical load. This lack of global plasticity due to localized shear flow has limited the application of BMGs in many traditional applications. Because of the strong shear-localization susceptibility in BMG, their use is currently under consideration for kinetic energy penetrators (KEP). It is known that the self-sharpening behavior in depleted uranium (DU), which is commonly used for this application due to its high density, is related to localized shear during high strain-rate deformation, which results in better performance when compared to tungsten heavy alloys (WHA). Therefore, it has been suggested that a combination of W with a BMG matrix would achieve the required combination of density and deformation behavior to compete with DU. However, the use of body-centered cubic metals to increase the density (especially W) presents another problem as they are notoriously resistant to shear localization because of their strong strain-rate sensitivity. In conventional BMG matrix composites, shear band formation in a BMG matrix does not necessarily mean that shear localized deformation will occur in the reinforcing phase. More often an increase of plasticity in BMG matrix composites is offset by a decrease in the ultimate strength of the matrix, and as a result the composites are easily blunted during high strain rate deformation. The effectiveness of a reinforcing phase in preventing shear bands depends to a large extent on the size of the reinforcement phase particles. It was reported that for certain bcc metals, such as Fe, Ta and V, strain rate sensitivity (m) decreases when the grain size is refined into the 1 μm range. Additionally, fine-grained tungsten metal (~500 nm scale) shows adiabatic shear localization flow when deformed under uniaxial dynamic compressive loading conditions. Therefore it should be more likely to find shear banding behavior in a homogeneously distributed nanometer scale reinforcing metal phase in the metallic glass matrix. Due to limitations in decreasing the reinforcement size as well as the fabrication process, most BMG matrix composites have not previously achieved nanometer scale uniformly. In the current study, we successfully fabricated uniformly-layered nanometer scale tungsten/metallic glass composites by a controlled milling process to yield composite powders that were consolidated by warm extrusion into fully dense rods. Deformation during quasistatic compression tests exhibited highly localized shear flow in the tungsten/metallic glass composites prepared with milled powder that is similar to that in DU materials.

Z5.24

Rocking-Beam Variable Coherence Electron Microscopy of Amorphous-Nanocrystalline Composite Alloys. Jing Li and

Ian M. Anderson; Metals & Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Variable coherence electron microscopy (VCEM) can be usefully regarded as an extension of hyperspectral imaging, with two real-space and one (tilted-beam, TB) or two (rocking-beam, RB) reciprocal-space coordinates, for the characterization of structural inhomogeneity. Such methods hold promise for the characterization of the amorphous-to-crystalline transformation in materials such as bulk amorphous alloys. In this study, we have performed RB-VCEM to characterize sputtered amorphous and partially crystallized tungsten thin films. Series of images were acquired with a CM200FEG operating at 200 kV in "rocking beam" mode, a beam current of ∼10 nA, "parallel" incident illumination, and an objective aperture semi-angle $Q = \sim 1.2\ \mathrm{nm}^{-1}$. The data indicate that local structural domains can be characterized with great angular precision. Strengths, limitations, and potential applications of the method will be discussed. Research at the SHaRE User Facility was sponsored by the Division of Materials Sciences and Engineering, U. S. Department of Energy, under Contract DE-AC05-00OR22725 with UT-Battelle, LLC.

Z5.25

Formation of Amorphous Al-Y-Fe-Ti Thin Films by Pulsed Laser Deposition. Lydia Grace Longstreth-Spoor[1,2], Y. T. Shen[1,2], K. F. Kelton[1,2] and Ramki Kalyanaraman[1,2]; [1]Physics, Washington University, St. Louis, Missouri; [2]Center for Materials Innovation, Washington University St. Louis, St. Louis, Missouri.

Al-based metallic glasses are interesting due to their favorable mechanical properties. In most cases, these glasses are prepared by rapid quenching; there have been relatively few studies of the formation of amorphous thin films. These could have numerous applications in areas requiring coatings with high mechanical strength. In this work, we show that amorphous thin film can be formed on Si substrates by pulsed laser deposition from targets with composition of Al87.5Y7Fe5Ti0.5. The amorphous nature of the film was determined by transmission electron microscopy investigations of the microstructure, complemented by x-ray diffraction studies. A detailed investigation of the film microstructure and elemental composition measured by energy dispersive x-ray spectroscopy will be presented as a function of growth conditions. It was determined that the critical growth parameter to stabilize the amorphous phase was a low growth temperature and deposition rate. Studies have shown that these Al-based glasses crystallize to form amorphous/nanocrystal composites with even more enhanced values of strength and hardness, without losses in ductility and toughness. The mechanisms responsible for nanostructure formation are unclear, however. This will be investigated further with these films, using them as laboratories for fundamental investigations of homogeneous and heterogeneous nucleation processes.

Z5.26

Amorphization and thermal stability of mechanically alloyed $Zr_{54}Cu_{19}Ni\ Al_8Si_5Ti_5O_1$. Vassilios Kapaklis[1], Athanasios Georgiopoulos[2], Peter Schweiss[3] and Constantin Politis[1,4]; [1]Engineering Science Department, University of Patras, Patras, Greece; [2]Materials Science Department, University of Patras, Patras, Greece; [3]Institut fuer Festkoerperphysik, Forschungszentrum Karlsruhe, Karlsruhe, Germany; [4]Institut fuer Nanotechnologie, Forschungszentrum Karlsruhe, Karlsruhe, Germany.

Zr- based bulk amorphous alloys have been the most investigated bulk amorphous alloys since the discovery of the latter in the early 1990s. Their remarkable engineering properties favored commercial applications. In the last years also a great variety of Zr- based alloys has been prepared by mechanical alloying methods and characterized. Mechanical alloying is considered to be a very competitive method because of the fact that it can be carried out at room temperature and for a large range of systems which may also exhibit poor glass forming ability or high melting points. One disadvantage of mechanical alloying may be the fact that during the process impurities are introduced to the sample, coming from the vial or the atmosphere under which the samples are prepared. These impurities in most cases are mainly iron or carbon from the steel vials and oxygen contained in small quantities in the inert gas atmosphere under which the alloys are milled. In the present work we have intentionally introduced significant amount of oxygen to Zr- based alloys. Samples were prepared either by high energy ball milling of the elemental powders and single phase α-Zr(O) at the appropriate stoichiometry, or by melting in an Zr-gettered arc melting facility, in both cases under purified argon atmosphere. The effect of small amounts of oxygen (1 at. %) on the amorphization process and the thermal stability of mechanically alloyed $Zr_{54}Cu_{19}Ni_8Al_8Si_5Ti_5O_1$ powders and arc melted bulk samples was studied by X-ray diffraction, differential scanning calorimetry and high resolution electron microscopy. It was found that the introduction of oxygen to the alloy composition does not inhibit the amorphization but enhances greatly the thermal stability of the mechanically alloyed amorphous powders. Compared to samples without oxygen prepared either by arc melting or mechanical alloying, samples with oxygen show an increase of the supercooled liquid region from $\Delta T_{x-g}=T_x-T_g=117$ °C to 141 °C, where T_x is the crystallization and T_g the glass transition temperature. The glass transition for the mechanically alloyed samples remains unaffected at 336 °C.

Z5.27

Comparison of Texture Evolution in Nickel Deformed by Equal Channel Angular Pressing and Rolling. Predrag Kisa and Nicholas G. Eror; MSE, University of Pittsburgh, Pittsburgh, Pennsylvania.

Considerable effort has been invested recently on the processing of second generation of superconductors. So far the rolling assisted biaxialy textured substrate approach (RABITS) has shown the best promise of achieving long lengths in coated conductors. In most of the current published literature nickel had been used as the substrate material. In this research we investigate the cube texture of severely plastically deformed and annealed nickel and the coating initially deposited as amorphous material ($YBa_2Cu_3O_7$ and CeO_2). Subjecting nickel and nickel alloys to a very high plastic strains using either equal-channel angular pressing (ECAP) or cryorolling usually give grain sizes in the submicrometer range of 100-200 nm although several reports had been made of grain sizes as small as 50 nm. Results of combined deformation ECAP and rolling will be presented with quantification of obtained texture and microstructures.

Z5.28

Radiation Damage Evolution in Helium Implanted Cu-Nb Multilayered Thin Films. Tobias Hoechbauer[1], Amit Misra[1], Khalid Hattar[2,1] and Richard G. Hoagland[1]; [1]Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico; [2]Materials Science and Engineering, University of Illinois, Urbana-Champaign, Illinois.

Our previous work has shown that sputter-deposited nanoscale Cu-Nb multilayer composites possess very high yield strength and morphological stability during elevated temperature annealing. In this investigation, we have explored the evolution of radiation damage in Cu-Nb multilayers and single layer Cu and Nb films subjected to 33 keV Helium ion implantation at room temperature. The samples were analyzed in their as-implanted state as well as after post-implantation annealing via Rutherford backscattering spectroscopy, elastic recoil detection and high-resolution transmission electron microscopy. In the as-implanted state, the implanted He content was retained and nanometer-scale bubbles precipitated preferentially at interfaces. During post-implantation annealing, significant blistering and He depletion occurred for both the single layer films and for composite multilayers with individual layer thickness of 40 nm. However, multilayers with 4 nm layer thickness showed a suppression of bubbles and He depletion. In all cases, the multilayer structure was retained during the ion-implantation process and post-implantation annealing of up to 600 C for 1 hour. The relation of the interfaces to the evolution of ion-radiation induced damage will be discussed. This research is supported, in part, by the DOE, Office of Science, Office of Basic Energy Sciences.

Z5.29

Transferred to Z3.3

Z5.30

Enhanced mechanical properties in ultrafine grained 7075 Al alloy. Yonghao Zhao and Yuntian Zhu; MST, Los Alamos National Lab., Los Alamos, New Mexico.

The high strength and high ductility for 7075 Al alloy were obtained by combining the equal-channel-angular pressing (ECAP) and natural aging. The tensile yield strength and ultimate strength of the ECAP processed and naturally aged sample were 103% and 35% higher, respectively, than those of the coarse-grained 7075 Al alloy counterpart. The tensile elongation to failure is about 12%. The enhanced strength resulted from high densities of the 2nd-phase particles (G-P zones and meta-stable phase) and dislocatons. The origin of the high ductility of the ECAP processed and agaed 7075 Al alloy will be discussed. This study shows that severe plastic deformation has the potential to significantly enhance the mechanical properties of precipitate hardening 7000 series Al alloys.

Z5.31

Local Atomic Structures of Amorphous / Nanocrystalline Aluminum Alloys. Tim Wilson[1], Hahn Choo[1], Cang Fan[1], Alex Hannon[2], Peter Liaw[1] and Laslo Kecskes[3]; [1]Materials Science and Engineering, University of Tennessee, Knoxville, Knoxville, Tennessee; [2]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, United Kingdom; [3]US Army Research Laboratory, Aberdeen Proving

Ground, Maryland.

The local atomic structures of Al-Y-Fe-Ni and Al-Y-Ni amorphous / nanocrystalline alloys were examined using neutron scattering. Two types of $Al_{85}Y_7Ni_8$, $Al_{85}Y_7Fe_5Ni_3$, and $Al_{81}Y_7Fe_5Ni_7$ alloys were examined. One set was produced by rapidly solidifying melt-spun ribbons, and another set was prepared by mechanical alloying of elemental powders. Atomic pair distribution function (PDF) analyses were performed on these alloys. Results showed that small changes in the composition affect the local atomic environment. The effect of the processing route and composition on the local atomic structures of these alloys was also investigated. This information was correlated to the results from differential scanning calorimetry (DSC), which showed that the onset of crystallization temperature for melt-spun ribbons was less than that of the mechanically alloyed powders with the same composition. The authors would like to thank Dr. C. Huber, the Program Director of the NSF International Materials Institutes (IMI) Program, for her support and encouragement of our IMI Program (DMR-0231320), at the University of Tennessee.

Z5.32

Micro- and Nanostructure Evolution with Exploding Wires. Vandana and P. Sen; Jawaharlal Nehru University, New Delhi, Delhi, India.

Advanced materials are often metastable, produced employing non-equilibrium methods. These are expected to have attractive mechanical, thermal and electrical properties associated with localized deformations. Here we employ electro-explosion of wires [1, 2] to introduce nonlinearities in a metal using a novel needle-plate geometry and show evolution of controlled micro and nanostructures. The exploding needle-plate system brings the plate instantaneously to its melting point. Hence shock wave generated in the plasma after the explosion [3], travels through the melt. Energy released by the shock waves gets stored in the melt and enhance the surface area of metal particles. As this process takes place far away from equilibrium, the configuration freezes in time scales shorter than the time available for the individual particles to coalesce into a single mass again. The molten plate metal re-crystallizes producing rings, modifying the metal surface at nanometer to micrometer scale as confirmed by our atomic force microscope (AFM). Grain size analysis reveals that the influence of applied electro-explosion voltage does not have any major influence on the grain size, whereas grain size scales with tip diameter, altering the nanostructure. The smaller exploding tips produce reasonably normal grain size distribution while the size distribution obtained with the large tip is skewed, with a long exponential tail. Time evolution of current during the electro-explosion process shows existence of melt for longest times for thick wires, allowing any small particle produced due to the shock waves to coalesce, leading to larger particle size. Reference [1] P. Graneau, Phys. Lett. A 97, 253 (1983). [2] P. Sen, J. Ghosh, A. Alqudami, P. Kumar, and Vandana, Proc. Indian Acad. Sci. (Chem. Sci.) 115, 499 (2003). [3] Igor V. Lisitsyn, Taishi Muraki, and Hidenori Akiyama, Appl. Phys. Lett. 70, 1676 (1997).

Z5.33

Processing and Properties of Nanostructured Alloy Coatings in the Binary Ni-Cr System. Pablo A. Castro[2,1], Hong Liang[3] and Christopher A. Schuh[1]; [1]DMSE, MIT, Cambridge, Massachusetts; [2]CINI Tenaris, Campana, Argentina; [3]Mechanical Engineering, Texas A&M, College Station, Texas.

Using a scalable electrodeposition process, Ni-Cr alloy coatings have been produced on copper and steel substrates, and the role of various processing variables on the resulting coating structure and properties has been investigated. Composite coatings of wear resistant nanostructured Ni-Cr alloys containing MoS2 particles have also been produced and characterized. Pin-on-disk testing showed that the co-deposition of solid lubricant particles improved the tribological performance of the coatings. The combination of a hard material such as Ni-Cr nanoalloys with a solid lubricant has a great potential for new surface modification developments.

Z5.34

The Influence of Equal Channel Angular Extrusion Route on the Mechanical Behavior of Commercial Purity Aluminum. Peiling Sun, Ellen Cerreta and George T. Gray; MST-8, Los Alamos National Laboratory, Los Alamos, New Mexico.

Changes in the deformation route during equal channel angular extrusion (ECAE) are known to result in different microstructures. Three ECAE routes: route A, no rotation between extrusion passess; route BC, 90° roation along the same direction between extrusions; and route C, 180° rotation between extrusion passes, were adopted to obtain different microstructures. The resulting microstructures have a submicron grain size, but with different morphologies and boundary structures. The three samples have been deformed in compression at deformation temperatures ranging from 77 to 298K and strain rates ranging from 0.001 to 3000/s. The effect of ECAE microstructures on the constitutive response of aluminum will be discussed.

Z5.35

Abstract Withdrawn

Z5.36

Investigation of the nature and the structure of truly amorphous nanosize metals, synthesized by means of nonequilibrium quantum chemical technology. Razmik Malkhasyan[1], David Ginley[2], Tatjana Kaydanova[2], Hans-Joachim Kleebe[3] and Sergo Kamanchadgyan[1]; [1]Scientific production enterprise "ATOM", Yerevan, Armenia; [2]NREL SERF W 102, Golden, Colorado; [3]Colorado School of Mines, Golden, Colorado.

The new non equilibrium method of transformation of materials, for example, metallic oxides, sulfides is developed for the last 15 years at SPE ATOM, Armenia. Non equilibrium chemical processes are carried out at the expense of the inner energy of reagents, for example, the energy of excitation of particles, when the thermal sources of energy excluding completely. Renunciation of temperature for the first time has enabled to synthesize truly amorphous metals (not alloys) in nanosize state. The powders of nanoamorphous tungsten, molybdenum etc. synthesized in Armenia in the main were investigated at NREL and Colorado School of Mines. The results of the investigation of nature and structure of nanoamorphous tungsten are presented in the given paper. The researches have confirmed the presence of the amorphous phase of metal in samples. The average size of the grain of developed nanosize metal is within the limits of 2-20 nm. Using transmission electron microscope the amorphous halo was being observed in all samples, irrespective of grain size, at the diffraction of electrons. It is shown that diffractional halos correspond exactly to metallic phase itself, but not to the oxides in possible core-shell structure. At the same time it is shown that there are marked concentration of nanocrystalline metals and their oxides in investigated powders. The methods are shown on increase of the purity of synthesized truly amorphous nanosize metals (not alloys).

Z5.37

Abstract Withdrawn

Z5.38

Crossover in Growth Exponent upon Nanocrystallization of Amorphous FeZr Thin Films. Mukul Gupta, Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institute, Villigen, Switzerland.

Thin films of $Fe_{75}Zr_{25}$ alloy were deposited by cosputtering of Fe and Zr targets using magnetron sputtering technique in the thickness range of 7-85 nm. It was found that at a critical thickness of about 40 nm, nanocrystallization of initially deposited amorphous phase takes place. A crossover occurs in the growth exponent β upon nanocrystallization giving a direct evidence for different growth behavior for amorphous and nanocrystalline phases. In case of amorphous film self-shadowing and energy minimization occurs and since the structure is spatially isotropic, the value of growth exponents remain small. On the other hand for nano grain structure, the spatial anisotropy may impose additional shadowing giving rise to an increased value of growth exponents as observed in this work. A mechanism leading to influence of microstructure on topology of the film is discussed.

Z5.39

A Microgravity Investigation of the Solidification Behavior of $Zr_{52.5}$ $Cu_{17.9}Ni_{14.6}$ $Al_{10}Ti_5$ (Vit-105). James J Wall[1], Won-Kyu Rhim[2], John Li[2], Peter K Liaw[1], Chain T Liu[3,1], Hahn Choo[1,4] and William L Johnson[2]; [1]Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee; [2]Division of Engineering and Applied Science, California Insitiute of Technology, Pasadena, California; [3]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [4]Diffraction and Thermophysical Proporties Group, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Using high-vacuum electrostatic levitation, specimens of a $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ glass forming alloy (Vit-105) with high (3000 ppm) and low (690 ppm) oxygen concentrations were processed in a containerless environment. Free cooling of the specimens from the liquid state resulted in recalescence in the supercooled liquid region for both oxygen levels, with larger undercoolings possible in the high-purity specimens. The thermal history of the high-purity specimens in both the liquid and supercooled liquid states was found to strongly affect their crystallization behavior. The low-oxygen specimens were found to exhibit a relatively small, negative volume change ($V_{crytalline} < V_{liquid}$) during the recalescence when held at, then free cooled from above the threshold temperature, T_T, the temperature required to decompose impurity-oxide particles in the molten alloy specimen. Holding the molten specimens at an incubation temperature (variable, below the threshold temperature), then free cooling, was found to increase the magnitude of the negative volume change during recalescence. Rapid heating of the specimens to near T_T and subsequently free cooling with no hold period was found to induce an anomalous crystallization behavior. This recalescence resulted in the formation of different phases, as seen by ex-situ neutron-diffraction experiments, with a different exothermic heat signature as compared to specimens held at temperature and then free cooled. Furthermore, this anomalous recalescence resulted in an increase in specimen volume during solidification ($V_{crytalline} > V_{liquid}$). This work has benefited from the use of the Intense Pulsed Neutron Source (IPNS), Argonne National Laboratory, Argonne, IL, which is funded by the U.S. Department of Energy (DOE). This work is supported by the NSF International Materials Institutes (IMI) Program DMR-0231320 with Dr. Carmen Huber as the Program Director. Further support was by the Division of Materials Sciences and Engineering, US DOE , under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

Z5.40
A Novel Submicron/Nanograined Stainless Steel with Superior Mechanical Properties. Shreyas Rajasekhara[1], Paulo J. Ferreira[1], Mahesh Somani[2], Leo Pentti Karjalainen[2], Koljonen‘ Mikko[2] and Antero Kyrolainen[3]; [1]Materials Science and Engineering, The University of Texas at Austin, Austin, Texas; [2]Department of Mechanical Engineering, University of Oulu, Oulu, Finland; [3]Outokumpu Stainless Oy, Tornio, Finland.

Metastable austenitic stainless steels transform into martensite on being subjected to cold rolling. Upon subsequent annealing, the martensite reverts into ultra-fine grained austenite. With this concept in mind, we produced nano/submicron austenitic grains in commercially available AISI 301LN stainless steel. AISI 301LN was first cold-reduced to 63% to obtain an approximately 90% conversion from austenite to martensite. Various specimens were then subjected to annealing treatments of 600°C, 700°C and 800°C for 1, 10 and 100 seconds. X-ray diffraction (XRD) analysis of samples annealed at 600°C indicates a partial martensite reversion to austenite for all annealing times. However, for samples annealed at 700°C a more efficient reversion is obtained, while at 800°C, practically all the martensite has reverted to austenite. These XRD results are confirmed by transmission electron microscopy (TEM) studies. TEM observations show that equiaxed austenitic grains as small as $\sim$ 200 nm can be obtained in samples annealed at 700-800°C. Tensile tests carried out on the aforementioned specimens indicate that samples annealed at 750°C for 1 and 10 seconds have a yield strength of about 900 MPa and a elongation of $\sim$ 35%. This is a substantial improvement in the mechanical properties when compared to both conventional fully annealed AISI 301LN stainless steels, which typically exhibit a yield strength of 240 MPa and a ductility of $\sim$ 60%; and cold-rolled AISI 301LN stainless steels, which possess an yield strength of 900 MPa and a ductility of 20%. The combination of nano/submicron grained austenite and tempered martensite is responsible for greatly enhancing the mechanical properties observed in these materials.

Z5.41
Synthesis and Properties of Nanocrystalline BCC Iron-Based Alloys. Jason R. Trelewicz and Christopher A. Schuh; Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Among the various techniques for synthesizing nanocrystalline metals and alloys, great progress has been made in aqueous electrodeposition. While this approach has been widely applied to the fabrication of alloys with FCC crystal structures, electrodeposition of nanocrystalline BCC metals has been considerably more limited. In this work, we describe recent progress in the electrodeposition of nanocrystalline iron alloys containing secondary transition metal components in solid solution. Through the manipulation of deposition conditions, the system composition can be altered and the structure tailored from the amorphous state up through the nanocrystalline regime, in specimens without porosity or other significant processing artifacts. Preliminary mechanical test data for these BCC nanocrystalline alloys are also compared and contrasted with the existing literature for FCC alloys produced by similar means.

Z5.42
Molecular Dynamics Study of the Effect of Dopant Atoms on Grain Boundary Sliding. Paul Christopher Millett[1] and R. Panneer Selvam[1]; [1]Civil Engineering, University of Arkansas, Fayetteville, Arkansas; [2]Mechanical Engineering, University of Arkansas, Fayetteville, Arkansas.

Nanocrystalline materials (NCMs) exhibit numerous attractive properties including increased mechanical strength, electrical resistivity, and magnetic permeability when compared with their coarse-grained counterparts. These properties are now known to be directly attributed to the high density of grain boundary regions, resulting in a significantly high fraction of miscoordinated atoms. The disparity in the observed macroscopic behavior of NCMs indicates that the fundamental processes involved at the microstructural level are unique as well. In regards to plastic deformation, NCMs have been shown to exhibit large increases in strength levels (which level off and slightly fade with $d < 30$ nm) accompanied by disappointingly low ductility values. Due in large part to computational studies, with support from experiment, it is now understood that the majority of deformation in these ultra-small grains is realized by grain boundary sliding and migration rather than unit dislocation glide throughout the crystalline regions. If the resistance of the grain boundaries to sliding can be either increased or decreased, it follows that the macroscopic tensile properties will as well be altered. This provides an opportunity to engineer these materials in order to optimize their strength and ductility. For instance, if grain boundary sliding can be increased, perhaps the ductility of the material will improve. Likewise, if grain boundary sliding can be decreased, the inverse Hall-Petch effect may be overcome. In this paper, molecular dynamics simulations are used to study grain boundary sliding in pure and doped Cu bicrystals using both Lennard-Jones and Embedded-Atom Method potentials. Two tilt [100] grain boundaries are considered: the coincident site lattice 5 interface and a random high angle interface. Shear stress between 0.69 GPa and 1.61 GPa was applied to the bicrystals for a duration of 10 ps at ambient temperature (300K) and high temperature (800K). For the pure bicrystals, the sliding of the 5 interface with respect to the random interface was lower at 800K and higher at 300K. For the doped bicrystals, interstitial dopant atoms and substitutional dopant atoms with larger atomic radius were effective in retarding grain boundary sliding. These simulations will aid further work to determine how segregated dopant atoms alter the tensile properties of nanocrystalline metals.

Z5.43
Three Dimension Characterization of Electrodeposited Samples. Alice Bastos da Silva, Stefan Zaefferer and Dierk Raabe; Microstructure Physics and Metal Forming, Max Planck Institute fuer Eisenforschung, Duesseldorf, Germany.

A detailed studied of the microstructure of electrodeposited samples is of great interest for understanding and developing nanostructured metals. Electrodeposited samples were investigated in planar and cross sections using orientation microscopy in a high resolution scanning electron microscope. The local crystallographic texture, grain size, amount of phases, and grain boundary character were characterized by Electron Backscatter Diffraction (EBSD). The combination of the microstructure observations on the e planar surface close to the substrate, on the growing surface and on the cross section allows a three dimension understanding of the deposit growth and the study of development of local texture and microstructure depending on the deposit thickness. Additionally a combination of well-controlled material removal by sputtering with a focused ion beam and subsequent analysis of the sputtered surfaces by orientation microscopy (EBSD) was carried on the samples to obtain detailed information on the bimodal grain structure that was observed on both planar and cross section microstructure of the deposit.

SESSION Z6: Deformation and Fracture of
Nanostructured Metals II
Tuesday Morning, November 29, 2005
Constitution A (Sheraton)

8:15 AM Z6.1
Grain Growth in Nanocrystalline Cu under Compressive Stress. Julia R. Weertman and Kai Zhang; Materials Science and Engineering, Northwestern University, Evanston, Illinois.

Extensive and prolonged indenter creep has been observed in high purity nanocrystalline Cu in microhardness tests as the result of rapid grain growth. New results will be reported on the influence of compressive stresses on grain growth, including the effects of grain size distribution and temperature. Research is sponsored by US DoE grant DE-FG02-02ER46002.

8:30 AM *Z6.2
Interplay between Plastic Deformation and Grain growth in Nanocrystalline Materials by Molecular-Dynamics Simulation. Dieter Wolf, Argonne Natl Lab, Argonne, Illinois.

We describe recent atomic-level simulations of the plastic-deformation and grain-growth behavior of nanocrystalline materials. These simulations have now become large and sophisticated enough where they begin to provide novel, materials-physics based insights into the intricate interplay between dislocation and grain-boundary processes controlling the thermo-mechanical behavior of these materials. In particular, such simulations now capture, with atomic-level resolution, the entire range of grain sizes in which the experimentally suggested transition from a dislocation-based deformation mechanism to one involving grain-boundary processes takes place as the grain size approaches dimensions of the order of tens of nanometers. By investigating the intricate coupling between grain growth and grain-boundary diffusion creep, these simulations also provide insight into the processes that control the high-temperature stability of these materials. Work supported by the U.S. Department of Energy, Basic Energy Sciences-Materials Sciences, under Contract W-3l-l09-Eng-38.

9:00 AM Z6.3

Influence of Room Temperature Stress-Assisted Grain Growth on the Mechanical Behavior of Nanocrystalline Al Thin Films. Daniel S. Gianola[1], Xuemei M. Cheng[2], Helena Van Swygenhoven[3], Chia-Ling Chien[2] and Kevin J. Hemker[1]; [1]Department of Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland; [2]Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland; [3]Paul Scherrer Institute, Villigen, CH-5232, Switzerland.

Recent evidence has been put forth to emphasize the importance of microstructural evolution during the deformation of fully dense nanocrystalline materials. Coupling of the applied stress to low and high angle grain boundaries has been shown to allow grain boundaries in nanocrystalline Al to break free of their original metastably pinned state during loading at room temperature, but the effect that this phenomenon has on the overall mechanical response is still being elucidated. To investigate these unique deformation mechanisms, submicron free-standing aluminum thin films with thicknesses of 80-380 nm and average grain sizes of 40-100 nm were fabricated using DC magnetron sputtering. Surface and bulk micromachining techniques were used to fabricate micro-tensile test structures that alleviate the challenges usually associated with the direct mechanical testing of submicron free-standing thin films. The gage section of the resultant film spans across a frame of (001) Si with an etched backside window and support strips on the periphery. Results obtained from these films demonstrate unique mechanical behavior, where discontinuous grain growth results in a fundamental change in the way in which the material deforms. In contrast to the low tensile ductility generally associated with nanocrystalline metals, these nanocrystalline films demonstrate extended tensile ductility. In situ X-ray diffraction and post mortem transmission electron microscopy point to the importance of stress-assisted room temperature grain growth in transforming the underlying processes that govern the mechanical response of the films; nanoscale deformation mechanisms give way to microscale plasticity. The starting microstructure and film thickness have been found to determine the extent of grain growth, and reactive sputtering with controlled amounts of oxygen is being employed to investigate the role of grain boundary pinning during deformation. The efficacy of these pinning processes and the effect of applied strain rate will also be discussed.

9:15 AM Z6.4

Deformation Behavior of Polycrystalline Ni Nanowires by Computer Simulation. Diana Farkas and Joshua Monk; Materials Science, Virginia Tech, Blacksburg, Virginia.

The deformation response to tensile loading was studied for digital polycrystalline Ni nanowires. The studies were performed using empirical embedded atom potentials and random grain orientations. The average grain size of the samples is 12 nm, and wire diameters of 10 to 16 nm were investigated. The simulations were performed at various strain rates and room temperature conditions. Significant grain boundary activity was observed as a deformation mechanism, resulting in ductile behavior of the wires. In particular grain boundary motion was found to be a main mechanism of accommodating the plastic deformation in the wires. The grain boundary motion observed was seen to be mainly driven by the stress and only weakly dependent on the strain rate. The development of necking and final failure was found to be controlled by the grain boundaries.

9:30 AM Z6.5

Grain Boundary Structure Evolution in Nanocrystalline Al by Nanoindentation Simulations. Virginie Dupont and Frederic Sansoz; Dept. of Mechanical Engineering, University of Vermont, Burlington, Vermont.

It has been demonstrated recently that grain boundary (GB) structure has a profound impact on the deformation of nanocrystalline metals. For example, Sansoz and Molinari [1] have predicted by atomistic simulations that the GB behavior of sliding and migration, which are key deformation mechanisms at small grain size, can be controlled by tailoring the GB structural units. Moreover, new evidence of grain growth via GB movement mechanisms has been found in nanocrystalline Al via in-situ TEM nanoindentation [2]. This atypical GB structure evolution however is not fully understood at present time. The objective of the current study is to examine the evolution of different nanocrystalline GB networks in Al deformed by nanoindentation. Molecular statics and dynamics were used to simulate a 15nm-radius single crystal cylinder indenting nanocrystalline Al surfaces with grain sizes less than 12 nm. The GB networks were made of vicinal and randomly-oriented <110> tilt GBs and the simulations were performed at 0K and 300K. The findings of this investigation can be drawn as follows: (1) friction and adhesion at the tip/surface interface have a strong influence on the grain boundary structure evolution; (2) GB movement and deformation twins are found to be the predominant deformation modes at small grain size. References: 1. F. Sansoz and J.F. Molinari: Mechanical Behavior of Sigma Tilt Grain Boundaries in Nanoscale Cu and Al: a Quasicontinuum Study, Acta Materialia, 53, 7, 1931-1944 (2005). 2. M. Jin, M, A.M. Minor, E.A. Stach, and J.W. Morris: Direct observation of deformation-induced grain growth during the nanoindentation of ultrafine-grained Al at room temperature, Acta Materialia, 52, 18, 5381-5387 (2004)

SESSION Z7: Deformation and Fracture of Amorphous Metals II

Tuesday Morning, November 29, 2005
Constitution A (Sheraton)

10:15 AM Z7.1

A Model for Liquid Rheology based on Shear Softening. Marios Demetri Demetriou[1], Mary-Laura Lind[1], Gang Duan[1], Konrad Samwer[2] and William L. Johnson[1]; [1]Materials Science, California Institute of Technology, Pasadena, California; [2]I. Physikalisches Institut, Universitaet Goettingen, Goettingen, Germany.

A cooperative shear model was recently developed to explain the universal yielding behavior of metallic glasses. The model is inspired by the Frenkel analysis of the shear strength of solids and is based on the concept of inherent states and potential energy landscapes. In the model, yielding is taken to occur by the cooperative shear motion of large atomic clusters of randomly varying shear modulus, referred to as shear transformation zones. This interpretation points to a new universal viscosity law for liquids based on shear softening, rather than free volume creation, as had been presumed over the last two decades. In this law, the state variable for flow is identified to be the shear modulus, which contrary to free volume, it constitutes a physical and quantifiable material property that can be assessed experimentally. In fact, sound velocity measurements on amorphous Zr46.75Ti8.25Cu7.5Ni10Be27.5 samples that were vitrified from either an equilibrated or deformed supercooled liquid state produce shear modulus data that can be directly converted to the corresponding experimental viscosity data over a range of temperatures and shear rates. The viscosity law produces a broad fit to Newtonian viscosity data over the entire liquid region, and appears to tie in better than the two most prominent free-volume viscosity models: the Vogel-Fulcher and Cohen-Grest models. Moreover, a constitutive flow law that assumes the shear modulus as the structural order parameter succeeds in capturing non-Newtonian viscosity data as well, and produces a fit that is comparable to previously established constitutive laws based on free volume.

10:30 AM *Z7.2

Homogeneous Flow of Bulk ZrTiAlCuNi Glasses. Pierre Guyot[1], Marc Bletry[1] and Jean-Jacques Blandin[2]; [1]LTPCM, Institut National Polytechnique, Grenoble, France; [2]GPM2, Institut National Polytechnique, Grenoble, France.

The homogeneous deformation of a bulk Zr52.5Al10Cu22Ti2.5Ni13 glass is investigated in the glass transition temperature range, using constant strain-rate compression tests, strain-rate jumps and stress relaxation mechanical tests. The results are analyzed and discussed in terms of a free volume model, where the plastic deformation results from the stress assisted diffusional motion of density fluctuations or flow defects. A mechanical strain-rate constitutive equation of the Spaepen type, in which the internal variable is the flow defect concentration, is coupled with a kinetic evolution of the flow defect density. This flow defect density variation rate is controlled by two opposite atomistic processes: a plastic strain-driven creation term and a recovery by defect mutual annihilation. The numerical resolution of these two coupled differential equations allows describing the different regimes of deformation observed: i) steady-state flow where the flow defects concentration is dynamically kept constant, and from which a scaling law of the glass viscosity versus temperature and strain-rate results. ii) transient deformation regimes as for instance for the formation of stress over/undershoots on the stress-strain curves at large strain rates and low temperatures, or during stress relaxation experiments. The values measured for the activation energy and volume of the strongly thermally activated plastic deformation, as well as the physical parameters involved in the free volume characteristics, are discussed. At last a partial crystallization of the glass has been observed during the mechanical tests. Such a crystallization produces a noticeable hardening which is explained in terms of a back stress effect originating in the undeformability of the formed crystallites.

11:00 AM *Z7.3

Mechanical behavior of bulk metallic glasses. L. Anand, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

In recent years, certain amorphous metallic alloys which can be solidified in relatively large section sizes under moderate cooling rates have been developed. Such disordered metals are referred to as bulk metallic glasses. When a metallic glass is deformed at ambient temperatures, well below its glass transition temperature, its inelastic deformation is characterized by strain-softening which results in the formation of intense localized shear bands; fracture typically occurs after very small inelastic strain in tension, but substantial inelastic strain levels can be achieved under states of confined compression, such as in indentation experiments. The micro-mechanisms of inelastic deformation in bulk metallic glasses are not related to dislocation-based mechanisms that characterize the plastic deformation of crystalline metals. The plastic deformation of amorphous metallic glasses is fundamentally different from that in crystalline solids because of the lack of long-range order in the atomic structure of these materials. Computer simulations in the literature show that at a micromechanical level, inelastic deformation in metallic glasses occurs by local shearing of clusters of atoms (_ 30 to 50 atoms), this shearing is accompanied by inelastic dilatation that produces strain-softening, which then leads to the formation of shear bands. An important consequence of the micro-mechanism of inelastic deformation in amorphous metals is that at the macroscopic level, experimentally-determined yield criteria for inelastic deformation are found not to obey the classical pressure-insensitive forms, but show a significant pressure sensitivity of plastic flow, which may be approximated by the Coulomb-Mohr yield criterion. In this talk I will present a complete three-dimensional constitutive model for the elastic-viscoplastic response of pressure-sensitive and plastically-dilatant isotropic materials. The flow-rule in this model is a generalization of a two-dimensional (plane-strain) “double-shearing” constitutive model (used in soil mechanics) to three-dimensions. The constitutive model has been implemented in a finite element program, and the numerical capability is used to study the deformation response of amorphous metallic glasses. Specifically, the response of an amorphous metallic glass in tension, compression, strip-bending, and indentation is studied, and it is shown that results from the numerical simulations qualitatively capture major features of corresponding results from physical experiments available in the literature.

11:30 AM Z7.4

Non-Newtonian flow in Zr-Ti-Cu-Ni-Be bulk metallic glass forming alloys above the liquidus temperature. Ralf Busch, Tyler Shaw and Christopher Way; Mechanical Engineering, Oregon State University, Corvallis, Oregon.

In this study the viscosity of Zr41.2Ti13.8Cu10.0Ni12.5Be22.5 as a function of temperature and shear rate has been measured above the liquidus temperature, Tliq = 1026 K, using a high temperature Couette Rheometer. It has been discovered that there exists a pronounced decrease in viscosity with increasing shear rate. This is contrary to the general belief that metallic systems above the liquidus temperature should show Newtonian behavior. It has also been discovered that this shear rate dependence of the viscosity gets less pronounced with increasing temperature and approaches the Newtonian behavior and viscosities of simple monatomic and binary alloys at approximately 1325 K. These results will be discussed in terms of configurational entropy, Sc, by using the Adam-Gibbs entropy model for viscous flow, ? = ?o exp(C/T Sc) [1]. The enthalpic energy barrier for cooperative atomic rearrangement, C, for an estimated zero shear is determined by fitting the Adam-Gibbs entropy model to a viscosity study with a shear rate of 10-5 Pa s [2]. In this fit the functional form of the entropy is obtained by integrating the specific heat difference between the crystal and liquid of this alloy [3]. The entropy model is then used to convert viscosity and temperature data at different shear rates directly into configurational entropy. It can be shown from this analysis that above the liquidus temperature a large amount of order still exists. At high shear rates this order is destroyed causing the configurational entropy to increase by a magnitude that is on the order of the entropy of fusion. References [1] G. Adam, J.H. Gibbs, J. Chem. Phys. Vol 43 (1965), p. 139 [2] T.A. Waniuk, R. Busch, A. Masuhr and W.L. Johnson, Acta Mater. Vol. 46 (1998), p. 5229 [3] R. Busch, Y.J. Kim, and W.L. Johnson, J. Appl. Phys. Vol 77 (1995), p. 4039

11:45 AM Z7.5

High-Energy X-Ray Measurements of Anisotropic Free Volume Creation in Metallic Glasses During Homogeneous Deformation. Ryan T. Ott[1], Matthew J. Kramer[1,2], Matthew F. Besser[1], S. Bulent Biner[1,2,3] and Daniel J. Sordelet[1,2]; [1]Materials Engineering Physics, Ames Laboratory, Ames, Iowa; [2]Materials Science and Engineering, Iowa State University, Ames, Iowa; [3]Aerospace and Engineering Mechanics, Iowa State University, Ames, Iowa.

Inhomogeneous flow in metallic glasses is accompanied by a deformation-induced disordering of the atomic structure, which is characterized by localized shear-induced dilation. For higher temperatures and lower applied stresses, the deformation mode is homogeneous. Previous work on metallic glasses deformed in the homogenous flow region has confirmed the presence of strain-induced structural disordering through the observation of a drop in the flow stress for constant strain rate experiments and accelerating strain rates for constant stress experiments. Here we report the use of high-energy X-ray scattering to examine strain-induced structural disordering in a Zr-based metallic glass that has been homogenously deformed under isothermal creep conditions. The dependence of the excess free volume on the macroscopic plastic strain in the creep samples is emphasized together with the dependence of the free volume on the stress state. For simple uniaxial tensile loading, we find that the free volume distribution is anisotropic. The free volume parallel to the loading axis increases with increasing macroscopic strain, while the free volume in the direction normal to the loading axis remains essentially constant. Moreover, the X-ray scattering results are compared to DSC data to discuss the effects of homogeneous deformation on the atomic structure.

SESSION Z8: Deformation and Processing of Nanostructured Metals

Tuesday Afternoon, November 29, 2005
Constitution A (Sheraton)

1:30 PM Z8.1

Fabrication of Bulk Nanostructured Zr Alloys by Severe Rolling. Francis Salort[1], Michael Kassner[2], Oscar Ruano[1] and Teresa Perez-Prado[1]; [1]Physical Metallurgy, CENIM, CSIC, Madrid, Spain; [2]Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, California.

Zr and Zr alloys are envisioned as potential biomaterials due to their excellent biocompatibility. Their application for the fabrication of implants require that, additionally, these metals have improved mechanical properties, such as good fatigue resistance and good room temperature strength, that can compete with those of titanium. An alternative way to enhance the mechanical behavior of Zr alloys is to develop cost-effective processing routes leading to the build up of nanostructures. This work focuses on the fabrication of bulk Zr nanomaterials by the application of severe plastic deformation through rolling. Processing was carried out at three different temperatures, -175°C, 25°C, and 300°C. The evolution of the microstructure with increasing rolling reductions is investigated by texture analysis and transmission electron microscopy (TEM). Rolling at high thickness reductions results in the development of heterogeneous nanostructures, formed by dislocation tangles, cell and subgrain boundaries, and high angle boundaries. Increasing rolling temperature contributes to accelerate dynamic recovery, leading to better defined boundaries together with a slight increase in the overall size of the structural features. The thermal stability of the rolled samples at different temperatures is investigated.

1:45 PM *Z8.2

Experimental Observations on the Deformation and Fracture of Nanocrystalline and Ultrafine-grained Nickel and Copper. Sharvan Kumar[1] and Subra Suresh[2]; [1]Division of Engineering, Brown University, Providence, Rhode Island; [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

A combination of experiments and computations have been used in recent years to understand flow and fracture of nanocrystalline (and ultrafine-grained) metals, in particular Ni and Cu. Experiments have focused on measuring monotonic and cyclic properties and deducing underlying mechanisms based on the response, as well as direct observations of deformation modes (in-situ TEM) such as dislocation-mediated plasticity, twinning, grain boundary sliding and diffusional processes. While the mechanisms governing the early stages of deformation in these materials are reasonably well-documented, the process of damage evolution that eventually leads to fracture is not understood. Fracture surface observations have consistently illustrated that at least in monotonic loading, dimpled rupture dominates with dimples on a scale that is an order of magnitude larger than the grain size; more recent results however confirm that this is not the case in cyclic loading. In addition, cyclic hardening and frequency dependence of life have been noted and remain to be explained. These results, along with structural size dependence of ductility and damage tolerance, as they pertain to nanocrystalline Ni and Cu will be discussed and unresolved issues will be highlighted.

2:15 PM Z8.3
Densification of Monosdisperse Iron Nanoparticles from a Colloidal Dispersion at Moderate Heating Rates and Temperatures. Nathan B Crane[1], Emanuel Sachs[1] and Samuel M. Allen[2]; [1]Mechanical Engineering, Massahusetts Institute of Technology, Cambridge, Massachusetts; [2]Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

The reduced melting and sintering temperatures or nanoparticles have been used to deposit metals at reduced temperatures, particularly for electronic applications by printing suspension of nanometer particles. The particles are typically solidified by rapid heating, but in most cases, the material properties such as electrical conductivity are inferior to bulk material. Alternatively, sintering the nanoparticles at slower rates may maintain or improve the material properties and can be more easily implemented, particularly on nonplanar substrates. We report on tests of iron particle consolidation by drying and sintering. These particles and the structures formed from them are useful for magnetic and structural applications. The same process may be applied to other material for electronic applications. The particles and their evolution during sintering is examined by TEM imaging, gas adsorption pore size measurement, and X-ray diffraction. The nanoparticles are shown to form both superlattice and glassy structures on drying. Large changes in drying rate had a modest impact on the pore structure when using a high temperature (286 C) solvent. However, fast drying at a lower temperature creates large pores that lead to pore coarsening during sintering. When heated, the nanoparticle structures densify by sintering reaching densities above 80% after heating to 700 C. Residual carbon from the coating ligands retards densification. The residual carbon can be reduced by oxidation of the particles to increase the sintering rate.

SESSION Z9: Processing of Amorphous Metals I
Tuesday Afternoon, November 29, 2005
Constitution A (Sheraton)

3:30 PM *Z9.1
Amorphous Steel, Light Metals, and Composites. S. Joseph Poon[1], Gary J. Shiflet[2] and Faqiang Guo[1]; [1]Physics, University of Virginia, Charlottesville, Virginia; [2]Materials Science & Engineering, University of Virginia, Charlottesville, Virginia.

In recent years, amorphous steels and several amorphous light metals have been obtained as non-magnetic structural materials. They exhibit some outstanding physical properties, including high specific strength, high elastic moduli, good corrosion resistance and various degrees of ductility, as well as having a relatively low cost. In this talk, we will discuss current studies of these structural amorphous metals and their composites with a focus on the synthesis, properties, and basic knowledge. Research sponsored by DARPA/ONR.

4:00 PM *Z9.2
Amorphous Metallic Foams. David C. Dunand and Alan H. Brothers; Northwestern University, Evanston, Illinois.

Only recently have foamed (or high-porosity) amorphous alloys been created. Various processing options will first be presented, with emphasis on retaining a glassy structure. Microstructure and architecture of existing amorphous foams will then be reviewed, in particular the connectivity of the porosity (open vs. close cells). Third, the recent discovery that extensive compressive ductilities (>80%) are being displayed in amorphous metal foams will be discussed in the light of two possible mechanisms: (i) shear band arrest in closed-porosity architectures and (ii) strut bending in cellular/reticulated architectures. Finally, recent results on mechanical properties of amorphous Zr-based Vit106 foams will be presented and discussed, in particular damage accumulation evaluated through acoustic emission, stiffness measurements and microscopy.

4:30 PM *Z9.3
Glass Formation in Eutectic Systems: Where are the Best Glass Formers? Z. P. Lu[1], D. Ma[2], C. T. Liu[3] and Y. A. Chang[2]; [1]Metals and Ceramic Division, Oak Ridge National Lab, Oak Ridge, Tennessee; [2]Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee; [3]Materials Science and Engineering, University of Wisconsi-Madison, Madison, Wisconsin.

Two long-standing problems of metallic glasses, i.e., where are the best compositions for glass formation and glass-matrix composites and what determines the glass-forming composition range in a given alloy system, have challenged materials scientists ever since the first metallic glass produced from the undercooled liquid was reported. A number of theories have been proposed; however, a universal understanding on these scientific issues with considerations of nucleation and crystal growth effects is still not fully realized. In this talk, we will present a unique approach to solving these two mysteries based on the competitive formation between the amorphous phase and its competing crystalline phases. As a result, a microstructure/phase selection diagram as a function of cooling rate in both regular and irregular eutectic systems has been constructed, which can be utilized as design guidelines/principles for exploring new metallic glasses. Experimental data from various alloy systems have validated our conceptual approach and model analysis. In addition, our analysis suggests that the use of the classical crystallization theory alone to rationalize and predict glass formation from undercooled liquids is insufficient and the composition effect on crystallization has to be taken into account. This research was sponsored partly (Lu and Liu) by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, US Department of Energy under contract DE-AC05-00OR-22725 with UT-Battelle, LLC. Ma and Chang, gratefully acknowledge financial support for this work from the Defence Advanced Research Projects Agency (DARPA), under ARO Contract No. DAAD 19-01-1-525, and with Dr. Leo Christodoulou as Program Manager.

SESSION Z10: Deformation and Fracture of Nanostructured Metals III
Wednesday Morning, November 30, 2005
Constitution A (Sheraton)

8:15 AM *Z10.1
Processing and Mechanical Properties of Artifact-Free Nanocrystalline Metals and Alloys. Carl C. Koch, Khaled M. Youssef, Ronald O. Scattergood and K. Linga Murty; Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina.

In the last several years processing methods have been refined which enable the synthesis of bulk nanocrystalline materials with grain sizes less than 50 nm and without artifacts. The availability of these materials has allowed for the measurement of presumably the inherent mechanical properties of several nanocrystalline metals and alloys. These results indicate that the consensus opinion regarding the low ductilities of fine grained nanocrystalline materials is no longer valid and that optimized high strength along with good ductility are possible. This talk will present results on the structure and mechanical properties of a variety of artifact-free nanocrystalline metals and alloys from the authors' laboratory and from the literature.

8:45 AM *Z10.2
Fracture of Face Centered Cubic (FCC) Nanostructured Metallic Materials. Fereshteh Ebrahimi, Materials Science and Engineering, University of Florida, Gainesville, Florida.

Conventional FCC metals fracture in a ductile manner by the microvoid coalescence mechanism. The absence of the "ductile-to-brittle" transition in these materials stems from their temperature insensitive yield strength, which causes dislocation generation and motion take place in preference to breaking atomic bonds at all temperatures. However, in nanostructured metals, the significant constraint on dislocation generation and motion allows the local stresses to be raised high enough for breaking atomic bonds, i.e. cleavage fracture. In this presentation the tensile properties and fracture of nanocrystalline as well as nanolayered metallic materials produced by electrodeposition is discussed. It is shown that in addition to the microstructural scale, i.e. grain size or layer width, the stress state and boundary structures contribute significantly to the fracture behavior.

9:15 AM Z10.3
Dynamic Instability in Inter-Granular Fracture in Aluminum. Vesselin I. Yamakov[1,2], Erik Saether[2], Dawn R. Phillips[3,2] and Edward H. Glaessgen[2]; [1]National Institute of Aerospace, Hampton, Virginia; [2]NASA Langley Research Center, Hampton, Virginia; [3]Lockheed Martin Space Operations, Hampton, Virginia.

The failure of nanocrystalline metals is dominated by failures within the dense network of grain boundaries in the microstructure. The properties of these grain boundaries dominate the fracture processes of the material. A molecular-dynamics model for inter-granular crack propagation under steady-state conditions is developed to study the strength of representative portions of the grain boundaries and determine the characteristics of the fracture processes including dynamic instabilities along a flat high-angle grain-boundary in aluminum that occur when the crack speed approaches 1/3 of the material's Rayleigh wave speed. Instead of crack branching, as is characteristic for a crack propagating in a homogeneous environment, the instability of an intergranular crack results in a periodic series of dislocation bursts. These bursts limit the crack speed, produce velocity oscillations and result in a large increase in energy dissipation compared to crack propagation occurring at a lower speed. Understanding the mechanism of inter-granular crack propagation at high velocity will help understanding the mechanism of failure in nanocrystalline metals at high loads and strain rates.

9:30 AM Z10.4

Deformation of Micron-Sized Amorphous and Nanocrystalline Metal Samples. Cynthia A. Volkert[1], Gerhard Wilde[1], Alex Donohue[2] and Frans Spaepen[2]; [1]Forschungszentrum Karlsruhe, Karlsruhe, Germany; [2]Harvard University, Cambridge, Massachusetts.

Both amorphous and nanocrystalline metals exhibit shear localization during deformation. In amorphous metals, shear band formation is attributed to the deformation-induced creation of free volume. In nanocrystalline metals, the underlying mechanisms for shear localization are less clear, but localization is associated with decreasing grain size and the absence of strain hardening. In this study, micron sized specimens of a-PdSi and nc-Ni (two samples with different average grain sizes) have been deformed under compression using a flat punch in a nanoindenter. The goal was to look for effects of sample dimensions on shear localization. The specimens were columns with diameters ranging form 0.3 to 8 μm that had been milled from the surface of an a-PdSi film on Si and nc-Ni foils using a focused Ga beam. The a-PdSi columns exhibit shear band formation at roughly 45° to the compression axis and a flow stress that decreases markedly with the column diameter, from 1.8GPa at 4 μm to 800 MPa at 0.5 μm. The clearest evidence of strain localization in the nc-Ni columns is their propensity for plastic buckling. When this is avoided, deformation appears homogeneous with no clear dependence on the column diameter. Reasons for these different modes of deformation will be discussed.

SESSION Z11: Deformation and Fracture of Amorphous Metals III

Wednesday Morning, November 30, 2005
Constitution A (Sheraton)

10:15 AM *Z11.1

Shear Band Nucleation and Propagation in Metallic Glasses. Michael Atzmon[1] and Wenhui Jiang[2]; [1]Depts. of NERS & MSE, University of Michigan, Ann Arbor, Michigan; [2]Department of MSE, The University of Tennessee, Knoxville, Tennessee.

At high strain rates and low temperature, deformation of metallic glasses is inhomogeneous – a result of an instability due to softening by shear. Such an instability is believed to be initiated at "weakened bands" [1,2] present in the material, due to fluctuations in the free volume. Shear bands formed by prior plastic deformation have been known to be likely sites for further deformation. Using nanoindentation, we have observed that prior cold-rolling of an Al-rich metallic glass leads to softening, and the deformation mechanism during indentation is based on propagation of previously-created shear bands. While the creation of new shear bands by indentation leads to significant pileups and serrations when indenting as-quenched samples, these are nearly absent in the cold-rolled samples. Low-temperature annealing of cold-rolled samples leads to a recovery of pileup and serrated flow, and hardness values greater than for the as-quenched material. The observed behavior is consistent with free-volume creation by cold rolling, and its annihilation by low-temperature annealing. In this paper, the experimental results will be reviewed. The dependence of shear-band nucleation and propagation on strain rates will be discussed and compared with theoretical, atomistic, predictions. 1) A.S. Argon, Acta Metall.27, 47 (1979). 2) P.S. Steif, F. Spaepen, and J.W. Hutchinson. Acta Metall. 30, 447 (1982).

10:45 AM Z11.2

Statistical Analysis of the First Shear Band Event during Nanoindentation of Metallic Glass. Corinne E. Packard and Christopher A. Schuh; Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Nanoindentation methods have been widely used to study shear bands in metallic glasses, and until now, most work has focused on the collective effects of many shear bands. In the present work, the conditions required to initiate the earliest shear band are studied in a statistical framework. By performing nanoindentation experiments at ambient and elevated temperatures and analyzing the first plastic event in the load-depth curves, we have gathered statistical distributions for the stress state at yield in $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass. Building from a shear-assisted thermal activation model, the activation volume and energy have been assessed for the rate-limiting step of shear band formation under the indenter.

11:00 AM *Z11.3

Shear Band Evolution in Amorphous Alloys Beneath a Vickers Indentation. Hongwen Zhang[2], Xiaoning Jing[3], Ghatu Subhash[3], Laszlo Kecskes[1] and Robert Dowding[1]; [1]US Army Research Laboratory, Aberdeen Proving Ground, Maryland; [2]Materials Science and Engineering, Michigan Technological University, Houghton, Michigan; [3]Mechanical Engineering-Engineering Mechanics, Michigan Technological University, Houghton, Michigan.

Shear band formation has been known to be the dominant deformation mechanism at room temperature in bulk metallic glasses. However, many indentation studies have revealed only a few shear bands surrounding the indent on the top surface of the specimen. This small number of shear bands cannot account for the large plastic deformation beneath the indentations. Therefore, a bonded interface technique has been used to observe slip-steps due to shear bands evolution. Vickers indentations were performed along the interface at increasing loads. At small indentation loads, the plastic deformation was primarily accommodated by semi-circular primary shear bands surrounding the indentation. At higher loads, secondary and tertiary shear bands were formed inside this plastic zone. A modified expanding cavity model was used to predict the plastic zone size characterized by the shear bands and to identify the stress components responsible for the evolution of various types of shear bands.

11:30 AM Z11.4

Shear-band formation and mechanical softening of different bulk metallic glasses during nanoindentation. Amadeu Concustell[1], Jordi Sort[1], German Alcala[2], Sonia Mato[2], Annet Gebert[2], Juergen Eckert[3] and Maria Dolors Baro[1]; [1]Dept. Physics, UAB, Bellaterra, Spain; [2]IFW Dresden, Institute of Metallic Materials, P.O. Box 27 00 16, D-01171, Dresden, Germany; [3]Physical Metallurgy Division, Department of Materials and Geo-Sciences, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany.

Nanoindentation tests on Pd-, Zr- and Cu-based bulk metallic glasses were performed over a wide range of indentation rates (from 0.04 up to 6.4 mN s-1) under the standard load control mode. The dependence of the pop-in formation on the loading rate is investigated and variations in hardness and reduced elastic modulus as a function of the indentation rate are observed. Furthermore, indentations in a displacement control mode were also performed and different displacement rates were applied to investigate the shear band formation (from 2.5 up to 20 nm s-1). The displacement control mode was used to minimize the shear localization of the free volume, although the formation of individual shear bands could still be observed. However, in the displacement control mode, the shear band formation depends on the composition of the bulk metallic glass. While for the Pd-based alloy pop-ins are easily formed and jumps of 1 to 4 nm are observed, in the Zr- and Cu-based alloys the pop-ins do not exceed 1 nm. Interestingly, a softening effect occurs in all the alloys in both control modes which is more pronounced for higher loading rates. This is explained by the differences in plastic deformation at different indentation rates. The obtained results confirm that plastic flow in bulk metallic glasses is governed by the rate of creation of free volume, which depends on the strain rate and its localization into shear bands.

11:45 AM Z11.5

Nanoindentation Study of Deformation In Sputter Deposited Cu-Nb Alloy Thin Films. Suman Vadlakonda[1], Rajarshi Banerjee[1,2], Arda Genc[2], Dan Huber[2] and Reza Mirshams[1]; [1]Materials Science and Engineering, University of North Texas, Denton, Texas; [2]Materials Science and Engineering, The Ohio State University, Columbus, Ohio.

In recent years there has been considerable interest exploring the study of the early stages of deformation and incipient plasticity in both amorphous and crystalline materials via nanoindentation based techniques. Nanoindentation studies have been conducted on metastable Cu-Nb alloy thin films deposited by UHV magnetron sputtering. The Cu-Nb system is rather interesting since Cu and Nb are virtually immiscible in the solid state and therefore, can only be alloyed in a highly metastable form by vapor quenching techniques such as sputtering. Also, by changing the composition in this system it is possible to achieve both nanocrystalline as well as amorphous structures and consequently compare and contrast their respective deformation mechanisms during nanoindentation. The influence of the micro- and nano-structure, as well as the strain rate, on the deformation behavior of these metastable Cu-Nb alloy thin films will be discussed in this presentation.

SESSION Z12: Structural Evolution I
Wednesday Afternoon, November 30, 2005
Constitution A (Sheraton)

1:30 PM Z12.1
Experimental and Numerical Evaluation of Deformation Mechanisms in Bulk Metallic Glasses. Antonia Antoniou[1], Patrick Onck[2], Bulent Biner[1] and Ashraf Bastawros[1]; [1]Aerospace Engineering, Iowa State University, Ames, Iowa; [2]Applied Physics, University of Groningen, Groningen, Netherlands.

A novel experimental configuration is devised to monitor the onset and evolution of plastic deformation in metallic glasses on a microscopic scale. The experiment is comprised of a cylindrical indenter while monitoring the evolution of the associated plastic zone by a microscopic digital image correlation system. The plastic zone beneath the indenter is comprised of near orthogonal sets of shear band traces. The shear band spacing to thickness ratio is about 20. The shear band traces almost follow the α and β characteristic lines of the Prandtl slip line field for a cylindrical indenter. It is remarkable that the whole field evolved in an essentially self-similar way. The observed experimental trend has been examined by finite element simulation using Drucker Prager yield surface including softening to understand the underlying mechanisms of shear band nucleation and interactions.

1:45 PM *Z12.2
New Insight into the Chemical Mixing Forced by Plastic Deformation from a Convection Flow Analysis.
Pascal M. Bellon, Robert S. Averback, Pavel Krasnochtchekov, Younhong Li and Samson Odunuga; Materials Science and Engineering, University of Illinois, Urbana, Illinois.

Materials are commonly subjected to sustained plastic deformation while in service or in processing. Examples include fatigue, wear, rolling, extrusion, high-energy ball milling, and more recently friction stir welding. At low temperatures plastic deformation can cause interdiffusion of chemical species, which, in turn, can lead to the dissolution of precipitates and stabilization of supersaturated solutions. At intermediate temperature, such forced mixing can compete with dynamics driven by thermodynamic forces, and produce self-organized microstructures. Despite the wealth of information presently available on forced mixing, its characteristics are still not well understood, particularly for nanocrystalline and amorphous alloys, for which the mechanisms of plastic deformation remain unresolved. We present here a new method for analyzing chemical mixing forced by plastic deformation that offers new insight into the mixing process. The method, which is similar to one used to characterize turbulent flows, monitors the evolution of the separation distance between pairs of atoms, R. The temporal evolution of R can be described by an effective diffusion coefficient. As in the case of turbulent flows, the effective diffusion coefficient is predicted to increase with R, and to saturate when R reaches a characteristic value Rc. We show for solids that Rc corresponds to the length scale of the defects responsible for plastic deformation. In particular, in the case of crystalline systems deformed by dislocation glide, Rc represents the length of mobile segments. For nanocrystals, this might be the grain size. In the case of amorphous material, Rc provides a direct measure of the size of the structural units responsible for plastic deformation. Once the R-dependence of the effective diffusion coefficient is known, it can be utilized to calculate the time evolution of the mean square relative displacement of atoms and, for instance, the time required to dissolve precipitates. We will also show how the R-dependence of the effective diffusion coefficient can be used to predict when nanocomposites will form during forced mixing, and their length scales. Our predictions are tested by 3D molecular dynamic simulations of materials cyclically deformed in compression at low temperature. We calculate the effective diffusion coefficient for single crystalline, polycrystalline and amorphous alloy systems. Our approach, in particular, makes it possible to identify the defects responsible for plastic deformation without the need to visualize them. In the case of amorphous systems, the size of the sheared zones is determined to be about 0.8 nm. In the case of crystalline systems, the evolution of the length scale of the microstructure is tracked through the R-dependence of Deff.

2:15 PM Z12.3
The Effect of As-quenched Structure on Primary Phase Crystallization in Amorphous Aluminum Alloys.
Joseph Hamann and John H. Perepezko; Materials Science and Engineering, University of Wisconsin - Madison, Madison, Wisconsin.

From the reported experience, primary nanocrystallization in amorphous Al alloys involves transient kinetic behavior that is sensitive to the initial as-quenched structural arrangements. In order to examine the precursor effects, systematic studies outlining the evolving growth kinetics of primary aluminum nanocrystals during pre-crystallization annealing treatments, and investigations on the microstructure refining effect of specific alloying substitutions represent new approaches for an analysis of primary phase crystallization kinetics. In Al88Ni8Sm4 melt-spun ribbon (MSR), incremental substitutions of Cu for Ni (0 - 1at%) affect the thermal stability of the material (crystallization onset shifts to lower temperature) and refine the size of the primary phase nanocrystals. However, continuous heating calorimetry measurements indicate that the primary crystallization enthalpy is not significantly changed with Cu substitution. From a structural analysis standpoint, quantitative microstructure examinations applied in parallel with calorimetry measurements have been employed to characterize the as-quenched volume of MSR samples. The increased primary Al nanocrystal particle density with Cu substitution reflects the modification of local structural arrangements, necessitating an understanding of the local structure of the as-quenched sample in order to develop a description of primary phase nanocrystal growth kinetics. The support of the ARO (DAAD19-02-1-0245) is gratefully acknowledged.

SESSION Z13: Processing of Amorphous Metals II
Wednesday Afternoon, November 30, 2005
Constitution A (Sheraton)

3:30 PM Z13.1
Multiple Zones of Glass Formation in the Eutectic Zr-Cu-Al System. D. Wang, H. Tan and Yi Li; Department of Materials Science and Engineering, National University of Singapore, Singapore, Singapore.

We demonstrate that three best glass forming regions up to 8 mm in diameter, $Zr_{48}Cu_{45}Al_7$, $Zr_{45}Cu_{49}Al_6$ and, $Zr_{54}Cu_{38}Al_8$ and $Zr_{56}Cu_{36}Al_8$ in three adjacent Zr_2Cu-τ_3-ZrCu, ?τ_3-τ_5-ZrCu and ?τ_5-ZrCu-$Cu_{10}Zr_7$ eutectics in the ternary Zr-Cu-Al system can be obtained via a metallographic way. The narrow bulk-glass-forming range was found to require composition pinpointing to 1 at. % and a phase selection concept is developed to explain the success of our microstructure-based approach to pinpoint the best glass former in a given system. The significance of this method in discovering new BMGs is discussed.

3:45 PM *Z13.2
Possibility of Using Late Transition Metal-Based Bulk Glassy Alloys as Structural Materials. Akihisa Inoue, Wei Zhang, Baolong Shen and Kazutaka Fujita; Institute for Materials Research, Tohoku University, Sendai, Japan.

Since the first synthesis of Fe-based bulk glassy alloys as a kind of late transition metal (LTM) base systems in 1995, a number of LTM-based bulk glassy alloys have been developed in Fe-, Co-, Ni and Cu-based systems up to date because their alloys are expected to exhibit high mechanical strength, high corrosion resistance and good viscous flow deformability, in addition to good soft magnetic properties for Fe- and Co-based glassy alloys. The maximum diameter of the LTM-based bulk glassy alloys exhibiting high mechanical strength is about 7 mm for Fe-based alloys, 3 mm for Co-based alloys, 5 mm for Ni-based alloys and 7 mm for Cu-based alloys. The tensile fracture strength is about 2800 MPa for Ni-based alloys and 2100 MPa for Cu-based alloys, while the fracture strength under compressive deformation mode reaches as high as 4200 MPa for Fe-based alloys, 5600 MPa for Co-based alloys, 3100 MPa for Ni-based alloys and 2400 MPa for Cu-based alloys. In particular, the Co-based bulk glassy alloys also exhibit very high elevated temperature strength of about 2000 MPa at 873K. The fracture strength has a good linear relation with Young's modulus, glass transition temperature and liquidus temperature. In addition, the fatigue strength limit defined by the ratio of maximum applied stress amplitude to fracture strength after 107 cycles under tensile-compressive stress and rotating bending beam conditions was measured to be 0.24 for Cu-based alloys and 0.20 for Pd-based alloys, being higher than those (0.04-0.13) for various Zr-based bulk glassy alloys. These LTM-based bulk glassy alloys also exhibit rather good corrosion resistance in various chemical solutions and its resistance is the greatest for Ni-based alloys, followed by Co-based alloys, Fe-based alloys and then Cu-based alloys. The present good combination in various engineering properties allows us to expect that these LTM-based bulk glassy alloys are used as structural practical materials.

4:15 PM *Z13.3
Discovering Large Mg-based Metallic Glasses in Three-Dimensional Composition Space. Jian Xu, Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, Liaoning, China.

Liquid alloys of certain compositions can be cast directly into bulk metallic glasses (BMGs) with a critical size (D_c, in the smallest dimension) larger than 1 mm, raising tremendous expectations for exploiting the superior mechanical properties of amorphous metals and the processing advantages in the supercooled liquid state. Industrial production and widespread applications of BMGs, however, demand much larger sizes (e.g., Dc of the order of 20 mm) that so far only a handful of BMGs can reach. Those that do, unfortunately, are all Be-bearing and/or based on expensive metals (e.g., in Pd-, Pt-, Zr-, Y-based systems). Here we report the discovery of low-cost BMGs with D_c=16 to 25 mm based on the ordinary engineering metal Mg. We also use this example to illustrate a practical strategy to pinpoint the best BMG-forming compositions in multi-component composition space, a "mission impossible" using the existing criteria of glass forming ability. Our work not only offers a light-weight BMG that has been sought after for many years, but also has implications for locating commercially viable alloys in other multi-component systems. Using composition pinpointing, the best glass-forming alloys in the Mg-Cu-Y ternary system were found at off-eutectic compositions, $Mg_{58.5}Cu_{30.5}Y_{11}$. The critical size for BMG formation was more double than that of the previously discovered eutectic $Mg_{65}Cu_{25}Y_{10}$ alloy, leading to fully glassy rods of 9 mm in diameter upon copper mold casting. Based on this ternary system, we introduced Ag to partially substitute for Cu in the Mg-(Cu,Ag) -Y pseudo ternary system. A new strategy has been developed to guide the search in three-dimensional composition space to locate the best glass-forming compositions, and to systematically examine the effects of an alloying element. The largest diameter for glass formation reached 16 mm in the Mg-(Cu,Ag)-Y system. The fact that D_c can be doubled by minor composition excursions on the Mg-Cu-Y ternary system and re-doubled through our search strategy in the 3D composition space clearly emphasizes the dramatic composition dependence of GFA. The authors are with the Multi-component Amorphous and Nanocrystalline Systems (MANS) research team, supported by the Chinese Academy of Sciences.

4:45 PM Z13.4

Computational Design of Iron-based Bulk Metallic Glass. James Wright[1], Gregory Olson[1], Weijia Tang[1], Mike Miller[2] and Kjetil Hildal[3]; [1]QuesTek Innovations, Evanston, Illinois; [2]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [3]University of Wisconsin, Madison, Wisconsin.

Structural amorphous metals have the potential for application in demanding engineering components due to the inherently high elastic limit of the amorphous state. However, currently available alloys are constrained to small cross-section components, and suffer from poor toughness and fatigue resistance. The maximum amorphous thickness that can be achieved is limited by a combination of the glass formability of the alloy as well as the cooling rate that can be achieved for a given processing method. Furthermore, the toughness and fatigue resistance of these alloys must be improved before their application can be realized. It may be possible to improve the toughness of such alloys through partial devitrification to precipitate toughening phases. With the goal of producing low-cost, iron-based, amorphous sheet, computational design models were developed and applied to design a new iron-based amorphous alloy. Parametric design goals were established to maximize the glass formability. A thermodynamic database and a glass transition temperature model were developed using the concept of molecular associates. Twin-roll casting was selected as a low-cost, scalable process that can achieve very high cooling rates while producing sheet product. The devitrification kinetics of two bulk metallic glasses were studied using differential thermal analysis and atom probe tomography, and the devitrification process was simulated using PrecipiCalc™ and the newly developed thermodynamic database. The design of high-performance structural amorphous metals will require a careful balance of alloying elements to maximize the glass formability while being able to partially devitrify the alloy to achieve the optimum microstructure that provides the desired mechanical properties.

SESSION Z14: Poster Session: Structure and Properties

Wednesday Evening, November 30, 2005
8:00 PM
Exhibition Hall D (Hynes)

Z14.1

In-Situ Diffraction: Looking For The Signatures of Polycrystal Deformation in Nano-Composites. Can Cahit Aydiner[1], Sven C. Vogel[1], John Almer[2], Don W. Brown[1], Bjorn Clausen[1], Amit Misra[1], Tarik A. Saleh[1] and Mark A. M. Bourke[1]; [1]MST-8, Los Alamos National Laboratory, Los Alamos, New Mexico; [2]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois.

In this study, high energy synchrotron X-ray diffraction (HESXRD) was utilized for the first time to probe the deformation of metallic nanostructured multilayers under tensile loading. These material systems are composed of alternating layers of two different metals and ideal for studying mechanical behavior at micrometer, submicrometer and nanometer length scales via the precise control of layer thickness. Accordingly, previous studies with nanoindentation revealed an alteration of deformation mechanisms when the layer thicknesses are reduced to tens of nanometers, as depicted by the breakdown of the Hall-Petch model. HESXRD offers a unique opportunity to further study this transition in mechanical behavior since it allows in-situ probing of crystal lattice strains with the ability to distinguish phases as well as crystallographic planes. For this study, polycrystalline Cu-Nb multilayers were synthesized by DC magnetron sputtering at uniform layer thicknesses of 20, 40, 100 and 1000 nm. Overall deposition thickness was 20 micrometers for each multilayer and dog bone shaped samples were cut out for tensile testing. Experiments were conducted at 1-ID-XOR beamline at Advanced Photon Source, Argonne National Laboratory with 80 keV X-rays. In addition to the diffraction analysis, macroscopic strain fields have been determined by an image correlation technique. For this geometry, the conventional deformation pattern comprises a co-deformation regime at low loads, where Cu and Nb have equivalent lattice strains. Subsequently with higher loads, plastic deformation commences in the softer Cu, and it 'transfers load' to Nb. This results in an excess of lattice strains in Nb in comparison to those in Cu. Preliminary analysis shows that there is a typical co-deformation regime in 100 and 1000 nm samples followed by the load transfer. Indeed, comparison of diffraction data and continuum finite element analysis corroborates that nano-scale effects on mechanical behavior are not observed at the 100 nm scale. On the other hand, 20 nm and 40 nm samples exhibit very limited co-deformation and the extent of load transfer from Cu to Nb increases with decreasing layer thickness; pointing to size effects. Additional evidence of nanometer scale deformation mechanisms in 20 nm and 40 nm samples will be presented such as the peculiar partial release of intergranular strains upon unloading. Deformation mechanisms that explain the nano-scale trends will be proposed.

Z14.2

Grain-boundary Accommodated Plasticity in A Bulk Nanocrystalline Ni(Fe) Alloy: The Experiment and Implication. Guojiang Fan, Gongyao Wang, Hahn Choo and Peter Liaw; Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee.

Intense efforts, by using molecular dynamics (MD) simulations as well as various experimental techniques, have been made in order to understand the mechanisms by which nanocrystalline (nc) metals and alloys deform plastically at room temperature, particularly for the nc metals and alloys with grain sizes less than 30 nm. MD simulations have indicated that grain-boundary (GB) accommodated deformation plays a major role during the plastic deformation of nc metals and alloys, in contrast to the dislocation pile-ups at the GBs for their coarse-grained counterparts. However, experimental evidences supporting the GB accommodated plasticity are limited, primarily in the thin nc foils. So far, GB accommodated deformation mechanism was not confirmed in the bulk nc metals and alloys, while nc materials virtually did not show any tensile ductility in the bulk form. We will present experimental data that correlate plastic deformation of the bulk nc-Ni(Fe) alloy to the GB sliding. The bulk nc-Ni(Fe) was synthesized by electrodeposition. The as-deposited sheets, with 3 mm in thickness, have an average grain size of 23 nm, allowing the determination of mechanical properties in a bulk form. We will demonstrate that substantial grain growth occurs in the nc-Ni(Fe) after the tensile tests at various strain rates. The observed grain growth can be attributed to the grain reorientation via GB sliding. The original grains separated by high-angle GBs reorient and agglomerate into groups of subgrains separated by small-angle GBs. The implication of the observed grain growth, as well as a good combination of strength and tensile ductility of the present bulk nc-Ni(Fe) alloy will be discussed. Acknowledgements: The authors were grateful for the financial support of the National Science Foundation (NSF): the International Materials Institutes (IMI) Program (DMR-0231320), with Dr. C. Huber as Program Director.

Z14.3

In-Situ Synchrotron Measurements of Intergranular Strains in Nanocrystalline FCC Nickel Alloys. Hongqi Li[1], Hahn Choo[1,2], Tarik Saleh[3], Ulrich Lienert[4], Peter K. Liaw[1] and Fereshteh Ebrahimi[5]; [1]Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee; [2]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [3]MST-8, Los Alamos National Laboratory, Los Alamos, New Mexico; [4]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois; [5]Materials Science and Engineering, University of Florida, Gainesville, Florida.

In this study, the intergranular-strain development and peak broadening as a function of applied stresses were investigated in nanocrystalline nickel alloys using a high-energy synchrotron X-ray diffraction technique. The full diffraction patterns including at least the first five rings of the fcc nickel phase were simultaneously recorded during in-situ loading. The average grain size of the various nanostructured nickel alloys investigated ranged from 10 to 50 nm. The results show that the microscopic deformation behavior and intergranular-strain evolution are dependent on the grain size. It is well known that the deformation mechanism depends on the grain size and changes from dislocation-controlled to grain-boundary-sliding controlled mechanisms below a critical grain size. As a result, the dependence of microscopic deformation behavior on the grain size is suggested to be associated with the changes in the deformation mechanisms with the grain size. (This work was supported by the National Science Foundation (NSF) International Materials Institutes (IMI) Program under the grant No. DMR-0231320, with Dr. Carmen Huber as the Program Director.)

Z14.4

Mechanical Properties of Nano-Scale Cu/Ag Composites. Bjorn Clausen[1], Donald W. Brown[2], Tong D. Shen[2], C. Can Aydiner[2] and Ricardo B. Schwarz[2]; [1]LANSCE-12, Los Alamos National Laboratory, Los Alamos, New Mexico; [2]MST-8, Los Alamos National Laboratory, Los Alamos, New Mexico.

Cu-Ag composite alloys (Cu40Ag60) were produced using the flux-melting technique, which facilitates the undercooling of the eutectic Cu-Ag melt by approximately 250°C. At this large undercooling, the rate of crystal nucleation dominates over the rate of crystal growth, resulting in the formation of a lamellar nanocrystalline microstructure. The as-quenched alloys are composed of nano-scale Cu and Ag lamellae, with an average lamellar spacing of 50 nm and an average crystallite size of 40 nm. Neutron diffraction offers a unique opportunity to investigate the properties of composites, as the large penetration depth of neutrons allows for simultaneously measurements of internal strains in all crystalline phases of bulk composites. Results from in-situ neutron diffraction measurements during room temperature tension tests of as-quenched and heat treated Cu-Ag composites will be presented. Normally, the onset of plasticity is easily seen as non-linearity in the elastic lattice strain data long before non-linearity is evident in the macroscopic data (measured by an extensometer). However, preliminary analysis for the as-quenched sample shows that macroscopic yield is observed at 120 MPa, whereas linear behavior is observed for the lattice strains up until 250 MPa. The heat treated and non-quenched samples show similar trends, but not to the same degree.

Z14.5

Study on fatigue properties of nanolayered Cu/Nb thin laminate films. Yun-Che Wang, John Greg Swadener, Tobias Hoechbauer, Tim Darling, Richard Hoagland and Amit Misra; Los Alamos National Laboratory, Los Alamos, New Mexico.

Nanolayered thin films exhibit unusual mechanical properties, such as ultra-high yield strength and large plastic deformation without formation of dislocation cell structures. The mechanism for these unusual phenomena has been explained by dislocation theory in confined layers at submicron length scales. Primarily, the limited space for dislocation storage and creation of dislocation sources is responsible for nano-layered films behaving differently from their bulk counterparts. In this study, we experimentally determine the fatigue properties of the magnetron sputtered Cu and Nb thin films in the form of composite laminates. Our method is to determine the curves of stress versus the number of cycles. Moreover, fracture surfaces are studied with scanning electron microscopy (SEM). We obtain S-N curves for thin films with different individual layer thicknesses. By systematically studying the S-N curves versus individual layer thickness and comparing results from bulk materials, the effects of nano-size layers on fatigue endurance in thin films can be obtained. We have developed a novel experimental method for fatigue and internal friction measurements. Our experimental method employs a bimorph piezo actuator to drive a cantilever beam sample in a moderate vacuum environment. The quality of vacuum determines the Q-factor of the dynamic system of a vibrating cantilever beam, and hence the maximum deformation at resonance. Since stress in the sample is proportional to deformation, the study of mechanical properties of the films under different applied force is closely influenced by the Q-factor. Maximum stress in the sample is determined by a curve-fitting method based on pictures of the deformed sample. A fiber-optic system is used to measure the deflection of the sample at desired locations along the specimen, and a feedback control mechanism is adopted to maintain deformation. Since large deflection is required to achieve a certain stress level, the effect of geometric nonlinearity is included in the stress calculations. We identify the phenomena of amplitude-dependent frequency responses and hysteresis in frequency scans, similar to the behaviour of Duffing oscillators, and present strategies that allow us to solve for the fatigue properties in the presence of nonlinear deformation.

Z14.6

Footprints of the thermal component in deformation mechanisms of nanocrystalline Ni: an in situ x-ray diffraction study. Steven Van Petegem, Stefan Brandstetter, Zeljka Budrovic, Bernd Schmitt and Helena Van Swygenhoven; Paul Scherrer Institution, Villigen PSI, Switzerland.

In-situ deformation of nanocrystalline metals at the materials science beamline of the Swiss Light Source allows tracking of the angular position and width of several diffraction peaks as a function of applied stress and strain, from which information on elastic and plastic properties can be obtained. It was previously shown that the broadening of the diffraction peaks observed during room temperature plastic deformation under tension is reversible upon unloading for electrodeposited (ED) nanocrystalline Ni, demonstrating the lack of a developing permanent dislocation network (Science 304 (2004) 273). In order to evidence a thermal component in the nanocrystalline deformation mechanisms in-situ tensile measurements were performed as function of temperature. We find that at 180K the peak broadening is not fully reversible upon unloading. However this additional broadening recovers completely after heating up the sample to room temperature. Furthermore after additional plastic deformation at room temperature the peak broadening remains fully reversible. Additionally, stress relaxation experiments reveal a strong temperature dependence of the thermal activation volume. TEM observations reveal no significant differences between the microstructure after deformation at 180K and room temperature. These observations in combination with results from molecular dynamics simulations suggest the freezing-in of dislocations at low temperature due to a restriction in the atomic activity within the surrounding grain boundary network. In order to achieve larger deformation strains the experimental setup was extended so that in situ compression tests could be performed. For ED Ni plastic strains up to 20% could be achieved. The microstructures after tensile and compression deformation are compared using TEM and related to the x-ray diffraction results.

Z14.7

Abstract Withdrawn

Z14.8

Modeling elastic and plastic deformation of nanostructured materials. Peter Stefanovic[1], Mikko Haataja[2], Sami Majaniemi[3] and Nikolas Provatas[1]; [1]Materials Science and Engineering, McMaster University, Hamilton, Ontario, Canada; [2]Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey; [3]Physics, McGill University, Montreal, Quebec, Canada.

Nanostructured materials (e.g., quantum dots, nanocrystalline materials, and nanoparticles) can have physical and mechanical properties that are strikingly different from their corresponding bulk counterparts. Consequently, unraveling the physical mechanisms that give rise to their behavior at the atomic scale is essential in order to exploit and harness their unique properties. From a theoretical perspective, capturing dynamic phenomena across very long time scales with direct atomistic simulation methods becomes a very challenging task due to inherent time scale limitations – indeed, brute-force Molecular Dynamics (MD) simulations can probe dynamics of the system only on very short time scales ($\sim$100ns). In contrast, deformation experiments typically take place across macroscopic time scales. In order to overcome some of these limitations, a continuum field theory approach is presented for modeling both elastic and plastic deformation, free surfaces, and multiple crystal orientations in systems with both hexagonal and cubic symmetry in two spatial dimensions. The model is based on a free energy for the local atomic density, which is minimized by spatially periodic structures. Hence, it incorporates, by construction, both elastic phenomena (deviations from the preferred spatial period cost energy) as well as defects in the form of, e.g., vacancies, dislocations, and grain boundaries. Furthermore, its dynamics is constructed such that it incorporates both diffusive and elastic relaxation phenomena. By introducing a variable elastic time scale, we are able to maintain mechanical equilibrium while simulating microstructural evolution on time scales well beyond those accessible by conventional atomistic MD simulation methods. We apply this model to elucidate the role of dislocations during deformation of nanocrystalline materials.

Z14.9

Dislocation Instability in Nanoscale Particles. Christopher Earl Carlton and Paulo Ferreira; Materials Science and Engineering, University of Texas at Austin, Austin, Texas.

Understanding the mechanical behavior of nanoparticles has become a key factor for the success of many engineering applications. Classically, for polycrystalline materials one would expect an increase in the yield strength for smaller grain sizes according to the empirical Hall-Petch equation. However, at the nanoscale, this mechanism seems to break down. Despite the number of interesting papers published on this topic, controversy persists and consensus is still lacking. While this discussion is of great interest for polycrystalline nanoparticles, contemporary models for strengthening are inappropriate for single-crystal nanoparticles, which pose an altogether, a very different problem: the absence of grain boundaries to inhibit dislocations. In this context, we present a new model wherein the change in Gibbs Free Energy of an edge dislocation in a single-crystal particle provides a driving force for dislocation motion. Specific results for nanoparticles with different sizes, along with spherical and hexagonal prism geometries are provided. These results show that, for both geometries, dislocations become unstable and are spontaneously ejected from the particles below a certain critical size. Discussion of the importance of this result and its implications for the mechanical properties of both bulk and powder nanomaterials are also included.

Z14.10

Statistical Characteristics of the Indentation-induced Strain Bursts in a Zr-based Metallic Glass. Han Li and Alfonso H. W. Ngan; Mechanical Engineering, The University of Hong Kong, Hong Kong, Hong Kong.

Plastic deformation of amorphous metals or metallic glasses can be homogeneous or inhomogeneous depending upon the stress and temperature. Nanoindentation tests in this family of materials reveal that discrete strain bursts, or serrated flow, can occur well below their glass transition temperature, suggesting the operation of localized shear bands being the deformation mechanism. The formation and propagation of these plastic instabilities appear to be rate-sensitive in nature. Considering that these discrete bursts occur in an apparently random form, a statistical analysis of the burst series is crucial for a deeper understanding of the deformation physics. In this work, we performed room-temperature nanoindentation experiments on the deformation behavior a Zr-based metallic glass sample to study the statistical characteristics of the induced strain bursts. A dimensionless parameter $\Delta h/h$, where h is displacement,is used to quantify the strain increment in an individual strain burst.Δh is obtained by subtracting the average elastoplastic behavior from the noisy displacement data through a curve fitting process. The results show that, surprisingly, the statistical distribution of the parameter $\Delta h/h$ cannot be satisfactorily described by a power-law distribution corresponding to self-organized critical (SOC) behavior. Instead, an exponential decay distribution seems to fit the data much more satisfactorily. Similar experiments in Ni3Al, Al, Cu, Zn, Nb and Al-Mg also reveal that the bursts in these materials are better fitted by an exponential distribution. Finally, it is noted that the exponential distribution corresponds to maximum Shannon entropy, or likelihood, of arranging the burst sizes to correspond to a fixed mean burst size. We therefore conclude that the occurrence of discrete bursts in the indentation situation for a wide range of materials can be better described by an exponential law rather than a power law as in self-organized criticality.

Z14.11

Modeling of Microhardness for Nanocrystalline Material with Nano-sized Twin Bends. Yueguang Wei and Bo Wu; Institute of Mechanics, Chinese Academy of Sciences, Beijing, Beijing, China.

A theoretical model based on both cell model and strain gradient plasticity theory is used to characterize the microhardness of the nanocrystalline material. Within each nanocrystalline grain region, a series of nano-sized twin bends are included. In the theoretical model, the indented crystal grain is treated with a plastic material, while each twin bend is described by the shear bend model, within which a shear strain hardening model is adopted to describe material behavior in the shear bend region. Outer boundary of the indented nanocrystal corresponds to grain boundary, by which the dislocations and twin bends within the grain region moving across the grain boundary are constrained during the nanostructure material deformation . The grain region outside the indented grain keeps elastic deformation. So, in the present study, the grain region outside the indented grain is homogenized into an equilvalent elastic medium by using the Hill consistent method. Modeling and simulation results show that for the case of a nanocrystalline grain with a series of twin bends inside the grain region, the material displays a very higher microhardness value than the case without the twin bends included inside the grain. Microhardness varying with volume fraction of the twin bends and with hardening property of the twin bend material. Finally, the modeling results are compared to the experimental ones given in literature.

Z14.12

Molecular Dynamics Simulation of Mechanical Properties in Amorphous and Nanocrystalline Metals. Yoshiaki Kogure and Masao Doyama; Teikyo Univ. of Science & Technology, Uenohara, Yamanashi, Japan.

Materials of amorphous or nanocrystalline states are known to show peculiar mechanical properties, which may be related with the disordered configuration of atoms. Elastic responses and plastic deformation of these materials are simulated by means of molecular dynamics simulation. The embedded atom method potential developed by the present authors are used to express the interaction of atoms. As the model systems pure copper and Ag-Cu alloys are adopted. The simulation systems contain several thousands of atoms. As an initial condition atomic systems are kept in molten state, then the systems are quenched to make amorphous states. The structure of the systems is examined through the radial distribution function. The external stresses are applied and displacements of atoms are monitored to investigate the elastic and plastic deformation. The strains are calculated from the displacement of individual atoms, then the elastic constants are evaluated. The distribution of internal stress is also evaluated from the configuration of the nearest neighbor atoms and the potential energy of individual atoms. The temperature of the material is increased and the relaxation of internal stress is monitored. The crystallization from the amorphous state is one of the useful processes to produce a nanophase material. The annealing of the model system is also tried to realize the nanocrystallization, and the changes of atomistic structure in the system are investigated.

Z14.13

Effects of Glass-Forming Metallic Film on the Fatigue Behavior of Structural Materials. F.X. Liu[1], C. L. Chiang[1,2], D. Smith[1], J. P. Chu[2], P. Rack[1] and P. K. Liaw[1]; [1]Department of Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee; [2]Institute of Materials Engineering, National Taiwan Ocean University, Keelung, Taiwan.

Metallic glass-forming materials exhibit excellent wear and corrosion resistances, and good surface finishes. They also show improved mechanical properties in the form of thin films, making them ideal candidates as coating materials to improve mechanical properties, especially fatigue properties of structural material. The Zr- and Cu-based metallic glass-forming films (∼200nm thick) were deposited on the 316L stainless steel and Ni-based alloy substrates, using magnetron sputtering. Four-point-bending fatigue tests were conducted on these coated materials. It was shown that the fatigue life and the fatigue- endurance limit of the materials could be considerably improved. Depending on the maximum applied stresses and the substrate materials, the fatigue life was enhanced by at least 30 times. Fractographic studies showed that the film maintained good adhesion to the substrate even after the severe plastic deformation. The surface-roughness measurements indicated the improved surface conditions due to the film deposition. The residual stresses were measured, based on the curvature change of the substrate before and after the film deposition. Analyses showed that the excellent adhesion of the film to the substrate, the improved surface roughness, and the compressive residual stress played beneficial roles in enhancing the fatigue properties of the coated systems, revealing the deposition of glass-forming films on structural materials as a novel and effective method to enhance fatigue properties.

Z14.14

Atomic Mixing in Immiscible Binary Alloys subjected to sustained Plastic Deformation. Samson Olusikunanu Odunuga, Youhong Li, Pavel Krasnochtchekov, Pascal Bellon and Robert S. Averback; Materials Science and Engineering, University of Illinois Urbana Champaign, Urbana, Illinois.

Molecular dynamics simulations were performed to understand the mechanisms of atomic mixing in crystalline immiscible binary alloy systems subjected to sustained plastic deformation. In this work, alloys based on Cleri-Rossato's Cu and Ag potentials, were cyclically deformed with a constant strain rate of $5 \times 10^{9}\ s^{-1}$ at 100K. The repulsive term of the potential was systematically varied to study the effect of the heat of mixing, lattice mismatch, and the relative shear modulus on the efficiency of atomic mixing between a precipitate and it bounding matrix. Short-range order was used to characterize the evolution of the forced mixing and it reveals nearly complete mixing in all the systems studied except where a hard (higher shear modulus) precipitate was embedded within a soft matrix. Common neighbor analysis shows that the deformation occurs by dislocation glide. The sources and development of partial and full dislocations and nanotwins are observed by a Burgers vector analysis, which details the changes in the atomic pair separations in the systems. The efficiency of atomic mixing was characterized by a similar novel procedure based on the mean squared relative displacements (MSRD) between pairs of atoms. This involves taking an average of the square change in the atomic pair separation as a function of their distance apart. The analysis shows the interesting result that the diffusion coefficient is linearly proportional to their separation. For initially first nearest neighbors, this results in their mean squared separation growing in time according to a power-law dependence, with an exponent $n \sim 1.5$.

A simple analysis predicts an exponent 2 for a mixing purely due to dislocation glide, in contrast to the standard exponent 1 for diffusive mixing. This finding provides further support to the conclusion that dislocation glide is the main mechanism responsible for mixing, in particular for large pair separation distances. Our procedure also provides a simple phenomenological rationalization for the compositional patterning that is observed in ball milling experiments.

Z14.15

Structure and Mechanical Properties of Monolithic Nanoporous Cu. J. R. Hayes, A. M. Hodge, J. Biener, Y. M. Wang and A. V. Hamza; Chemistry and Materials Science, Lawrence Livermore National Lab, Livermore, California.

Nanoporous materials offer many unique properties which can be exploited in scientific and engineering applications. The extremely high surface areas of nanoporous materials make them ideal for catalytic and sensor applications. Low density nanoporous materials have demonstrated increased yield strength due to the small dimensions of the interconnecting ligaments. This suggests the ability to form a low density nanoporous metal with high tensile and compressive strength. For a nanoporous material to have uniform macroscopic mechanical properties, its internal structure must be homogeneous and without flaws and defects throughout the bulk dimensions of the sample. Such a structure can be achieved through the electrochemical process of dealloying, whereby one component of an alloy is removed and the remaining component restructures into a bicontinuous open pore structure. However, the alloy starting composition and microstructure are of critical importance to the formation of a homogeneous porous structure. An ideal system is Ag/Au, which produces nanoporous Au, but the formation of a low density, homogeneous nanoporous copper has not been achieved. Nanoporous copper offers several advantages over Au, such as lower density, larger modulus of elasticity, and lower cost. We report here on the formation of monolithic nanoporous copper by dealloying Cu/Mn alloys. The Cu/Mn alloy formation and heat treatment are critical since precipitates, second phases, and inhomogeneities in the Cu/Mn alloy develop into flaws in the dealloyed structure. Specifically, we discuss the synthesis, structure, and mechanical properties of nanoporous copper. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under contract of No.W-7405-Eng-48.

Z14.16

Simulated x-ray diffraction spectra of nanocrystalline materials: the effect of lattice dislocations in a high interface density material. Peter Derlet, Stefan Brandstetter, Steven Van Petegem and Helena Van Swygenhoven; Paul Scherrer Institution, Villigen PSI, Switzerland.

Large scale molecular dynamics simulation of bulk metallic nanocrystalline systems have revealed that slip contributes to their plastic deformation behaviour, through the nucleation and absorption of dislocations at grain boundaries. This important result has also been recently confirmed with an in situ deformation x-ray experiment which has demonstrated that the footprint of dislocations in terms of the broadening of Bragg diffraction peaks during plastic deformation disappears upon unloading indicating no dislocation debris are accumulated in nanocrystalline plasticity (Science 304 (2004) 273). The ability to understand the contribution of dislocations to the x-ray spectra is hindered by the fact that many theoretical approaches consider simplified distributions of lattice dislocations and do not consider the presence of a high density of missorientation interfaces and its associated strain signature. The present work takes an alternative approach (Phys. Rev. B. 71 (2004) 024114) by employing a numerical algorithm that allows the calculation of the x-ray powder diffraction spectrum for a multi-million atom computer generated nanocrystalline sample. In particular we investigate the influence of special grain boundaries, twin lamella, and lattice dislocation content on the x-ray diffraction spectra using photon wavelengths in synchrotron regime.

Z14.17

Abstract Withdrawn

Z14.18

Transferred to Z12.1

Z14.19

Crystallization and Mechanical Behaviour of a Mg-Cu-Gd Bulk Metallic Glass. Sylvain Puech[1,2], Jean-Jacques Blandin[1], Jean-Louis Soubeyroux[2] and Patricia Donnadieu[3]; [1]GPM2, INP Grenoble, Saint-Martin d'Heres, France; [2]CRETA, CNRS Grenoble, Grenoble, France; [3]LTPCM, INP Grenoble, Saint-Martin d'Heres, France.

Bulk metallic glasses with Mg65Cu25Gd10 composition were elaborated and their resistance to crystallization was investigated by differential scanning calorimetry, X-ray analyses and transmission electron microscopy with a particular attention given to the kinetics of crystallization, the nature and the average size of the produced crystals. Mechanical properties at room temperature and nearby the glass transition were studied in compression. In both cases, the introduction of nanocrystals in the amorphous matrix modifies the mechanical behaviour of the material. At room temperature, even with no additional crystallization treatment, a particular fragility of the glass is observed and interpreted in relation with relaxation processes. Increasing the quantity of crystals induces a systematic decrease of the fracture stress whereas a continuous increase of hardness is measured. At high temperature, partial crystallization results also in important changes in the rheology of the alloy. The hardening associated to crystallization is discussed in terms of the respective contributions of on the one hand, the "composite" effect resulting from the presence of rigid particles in a viscoplastic matrix and, on the other hand, the variations in properties of the residual glass.

Z14.20

Transferred to Z16.1

Z14.21

Elastic Properties in Liquid and Glassy States of Metallic Glass. Gang Duan[1], Marios Demetriou[1], Konrad Samwer[2], Tahir Cagin[3], William Goddard[1] and William Johnson[1]; [1]California Inst. of Tech, Pasadena, California; [2]University of Gottingen, Gottingen, Germany; [3]Texas A&M University, College station, Texas.

Recently it is shown that plastic yielding of metallic glasses at room temperature can be roughly described by an average elastic shear limit criterion based on the data for $\sim$ 30 bulk metallic glasses. A Cooperative Shear Model (CSM) combined with a scaling relationship among plastic flow barrier, the elastic strain and the shear modulus is proposed to explain this universal behavior. However, it remains unclear how the temperature dependence of elastic properties influences the plastic yielding of metallic glasses. Unfortunately, owing to apparatus setup difficulties, experimental determination of the full temperature dependence of elastic properties for amorphous metals has not been accomplished yet. In this work, we provide the elastic properties in liquid and glassy states of metallic glasses based on molecular dynamics simulations.

Z14.22

Length Scale of Flow Defects in Amorphous Solids Derived from Diffusion Analysis. Youhong Li, Pascal M. Bellon and Robert S. Averback; Materials Science and Engineering, University of Illinois, Urbana, Illinois.

A fundamental understanding of plastic deformation in amorphous solids has been rather slow to evolve, owing in large part to the complexity of the amorphous structure. While computer simulations are becoming an increasing important tool in this field, providing a direct view the deformation process, most work is performed in two dimensions to make the underlying mechanisms more transparent. Such visual observations mimic the early work on grain sliding using bubble rafts. We have recently demonstrated in crystalline materials that much about the deformation process can be gleaned without directly viewing the atomic motions, but rather by characterizing how atoms move relative to one another. Our method examines an effective diffusion coefficient, which is the time derivative of average mean square relative displacement, $\sigma\hat{2}$, of pairs of atoms as a function of time and their separation distance, ri,j. For crystals under cyclic plastic deformation, for example, D(r) is linearly proportional to r/L where L is the length scale of the system. In the present study we determine D(r,t) using fully three dimensional, constant strain rate, constant temperature (100 K), molecular dynamics simulations of amorphous Cu-Ti, which we represent with a many body Cu-Ti potential in the form of second moment approximation to Tight Binding scheme. Unlike crystalline systems, we find that the diffusion coefficient exponentially approaches a constant value with a characteristic decay length given by Rc $\approx$ 1 nm. This analysis thus suggests that the deformation process takes place locally, and involves some tens of atoms. As a consequence of this scale-dependent forced mixing, composition patterns can form at a mesoscopic scale when thermally activated decomposition acts in competition. The maximum scale of these amorphous patterns, however, is given by Rc and thus will remain small. This is in contrast with crystalline materials for which the patterning scale is bounded by dislocation glide distance, which can reach large values. This prediction will be compared with available experimental data.

Z14.23

Room-Temperature Embrittlement of Mg-based Amorphous Alloys. Alberto Castellero, Dirk I. Uhlenhaut and Jorg F. Loffler; Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Zurich, Switzerland.

Mg-Cu-Y alloys can be amorphised in a wide range of compositions. When these alloys are produced in bulk form they exhibit high mechanical strength but no ductility. Rapidly quenched ribbons and thin foils show plastic deformation upon bending. However, a dramatic deterioration of the mechanical properties is observed after aging at room temperature. A sharp transition from ductile to brittle behaviour can be observed in Mg65Cu25Y10 a few hours after the alloy has been produced. The process becomes slower when Cu is substituted by Mg. Corresponding to this time-dependent embrittlement, the DSC curves show a reduction in the relaxation enthalpy that is associated with a structural relaxation of the metallic glass. Oxidation as a cause of the embrittlement has been ruled out, since the same behaviour is observed when the samples are stored in a protective atmosphere. The bent as-quenched samples exhibit shear bands on the surface, indicating that the material is able to deform plastically. The aged metallic glass exhibits only elastic deformation, followed by catastrophic failure at a certain critical bending strain which progressively decreases with time. The latter may be explained by a time-dependent increase in the stiffness of these aged Mg-based metallic glasses.

Z14.24

Characterization of Plasticity-Induced Free Volume Changes in Bulk Metallic Glass. Katharine M. Flores, Materials Science and Engineering, The Ohio State University, Columbus, Ohio.

Improving the structural reliability of bulk metallic glass components requires a detailed understanding of the relationship between glass structure and plastic flow behavior. The free volume theory for flow in metallic glasses indicates that the average free volume increases during plastic deformation, and prior positron annihilation spectroscopy (PAS) studies of free volume distribution suggest that the sizes of free volume sites range from inherent interstitial-like defects to larger defects capable of flow. However, the precise flow mechanism and the evolution of the free volume distribution during flow remain unclear. An examination of structural changes during plastic deformation is therefore of interest. In this study, a Gleeble thermomechanical test system was used to investigate the homogeneous flow behavior of a Zr-based bulk metallic glass. The tensile and compressive deformation behavior was characterized near the glass transition temperature. Structural changes were observed as a function of total plastic strain using x-ray diffraction and DSC techniques. XRD results indicate a change in the width of the second amorphous peak consistent with an increase in the nearest neighbor separation distance. These results are compared with the structural changes observed following inhomogeneous deformation over a similar range of total plastic strains. Previous results revealed that $\sim$30% inhomogeneous plastic strains achieved by rolling increased the average free volume by $\sim$4%, consistent with the free volume theory of flow. More detailed information about the evolution of the free volume distribution was obtained using PAS, where an increase in the concentration of flow defects was observed following deformation. For very large inhomogeneous plastic strains, PAS data suggests that the flow defects coalesce to form larger scale defects, consistent with the nanovoids observed in shear bands by other researchers. Finally, in order to assess the impact of prior thermomechanical processing on component performance at room temperature, shear band formation and inhomogeneous flow behavior following structural relaxation and homogeneous deformation near the glass transition were also investigated and will be discussed.

Z14.25

An Investigation on the Plasticity of a Zr-based Bulk Metallic Glass. Wenhui Jiang, Guojiang Fan, Hahn Choo and Peter K. Liaw; Materials science and Engineering, The University of Tennessee, Knoxville, Tennessee.

Bulk metallic glasses deform inhomogeneously at low temperature and high strain rates. The deformation is highly localized in a few shear bands, resulting in very limited bulk plasticity and a premature fracture. Recently, however, high-resolution scanning electron microscopy observations showed that a substantial deformation occurred on the fracture surface of a Mg-based bulk metallic glass, indicating a ductile fracture [1]. This presentation will report our investigation on the plasticity of Zr 52.5 Ti 5 Cu 17.9 Ni 14.6 Al 10 (Vit 105) bulk metallic glass under uniaxial loading. The significant plastic deformation can happen under constrained conditions. We will discuss the various plastic-deformation behaviors of this Zr-based bulk metallic glass. This work is supported by the National Science Foundation through the International Materials Institutes (IMI) Program on Advanced Neutron Scattering Network for Education and Research under DMR-0231320, with Dr. Carmen Huber as the program director. [1] X.K. Xi, D.Q. Zhao, M.X. Pan, W.H. Wang, Y. Wu, J.J. Lewandowski, Fracture of brittle metallic glasses: brittleness or plasticity, Physical Review Letters, 2005, 94:125510.

Z14.26

Abstract Withdrawn

Z14.27

Abstract Withdrawn

Z14.28

Nanomechanical Properties and Deformation Behavior of Amorphous Nickel-Phosphorous Films under Nanoindentation Test. Shou-Yi Chang, Yu-Shuien Lee, Ting-Kui Chang and Hsiang-Long Hsiao; Department of Materials Engineering, National Chung Hsing University, Taichung, Taiwan.

Electrolessly plated nickel-phosphorous (Ni-P) films with good mechanical and anticorrosion properties have been widely used in molding, tool, micro-electromechanical systems and many other industries as wear- and corrosion-resistant coatings. Most of previous studies are emphasized on the effects of processing parameters, like plating solution and pH value, on the structure and corrosion resistance of the plated Ni-P films. However, the mechanical properties of the Ni-P films with an amorphous structure, especially the deformation mechanism different from dislocation activity, have not been clarified. Therefore in this study, the nanomechanical properties and deformation behavior of the electrolessly plated Ni-P films have been investigated using instrumented nanoindentation for the evaluation of more representative reliability during practical application. Electroless plating solutions of different pH values were applied to deposit Ni-P films with different P contents and to investigate the effect of P content on the mechanical properties of the films. The hardness and elastic modulus of the Ni-P films deposited at a pH value of 3.75 were measured as about 6.2 and 157 GPa, respectively. With increasing pH value to 6.0, the P content decreased from 12 wt% to about 9 wt%, and the hardness and elastic modulus slightly increased to 7.5 and 168 GPa, respectively. From the load-indentation depth curve and converted true stress-depth curve, it was observed that the Ni-P films deformed elastically at first and then yielded at an indentation depth of about 10 nm. The critical stress for the initiation of plastic deformation in the Ni-P films was measured as about 8 GPa, and no strain hardening or dislocation activity was recognized. By using atomic force microscopy and transmission electron microscopy (TEM), plastic deformation was observed through the formation and extension of shear bands rather than the nucleation and sliding of dislocations. Inside the highly deformed shear bands around the indent mark, few diffraction spots were observed by TEM selective area diffraction analysis, implying the nucleation of nanocrystallites in the amorphous matrix probably through flow dilatation under the atomic-scale contact of nanoindentation. Moreover, the creep behavior of the electrolessly plated Ni-P films was also analyzed by nanoindentation test and showed a creep strain rate of about 10-4 1/sec under a high stress intensity of 4 GPa. The creep strain-stress relationship exhibited a typical power law expression with a stress exponent of only 0.24. The higher creep strain rate but lower stress exponent of the amorphous Ni-P films than typical crystalline metal films suggests the high but constant atomic mobility caused by the flow dilatation induced intense shear localization within the shear bands under nanoindentation.

Z14.29

Abstract Withdrawn

Z14.30

Effect of AlN addition on the sintering of SiC nanopowder with stacking disordered structure. Kenshiro Shirai[1], Takeshi A. Yamamoto[1], Manshi Ohyanagi[1] and Zuhair A. Munir[2]; [1]High-tech Research Center, Ryukoku University, Otsu, Japan; [2]Chemical Engineering and Materials Science, University of California, Davis, Davis, California.

Silicon carbide (SiC) is one of the promising candidate materials for high-temperature structural application because of its many excellent properties, including strength retention, oxidation resistance at high temperature and so on. The consolidation of SiC is generally difficult without the grain growth because it can be sintered at higher temperature than 2000°C. The sintering additives have been usually used for performing it at the lower temperature. However, the precipitation of sintering additives in the grain boundary often makes decrease the mechanical properties of sintered compact. We have already reported that SiC nanopowder with stacking disordered structure prepared by mechanical alloying (MA), so-called MA-SiC powder, could be consolidated without sintering additives by spark plasma sintering (SPS) at 1900°C. The consolidation was concluded to take place due to the ordering process of the stacking disordered structure. According to phase diagram of AlN and SiC, its solid solution is stabilized easily at lower temperature with a small amount of AlN. Therefore, it is expected that a solid solution of AlN into SiC accelerates the consolidation of MA-SiC nanopowder with disordered structure without the precipitation of sintering additive in the grain boundary. In this work, the MA-SiC powder with a small amount of AlN milled by planetary ball milling was consolidated by SPS. And those samples were compared to the reference samples which consisted of SiC nanopowder without AlN. The MA powder was prepared by planetary ball milling (Fritch, P-5, 300 rpm, weight ratio of pulverizing ball against powder of 40, 24hours) under Ar atmospheric pressure. The sintering and consolidation was accomplished by spark plasma sintering at 1500 to 1900°C for 10min under applied pressure of 70MPa while monitoring the displacement change of pressing axis. The characterization was performed by X-ray diffraction analysis, measurement of density, shrinkage rate and electron microscopy by TEM and SEM. The X-ray diffraction patterns indicated that MA-SiC powder with a small amount of AlN has disordered structure without pure AlN. In the sintering of MA-SiC powder with a small amount of AlN, the shrinkage phenomenon was observed at lower temperature compared to reference powders and its sintered compact prepared at 1700°C for 10min had the relative density of 99.2% against theoretical density (3.215g/cm^3). And the shrinkage rate was also higher than that of reference samples. The results suggest that the AlN addition has extremely an effect on MA-SiC sintering. From TEM and SEM observations, the grain size of sintered compact with relative density of 99.2% was approximately 50nm corresponding to grain size of reference sample. This indicated that consolidation was performed while preventing the grain growth by solid solution of AlN into SiC. Those results will be described at presentation in detail.

Z14.31

Poisson's ratio and the fragility of bulk metallic glasses.

Jong Hyun Na[1], Jin Man Park[1], Won Tae Kim[2] and Do Hyang Kim[1]; [1]Center for Non-crystalline Materials, Yonsei University, Seoul, South Korea; [2]Department of Physics, Chongju University, Chongju, South Korea.

Most of the bulk metallic glasses(BMGs) reported so far exhibit a plastic strain of $\sim$2% when deformed under compression mode. The very low level of plasticity and absence of strain hardening in the metallic glass alloys restricts the range of their application as structural components. But, recently, the pronounced global plasticity in monolithic BMG alloy has been reported the several systems including the Pt57.5Cu14.7Ni5.3P22.5 alloy. In the present study, the correlation among the apparent global plasticity, Poisson's ratio and the fragility in monolithic bulk metallic glass alloys has been investigated. The relative strength of shear and bulk moduli in monolithic Zr- and Ti-based BMG alloys has been investigated by resonant ultrasound spectroscopy(RUS) and ultrasonic measurement. The Zr41Ti20Cu9Ni10Be20 alloy showing a large apparent global plasticity($\sim$8%) exhibits a high Poisson's ratio of 0.42 when compared with that of Zr41Ti14Cu12Ni10Be23(Vit1) BMG alloy. Similarly, the Ti45Zr16Cu10Ni9Be20 BMG alloy with large plastic strain($\sim$7%) before failure shows higher Poisson's ratio of 0.43 that exceeds the value of conventional BMG alloys. In addition, the fragility of the BMGs obtained by the differential scanning calorimetry(DSC) is linked to the Poisson's ratio of the corresponding glass phase. Moreover, the correlation between Poisson's ratio and apparent global plasticity in monolithic bulk metallic glass alloys has been investigated. The Poisson ratio might be regarded as an important parameter that controls the fragility and global plasticity of glass-forming alloys.

Z14.32

Synthesis of in situ Fe-base nano/ultrafine eutectic structured alloys with high strength.

Jin Man Park[1], Jong Hyun Na[1], Won Tae Kim[2] and Do Hyang Kim[1]; [1]Center for Noncrystalline materials, Yonsei University, Seoul, South Korea; [2]Division of Applied Science, Chongju University, Chongju, South Korea.

The novel functional and structural properties of nanocrystalline materials have accelerated developement of Fe-based nanocrystalline alloys in terms of their large potential applications. However, applications of bulk nanocrystalline alloys are limited by their limited scale and brittle nature. Moreover, generally complex and multiple manufacturing processes are required for synthesis of bulk form. In this study, we found Fe-based alloys can be cast into in situ nano/ultrafine structured states with bulky sizes by using conventional injection casting method. There structures and properties have been examined in detail using X-ray diffraction (XRD), secondary electron microscopy (SEM), transmission electron microscopy (TEM) and Instron-type tester. These new Fe-based bulk nano/ultrafine structured alloys show excellent mechanical properties such as high strength and good ductility. The nanostructured matrix is achieved by the reduction of eutectic lamellar spacing down to nano/ultrafine scale. The Fe-(Ti, Zr, Nb) binary or Fe-(Ti, Zr, Nb)-B ternary eutectic structured alloys with nano/ultrafine scale lamellar spacing exhibit high strength of about 2$\sim$2.7 GPa and a plastic strain of 2$\sim$6 %. Moreover, Fe83Ti7Zr6B4 alloy among Fe-Ti-Zr-B quaternary alloys investigated exhibit high compressive strength of about 3.1 GPa and ductility to fracture of about to 6 %. The as-cast nano/ultrafine eutectic lamellar structure consists of Fe2Ti (P63/mmc) and α-Fe solid solution (Im3m) phases. The fabrication of Fe-based nanocrystallined alloys with fine eutectic structure appears to be a promising structural alloy with high strength and large ductility.

Z14.33

Binormal Nanohelices.

Alexandre F. da Fonseca[1], Douglas S. Galvao[2] and Coraci P. Malta[1]; [1]Physics Institute, University of Sao Paulo, Sao Paulo, Sao Paulo, Brazil; [2]Applied Physics, State University of Campinas, Campinas, Sao Paulo, Brazil.

Helical nanowires and nanobelts are promising nanostructures due to their great potential applications in nanoelectronics, nanomechanics and nanoelectromechanical systems. Recent works have been published in the literature on the growth of both amorphous and crystalline nanohelices, but some fundamental questions remain not completely understood. Physically a helical rod can be classified in accordance to the orientation of its cross-section with respect to the normal or binormal vectors. While common and binormal helical nanostructures have been reported in the literature, it seems that normal nanosprings do not exist. In this paper we explain using analytical models why amorphous and crystalline normal nanosprings should not exist. For the case of nanosprings grown without the presence of catalytic particles, we have applied the stability analysis developed by Goriely and Shipman to show that only binormal nanohelices with flat cross-sections are stable structures. Normal helices are always unstable, and consequently should not exist. One important function of the catalytic particles (used in the process of growing helical amorphous nanostructures) is to produce intrinsic curvature that provides dynamical stability to the structures. The vapor-liquid-solid (VLS) growth model, first proposed by Wagner and Ellis, to explain the whisker formation, and recently modified by Mcllroy et al. to explain the growing process of a helical nanowire, is used here by us to show why a normal helical nanostructure is difficult to obtain. We show that the shape and the orientation of the catalytic particle can explain not only the difficulty of growing a normal nanospring but also the growing of a binormal nanospring.

Z14.34

Mechanical Behavior of Multi-Principal-Element Fe-Co-Ni-Cr-Al-Mn Alloy System.

Wei-Jen Wang, Hung Cheng Jack Chen, Chin-Pang Tu and Jiun-hui Lai; Material Reserch Lab., Industrial Technology Research Institute, Tainan, R.O.C, Taiwan.

Design of metallic alloy is an experience science and engineering. Other than the conventional concept of alloy design based on principal metallic element (>40 at.%), to synthesize several (5$\sim$7) principal elements, i.e. equal or near-equal molar ratio, for a new alloy design is novel and as similar as the metallic glass or called bulk amorphous materials. The multi-principal-element alloy presents high entropy. At meanwhile, the properties and performance of this multi-principal-element alloy are discovered. Here, this paper will disclose the behaviors of three types of alloy, Fe0.5Co0.5NiCr0.1Al0.3Mn0.1, FeCo0.5NiCr0.5Al0.3Mn and Fe1.5Co0.5NiCrAl0.3Mn0.5 in molar ratio, between normal and high temperature condition for the comparison. These three alloy commonly possess the FCC crystal structure, and the melting points are all over 1200 degree C. Also the hardness of them does not decrease after high temperature (1000 degree C) annealing. The ultimate tensile strength (UTS) of Fe0.5Co0.5NiCr0.1Al0.3Mn0.1 can be elevated to 1115 MPa as twice as original through cold wrought.

Z14.35

Fabrication of Metal/Ceramic Co-continuous Nanocomposites.

Charlotte N. Sisk, Louisa Hope-Weeks and Yamini Kasturi; Chemistry & Biochemistry, Texas Tech University, Lubbock, Texas.

Fabrication of metal/ceramic co-continuous nanocomposites can exhibit enhanced strength, plasticity, and hardness due to limited displacement mobility. Silver-containing porous frameworks demonstrate unique properties, they are readily used in biofiltration, catalysis, and electrochemistry applications. This paper describes the novel approach to the synthesis of a nanograin silica ceramic compact filled with a continuous silver metallic nanowire network. The high capacity metal loading can be readily achieved using a modified room temperature sol-gel procedure. The structure of the silver-silica nanocomposites are evaluated as a function of metal loading and the resulting effect on the electronic and mechanical properties are assessed.

Z14.36

Deformation twinning in nanocrystalline, high-strength tantalum.

Yinmin Wang[1], A. M. Hodge[1], J. Biener[1], A. V. Hamza[1], D. E. Barnes[2], K. Liu[2] and T. G. Nieh[3]; [1]Nanoscale Synthesis and

Characterization Lab, Lawrence Livermore National Laboratory, Livermore, California; [2]Department of Physics, University of California, Davis, California; [3]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee.

Body-centered-cubic (bcc) nanocrystalline (nc) materials have unique strength advantage in compared with face-centered-cubic (fcc) nc equivalents. Despite this strength advantage, bcc nanocrystalline materials are hard to synthesize. Furthermore, the deformation mechanisms of these interesting materials are very poorly understood. In this presentation, we will exhibit our strategy to fabricate these high-strength materials, using nanocrystalline Ta as an example, as well as our experimental investigation results on deformation behavior of bcc nanocrystalline materials. In a deviation from the molecular dynamics simulations and the existing experimental observations on BCC nanocrystalline materials, the deformation of nanocrystalline Ta proceeds by partial dislocation mechanisms. We will discuss the implications of this surprising behavior in BCC nanocrystalline materials. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under contract of No.W-7405-Eng-48.

Z14.37
Rate-controlling deformation mechanism in nanocrystalline Ni. Yinmin Wang[1], E. Ma[2] and A. V. Hamza[1]; [1]Nanoscale Synthesis and Characterization Lab, Lawrence Livermore National Laboratory, Livermore, California; [2]Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, Maryland.

Electrodeposited nanocrystalline nickel with grain sizes well below 100 nm is a model material for investigating the deformation mechanism of nanocrystalline materials. Numerous studies have indicated that such deformation mechanisms are rate-related. In this poster, we will present the results of our analysis of repeated transition tests to monitor the coupled evolution of dislocation velocity and mobile dislocation density in plastically deforming nanocrystalline Ni. The stress relaxation series allow the determination of the activation volume in nanocrystalline Ni, indicating a rate-controlling mechanism different from that in coarse-grained Ni and those expected from grain boundary diffusion controlled processes. The high mobile dislocation exhaustion rates observed are also correlated with the unusually high apparent work hardening rate during the early stage of plastic deformation. It is proposed that the grain boundary diffusion controlled processes such as Coble creep and grain boundary sliding can be ruled out as a dominant mechanism for the nanocrystalline nickel studied.

Z14.38
A Study on the Tribological Properties of DLC Films Deposited with Different Reaction Gases. Yong Ki Cho, Kang Sam Kim, Woo Soon Jang, Kyoung Il Moon and Sung Wan Kim; Plasma Enhanced Technology Development Team, Korea Institute of Industrial Technology, Incheon, South Korea.

The effects of precursor gas composition and gas pressure on the structural and mechanical properties of DLC films has been studied by plasma enhanced CVD (PECVD) method. The effect of deposition temperature and gas composition on the hydrogen content in DLC films and the resulting tribological properties has been also reviewed. DLC films were deposited on D2, H13, M2 steels and various interlayers such as Si, Cr, Ti, nitriding were added to improve adhesion of DLC on steel substrates and to prevent diffusion at DLC/steel interfaces. The structural properties were evaluated by Raman spectroscope and RBS. The tribological behaviors of DLC films were investigated using a scratch tester and ball on disk tribometer. The failure mechanism of DLC deposited on steel substrates was examined using optical microscope and SEM/EDS. The results show that the best adhesion is achieved in Si interlayer and the friction coefficient improve with decrease hydrogen content in DLC films.

SESSION Z15: Deformation and Fracture of Nanostructured Metals IV
Thursday Morning, December 1, 2005
Constitution A (Sheraton)

8:00 AM *Z15.1
Deforming Inert-Gas Condensed Nanocrystalline Metals. Jurgen Markmann[2,1], Harald Rosner[1], Rainer Birringer[2] and Jorg Weissmuller[1,2]; [1]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany; [2]Technical Physics, Universitat des Saarlandes, Saarbrucken, Germany.

Recent experiments have brought new insights into the mechanisms which govern the plasticity of nanocrystalline metals. In particular, new opportunities have arisen from the finding that bulk nanocrystalline samples with extremely small grain size, between 8 and 30nm, prepared by the inert gas condensation technique, can be deformed to large true strain. The findings elucidate the roles of creep, partial dislocation activity along with its consequences, faulting and twinning, as well as grain boundary sliding and grain rotation. An emerging insight is that there is not 'the' deformation mechanism at small grain size; instead, deformation mechanism maps in, for instance, the parameter space spanned by the strain rate and the grain size, are more appropriate representations of the various processes that control the materials behavior. The talk will focus on some open questions which have arisen from the recent experiments, specifically the conditions for dislocation nucleation at grain boundaries and in the confined geometry of nanograins, and the issue of slip system selection and alignment in twinned grains.

8:30 AM *Z15.2
A Continuum Investigation on the Effect of Grain Size Distribution in Nanocrystalline Metals.
Jean-Francois R. Molinari and Derek H. Warner; Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland.

The ability to create fully dense nanocrystalline metals has led to materials with significantly higher strengths than their coarse-grained counterparts. Nevertheless, there are still major hurdles to overcome if these metals are to be used in a wide range of structural applications. Two of these hurdles are the large variability of strength and the lack of ductility observed in experimental tests. A possible solution may lie in the grain size distribution of the nanocrystalline samples. Through numerical simulations, the aim of this work is to model various grains size distributions and explain their influence on macroscopic behavior. A large spatial domain is required to accurately model microstructures with a wide range of grain sizes. A computationally inexpensive continuum approach must thus be utilized. The finite-element method is chosen as the core technique. The identification and implementation of the non-traditional constitutive properties associated with these materials are addressed through a hierarchical multiscale modeling and atomistic simulations. Competing deformation mechanisms that are incorporated in the model include grain boundary sliding, grain boundary migration and discrete dislocation events at the grain level. Results obtained for various widths of log-normal grain size distributions and several bi-modal distributions are exposed. We discuss the mechanical implications of stress-activated microstructure evolution. In particular, by allowing the microstructure to evolve during mechanical testing to mirror experimental data, insight is gained into the relationship between stress activated grain growth and the macroscopic mechanical response. In addition, numerical simulations reveal the interplay between localization of intragranular plasticity and grain boundary fracture. Finally, we conclude by suggesting optimum mixtures of grain sizes to achieve both high strength and ductility.

9:00 AM Z15.3
TEM studies of deformation and fracture of copper with high density nano-scale twins. Zhiwei Shan[1,2], Lei Lu[3], Minor Andrew[2] and Scott Mao[1]; [1]Mechanical Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania; [2]National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, Pennsylvania; [3]Institute of Metal research, Shenyang, China.

It has been experimentally established that the presence of high density nanoscale growth twins in pure copper can impart extremely high tensile strength and hardness relative to their coarse-grained counterpart. This suggests that unique plastic deformation mechanisms which are different from that in coarse-grained materials are operating. In this study, the deformation and damage evolution in electrodeposited pure copper with a high density of nanoscale growth-in twins were investigated by means of tensile straining in transmission electron microscope. The real time observations clearly reveal that twin boundaries serve as main dislocation source during the plastic deformation; twin boundary strength has been evaluated based on classical dislocation nucleation model; steps and jogs are observed to form through the interactions of dislocation and twin boundary; crack nucleate mainly from twin boundaries and follow a zigzag path; multi-twin ligaments which are formed along twin boundaries are observed to undergo extensive plastic deformation to the extent that many of them neck down to a chisel point. All of above observations are synthesized to formulate a mechanistic framework that provides new insights into the deformation and fracture mechanisms of copper with high density nanoscale twins.

9:15 AM Z15.4
3-D Atomistic Pathways of Slip Transmission across Twin Boundaries. Ting Zhu[1], Hyoung Gyu Kim[3,2], Amit Samanta[2] and Ju Li[2]; [1]Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts; [2]Department of Materials Science and Engineering, Ohio State University, Columbus, Ohio;

[3]Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology, Taejon, South Korea.

Recent experiments show that the introduction of nano-scale twins within ultrafine crystalline metals leads to significant increases in the strain-rate sensitivity. We explore in this work the role of twin boundaries in 3-D thermally activated dislocation motions and the consequent influences on the rate dependence of plastic flow. Using the reaction pathway sampling scheme of nudged elastic band and dimer methods, we identify the atomistic pathways of slip transmissions of both perfect and partial dislocations across the coherent twin boundaries. The corresponding activation energies and activation volumes are quantified, thus making contact with previous continuum analyses and experimental measurements.

SESSION Z16: Deformation and Fracture of Amorphous Metals IV

Thursday Morning, December 1, 2005
Constitution A (Sheraton)

10:00 AM Z16.1
Approaching the Universal Yield Point of Bulk Metallic Glasses from Molecular Dynamics Simulations. Futoshi Shimizu[1,2], Shigenoube Ogata[3], Hideo Kaburaki[2], and Ju Li[1], [1]Department of Materials Science and Engineering, Ohio State University, Columbus, Ohio; [2]Center for Promotion of Computational Science and Engineering, Japan Atomic Energy Research Institute, Tokyo, Japan; [3]Department of Mechanical Engineering, Osaka University, Osaka, Japan.

Most bulk metallic glasses (BMG) yield at about 2% strain in uniaxial tension/compression test. A careful analysis of the elementary shear behavior in contrast to crystalline concepts such the generalized stacking fault (GSF) energy reveal a particularly simple and direct explanation. We perform molecular dynamics (MD) simulations on 2-component model systems and a 5-component BMG system, observing and characterizing the nucleation and evolution of shear bands. Despite gross uncertainties in the interatomic interactions and the pre-deformation glass structure, our MD results give a reasonable account of the 2% universal yield point. The general concepts of glass rejuvenation and aging, which we call alienation and recovery process in the context of intense localized shear, and occurring mainly within a timescale of 1-100 atomic vibration periods, is postulated to play a critical role. This theory (various points has also been proposed by others) can explain why the yield point is relatively insensitive to the interatomic potential and the structure of the pre-deformed glass.

10:15 AM *Z16.2
Phase separation and nanocrystallization of bulk-forming metallic glasses. K. Hono, Natl Inst Mater Sci, Tsukuba, Japan.

To explain the nanocrystalline microstructure observed in Zr and Cu based bulk metallic glasses (BMG), many previous investigations reported glass phase separation prior to the crystallization of amorphous alloys. To verify such precursor reactions, we have carried out systematic investigations on the early crystallization stages of Pd-Si-Au, Cu-Zr-Ti, Zr-Ti-Be, Zr-Cu-Ni-Al-Ti, Zr-Ti-Cu-Ni-Be, and Al-Gd-Er-Ni metallic glasses, all of which used to be interpreted to phase separate into two glass phases. The amorphous alloys of the above systems were annealed right above the glass transition temperatures, and the microstructure evolution was studied. Utmost attention has been paid to separate chemical decomposition and structural transformation by the complementary use of TEM, 3DAP, and SAXS. No evidence for the glass phase separation has been obtained in the above systems. However, we found the systems that contain a pair of elements with positive heat of mixing can phase separate into two glassy phases without crystallization if alloy composition is carefully selected so that crystallization can be suppressed during solidification or post annealing. The La-Zr-Al-Cu-Ni system is one example of strong phase separating system, which decomposes into two phases during rapid solidification from a melt. Because of this dynamic phase separation, the microstructural scale scatters in a wide range, forming a surface fractal microstructure. Another example is the Cu-Zr-Al-Ag system, which can be melt-spun to a single phase amorphous and can phase separate by the post annealing process. Detailed microstructural characterization results as well as possible applications of two phase metallic glasses will be demonstrated.

10:45 AM *Z16.3
Search for Microscopic Mechanisms of Deformation and Shear Banding in Amorphous Metals. Mo Li, Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia.

Shear banding and shear localization are known for centuries. They occur typically in metals when severe plastic deformation is accumulated or if the deformation rate is high. For non-crystalline materials such as metallic glasses shear banding and shear localization are the normal deformation mode. They occur under a wide range of loading rates from the quasi-static to shock loading conditions and without much prior accumulation of plastic deformation. The purpose of our research is to discover the microscopic mechanisms and structural entities that are responsible for the phenomena. In this talk, I will focus on our recent efforts using extensive atomistic simulations. Intrinsic deformation behaviors are investigated with an aim to uncover material strength and ductility; and extrinsic deformation behaviors are also studied in samples with the presence of various imperfections. Significant (dynamic) hardening and exceedingly large intrinsic ductility were observed for metallic glasses. Local deformation and free-volume defects are characterized. From these findings, we developed a phenomenological theory to model the deformation and shear banding in mesoscopic scales. I will also discuss the microscopic mechanisms for initiation of shear banding.

11:15 AM Z16.4
Damage Initiation and Growth during High Cycle Fatigue in Zr-Based Bulk Metallic Glass. Brian C. Menzel and Reinhold H. Dauskardt; Materials Science and Engineering, Stanford University, Stanford, California.

A high-cycle stress-life fatigue study was conducted on a Zr-based bulk metallic glass to elucidate the anomalously low endurance limits that have been reported. The effect of stress state on damage initiation and propagation were investigated using uniaxial tension-tension, compression-tension and compression loadings. Distributed damage was observed to initiate very early in the fatigue process as either shear bands or mixed mode surface cracks under tension-tension loading. Damage initially grew under mixed mode loading conditions in the maximum shear stress direction. On reaching a characteristic size, they abruptly changed orientation and continued to grow as mode I cracks. Stable fatigue crack growth similar to that observed in the tension-tension tests was observed in specimens tested under tension-compression. Under compression loading failure occurred by unstable fracture along a shear band. A focused ion beam (FIB) was used to introduce well-defined distributions of initial defects to systematically elucidate damage initiation and growth processes. High-resolution techniques were used to characterize the effect of defect size, shape and orientation on damage initiation and the early stages of damage growth. FIB cross sections were taken of surface cracks to reveal subsurface growth behavior.

11:30 AM Z16.5
Localization and Percolation of Short Range Ordering in Bulk Metallic Glasses. Yunfeng Shi and Michael L. Falk; Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan.

Bulk metallic glasses (BMGs) have attractive mechanical properties but are prone to strain localization. Understanding this deformation mechanism is crucial for designing alloys with higher ductility and for incorporating BMG as a component in nano-phase composites. We have performed a large number of molecular dynamics simulations using one 2D and several 3D models of metallic glasses under both uniaxial tension and compression. These simulations indicate that the rate of quenching can have a significant effect on the degree of localization. By analyzing the strain rate dependence of the localization we note that there is a transition in the strain rate dependence at a critical degree of structural relaxation as indicated by the potential energy of the system prior to mechanical testing. This change in strain rate dependence corresponds to a structural transition from glasses that deform homogeneously to those that deform inhomogeneously in the low strain rate limit. Structural analysis indicates that this transition also corresponds to the onset of percolation of short-range order (SRO) in the glass. In all systems studied an increased degree of SRO promotes the development of shear bands. The nature of the percolation transition appears to be that of k-core percolation where each atom with high SRO must connected to a number of other high SRO atoms equal to one more than the spatial dimension.

11:45 AM Z16.6
Characterization of Shear Banding in Bulk Metallic Glasses using Full-Field Strain Measurements. Sven Bossuyt[1,2], R. Dale Conner[2], Danny Van Hemelrijck[1] and William L. Johnson[2]; [1]Mechanics of Materials and Constructions, Vrije Universiteit Brussel, Brussel, Belgium; [2]Engineering and Applied Science, California Institute of Technology, Pasadena, California.

Full-field strain measurement methods are powerful investigative tools for studying inhomogeneous deformation of materials. Digital image correlation algorithms allow full-field strain measurements from a series of images of a random speckle pattern applied to the surface of the material. Provided that the geometric relationship between the image and the object can be characterized, any imaging technique is suitable. We will present preliminary investigations of strain field measurements based on a digital image correlation technique, applied to shear banding in bulk metallic glass by means of multiple imaging methods (optical, scanning electron, and scanning probe) at different length scales. The digital image correlation technique will be compared to other full field strain measurement methods, such as optical interferometric techniques, and to discrete strain measurement techniques. Specific issues in the analysis of deformation fields with shear bands -especially at the macroscopic scale, where the shear band presents itself as a discontinuous displacement- will be adressed, and linked to related issues in computer simulation of shear banding behaviour.

SESSION Z17: Amorphous Metals: Ductility and Dual Phase Systems I

Thursday Afternoon, December 1, 2005
Constitution A (Sheraton)

1:30 PM *Z17.1

Flow and Fracture Toughness Investigations on Metallic Glasses. John J. Lewandowski, Department of MS&E, Case Western Reserve University, Cleveland, Ohio.

The flow and fracture behavior of a variety of different bulk metallic glasses has been investigated under a wide range of stress states and temperatures. The effects of superimposed hydrostatic pressure on the flow and fracture behavior will be described from experiments conducted at room temperature and elevated temperatures, followed by a summary of the effects of notches on the toughness of a number of different metallic glass systems in comparison to the behavior of conventional structural materials. Differences in the toughness between different metallic glass systems will be correlated with their elastic constants in order to demonstrate intrinsic differences between the behavior of some bulk metallic glasses. The implications of these observations will be discussed.

2:00 PM Z17.2

Enhanced Low-Temperature Ductility of Nanoscale Metallic Glasses. Alex S. Donohue[1], Frans Spaepen[1], Amit Misra[2] and Richard G. Hoagland[2]; [1]Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts; [2]MST-8, Los Alamos National Laboratory, Los Alamos, New Mexico.

Metallic glasses have high yield strengths but their ductility at low temperatures is often limited by plastic instabilities (shear bands). We have investigated the room-temperature deformation of nanoscale metallic glasses as a component in a crystal/glass multilayer composite. Self-supported foils of alternating 90 nm Cu and 10 nm Pd-Si layers were deposited by ion-beam sputtering. The samples were deformed at room temperature in tensile tests and by rolling. Rolled foils exhibited plastic strains greater than 200% in the rolling direction. Cross-sectional TEM showed uniform reduction in thickness of both layers. The evolution of the initial strong [111] texture of the Cu layers was studied by X-ray diffraction. The metallic glass layers deformed uniformly, without any evidence of shear bands. The enhanced plastic stability of the constrained metallic glass will be discussed, along with the mechanism of slip transfer from one crystalline layer to another through the intervening nanoscale glassy layer.

2:15 PM *Z17.3

Phase Separation and Enhancement of Plasticity in Glass Forming Alloys. Eun Soo Park, Hye Jung Chang, Byung Joo Park, Eun Young Jeong and Do Hyang Kim; Dept. of Metall. Eng., Yonsei University, Seoul, South Korea.

Addition of alloying element having positive enthalpy of mixing with constituent elements can induce the two-glass phase separation in glass forming alloys. In the multi-component systems with high glass forming ability, there is a high possibility for phase separation due to the difference in the values of the heat of mixing between the binary combinations. Recently, it has been shown that phase separation into two-glass phases occurs in (Zr, La)-Al-Cu-Ni and (Ti,Y)-Al-Co glass forming alloys [1,2]. In the present study, results on the phase separation in Ni-Nb-(Co, Nd, La), (Nd, Gd, Ti, Nb)-Al-Fe, (Cu, Ag, Co)-(Zr, La, Nb, Ta)-Al and (Ti,Y)-Al-Co alloys will be presented. The alloys undergo liquid phase separation in the under-cooled liquid state and subsequently solidifies into two different amorphous phases. Besides the primary phase separation, secondary phase separation occurs due to the supersaturation of the primary separated liquids as the temperature decreases. We will also show that compositional inhomogeneity resulting from the positive heat of mixing between binary pairs can play a role in enhancing plasticity of the bulk metallic glasses. For example, the Zr-Y-Cu-Al bulk metallic glasses show enhanced plasticity in the limited composition range, i.e. when small amount of Y is added, indicating that addition of alloying element having positive enthalpy of mixing with the constituent elements can lead to the enhancement of plasticity. [1] A. A. Kundig , M. Ohnuma , D. H. Ping , T. Ohkubo and K. Honom, Acta Mater 52, 2441 (2004) [2] B.J. Park, W. T. Kim and D. H. Kim, Appl. Phys. Lett., 85 6353 (2004)

2:45 PM Z17.4

Novel Graphite-Reinforced Bulk Metallic Glass Composites with High Ductility. Marco E. Siegrist and Jorg F. Loffler; Laboratory of Metal Physics and Technology, ETH Zurich, Zurich, Switzerland.

Graphite particles were introduced into an amorphous Zr52.5Cu17.9Al10Ni14.6Ti5 (Vit105) matrix with the aim of increasing plasticity and improving the wear and friction properties of monolithic metallic glass. The graphite content was varied from 5-30 vol%. These samples were produced via a multi-step melt processing route, and good particle distribution was achieved using a levitation mixing procedure. By adjusting the processing parameters part of the graphite can be transformed into ZrC, which allows a systematic change in mechanical properties. This contribution describes the thermophysical and mechanical properties of these graphite/ZrC Bulk Metallic Glass matrix composites. The crystallization sequence of the matrix was studied using differential scanning calorimetry, and the amorphous structure was confirmed by x-ray diffraction. The effect on composite hardness, fracture strength and ductility of varying the reinforcement fractions and carbide content was investigated. We found that graphite causes a decrease in hardness, whereas carbide formation leads to an increase compared to the monolithic matrix material. The best mechanical properties were observed at low volume fractions of graphite where high plastic deformation combined with a fracture strength of 1.7 GPa was achieved. The effect of particle reinforcement on fracture behavior was studied using high-resolution scanning electron microscopy.

SESSION Z18: Amorphous Metals: Ductility and Dual Phase Systems II

Thursday Afternoon, December 1, 2005
Constitution A (Sheraton)

3:30 PM *Z18.1

Strain measurement in metallic glasses and metallic-glass-matrix composites by means of x-ray scattering. Todd Hufnagel, Materials Science and Engineering, Johns Hopkins University, Baltimore, Maryland.

X-ray and neutron diffraction have long been used to measure elastic strains (and thus stresses) in crystalline solids. More recently, the availability of high-energy synchrotron beamlines has made it possible to study the development of strain in crystalline materials in situ during loading, and to measure strain in amorphous materials as well. In this talk, we discuss the application of these techniques to the study of both metallic-glass-matrix composites and single-phase metallic glasses. Several groups have developed materials consisting of an amorphous metallic matrix reinforced by a ductile crystalline second phase, with the goal of achieving enhanced ductility by multiplication of shear bands. Our group (and others) have examined the development of strain in crystalline particles in these composites during uniaxial compression. In the case of a Zr-based metallic glass reinforced by Ta-rich bcc particles, the results show that the particles yield at a relatively low applied stress but do not strain harden significantly due to the constraint imposed by the surrounding amorphous matrix. At higher loads, a stress concentration resulting from the plastic misfit strain between the particles and matrix induces localized yielding of the matrix around the particles, releasing the constraint and allowing the particles to strain harden rapidly. The determination of strain in crystalline materials is relatively straightforward (because the interplanar spacings can be calculated directly from the Bragg equation). In amorphous materials the situation is more complex. One approach is to measure the scattered intensity to a large value of the scattering vector q, which, with the proper corrections and normalization applied, can be Fourier-transformed to yield a radial distribution function (RDF). In measurements done under load, the strain can be determined by measuring changes in the near-neighbor atomic spacing determined from the RDF. Alternatively, it has been proposed that the strain can be determined directly (and much more conveniently) from shifts in the position of the first scattering maxium. We discuss the relative merits of both approaches as applied to both single-phase metallic glasses and metallic-glass matrix composites. Recent experimental results on single-phase glasses suggest that the two approaches may yield somewhat different values for the elastic constants. We will discuss the reasons for the differences, as well as their physical implications.

4:00 PM *Z18.2
Microstructure Design for Ductilization of Nanocrystalline and Amorphous Metals. J. Eckert, J. Das, K. B. Kim and F. Baier; Materials and Geo Sciences, Physical Metallurgy Division, Darmstadt University of Technology, Darmstadt, Germany.

Nanocrystalline and amorphous metals and alloys are well-known to have attractive mechanical properties that are often superior to the performance of conventional coarse-grained crystalline alloys. As a result these metastable materials are attractive candidates for a variety of structural applications. However, one major drawback that still limits such applications is the pronounced tendency of amorphous and nanocrystalline materials for shear localization, especially upon room temperature deformation under unconstrained conditions. Accordingly, finding ways to improve their plastic deformability and toughening behavior are an urgent task for further materials development. To circumvent such limitations, over the last years the concept of creating heterogeneous materials with nanosructured or amorphous matrix and different type and length-scale of second phases has been followed to control the mechanical properties by proper alloy and microstructure design. The recent developments along this line will be summarized and new results for different types of alloys in Ti-, Zr-, and Cu-base systems will be presented to illustrate how the mechanical properties can be tuned by appropriate microstructure control. This will cover selected examples for nanostructured alloys with ductile primary precipitates in a eutectic matrix, simple eutectic structures as well as bulk metallic glasses with ultrafine-scale structural inhomogeneities. In all these cases the details of metastable phase formation are closely linked with otimized processing conditions required to form the desired microstructure. The possible mechanisms that govern the deformation behavior will be critically assessed and the microscopic processes will be linked with the overall plastic deformation and fracture of the material. This work is supported by the European Commission under contract MC-RTN-CT-2003-504692 "Ductile BMG Composites".

4:30 PM Z18.3
High-Strain-Rate Dynamic Mechanical Properties of a W-Reinforced Zr-Based Bulk Metallic Glass Composite. Morgana Martin[1], Naresh N. Thadhani[1], Laszlo Kecskes[2] and Robert Dowding[2]; [1]Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia; [2]Weapons and Materials Research Directorate, U.S. Army Research Laboratory, Aberdeen Proving Ground, Maryland.

The structural/mechanical behavior of zirconium-based (Vitreloy106) bulk metallic glass reinforced with tungsten particles are evaluated using elastic and plastic property measurements via static and dynamic compression tests performed on rod shaped samples. Reverse Taylor anvil-on-rod impact tests combined with high-speed digital photography and velocity interferometry are used to obtain qualitative and quantitative information about the transient deformation and failure response of the composites. The deformation and failure mechanisms of recovered impact specimens are also being characterized and correlated with their structure and tungsten phase distribution. The results of these experiments and initial attempts at validating constitutive equations based on homogeneous/inhomogeneous plastic/viscous flow in glassy and glassy-crystalline composites will be presented. Funded by ARO Grant No. E-48148-MS-000-05123-1 (Dr. Mullins program monitor)

4:45 PM Z18.4
Copper Fiber Reinforced Zr41.2Ti13.8Cu12.5Ni10.0Be22.5 Bulk Metallic Glass. Prashant Wadwa, Jochen Heinrich and Ralf Busch; Mechanical Engineering, Oregon State University, Corvallis, Oregon.

Highly conductive Cu fibers were introduced into Zr41.2Ti13.8Cu12.5Ni10Be22.5 (Vitreloy1TM) BMG of poor conductivity to produce a composite with a thermal anisotropy. The main challenge in processing was to avoid the dissolution of Cu fibers into the matrix because Cu has a negative heat of mixing with most of the matrix components. The composites with circular and square cross-sections with the volume fraction ranging from 7% to 60% were processed successfully by pressure-gravity infiltration. Differential scanning calorimetry (DSC) showed that the BMG matrix remained predominantly amorphous after adding up to 60% volume fractions of Cu fibers. The limited crystallization at the Cu/Vitreloy1TM interface observed under optical microscopy. This crystallization is attributed to the heterogeneous nucleation starting from the Cu/Vitreloy1TM interface due to the presence of Cu fibers, which act as nucleation sites, followed by the growth in the areas surrounding the fibers with enhanced Cu concentration. The concentration profile of Cu into the matrix was simulated and related to the crystallization. A combination of 2-dimensional triangular and square ordering of the fibers was observed in the composite samples. X-ray diffraction patterns of the composites showed the peaks from the reinforced fibers and crystals around the Cu/Vitreloy1TM interface superimposed on the broad diffuse maxima from the amorphous phase. Finally, the best processing parameters in terms of processing time and temperature were determined for the composite reinforced with 60 volume percent fibers. One promising application of this metallic glass matrix composite could be in the meso- and microscale heat exchanger, where high heat transfer in one direction is required.