

## MM 13: Liquid and Amorphous Metals III: Mechanical properties

Time: Monday 15:45–17:30

Location: H52

MM 13.1 Mon 15:45 H52

**Thermal relaxation of metallic glasses: Influence on mechanical properties and structure studied by molecular dynamics simulations** — ●TOBIAS BRINK and KARSTEN ALBE — Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Metallic glasses show a transition from homogeneous deformation to shear banding depending on temperature and strain rate, with shear banding being the typical mechanism at ambient conditions. The critical values for the transition are determined by the glass composition but should also depend on the structure of the glass. We use molecular dynamics computer simulations to investigate the deformation mechanism in as-quenched and annealed  $\text{Cu}_{64}\text{Zr}_{36}$  metallic glasses. Due to the very high strain rates in the simulation, the as-quenched glass only exhibits shear banding at low temperatures. In contrast, shear banding occurs at the same strain rates well above room temperature in samples that were annealed for several hundred nanoseconds near  $T_g$ . Additionally, properties like structure, short-range order, potential energy, free volume, and vibrational properties (boson peak) change with annealing time, indicating a more relaxed metallic glass, i.e., a decreased fictive temperature. We discuss the shear banding at elevated temperatures in terms of these structure-related changes. Furthermore, we investigate the influence of thermal relaxation on pre-existing shear bands and compare their structural relaxation to that of the matrix.

MM 13.2 Mon 16:00 H52

**Ductility changes in the bulk metallic glass former PdNiP due to micro-alloying by adding Cobalt and Iron** — ●NIKLAS NOLLMANN, ISABELLE BINKOWSKI, HARALD RÖSNER, and GERHARD WILDE — Universität Münster

Deformation of bulk metallic glasses (BMGs) at low temperatures and high stresses lead to an inhomogeneous plastic flow. During plastic deformation, bulk metallic glasses show almost no ductility and fail alongside shear bands where the strain is localized. This limited ductility has led to substantial effort in order to improve the plasticity of BMGs. We investigated PdNiP based glasses which feature a rather high ductility in bending, compared to other bulk metallic glasses. By the use of micro alloying, the mechanical properties of metallic glasses can be influenced. Adding Iron or Cobalt to the PdNiP BMG leads to a huge change in ductility. To investigate the reason for these changes, the Poisson's ratios were determined by ultrasonic measurements. Interestingly, the plasticity is not reflected by the high Poisson ratio, which remained unaffected by microalloying within the accuracy of the measurement. While analyzing the dependence of the ductility of the present glasses on relaxation treatments, we utilize the fictive temperature concept to investigate the impact of minor alloying on the relative amount of free volume. Also the critical fictive temperature was measured to characterize the ductility of the new BMGs.

MM 13.3 Mon 16:15 H52

**Synthesis and Mechanical properties of Cu-Zr metallic Nanoglasses** — ●SREE HARSHA NANDAM<sup>1</sup>, RUTH SCHWAIGER<sup>2</sup>, JULIA IVANISENKO<sup>1</sup>, XIAOKE MU<sup>1</sup>, and HORST HAHN<sup>1,3</sup> — <sup>1</sup>Institute for Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany. — <sup>2</sup>Institute for Applied Materials, Karlsruhe Institute of Technology, D-76344, Eggenstein-Leopoldshafen, Germany. — <sup>3</sup>KIT-TUD Joint Research Laboratory Nanomaterials, Institute of Materials Science, Technische Universität Darmstadt (TUD), Jovanka-Bontschits-Str. 2, D-64287 Darmstadt, Germany.

Bulk  $\text{Cu}_{50}\text{Zr}_{50}$  metallic nanoglass (NG) specimens were synthesized using a modified Inert Gas Condensation method fitted with magnetron sputtering instead of thermal evaporation of the starting alloy. As-sputtered powder had a particle size of about 5–8 nm as observed in a transmission electron microscope. X-ray diffraction of the synthesized pellet confirmed its amorphous nature and energy dispersive spectroscopy showed the equiatomic  $\text{Cu}_{50}\text{Zr}_{50}$  alloy. Differential scanning calorimetry revealed a crystallization temperature of the NG specimen of around 475°C. Vickers microhardness and compression tests of NG  $\text{Cu}_{50}\text{Zr}_{50}$  specimens were performed. Similar tests were also carried out on metallic glass ribbons of a similar composition. In order

to compare elastic modulus of the nanoglass samples and of the melt spun ribbons, nanoindentation tests were performed. Possible reasons for the differences in the mechanical behavior of the melt spun ribbons and nanoglass samples will be discussed in the present paper.

15 min. coffee break

MM 13.4 Mon 16:45 H52

**Size effects in the deformation behavior of metallic nanoglass pillars** — ●OMAR ADJAOUD and KARSTEN ALBE — Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Jovanka-Bontschits-Str. 2, D-64287 Darmstadt, Germany

Metallic nanoglasses (NGs) are amorphous materials with an inhomogeneous microstructure which consists of glassy grains connected by glass-glass interfaces. The metallic NGs can be produced by consolidating nanometer-sized glassy spheres which are prepared by inert-gas condensation. Glass-glass interfaces of metallic NGs are characterized by an excess free volume and a lack of short range order. This characteristics of the interfaces prevent the shear strain localization during the deformation of the metallic NGs, which leads to an enhanced plasticity in metallic NGs as compared to the bulk metallic glasses of the same chemical composition. In this contribution, we present the results of MD simulations on size effects in the deformation behavior of  $\text{Cu}_{64}\text{Zr}_{36}$  and  $\text{Pd}_{80}\text{Si}_{20}$  nanoglass pillars by varying systematically the diameter of the pillars from 4.5 nm to 54 nm. The results reveal that the pillars deform homogeneously due to their inhomogeneous microstructure. In contrast metallic glass pillars, with the same chemical composition, fail along a single shear band. Consequently, we assume that the deformation behavior of metallic glass pillars can be controlled by changing their microstructure rather than their size.

MM 13.5 Mon 17:00 H52

**Analysis of the impact of nanocrystalline precipitates on the deformation behavior of a ZrCu based metallic glass** — ●MARIUS GERLITZ<sup>1</sup>, TOBIAS BRINK<sup>2</sup>, MARTIN PETERLECHNER<sup>1</sup>, HARALD RÖSNER<sup>1</sup>, KARSTEN ALBE<sup>2</sup>, and GERHARD WILDE<sup>1</sup> — <sup>1</sup>Institut für Materialphysik, WWU Münster, Germany — <sup>2</sup>Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Due to the absence of dislocations in amorphous materials, plastic deformation of metallic glasses is carried by localized shear bands. In this work, the influence of nanocrystalline precipitates on the formation of shear bands is surveyed. To control the size and distribution of nanocrystallites within the amorphous phase, a crystallization study of the time and temperature dependence is carried out using differential scanning calorimetry (DSC). Structural analysis of partial crystallized samples is accomplished by transmission electron microscopy (TEM). Subsequently to the annealing procedure, the deformation of the material is enforced via cold rolling using a two-high rolling mill. By this means shear bands are induced inside the material. TEM analysis of the annealed and deformed metallic glass reveals the interaction between shear bands and nanocrystallites. Experimental results are compared to results of molecular dynamics simulations concerning different types of shear band particle interactions. The financial support of the DFG is gratefully acknowledged.

MM 13.6 Mon 17:15 H52

**Shear band diffusion in cold rolled Pd40Ni40P20 bulk metallic glass micro-alloyed with Co** — ●MIKHAIL SELEZNEV<sup>1,2</sup>, ISABELLE BINKOWSKI<sup>1</sup>, SERGIY DIVINSKIY<sup>1</sup>, and GERHARD WILDE<sup>1</sup> — <sup>1</sup>Institute of Materials Physics, University of Münster, Münster, Germany — <sup>2</sup>Togliatty State University, Togliatty, Russia

Bulk metallic glasses (BMGs) appear to be promising materials due to a unique combination of glass-like elastic limit, hardness, corrosion resistance but without a ceramic-like brittleness. Although BMGs show some plasticity, their application is hindered due to deformation localization in shear bands (SBs). The shear banding mechanism seems to be the main reason for early failure in deformation and a key parameter that governs plasticity of BMGs.

Micro-alloying of the master alloy Pd40Ni40P20 glass with Co (1 at.%) was found to increase the plasticity during compression by 13% [1]. This strong enhancement was accompanied by significant branch-

ing of SBs which could be due to a change in the work softening process and also by an increase of the free volume. To clarify a possible correlation between the micro alloying-induced plasticity increase and the SB structure changes, the atomic diffusivity was measured in deformed samples by the radiotracer technique and the results are discussed in

relation to the Co-free PdNiP glass.

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1. Nollmann N. et al. *Scr. Mater.* 111, 119 (2015)