MM 36 Amorphous and Liquid Materials IV

Time: Thursday 16:30–18:00 Room: IFW B

MM 36.1 Thu 16:30 IFW B

Heterogeneous dynamics in MD simulated constant-shear-rate deformations of amorphous $Ni_{50}Zr_{50}$ — •Kevin Brinkmann and Helmar Teichler — Institut für Materialphysik d. Univ. Göttingen, 37077 Göttingen

Molecular-dynamics simulations of viscoplastic deformation of amorphous $Ni_{50}Zr_{50}$ show — in agreement with experiments — a characteristic stress-strain curve with an elastic linear regime for small strains, a pronounced stress overshoot and a drop to a constant flow stress, the latter indicating the transition into the steady-state flow regime. From analyzing changes in the local topological short range order, it is found that at $T = 700$ K strains below the upper yield point induce moderate, spatially homogenous atomic rearrangements only. Most of them are reversible, accounting for (an)elastic contributions. The marked decrease in stress between upper and lower yield point is due to a growing number of local rearrangement centers in the Zr-matrix. These rearrangements appear spatially heterogenous in the simulation cell, gradually filling a plane of maximum shear stress and forming a (micro-)shear-band. The interior of the shear-band exhibit significantly altered properties compared to topologically unchanged regions indicating a structural change in the shear-band resembling rejuvenation. At $T = 1000$ K ($T_g = 1050$ K), stress localization, is depressed leading to a highly unorganized formation of the structurally altered regions, rapidly covering the whole sample.

MM 36.2 Thu 16:45 IFW B

Rheology of selected metallic glasses — •Andreas A. Kündig[1], Thomas Schweizer[2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Swiss Federal Institute of Technology (ETH) Zürich, Wolfgang-Pauli-Str. 10, CH-8093 Zürich, Switzerland — [2]Polymer Physics, ETH Zürich, CH-8093 Zürich, Switzerland

Metallic glasses exhibit a superplastic forming regime at temperatures above the glass transition temperature (T_g) and below the crystallization temperature (T_x). The formability in this range is limited by the onset of crystallization, which typically causes the characteristic properties of metallic glasses to deteriorate. In this work, the direct rheological parameters of selected low-temperature metallic glasses (Cu-, Mg-, and Au-based) were measured in parallel plate geometry. Using this technique, absolute values for the elastic modulus and the loss modulus as a function of the temperature are obtained, allowing us to compare formability in the different systems. Additionally, strain-rate sensitivity, dynamic viscosity and the onset of crystallization were measured to determine optimum forming parameters. The results are discussed with respect to more easily accessible estimates based on thermal values, such as the extension of the undercooled liquid regime $\Delta T(= T_x - T_g)$ or, normalized to the liquidus temperature (T_l), the value $S = \Delta T/(T_l - T_g)$.

MM 36.3 Thu 17:00 IFW B

Microscopic processes during shear transformation of metallic glasses - a Molecular Dynamic study — •Mareike Zink, Konrad Samwer, and Stefan G. Mayr — 1. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The atomic-scale processes which underlie shear transformation in the model glass, CuTi, were studied with classical Molecular Dynamic computer simulations. The formation of shear bands and dynamical heterogenities below the glass transition temperature could be investigated as well as the influence of boundary conditions. Microscopic results were compared with macroscopic behavior and elastic constants [1]. The shear rate dependence of the shear modulus for various temperatures relected time scales for alpha-relaxation and flow processes in the model glass.

Financially supported by the DFG - SFB 602.

[1] *W.L. Johnson and K. Samwer,*PRL 95, 195501 (2005)

MM 36.4 Thu 17:15 IFW B

Effect of mechanical deformation on the quasicrystallization of Zr-based metallic glasses — •Sergio Scudino[1], Hergen Breitzke[2], Klaus Lüders[2], Ludwig Schultz[3], and Jürgen Eckert[1] — [1]FB 11 Material- und Geowissenschaften, FG Physikalische Metallkunde, Technische Universität Darmstadt, Petersenstrasse 23, D-64287 Darmstadt, Germany — [2]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [3]IFW Dresden, Institut für Metallische Werkstoffe, Postfach 270016, D-01171 Dresden, Germany

The devitrification of melt-spun $Zr_{57}Ti_8Nb_{2.5}Cu_{13.9}Ni_{11.1}Al_{7.5}$ glassy ribbon is characterized by the formation of a metastable quasicrystalline phase during the first stage of the crystallization process. To investigate the effect of the mechanical deformation on the formation of quasicrystals, the glassy ribbon was submitted to ball milling. The mechanical treatment drastically affects both the thermal stability and the microstructure evolution upon heating. In particular, primary quasicrystal formation is progressively suppressed with increasing milling time. The results reveal that oxygen, which is introduced during milling, is responsible for the modified crystallization behavior by selectively reacting with zirconium. However, the suppression of quasicrystal formation can be reversed by an appropriate variation of the chemical composition. This indicates that quasicrystal formation from glassy precursors is governed by the chemical composition rather than by the occurrence of a special quenched-in short-range order. This work was supported by the German Science Foundation under grants Ec 111/10-1,2 and Lu 217/17-1.

MM 36.5 Thu 17:30 IFW B

Structure and electronic transport of a-$Cu_x(Mn_{50}Al_{50})_{100-x}$ — •Jan Rauchhaupt and Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

Amorphous phases are precursors of the cristalline state and hence interesting for investigating fundamental structure forming processes and the related evolvement of electronic transport.

In the last years we could show by many different classes of alloys (from e.g. metals, semiconductors, ionic glasses, to those containig transition metals) that the alloys organize themselves under the influence of a resonance interaction between two global systems, namely the electronic system of the valence electrons and the forming static structure. For TM-containing Al-alloys we discussed our results as a resonance interaction of the Al-p-electrons with the empty d-states of the TM via hybridisation. This model needs to be refined when a second transition metal comes in play.

The amorphous ternary alloys of Cu, Mn and Al were produced in situ at T=4 K in a HV-cryostate and were annealed up to the cristalline state. The static structure, by means of electron diffraction, the resistivity and the thermopower were measured as a function of temperature and composition.

MM 36.6 Thu 17:45 IFW B

Positron annihilation spectroscopy of glassy $Mg_{65}Cu_{25}Y_{10}$ ribbons — •Dirk I. Uhlenhaut[1], Alberto Castellero[1], Florian Dalla Torre[1], Carlos Palacio[2], Nikolay Djourelov[2], Danny Segers[2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Swiss Federal Institute of Technology (ETH) Zürich, Wolfgang-Pauli-Str. 10, CH-8093 Zürich, Switzerland — [2]Department of Subatomic and radiation physics, Gent University, Proeftuinstraat 86, B-9000 Gent, Belgium

The well-known Mg-Cu-Y amorphous alloys become brittle during quenching or ageing. The ductile state is obtained at high quenching speeds, while a low copper content delays embrittlement during room-temperature ageing. Here we report on positron annihilation spectroscopy of amorphous ribbons from the $Mg_{65}Cu_{25}Y_{10}$ bulk glass-former, measuring positron lifetime, Doppler broadening and coincidence Doppler broadening as a function of the alloy's room temperature age. A decrease in positron lifetime and changes in the Doppler peak width, corresponding to a reduction of free volume, were seen during the time the embrittlement takes place at room temperature. Coincidence Doppler broadening spectroscopy revealed changes in the immediate environment of the free volume during annihilation. Analogies with calorimetric measurments and mechanical tests are discussed.