MM 66: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses VI - mechanical properties

Time: Thursday 15:45–17:15 Location: IFW A

Topical Talk MM 66.1 Thu 15:45 IFW A

Molecular Dynamics Simulation On The Avalanche Dynamics and the microstructural evolution in the so called elastic region of the Cu50Zr50 — •Alexandra Lagogianni, Marius Milnikel, and Konrad Samwer — I. Physikalisches Institut, Georg-August Universität Göttingen,Göttingen,Deutschland

We present results on the study of the avalanche dynamics of a 3D Cu50Zr50 system by means of molecular dynamics simulations. The system is subjected to a finite strain rate deformation scheme and to the athermal quasistatic protocol. We find that the avalanches occur from the beginning of the so called elastic region. The critical exponents obtained by the stress drop sizes and time duration distributions for the elastic and plastic region are similar, indicating that the difference in the deformation mechanisms that govern the two regions are not depicted in these kind of statistical profiles of the avalanches. The two regions differ in the way that the number of the avalanches, their average size and the instantaneous shear modulus evolves with strain. Additionally the stress drops are accompanied by the appearance of regions in the systems that undergo shear transformations and consist of characteristic categories of clusters. The percentage of the clusters in these regions evolves upon deformation in a correlated way with the stress and the energy of the system. The overall decrease/increase of their number upon deformation is taking place by a continuous structural loop where an initial type of cluster transforms into an intermediate one of the same coordination number and consecutively this new type transforms back again to the initial state.

MM 66.2 Thu 16:15 IFW A

Mechanical properties of Palladium based bulk metallic glasses during deformation — •Niklas Nollmann, Vitalij Hieronymus-Schmidt, 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 this plastic deformation the strain is localized in so called shear bands. Bulk metallic glasses show almost no ductility and fail alongside shear bands where the strain is localized. In our study we investigated PdNiP based glasses. PdNiP samples were deformed by cold rolling in several steps and the wave velocity was measured with an ultrasonic device after each step. Thus the dependence of the Poisson's ratio on the deformation state was observed. We also analyzed modifications of the mechanical properties of the metallic glass by micro alloying. Adding Iron or Cobalt to the PdNiP BMG leads to a huge change in ductility. 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 [1].

[1] G. Kumar, P. Neibecker, Y. H. Liu and J. Schroers, Nature communications 4, 1536 (2013).

MM 66.3 Thu 16:30 IFW A

microstructural fluctuations at equilibrium and under tensile deformation of a Cu-Zr model glass by molecular dynamics simulations — •pablo palomino rico[1], dimitris papageorgiou[2], and giorgos evangelakis[1] — [1]Department of Physics, University of Ioannina, Ioannina 45110 Greece — [2]Department of Materials Science and Engineering, University of Ioannina, Ioannina 45110, Greece

We present Molecular Dynamics Simulations results referring to microstructural fluctuations of a Cu65Zr35 computer glass at equilibrium and under tensile deformation. We found that at equilibrium the atoms perform short distance atomic displacements, which are not homogeneously distributed along the system, showing high and low mobility zones, and take place with the concomitance of 2 or 3 neighboring atoms, resulting in local changes of the microstructure. Inspection of the potential energy landscape of the process indicates the presence of a β-relaxation event. Under tensile deformation, those movements increase in number and distance, the high mobility zones group larger number of particles participating in such displacements and furthermore, they contribute by as much as 40% in the accommodation of the volume gain that takes place during the straining process through clusters* transformations of Icosahedra to Dodecahedra or Cuboctahedra. These results could be useful in the understanding of phenomena like aging and creep relaxation in Metallic Glasses.

MM 66.4 Thu 16:45 IFW A

Probing the mechanical properties of metallic glasses using avalanche dynamics — •Carlos Herrero-Gómez and Konrad Samwer — 1 Physikalisches Institut, Georg-August Universität Göttingen, Göttingen, Germany

Amorphous solids have been discovered, fabricated and used by mankind for more than 2000 years. Despite this fact the microscopic origin of the plasticity in such materials remain nowadays elusive. Recently such problem have been approached from the perspective of the avalanche dynamics, which allows to analyze correlations during deformation [1]. We report the avalanche analysis of several deformation experiments in metallic glasses. Based in creep tests of PdCuSi metallic glasses, we report a crossover on the deformation behavior that we associate to the strain rate [2]. In addition, we use creep tensile experiments on several amorphous materials to show that the avalanche statistics are reproduced in different systems. Finally we analyze the effect of an external magnetic field on the mechanical properties of a magnetostrictive magnetic metallic glasses, in order to study the magneto-mechanical coupling. Financial support from the ITN-FP7 Marie Curie program VitriMetTech N. 607080 is thankfully acknowledged.

Literature:

[1] Salje et al Annu. Rev. Condens. Matter Phys. 5.1 (2014): 233-254.

[2]C.Herrero-Gómez and Konrad Samwer. Scientific Reports 6 (2016).

MM 66.5 Thu 17:00 IFW A

Transformation-mediated ductility in bulk metallic glass composites — •Daniel Sopu[1], Mihai Stoica[1], and Jürgen Eckert[2] — [1]IFW Dresden, Helmholtzstr. 20, 01069, Institut für Komplexe Materialien, Dresden, Germany — [2]Erick Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, A-8700 Leoben, Austria

We investigate the influence of various critical structural aspects such as crystallite phase, size and distribution on the deformation behavior of Cu64Zr36 bulk metallic glass composites. By using molecular dynamics simulations we provide an effective strategy to control the strain localization in these composites. We show that the shear band nucleation and localization is strongly influenced by the martensitic transformation of the B2 CuZr nanocrystallites. Moreover, the martensitic transformation perturbs the local atomic strain around the nanocrystals leading to broadening of the shear bands when approaching these nanocrystals. The width increase of a shear band reduces the elastic shear stress in the vicinity of the nanoparticles, and thereby impedes the further propagation and formation of critical shear bands. This unique deformation mechanism promote ductility and work hardening in bulk metallic glass composites.