MM 61: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses V - dynamical response

Time: Thursday 11:45–13:15 Location: IFW A

Topical Talk MM 61.1 Thu 11:45 IFW A

Towards a dissipative atomic-scale theory of the dynamical response of metallic glasses — •Alessio Zaccone — University of Cambridge, U.K.

One of the most fruitful concepts to characterize the deformation of metallic glasses has been that of nonaffine displacements [1]-[3], defined as additional atomic motions on top of the affine displacements prescribed by the macroscopic strain tensor. Using this, and recognizing that nonaffine displacements ultimately originate from the breaking of local centrosymmetry on every atom in the amorphous lattice [4], opens up the possibility of formulating a "nonaffine lattice dynamics" of metallic glasses. I will show that new viscoelastic sum-rules can be derived from a system-bath Hamiltonian of the Zwanzig-Caldeira-Leggett type which leads to a low-temperature Generalized Langevin Equation for dissipative nonaffine motions. This approach can be combined with a mode-coupling result [5] for the atomic-scale damping coefficient (a non-Markovian friction which accounts for memory-effects) to give predictions of dynamic response in agreement with experimental results of mechanical spectroscopy. The approach also provides a robust connection with the vibrational density of states. Finally, a possible route to explain the beta-relaxation process with this approach is outlined.

[1] A. Zaccone & E. Scossa-Romano, Phys. Rev. B (2011). [2] T.C. Hufnagel, C.A. Schuh, M.L. Falk, Acta Mater. (2016). [3] S. V. Ketov, Y.H. Sun, et al., Nature (2015). [4] R. Milkus and A. Zaccone, Phys. Rev. B (2016). [5] L. Sjoegren and A. Sjoelander, J. Phys. C: Solid State Phys. (1979).

MM 61.2 Thu 12:15 IFW A

Plastic deformation mechanism of metallic glasses — •Vitalij Hieronymus-Schmidt[1], Harald Rösner[1], Alessio Zaccone[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Deutschland — [2]University of Cambridge, Cambridge, U.K.

Deformation of metallic glasses performed well below the glass transition temperature leads to the formation of shear bands, narrow regions in which the plastic flow is confined. It is believed that shear banding originates from individual stress concentrators having quadrupolar stress symmetry. To elucidate the underlying mechanisms of shear band formation, microstructural investigations were carried out on sheared zones using transmission electron microscopy. An evidence of a characteristic signature present in shear bands manifested in the form of sinusoidal density variations was found. On this basis we present an analytical solution for the observed post-deformation state derived from continuum mechanics using an alignment of quadrupolar stress field perturbations for the plastic events. Since we observe qualitatively similar features for three different types of metallic glasses that span the entire range of characteristic properties of metallic glasses, we suggest that the reported deformation behavior is generic for all metallic glasses, and thus has far-reaching consequences for the deformation behavior of amorphous solids in general.

MM 61.3 Thu 12:30 IFW A

The Effect of Glass Structure, Stress State and Strain Rate on Shear and Densification - A Nanomechanical Study on a Sodium-Boro-Silicate Glass — •Christoffer Zehnder[1], Niklas Peltzer[1], Doris Möncke[2], James Gibson[1], and Sandra Korte-Kerzel[1] — [1]RWTH Aachen University, Germany — [2]Alfred University, New York, USA

It is well known that the mechanical properties of glasses are closely related to their atomic structure. The exact structure-property-relationship, however, is only poorly understood even for fundamental mechanisms like shear and densification. Nanomechanical test methods like micropillar compression and nano-impact indentation can help fill this gap. In this study a sodium-boro-silicate glass is quenched from different temperatures to induce changes in the atomic structure. Micropillar compression was used to investigate the effect of uniaxial stresses and nanoindentation with different tip geometries enabled testing under different amounts of hydrostatic pressure. Finally, impact nanoindentation was utilised to observe the effect of high strain rates on the deformation of glass. It is shown that by changing the glass structure or the stress state one can influence the occurrence of shear and densification. Testing with different strain rates also revealed a strong strain rate dependence of the deformation mechanism. These findings are analysed against the background of the glass structure. The experimental techniques and analyses presented could easily be applied also to metallic glasses in order to investigate the effects of rate and stress state on their plastic deformation.

MM 61.4 Thu 12:45 IFW A

Yielding transition in a binary model glass under oscillatory shear: Molecular Dynamics computer simulation — •Juergen Horbach[1], Gaurav Prakash Shrivastav[1], and Pinaki Chaudhuri[2] — [1]Institut für Theoretische Physik II, Universität Düsseldorf, Germany — [2]The Institute of Mathematical Sciences, Chennai, India

Under shear, a glass may exhibit the transition from an elastically deformed state to plastic flow. The nature of the yield point at which this transition occurs is a highly debated issue. We use molecular dynamics simulation to study a model of a $Ni_{80}P_{20}$ glass under oscillatory shear. Recently, we have shown that the yielding in this system can be associated with a directed percolation transition of mobile regions [1-3]. Under oscillatory shear, the occurrence of a yielding transition depends on the maximal strain amplitude, γ_{max}, in each cycle. We show that the time scale at which the transition occurs diverges at a finite value of γ_{max}.

[1] G. P. Shrivastav, P. Chaudhuri, and J.Horbach, Phys. Rev. E **94**, 042605 (2016).

[2] G. P. Shrivastav, P. Chaudhuri, and J. Horbach, J. Rheol. **60**, 835 (2016).

[3] I. Binkowski, G. P. Shrivastav, J. Horbach, S. V. Divinski, and G. Wilde, Acta Mater. **109**, 330 (2016).

MM 61.5 Thu 13:00 IFW A

Effect of hydrogen on the pop-in behavior in a metallic glass — •Lin Tian, Moritz Hirsbrunner, Dominik Tönnies, and Cynthia Volkert — Institute of Materials Physics, University of Göttingen

Hydrogen is a detrimental element in structural materials which usually causes obvious reduction of fracture toughness. For example, hydrogen embrittlement is a well-known reason for failure of steels. In contrast, in metallic glasses, which are considered to be brittle materials, hydrogen (H) can play a beneficial roll by preventing shear band formation. In this contribution, the effect of H content on the pop-in behavior of a Zr based metallic glass (M) is studied. Samples are charged to different H content (H/M) with electrochemical hydrogen loading. Then, nanoindention with a spherical indenter is carried out on the surface of the samples. While the load of the first pop-in increases with increasing H content, the possibility of pop-ins occurring decreases. A transition from shear band dominated to homogeneous deformation is observed. This result is consistent with a study of the compression of submicron pillars in hydrogen gas environment. The suppression of shear band initiation is attributed to changes in the local environment induced by H doping, such as local strain.