MM 56: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses - kinetic transitions

Time: Thursday 10:15–11:30 Location: IFW A

Topical Talk MM 56.1 Thu 10:15 IFW A

anomalous atomic motion in metallic glasses revealed by coherent X-rays — •Beatrice Ruta — Institute of Light and Matter, Lyon 1 University-CNRS, France.

Metallic glasses display outstanding thermal, mechanical and chemical properties, which make them forefront materials for technological applications in many diverse fields such as medicine, environmental science and engineering. Their widespread use is, however, limited by their lack of stability over time due to ongoing relaxation processes and physical aging. X-ray Photon Correlation Spectroscopy (XPCS) has recently emerged as the very only technique able to measure the atomic motion in both crystalline and amorphous materials. By collecting series of diffraction data with coherent X-rays, XPCS measures the particle dynamics though the temporal evolution of the intensity fluctuations in the generated speckles patterns. Measurements on metallic glasses have revealed the existence of microscopic structural rearrangements, which cannot be explained by any current theory. In these systems, the dynamics evolves from a diffusive atomic motion in the supercooled liquid phase to a stress-dominated dynamics in the glass, characterized by a complex hierarchy of aging regimes. By combining dynamical (XPCS) and structural (XRD) studies we have been able to quantitatively link for the first time this anomalous atomic motion to microscopic structural mechanisms usually observed in diffraction studies, providing a broader unique view of the glassy state.

MM 56.2 Thu 10:45 IFW A

Structural origins of the boson peak in metals: From high-entropy alloys to metallic glasses — •Karsten Albe, Tobias Brink, and Leonie Koch — Fachgebiet Materialmodellierung, Technische Universität Darmstadt, Germany

Virtually all amorphous materials exhibit a boson peak, which is an excess of vibrational modes at low frequencies compared to the phonon spectrum of the corresponding crystal. Until recently, the consensus was that it originated from “defects” in the glass. However, the boson peak was also attributed to the first van Hove singularity of crystal lattices in alternative theories. A recent viewpoint is that the van Hove singularity is simply shifted by the decreased density of the amorphous state and is therefore not a glass-specific anomaly. In the current contribution, we aim to resolve this question for metallic systems. Using molecular dynamics computer simulations of high-entropy alloys and metallic glasses of the same composition, we show that the boson peak consists of additional modes which only arise in structurally disordered, softened regions [1]. Consistent with theoretical models, these regions are characterized by reduced stiffness and can be regarded as “soft spots”: The boson peak can serve as an indicator for the amount of such regions. This is consistent with observations that find an increased boson peak signal in mechanically deformed glasses in which an increase of the boson peak originates in the shear band [2].

[1] Brink *et al.*, PRB, accepted (2016)
[2] Bünz *et al.*, PRL **112**, 135501 (2014)

MM 56.3 Thu 11:00 IFW A

Fragile-strong liquid transitions and the underlying structural transitions in chalcogenide glassformer Ge15Te85 and bulk metallic glass-forming liquids — •Shuai Wei[1], Moritz Stolpe[2], Oliver Gross[2], William Hembree[2], Simon Hechler[2], Jozef Bednarcik[3], Ralf Busch[2], Pierre Lucas[4], and C.Austen Angell[1] — [1]Arizona State University, Tempe, USA — [2]Saarland University, Saarbruecken, Germany — [3]DESY, Hamburg, Germany — [4]University of Arizona, Tucson, USA

A striking anomaly in the viscosity of chalcogenide glass-forming alloy Ge15Te85 is reminiscent of the equally striking comparison of liquid tellurium and water. Applying the Adam-Gibbs viscosity equation to calorimetric data, we find a fragile-to-strong liquid transition (FS-transition), and then predict the ”strong” liquid course of the viscosity down to Tg at 406 K. The extrapolation is in good agreement with a direct measurement of fragility near Tg using differential scanning calorimetry. The in-situ X-ray scattering data reveal that the transition is not only related to short-range-order (SRO) structural change, but also linked to a remarkable development of medium-range-order (MRO). The latter manifests as an emerging pre-peak in total structural factor S(Q) and an atomic pair correlation on the length scale of ˜8 Å in the real-space G(r) function. The FS-transitions at high pressures are examined in terms of experimental data and the Ehrenfest relation. Finally, we compare the behavior of Ge15Te85 with the liquid-liquid transition in the bulk metallic glass-forming liquid, Zr58.5Cu15.6Ni12.8Al10.3Nb2.8 (Vit.106a).

MM 56.4 Thu 11:15 IFW A

Indications for a kinetic crossover in bulk metallic glasses — •Stefan Küchemann[1], Robert Maass[1], and Konrad Samwer[2] — [1]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, USA — [2]1. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

In the supercooled liquid, kinetic crossovers strongly alter the dynamics of glass-forming alloys leading, for instance, to the breakdown of the Stokes-Einstein relation and the emergence of a secondary relaxation mode. Measurements of the static structure factor during ultrafast heating experiments of metallic glasses reveal an underlying structural transition which occurs in the close vicinity of the kinetic crossover in the supercooled liquid [1]. In this contribution we provide evidence that a kinetic crossover also occurs in the glass state. By covering an extended range of heating rates from very slow to ultrafast we are able to show that the glass transition temperature as a function of heating rate deviates from the expected Vogel-Fulcher-Tamann behavior [2]. At this crossover the amorphous structure rejuvenates despite the exposure to elevated temperatures which changes the mechanical properties. The results are discussed in the framework of an underlying thermodynamic phase transition.

The authors acknowledge the financial support by the DFG within FOR1394 in P1.

[1] S. Küchemann and K. Samwer, Acta Materialia 104, 119 (2016). [2] S. Küchemann, G. Gibbins, J. Corkerton, E. Brug, J. Ruebsam, and K. Samwer, Philosophical Magazine Letters, 1 (2016).