MM 16: Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids

Time: Wednesday 10:15–13:00 Location: H10

Topical Talk MM 16.1 Wed 10:15 H10

Microstructure and transport in model isotropic amorphous solids — •Peter Derlet — Condensed Matter Theory Group, Paul Scherrer Institut, Switzerland

Amorphous solids lack long range order, however structural heterogeneity can exist over intermediate length scales suggesting the notion of a glassy microstructure. Such spatial variations, whatever they may be, can also be related to variations in thermally driven structural fluctuation time scales. In this talk, I will present atomistic simulations of model isotropic (metallic) binary glass systems spanning the microsecond timescale, and discuss the resulting amorphous structure in terms of bond frustration, demonstrating that despite the strong disorder, a percolative region containing strong medium range order emerges that fundamentally affects transport and dissipation. Particular focus will be given to how such simulations can give insight into experiments probing arrested colloidal glasses obtained through isotropic compression, and structural decorrelation in a metallic glass probed by long-time x-ray photon correlation measurements.

MM 16.2 Wed 10:45 H10

Liquid-like versus Stress-Driven Dynamics in a Metallic Glass Former Observed by Temperature Scanning XPCS — •Maximilian Frey[1], Ralf Busch[1], and Eloi Pineda[2] — [1]Chair of Metallic Materials, Saarland University, Campus C6.3, 66123 Saarbrücken, Germany — [2]Department of Physics, Institute of Energy Technologies, Universitat Politècnica de Catalunya - BarcelonaTech, 08019 Barcelona, Spain

Using high flux synchrotron radiation (ESRF, ID10), we study a Pt-based metallic glass former via X-ray photon correlation spectroscopy (XPCS) upon temperature scanning through the glass, glass transition and supercooled liquid (SCL). In the equilibrium SCL, the obtained intensity autocorrelation functions are well-described by a conventional Kohlrausch-William-Watts (KWW) model. Yet, in the glass and especially the glass transition region, this approach fails. Instead, we demonstrate that a multiplication of two KWW functions allows to describe the complex decay shape. Within the glass transition region, the fit parameters of the two separate KWW fits decouple massively. While one KWW component models the compressed shape of glass-typical non-equilibrium dynamics, the other fit maintains stretched liquid-like characteristics. We demonstrate that the compressed decay can be likely addressed to ballistic-like atomic motions while the stretched component apparently reflects (sub-)diffusive atomic motions, which are both superimposed in the non-equilibrium.

MM 16.3 Wed 11:00 H10

Non-monotonic hydrodynamic relaxations in a nanochannel — •Linnea Heitmeier[1,2], Thomas Voigtmann[1,2], and Jesper Schmidt Hansen[3] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, 51170 — [2]Heinrich Heine University, Universitätsstraße 1, Düsseldorf — [3]DNRF Center Glass and Time, IMFUFA, Department of Science, Systems and Models, Roskilde University, DK-4000 Roskilde

Nanotechnology is an active research field with applications in the everyday-life, electronics and medicine.

In my talk, I will present results of Molecular-Dynamics Simulations of a glass-forming liquid, which is confined in a nanochannel and excited with a sinusoidal force in order to probe the velocity relaxation on different lengthscales.

I show that the velocity relaxation behavior in different regions of the channel depends non-monotonically on the position of the fluid.

To explain the results, I will make use of the Maxwell-model for fluids, which states that a fluid behaves like an elastic solid on small timescales and like a viscous fluid on large timescales.

The simulation results can be recovered by this model, when using generalizations of this model:

On the one hand, a two-mode-Maxwell-model captures the contributions from the short-time dynamics and the slow structural relaxation to the viscosity. On the other hand, a spatially non-local generalization of the Maxwell-model allows to capture the velocity relaxation in the channel depending on different positions.

MM 16.4 Wed 11:15 H10

Structural Complexity and Atomic-Scale Dynamics in Metallic Glasses — •Emel Gurbuz and Elif Ertekin — University of Illinois Urbana-Champaign

Metallic glasses (MG) become prominent for their exceptional mechanical strength, corrosion resistance, and versatile processing capabilities, all strongly linked to their amorphous atomic structures. Despite extensive research, the interplay between structural motifs, their connectivity, and the resulting dynamic behavior during glass formation remains insufficiently understood.

This study uses molecular dynamics simulations to explore the dynamics of glass formation in MG systems with varying compositions (Fe_xZr_{100-x}, Co_xZr_{100-x}, Cu_xZr_{100-x}). By analyzing melt-quench trajectories, we identify key structural motifs, such as five-fold icosahedra, and examine their role in the "freezing in" process. Regions with rapid solidification and liquid-like behavior are characterized by tracking atomic diffusivity distributions over time. Remarkably, sequences of connected icosahedra persist as liquid-like regions even at low temperatures, facilitating ionic transport.

Our findings reveal critical insights into the mechanisms governing structural and dynamic complexity in MGs, advancing the understanding of their formation and potential for designing functionally optimized materials.

15 min. break

Topical Talk MM 16.5 Wed 11:45 H10

Structural relaxation and deformation of bulk metallic glasses — •Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

In metallic glasses, relaxation is discussed in the context of shear transformation zones, viscous flow, structural medium-range order (MRO) and even crystal nucleation. However, the structural origin of different relaxation modes and how these structures change during relaxation, rejuvenation or deformation is rather unclear. In order to address some of these related aspects, calorimetric measurements have been performed together with TEM-based analyses of the local medium range order structures before and after plastic deformation as well as after controlled thermal relaxation. The combined results of macroscopically averaging and spatially resolved analyses are discussed with respect of the correlations between relaxation, deformation and modifications of the MRO structure.

MM 16.6 Wed 12:15 H10

Tracing the Roots of Elastic Heterogeneity in Metallic Glass — •Reza Rashidi[1,2], Birte Riechers[1], and Robert Maass[1,2,3] — [1]Federal Institute of Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]Department of Materials Engineering, Technical University of Munich, 85748 Garchingen, Germany — [3]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

Metallic glasses (MGs) show structural and temporal heterogeneities over a broad range of time and length scales. With the aid of atomistic simulations, we can explain these dynamic and structural fluctuations at the nanometer scale. Here, our focus shifts to the larger length scale of property variations and the ongoing exploration of their origin. In past work, we suggested that cooling constraints during solidification could lead to elastic heterogeneities and therefor an elastic microstructure on the scale of ~100 nm (Materials & Design 229 (2023) 111929). In this presentation, we further support this idea by examining various casting geometries and thermal histories, tracking how elastic decorrelation lengths change with sample size and position within the MG. We also find that thermal annealing reduces decorrelation length-scale gradients and smooths out fluctuations in modulus values (Scripta Materialia 255 (2025)116380). In concert with the nano-elastic property assessment, we leverage spatially-resolved scanning nanobeam diffraction in the search for a structural origin of elastic microstructure.

MM 16.7 Wed 12:30 H10

Yield surfaces of glass-forming fluids — •Stephan Domann[1,2] and Thomas Voigtmann[1,2] — [1]Institut für Materialphysik im Wel-

traum, DLR Köln — [2]Heinrich-Heine-Universität

The yielding of amorphous solids depends in principle on the geometry of the deformation applied to the solid. This defines a "static" yield surface in the state of principal stresses that is typically described by empirical models (such as von Mises, Tresca, Drucker-Prager etc). In a similar vein, approaching the glass transition from the fluid side, the flow stresses approach a dynamical yield stress, defining the dynamical yield surface as the geometry of the flow is varied. Owing to the difficulty of imposing arbitrary steady deformation geometries, both experiment and simulation data are scarce.

We will discuss an approach to model yield surfaces that is rooted in a first-principle theory originally developed by Fuchs and Cates, the combination of mode-coupling theory of the glass transition with the integration-through transients framework (ITT-MCT). Using suitable simplifications, we recover some of the well-known empirical yield surface descriptions as limiting cases. It also sheds light on the qualitative differences arising between models of the upper-convected and the lower-convected type. We also performed non-equilibrium molecular-dynamics simulations of a model glass former to determine the dynamical yield surface. Surprisingly, this attains a shape that is in qualitative agreement with the lower-convected model, although common expectation is that upper-convected models are more canonical in emerging from microscopic descriptions of glass forming fluids.

MM 16.8 Wed 12:45 H10

Unveiling the Asymmetry in Density within the Shear Bands of Metallic Glasses — •Harald Rösner[1], Arabinda Bera[2], and Alessio Zaccone[2] — [1]Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]University of Milan, Department of Physics "A. Pontremoli", via Celoria 16, 20133 Milan, Italy

Plastic deformation in metallic glasses at room temperature leads to the development of shear bands due to shear localization. In many experiments, shear bands have shown local density variations along their path, with a distinct imbalance in magnitude between local densification and dilation. However, a comprehensive mechanistic understanding or theory to explain this asymmetry has been lacking until now. Here, we introduce a new model [1] that consists of a sequential arrangement of alternating topological charges, generating a dipolar field. The resulting microscopic displacement field, when integrated into the deformation gradient tensor, provides an accurate analytical solution for the observed imbalances in the density variations. The implications of this model are discussed, highlighting the potential to elucidate a broader range of observations in shear bands.

[1] H. Rösner, A. Bera, and A. Zaccone, Phys. Rev. B, 110(1), 014107 (2024).