CPP 21: Glasses and Glass Transition 2 (joint session DY/CPP)

Time: Wednesday 11:00–13:00 Location: DYc

CPP 21.1 Wed 11:00 DYc

Residual stress distributions and mechanical noise in athermally deformed amorphous solids — •Céline Ruscher[1,2], Daniel Korchinski[2], and Joerg Rottler[2] — [1]Institut Charles Sadron, Strasbourg, France — [2]Department of Physics and Astronomy and Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, Canada

Amorphous solids are yield stress materials whose flow consists of periods of elastic loading interrupted by rapid stress drops, or avalanches, coming from microscopic rearrangements known as shear transformations (STs). From the microscopic point of view, the density of STs, or density of local residual stresses, $P(x)$, governs the statistical properties of global collective failure events at the yielding transition.

Using atomistic simulations, we reveal the evolution of $P(x)$ upon deformation. A pseudogap form $P(x) \sim x^{\theta}$ is observed in the freshly quenched state and in the early stages of deformation. After a few percent strain, however, $P(x)$ starts to develop a system size dependent plateau in the small x limit. To explain the origin of the plateau we consider a mesoscopic elastoplastic approach. Our results show how the spatial extent of avalanches in the stationary regime has a profound effect on the distribution of local residual stresses x. While the entrance into the plateau is set by the lower cutoff of the mechanical noise produced by individual STs, the departure from the usually assumed power-law pseudogap form comes from stress fluctuations induced by collective avalanches.

CPP 21.2 Wed 11:20 DYc

Evaluation of Local Atomic Structural Changes in $Cu_{50}Zr_{50}$ Cluster Assembled Metallic Glasses through Molecular Dynamics Simulations — •Syamal Praneeth Chilakalapudi[1], Shyam Katnagallu[1], Wolfgang Wenzel[1], Penghui Cao[2], and Horst Hahn[1,2,3] — [1]Institute Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]Dept. Mat. Sci. & Engg., University of California-Irvine, USA — [3]KIT-TUD Joint Research Laboratory Nanomaterials, Technische Universität Darmstadt, Germany

Cluster assembled metallic glasses (CAMGs), synthesized by cluster (amorphous) ion beam deposition (CIBD), are a prominent bottom-up approach to tailor amorphous structures. Experimental control of amorphous structure and magnetic properties [1] was demonstrated with a custom-made apparatus which offers precise control on the size and the deposition energy of the clusters under ultra high vacuum [2].

To understand the underlying mechanisms of these structural changes in CAMGs, we performed atomistic molecular dynamics simulations of $Cu_{50}Zr_{50}$ cluster assembly using LAMMPS. Our simulations model the CIBD process and evaluate changes in the local short-range order in CAMGs as a function of the deposition energy of the clusters. We notice the presence of interfacial regions, formed between every adjacent cluster. The interfaces are most prominent in soft-landing cases. We also investigate the effect of quenching rate used to generate the amorphous clusters on CAMGs.

[1] C. Benel et al., Mat. Horizons, (2019) 6, 727
[2] A. Fischer et al., Rev. Sci. Instr. (2015) 86, 023304

CPP 21.3 Wed 11:40 DYc

X-ray computed tomography of glass foams with tailored hierarchical pore structure — •Cristine Santos de Oliveira[1], Richard Kohns[2], Felix Meyerhoefer[2], Simon Carstens[2], Dirk Enke[2], Ralf Boris Wehrspohn[1,3], and Juliana Martins de Souza e Silva[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Institut für Technische Chemie, Universität Leipzig, Germany — [3]Fraunhofer Gesellschaft, München, Germany

Glass foams are materials consisting of a light-weight porous glass structure of special importance in the fields of civil engineering and bio-implants. Typically, their synthesis involves the thermal foaming of a powder mixture of glass with a foaming agent that decomposes at the foaming temperature, resulting in a solid glass skeleton permeated by empty pores. In our work, we synthesized a series of glass foams with a hierarchical pore structure, obtained by combining pores generated through the foaming of a powdered mixture of silica-based glass, MnO_2 and C at 815 °C, with pores obtained by phase-separation (performed at circa 500 °C) followed by acid leaching and washing. Using a combination of mercury intrusion porosimetry, N_2 sorption and X-ray CT at the micro and nanometer scales we observed that slight changes in the preparation procedure resulted in foams with different porosity, surface area, pore size and pore volume. Furthermore, by applying machine learning segmentation to the X-ray CT data it was possible to map inhomogeneities, residues and cracks inside the foam walls.

CPP 21.4 Wed 12:00 DYc

Decelerated aging in metallic glasses by low temperature thermal cycling — •Fathollah Varnik — ICAMS, Ruhr-University Bochum, Germany

It has been recently proposed that deep temperature cycling of metallic glasses may lead to a rejuvenation and improve their ductility. Here, we investigate this issue via extensive molecular dynamics simulations of a generic model glass former. We disentangle the effects of aging from those of thermal treatment and show that aging is slowed down but not stopped – neither reversed – during thermal cycling. These observations are corroborated further by a survey of energy distribution, which continues narrowing, albeit with a smaller rate. Our results are in qualitative agreement with recent differential scanning calorimetry measurements on different bulk metallic glasses, which show no measurable rejuvenation upon deeply cooled (cryogenic) thermal cycling. This applies both to as-quenched and well-annealed samples.

CPP 21.5 Wed 12:20 DYc

Glassy dynamics in viscous liquids - Prospects of broadband NMR relaxometry — •Manuel Becher[1,2], Michael Vogel[2], and Ernst Rössler[1] — [1]Nordbayerisches NMR-Zentrum, Universität Bayreuth, Germany — [2]Institute of Condensed Matter Physics, TU Darmstadt, Germany

As the molecular dynamics of a liquid undergoing a glass transition features a wide range of timescales over many decades, it is beneficial to study these viscous liquids with broadband spectroscopic techniques. Besides well established methods such as dielectric spectroscopy (DS) and depolarized dynamic light scattering (DDLS) covering many decades in time/frequency, also nuclear magnetic resonance (NMR) offers detailed insights in molecular motion ranging from the boiling point of a liquid to its glassy arrest. However, in most recent publications the spectral shape of the main relaxation peak between DS, DDLS and NMR was readressed and the question of universality arised, rendering the prospect of broadband NMR experiments to a new importance. As NMR experiments can provide single-particle correlation functions of the probed molecular moieties, but are usually carried out at a single Larmor-frequency, interest lies in 'broadening' their frequency range. In this talk, ways to access the relaxation spectrum are presented, focussing on field-cycling (FC) NMR. Here, recent advances allow us to evaluate the concept of frequency-time superposition in molecular glass formers. Moreover, making use of NMR's isotope sensitivity, molecular site-dependent measurements are shown to reveal the impact of molecular flexibility on structural relaxation.

CPP 21.6 Wed 12:40 DYc

The dynamics of a glassforming Lennard-Jones system below the critical mode-coupling temperature — •Juergen Horbach — Heinrich Heine-Universitaet, Duesseldorf, Germany

We present molecular dynamics (MD) computer simulations of a polydisperse glassforming Lennard-Jones model. The equation of state of this model is very similar to that of the Kob-Andersen binary Lennard-Jones (KABLJ) mixture. At a comparable density, also the critical mode coupling temperature is similar as in the KABLJ mixture. Using the swap Monte Carlo technique in combination with MD, we are able to equilibrate supercooled liquids far below the critical mode coupling temperature. We analyze the properties of these deeply supercooled samples with respect to their dynamics in the beta relaxation regime and their response to external shear. In particular, we find the formation of shear bands at sufficiently low shear rates.