DY 13: Glasses and Glass Transition (joint session CPP/DY)

Time: Monday 16:15–17:45 Location: H 0107

Invited Talk DY 13.1 Mon 16:15 H 0107

The boson peak in the vibrational spectra of glasses — •Edan Lerner — Institute for Theoretical Physics, University of Amsterdam, Science Park 904, Amsterdam, Netherlands

A hallmark of glasses is an excess of low-frequency, nonphononic vibrations, in addition to phonons. It is associated with the intrinsically nonequilibrium and disordered nature of glasses, and is generically manifested as a THz peak — the boson peak — in the ratio of the vibrational density of state (VDoS) and Debye's VDoS of phonons. Yet, the excess vibrations and the boson peak are not fully understood. In my contribution I will provide direct numerical evidence that vibrations near the boson peak consist of hybridizations of phonons with many quasilocalized excitations; the latter have recently been shown to generically populate the low-frequency tail of the vibrational spectra of structural glasses quenched from a melt and of disordered crystals. I will next use a reanalysis of experimental data, extensive computer simulations and a mean-field model, to show that the nonphononic part of the VDoS itself features both a universal power-law tail and a peak, entirely accounted for by quasi-localized nonphononic vibrations. Our results provide a unified physical picture of the low-frequency vibrational spectra of glasses, and in particular shed basic light on the origin, nature and properties of the boson peak.

DY 13.2 Mon 16:45 H 0107

Dynamics and Timescales of Higher Order Correlations in Supercooled Colloidal Systems — •Nele N. Striker[1], Irina Lokteva[1,2], Michael Dartsch[1,2], Francesco Dallari[1], Claudia Goy[1], Fabian Westermeier[1], Verena Markmann[1], Svenja C. Hövelmann[1], Gerhard Grübel[1,2], and Felix Lehmkühler[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

There has been extensive research into the nature of the glass transition, however its mechanisms remain mostly unclear. Recent works show that long-living locally favored structures (LFS), such as icosahedral structures forming upon supercooling, may play a key role. We show results from a combined X-ray Photon Correlation Spectroscopy (XPCS) and X-ray Cross Correlation Analysis (XCCA) experiment on colloidal hard spheres in the vicinity of the glass transition [1]. We defined a new correlation function g_c probing the timescales of higher-order correlations by tracking the time evolution of the structural higher-order correlations within the sample. We observed an increase in the ratio of the relaxation times of g_c and the standard individual particle relaxation time from about 0.4 to 0.9. The increasing values suggest that the local orders within the sample are becoming more long-lived approaching the glass transition. These results indicate that not only the presence but also the lifetime of LFS grows close to the glass transition.

[1] N. Striker et al., J. Phys. Chem. Lett., 2023, 14(20), 4719-4725

DY 13.3 Mon 17:00 H 0107

What can MD simulations tell us about the micromechanics of deformation of glassy amorphous polymers? — •Pramod Kumar Patel[1] and Sumit Basu[2] — [1]Department of Mechanical Engineering, Indian Institute of Technology, Kanpur, India — [2]Department of Mechanical Engineering, Indian Institute of Technology, Kanpur, India

Under uniaxial compression, the stress-strain responses of glassy amorphous polymers exhibit a yield drop followed by hardening at large strains. The extent of the yield drop and the steepness of the hardening response seem connected to the polymer's molecular architecture. Moreover, these materials exhibit strain rate sensitivity, pressure-dependent yielding, and somewhat peculiar unloading behaviour. The connections between the molecular architecture of the glassy amorphous polymer and its uniaxial compressive response are not well understood.

Micromechanically motivated constitutive models proposed by various authors are often able to negotiate many of the subtle aspects of the stress-strain behaviour but need to incorporate several fitting parameters to do so. We attempt to probe the physical processes and the effect of the underlying macromolecular force fields that lead to the typical stress-strain response through well-designed molecular dynamics (MD) simulations. Moreover, using a recently developed probe for quantifying the entanglement structure of the polymer, we show that the large strain uniaxial behaviour is governed by disentanglements and entanglement slips that invariably accompany deformation.

DY 13.4 Mon 17:15 H 0107

Sampling energy landscapes through resistance fluctuations in germanium telluride glass — •Sebastian Walfort, Jakob Ballmaier, Nils Holle, and Martin Salinga — University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Str. 10, 48149 Münster

Germanium telluride (GeTe) is a fragile glass former with a large electrical property contrast between a conductive crystalline phase and highly resistive glass states. It is further possible to repeatedly amorphize and crystallize a nanoscopic, confined volume by applying short voltage pulses, which makes GeTe an interesting model system for observing glassy dynamics. For instance, physical aging following melt-quenching of GeTe glass seems to manifest in a continued evolution of the electronic properties, e.g. in a power-law-like increase of the resistivity. In this experimental study, resistance serves as the observable to probe the structural dynamics of the glass. We demonstrate that, as a consequence of reducing the nanoscopic amorphous volume, individual resistance states can be resolved in time. The fluctuations between these states are measured over a wide temperature range, six orders of magnitude in time and modeled as a (hidden) Markov process. The resulting attempt frequencies and activation energies reveal a complex free energy landscape, where transitions between states are governed by both energetic and entropic contributions to energy barriers. Beyond their relevance for electronic memory applications, these results illustrate the feasibility of the experimental approach to probe the energy landscape of a glass through a fluctuating resistance

DY 13.5 Mon 17:30 H 0107

A self-consistent current response theory of jamming and vibrational modes in low-temperature amorphous solids — •Florian Vogel, Philipp Baumgärtel, and Matthias Fuchs — University of Konstanz, Konstanz 78464, Germany

Topologically disordered solids exhibit characterisitc anomalies like sound attenuation in the absence of thermal fluctuation and deviations from Debye*s law in the density of states. We present a novel mode-coupling approach to the understanding of athermal amorphous solids, which goes beyond the usual self-consistent Born approximation. To successfully predict the correct sound attenuation, we had to take correlated fluctuations into account. The resulting first principle theory successfully describes the jammed phase. It can also be mapped to the schematic theory [1] of the Euclidean-random-matrix model introduced by Parisi and co-workers [2] and provides a sound description of the unjammed athermal phase and our predictions for the critical dynamics agree with simulations. Most importantly, we manage to describe the unjamming transition without having to rely on negative eigenvalues of the Hessian. The softness of our systems expresses itself as a vanishing dispersion relation, which always stays non-negative. Our theory is in qualitative and semi-quantitative agreement with the numerical solutions of the ERM-model.

References

[1] F. Vogel and M. Fuchs. Phys. Rev. Lett., 130:236101, 2023.

[2] M. Mézard, G. Parisi, and A. Zee. Nuclear Physics B, 559(3):689*701, 1999.