CPP 35: Glasses and Glass Transition (joint session DY/CPP)

Time: Wednesday 11:15–12:45 Location: ZEU/0118

Invited Talk CPP 35.1 Wed 11:15 ZEU/0118

Topological defects in 2D amorphous ensembles — •Peter Keim — Heinrich-Heine-Universität Düsseldorf

Topological defects are key to understand melting of crystals in two dimensions. A dilute gas of bound thus virtual pairs of dislocations cause the softening of a crystal in the vicinity of melting. If thermal energy is high enough to unbind dislocation pairs, translational order is destroyed and the crystal to melts due to the lack of shear resistance. In an amorphous solid, the concept of topology seems useless for the first glance due to the absence of order. Here, we discuss, how the definition of virtual dislocations can be generalized for a two-dimensional glass. Based on positional data of a binary colloidal monolayer we determine the fugazity of generalized virtual dislocations and measure elasticity close to the glass transition: Youngs modulus gets 16π at melting in surprisingly close analogy to Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) - theory for melting of 2D crystals.

CPP 35.2 Wed 11:45 ZEU/0118

Glass transition and universal scaling in ultra-low crosslinked microgels — Alessandro Martinelli[1], Rajam Elancheliyan[1], Andrea Scotti[2], Alexander V. Petrunin[3], •Domenico Truzzolillo[1], and Luca Cipelletti[1,4] — [1]Laboratoire Charles Coulomb (L2C), UMR 5221 CNRS-Universitè de Montpellier, F-34095 Montpellier,France — [2]Division of Physical Chemistry, Lund University, SE-22100 Lund, Sweden — [3]Institute of Physical Chemistry, RWTH Aachen University, Landoltweg 2, 52074 Aachen,Germany — [4]Institut Universitaire de France, F-75231 Paris, France

We investigate the glassy dynamics of Ultra-Low Crosslinked (ULC) poly(N-isopropylacrylamide) (PNIPAM) microgels. The glass transition is reached by varying either the temperature (modulating microgel swelling) or the colloidal number density. Our Dynamic Light Scattering (DLS) measurements confirm that the dynamic slowdown is solely governed by the effective volume fraction (φ), with ULC microgels behaving as fragile glass formers. Small-Angle X-ray Scattering data further indicates that the center-to-center inter-microgel distance is insensitive to temperature, scaling geometrically with mass fraction, while the height of the first peak of the static structure factor decreases with increasing concentration, suggesting structural melting above glass transition. We finally we report on the striking emergence of a universal dynamic behavior for the relaxation time (τ_α) dependence on the scattering vector (q) across the entire supercooled and glass regimes, allowing the data to collapse onto a master curve, whose features will be discussed.

CPP 35.3 Wed 12:00 ZEU/0118

Strain-rate dependent rheological memory in a model glass former — •Monoj Adhikari and Jürgen Horbach — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

We investigate the shear response of deeply supercooled liquids far below the mode coupling critical temperature of a model glass former. Our system is based on the Kob-Andersen binary Lennard-Jones mixture (KABLJM) model but incorporates polydispersity, allowing us to combine SWAP Monte Carlo (MC) with Molecular Dynamics (MD) simulations. This hybrid approach enables equilibration at temperatures far below the Mode-Coupling critical temperature, T_{MCT}, while maintaining an equation of state similar to the original binary KABLJM model. We examine the response of these equilibrated samples to shear deformation at finite temperature and strain rate. By combining MD with SWAP MC during shear, we demonstrate that states with stress far below the yield stress can be accessed, making Newtonian fluid behavior observable even at temperatures well below T_{MCT}. To characterize the Newtonian fluid states obtained from this hybrid approach, as well as the solid-like states from standard MD, we employ a strain-rate switching protocol on the steady states. When applying this protocol to the stationary states, we observe intriguing memory effects. In the transient regime, stress overshoots appear when increasing the strain rate, whereas a striking stress undershoot emerges when decreasing it, mirroring recent experimental observations in polymer glasses.

CPP 35.4 Wed 12:15 ZEU/0118

An Analytical Relation between Thermodynamics and Dynamics in a Trap-like Model of Supercooled Liquids — •Simon G. Kellers, Anshul D. S. Parmar, and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany

Recent studies on 2D non-network glass formers, enabled by the million-fold acceleration of Swap Monte Carlo, have revealed clear deviations from Gaussian behavior in the inherent-structure (IS) density of states and linked these features to the fragile-to-strong crossover (FSC) and the emergence of a low-energy depletion regime.

Here, we establish such a connection by introducing a direct analytical relation between thermodynamic PEL statistics and dynamical properties within a trap-like description of supercooled liquids. We illustrate this relation using a binomial distribution of IS states and show that it naturally yields a characteristic trap size for polydisperse systems. This trap size reflects the effective number of degrees of freedom that collectively determine the depth and barrier of a metabasin participating in an activated relaxation event, thereby offering a physically transparent measure of cooperativity.

By combining this analytical framework with simulation data for a polydisperse 2D glass former, we obtain a coherent and quantitatively consistent landscape-based interpretation of the FSC.

[1] Andreas Heuer, J. Condens. Matter Phys. 2008, 20, 373101

[2] Anshul D. S. Parmar, Andreas Heuer, 2023 arXiv preprint arXiv:2307.10143

CPP 35.5 Wed 12:30 ZEU/0118

Single particle vs. collective diffusion dynamics in a glass-forming ternary Lennard-Jones mixture — •Anna Pini and Jürgen Horbach — Institut für Theoretische Physik II: Soft Matter, Heinrich Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf

Ternary fluid mixtures exhibit a rather complicated diffusion dynamics compared to their binary counterparts. Apart from three self-diffusion coefficient, there are three interdiffusion coefficients. In this work, we study a ternary ABC Lennard-Jones mixture using molecular dynamics computer simulation. It is based on the Kob Andersen binary Lennard-Jones mixture (KABLJM) [1] to which we have added a third C component. While C-C and A-C interactions are respectively identical to A-A and A-B interactions, B-C interactions are different from those between A and B particles. We study the glassy dynamics of this system at a high density of $\rho = 1.2$ and compare it to that of the original KABLM. While the self-diffusion coefficient show a similar temperature dependence for the binary and the ternary system, the behavior of the interdiffusion coefficients in the ternary system is significantly different from that in the binary one; in particular, unlike the binary system, the Darken equation does not hold in the ternary one. [1] W. Kob and H. C. Andersen, Phys. Rev. Lett. **73**, 1376 (1994).