CPP 33: Glasses and Glass Transition (joint session DY/CPP)

Time: Monday 15:00–18:00 Location: ZEU 118

Invited Talk CPP 33.1 Mon 15:00 ZEU 118

Shearing of glasses: new insight from studying model glasses of different system sizes — •Andreas Heuer, Markus Blank-Burian, Lawrence Smith, and Moumita Maiti — Inst. Phys. Chemie, WWU Muenster, Germany

Upon shearing of glasses a large variety of different phenomena can be observed. This includes, e.g., the stress overshoot and the emergence of shear bands. Many properties have been related to the presence of shear transformation zones (STZs).

In previous work on quiescent glasses important information about the physical mechanisms could be extracted from studying the dependence of dynamical properties on the system size. Here it was essential to study system sizes between approx. 60 and a few thousand [1]. Furthermore, an appropriate discretization of the dynamics in terms of metabasins was essential.

Here we study the properties of sheared systems in an analogous setting. Formally, shearing corresponds to a time-dependent energy landscape, requiring a generalization of the metabasin concept [2]. Interestingly, when studying the size dependence upon shearing at low temperatures, it turns out that macroscopically relevant behavior starts to be observed for system sizes above (approx.) 10.000. Important properties of the dynamic heterogeneities as reflected, e.g., by the emergence of shear bands, is extracted from these dependencies and related to the STZs.

[1] C. Rehwald, A. Heuer, Phys. Rev. E, 86, 051504 (2012). [2] M. Blank-Burian. A. Heuer, Phys. Rev. E 98, 033002 (2018).

CPP 33.2 Mon 15:30 ZEU 118

Nonlinear dielectric response: molecular reorientation models — •Gregor Diezemann — Institut für Physikalische Chemie, JGU Mainz, Duesbergweg 10-14, 55128 Mainz

The nonlinear dielectric response of supercooled liquids has been intensively studied, both experimentally and theoretically during the last decade. Since an analogue of the well known fluctuation dissipation theorem for nonlinear responses is missing, one has to rely on the results of model calculations. A number of different models have been used for the calculation of the nonlinear (third order) response and some of them exhibit features also observed experimentally.

I will present the results of calculations of the third order and the fifth order response for models of molecular reorientations. Sofar, one important point in the interpretation of the peaks observed in the modulus of the nonlinear response was that rotational Brownian motion does not give rise to such a peak. However, it is well known that this model of isotropic rotational diffusion is also not able to reproduce important features of the linear dielectric response of glassforming systems.

Here, I will show that very simple models like the model of random rotational jumps or anisotropic rotational diffusion also exhibit a so-called hump in the modulus of the nonlinear response functions. Also the relation between the third order response and the fifth order repsonse is obeyed to some extent. What is missing in this kind of models is a temperature dependence of the features observed. I will discuss the results in the context of recent experimental observations.

CPP 33.3 Mon 15:45 ZEU 118

Efficient algorithm to study dynamics in the transition between quasiperiodic and disordered environments — •Alan Rodrigo Mendoza Sosa and Atahualpa Kraemer — Universidad Nacional Autónoma de México, Mexico City, Mexico

Crystals have translational and rotational symmetries while quasicrystals have rotational symmetry in a single point, and glasses have none. This is revealed in the diffraction pattern, where crystals and quasicrystals have a discrete pattern, but quasicrystals exhibit forbidden symmetries, while glasses have a continuous pattern. Increment the rotational symmetry of quasicrystals should produce a denser diffraction pattern, closer to the continuous pattern exhibit in glasses. Motivated with the previous arguments we propose to study the structure of a quasiperiodic array and the dynamics of particles in quasiperiodic environments when the folding symmetry increases. However, the usual techniques to produce quasiperiodic arrays are aimed at producing arrays of low symmetries and near to the center of symmetry, then it becomes time expensive to perform simulations. In this work, we present an algorithm to produce quasiperiodic arrays with arbitrary symmetry around any point in the space, based on the generalized dual method. Also, using the Voronoi tessellation of the quasiperiodic array, and the incremental algorithm to track particles, we made an algorithm to perform simulations of particles moving in a quasiperiodic potential with arbitrary symmetry. We apply this algorithm to a quasiperiodic Lorentz gas with high symmetry to study diffusion and compare it with the random Lorentz Gas.

CPP 33.4 Mon 16:00 ZEU 118

Interpreting the Types of Derivatives in Fractional Relaxation Models — •Tillmann Kleiner and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

The excess wing of α-relaxation peaks and the phenomenon of nearly constant loss that have been observed in dielectric spectra of glass forming materials [1] are predicted by susceptibility functions that involve stretching exponents derived from fractional dynamics [2,3]. The relaxation motions predicted by such models can be described by initial value problems involving fractional derivatives with a type parameter. Special choices for the type parameter yield Liouville-Caputo and Riemann-Liouville derivatives.

Using a translation invariant fractional derivative the fractional initial value problems are reformulated as linear response equations. The influence of the type parameter is then described by additional fractional derivative expressions. The reformulation brings the advantage that the mathematical external force term coincides with the physical external force term which is not guaranteed for all types in the initial value problem formulation. Further, predictions for realistic spectroscopy and relaxation experiments are now described in a unified way and physical predictions depend continuously and more transparently on the parameters of the model.

[1] F. Kremer and A. Loidl, The Scaling of Relaxation Processes, Springer, (2018)
[2] R. Hilfer, Analysis **36**, 49-64 (2016)
[3] R. Hilfer, J. Stat. Mech. (2019) 104007

CPP 33.5 Mon 16:15 ZEU 118

Dynamic properties of quasi-confined colloidal hard-sphere liquids near the glass transition — •Lukas Schrack, Charlotte Petersen, and Thomas Franosch — Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, 6020 Innsbruck, Austria

The complex behavior of confined fluids arising due to a competition between layering and local packing can be disentangled by considering quasi-confined liquids with translational invariance along the confined direction. We provide a mode-coupling theory (MCT) for quasi-confined liquids using multiple relaxation channels and elaborate an efficient method for the numerical implementation.

Investigating both the collective and tagged-particle motion near the glass transition we focus on the non-monotonic behavior of the glass-form factor as well as of the intermediate scattering functions comparing numerical MCT results and simulations. We also provide a non-equilibrium state diagram as a function of the confinement length.

CPP 33.6 Mon 16:30 ZEU 118

Broadband Dielectric and Nuclear Magnetic Resonance Spectroscopy Studies on Dynamics of Ethylene Glycol in Soft and Hard Confinement — •Melanie Reuhl, Max Weigler, and Michael Vogel — Institut für Physik kondensierter Materie, Technische Universität Darmstadt

As hydrogen-bond networks are often restricted or confined in nature and technology, we investigate the influence of the type of confinement on hydrogen-bonded systems. Using nuclear magnetic resonance (NMR) and broadband dielectric spectroscopy (BDS), we analyse the dynamics of ethylene glycol (EG) in nanoporous silica, elastin and Ficoll matrices over broad temperature ranges. For all investigated systems, BDS and NMR results consistently indicate a slowdown and an enhanced heterogeneity of dynamics due to confinement. For EG in silica pores, calorimetric studies reveal partial freezing at temperatures below the bulk freezing point, indicating substantial freezing point suppression. We study changes in the dynamical behaviour when the confined liquid evolves into coexisting liquid and solid phases upon

cooling. The dynamical behaviour of both EG phases in silica confinement is independent of pore size for diameters below 6 nm. In the studied soft confinements, fractional freezing does not occur. Still, two dynamically distinguishable EG species occur, which can be assigned to free EG and interfacial EG at elastin/sugar surfaces.

15 min. break.

CPP 33.7 Mon 17:00 ZEU 118

Dynamics of Ethylene Glycol Water Mixtures in Bulk and Mesoporous Silica Studied by Nuclear Magnetic Resonance and Dielectric Spectroscopy — •Philipp Monnard, Melanie Reuhl, and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Hydrogen bonds remain a topic of scientific interested because of their key role in countless chemical systems. Aqueous solutions of ethylene glycol (EG) create complex networks of hydrogen bonds, because of EGs ability to form both intramolecular and intermolecular bonds. Those solutions are also widely used in heating, cooling and deicing applications, since their freezing point is significantly lower than that of their components. Using nuclear magnetic resonance (NMR) and dielectric spectroscopy (DS), we analyze the effect of silica confinement on the dynamics of EG-water mixtures with different concentrations. In particular, we determine the dependence of correlation times on the pore diameter over a broad temperature range. In doing so, we exploit the isotope selectivity of NMR to observe only the partially deuterated EG-d4(C2D4(OH)2) molecules. Further, we prepared solutions, with heavy water and EG-d2(C2H4(OD)2) to measure the dynamics of the counterpart. We found that the dynamics depend on the mixing ratio, explicitly there is a slowdown with higher concentrations of EG. Moreover, we observe strong dynamical heterogeneity and, for solutions of 30 wt.% EG, the relaxation is even bimodal at intermediate temperatures.

CPP 33.8 Mon 17:15 ZEU 118

Aging of SiO_2: Scaling of Dynamic Heterogeneities and Cluster Analysis of Single Particle Jumps — •Katharina Vollmayr-Lee[1], Horacio E. Castillo[2], Christopher H. Gorman[3], and Taylor S. Cookmeyer[4] — [1]Bucknell University, Lewisburg, PA, USA — [2]Ohio University, Athens, OH, USA — [3]University of California, Santa Barbara, CA, USA — [4]University of California, Berkeley, CA, USA

We study the aging dynamics of the strong glass former SiO_2 via molecular dynamics simulations. We quench the system from a high to a low temperature, and then investigate the dynamics of the system as a function of waiting time, the time elapsed since the quench. For a system of 336 atoms, we find that both the dynamic susceptibility and the probability distribution of the local incoherent intermediate scattering function can be described by simple scaling forms in terms of the global incoherent intermediate scattering function. We also find for the scaling of these dynamic heterogeneities that the aging dynamics is controlled by a unique aging clock which is the same for Si and O atoms. Furthermore, we present results for a system of 115248 atoms for which we use single particle trajectories to identify single particle jump events when a particle escapes its cage formed by its neighbors. To study how these jump events are correlated in space and time, we find clusters of jumping particles. We will present cluster size distributions of both simultaneously jumping particles, as well as space-time clusters (jump events which are neighbors in space and time).

CPP 33.9 Mon 17:30 ZEU 118

Residual stress distributions and mechanical noise in athermally deformed amorphous solids from atomistic simulations — •Céline Ruscher[1,2] and Jörg 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

The distribution $P(x)$ of local residual stresses in amorphous packings governs the statistical properties of global collective failure events at the yielding transition. We reveal the evolution of $P(x)$ upon deformation by combining atomistic simulations with the frozen matrix approach. 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 plateau p_0 in the small x limit, where $p_0 \sim L^{-p}$ with L the system size. A direct comparison with the system size scaling of the stress drops shows that the distribution of avalanche sizes are controlled by θ in the transient regime and the plateau exponent p in the steady state flow. The broad distribution of mechanical noise $P(\Delta x) \sim |\Delta x|^{-1-\mu}$ is characterized by a Levy-exponent μ and can be related to the behavior of $P(x)$ via a mean-field description.

CPP 33.10 Mon 17:45 ZEU 118

AGE-INDEPENDENT PROCESS IN AGING HARD-SPHERE SUSPENSIONS: THE BETA PROCESS AND ITS RAMIFICATIONS — •Hans Joachim Schöpe[1] and William van Megen[2] — [1]Universität Tübingen — [2]RMIT University Melbourne

We consider the dynamics of a suspension of hard sphere-like particles in the proximity of its glass transition, the region where the intermediate scattering functions show significant aging. The time correlation function of the longitudinal particle current shows no dependence on age and reveals behaviour of ideal super-packed fluid and glass. The power laws of the beta process of the idealised mode coupling theory are exposed directly without reliance on fitting parameters. We proffer a mechanism linking the reversible/ageless dynamics, which constitutes the beta-process, and the irreversible aging dynamics.