DY 52: Glasses and Glass transition (joint session DY/ DF/ CPP)

Time: Thursday 15:00–17:30 Location: BH-N 128

DY 52.1 Thu 15:00 BH-N 128

Binary colloidal mixtures investigated by differential dynamic microscopy — •Tatjana Sentjabrskaja, Marco Laurati, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich-Heine University, D-40225 Duesseldorf, Germany

We investigate dynamics of colloids in binary mixtures of hard spheres with large size asymmetry, using confocal differential dynamic microscopy (con-DDM). This technique allows to study wave vector dependent dynamics of particles by analysing time series of confocal microscopy images. Analysis of the Fourier spectra of image differences acquired at different delay times allows to determine the time-dependent density-density correlation functions and, from its shape and decay time, the nature and characteristic times of particles' dynamics. To benchmark con-DDM, we investigate one-component systems of colloidal particles at different volume fractions. Diffusion coefficients of particles as a function of volume fraction obtained from con-DDM measurements are found to be in good agreement with those obtained using dynamic light scattering experiments. We additionally show that con-DDM can be used to separately study the dynamics of single species in multicomponent systems using fluorescent labeling. In particular, we are able to determine the dynamics of sub-resolution tracer particles in binary colloidal mixtures with large size asymmetry, as a function of increasing volume fraction of the large particles. The motion of the tracer, small particles becomes increasingly constrained by the dense matrix of large spheres, resulting in complex, non-diffusive motion of the tracers.

DY 52.2 Thu 15:15 BH-N 128

Critical-like behaviour in non-crystalline solids caused by angular correlations — •Mariya Rasshchupkyna[1,2,3], Volodymyr Bugaev[3,4], Johannes Roth[5], Gerhard Grübel[6,1], and Peter Wochner[3,4] — [1]The Hamburg Centre for Ultrafast Imaging (CUI) — [2]University of Hamburg — [3]Max Planck Institute for Intelligent Systems, Stuttgart — [4]Max Planck Institute for Solid State Research, Stuttgart — [5]Institute for Functional Materials and Quantum Technologies, University of Stuttgart — [6]DESY

Modern experimental techniques on the basis of coherent scattering data, such as X-ray cross-correlation analysis (XCCA) [1] allow the direct determination of angular correlations (and their modes) in molecular disordered systems. We performed molecular dynamics (MD) simulations for model systems with Dzugutov-type [2] interaction adjusted for the creation of glassy-type quasi-equilibrium states. XCCA applied to the simulated coherent scattering patterns of the MD samples reveals a four-point dodecagonal dominant mode responsible for the formation of non-commensurate structures, as found in glasses and quasicrystals. Strikingly, this mode exhibits a pronounced temperature-dependence indicating a critical-type behavior in the vicinity of the glassy-type transition.

References

1. P. Wochner, C. Gutt, T. Autenrieth, T. Demmer, V.N. Bugaev, A. D. Ortiz, A. Duri, F. Zontone, G. Grübel, H. Dosch, Proc. Natl. Acad. Sci. USA 106, 11511 (2009).

2. M. Dzugutov, Phys. Rev. Lett. 70, 2924 (1993).

DY 52.3 Thu 15:30 BH-N 128

Nonaffine deformations, glass transition, and yielding in disordered solids — •Alessio Zaccone — Physics-Department, Technische Universität München

A new approach to the glass transition has been recently developed from the angle of nonaffine elasticity. Due to structural disorder, the particle motions in glasses under shear do not merely follow the imposed affine pathways prescribed by the strain tensor of standard continuum linear elasticity, but deviate significantly to undergo additional nonaffine displacements. Importantly, these nearest-neighbour forces would exactly cancel out mutually in any ordered lattice with local center-inversion symmetry. The concept of nonaffine free energy of deformation can be applied to molecular and atomic glasses. The resulting scheme has been implemented to predict the T-dependence of the shear modulus of polymer glasses and its vanishing at the glass transition. The main effect leading to vanishing of rigidity can be identified with the decrease of the average effective intermolecular connectivity as the material expands upon increasing T. In turn, this makes the negative nonaffine contribution to free energy become increasingly more important as T rises, until the free energy of deformation vanishes at a critical temperature for mechanical instability, which is very close to the calorimetric glass transition. Besides nonaffinity, an important role is played by anharmonic interactions which control the thermal expansion coefficient of the glass, which in turn controls how connectivity decreases with increasing T.

DY 52.4 Thu 15:45 BH-N 128

The Potential Energy Landscape of microrheologically driven supercooled liquids — •Carsten F. E. Schroer[1,2] and Andreas Heuer[1,2] — [1]Westfälische Wilhelms-Universität, Münster, Germany — [2]NRW Graduate School of Chemistry, Münster, Germany

We perform computer simulations of a fragile model glass-former in which a single particle is driven by an external force through the liquid. Thereby, we track the path the system takes through its underlying Potential Energy Landscape (PEL) and aim for understanding how this is altered by the external field[1,2] and how the altering is related to the nonlinear responses of dynamic quantities.

In the PEL approach, the dynamics of undriven (strong *and* fragile) glass formers have found to be very well described in terms of an improved trap model, the Gaussian Glass Former (GGF)[3]. In this talk we want to demonstrate, how the GGF can be extended to driven supercooled liquids. This enables one to predict typical nonlinear responses like the nonlinear decay of the local friction coefficient as well as highly nontrivial effects like the occurrence of effective temperatures. Within this framework we can quantitatively predict the numerically observed effective temperatures in terms of the kinetics of the force-dependent hopping processes in the PEL. This establishes an intimate relation between the thermodynamics and the kinetics also in the highly non-equilibrium regime.

[1] C. F. E. Schroer, A. Heuer, *J. Chem, Phys* **138**, 12A518 (2013)
[2] C. F. E. Schroer, A. Heuer, *Phys. Rev. Lett* **110**, 067801 (2013)
[3] A. Heuer, *J. Phys.: Condens. Matter* **20**, 373101 (2008)

DY 52.5 Thu 16:00 BH-N 128

Physical mechanisms of nonlinear conductivity: A model analysis — •Andreas Heuer and Lars Lühning — Institute for Physical Chemistry, University of Münster, Germany

Nonlinear effects are omnipresent in thin films of ion conducting materials showing up as a significant increase of the conductivity upon increasing electric field. For a disordered hopping model general physical mechanisms are identified giving rise to the occurrence of positive or negative nonlinear effects, respectively. Analytical results are obtained in the limit of high but finite dimensions [1]. They are compared with the numerical results for 3D up to 6D systems. A very good agreement can be found. The results can also be used to rationalize previous numerical simulations. The implications for the interpretation of nonlinear conductivity experiments on inorganic ion conductors are discussed.

[1] A. Heuer, L. Lühning, J. Chem. Phys. 140, 094508 (2014).

15 min. break

DY 52.6 Thu 16:30 BH-N 128

Where to go in a rough free-energy landscape? — •Stefan Schnabel and Wolfhard Janke — Universität Leipzig

Frustrated spin systems like the Edwards-Anderson spin glass are notorious for disorder-induced frustration. Sampling their rough free-energy landscape is very challenging and only small systems can be investigated. Over the years great efforts have been made to improve both hardware and implementation, yet the basic method for the investigation of 3d spin glasses is and has been parallel tempering [1]. Here, we explore the possibility of using additional information obtained by a local minimization procedure similar to the basin-hopping algorithm [2]. Altering the statistical weight of conformations according to the depth of nearby local minima can reduce autocorrelation time. We investigate whether this improvement outweighs the additional computational cost.

[1] K. Hukushima and K. Nemoto, J. Phys. Soc. Japan 65 (1996) 1604. [2] D. J. Wales, J. Phys. Chem. A 101 (1997) 5111.

DY 52.7 Thu 16:45 BH-N 128

Evidence for a Novel Relaxation Mechanism in Glasses at Very Low Temperatures — •Marius Hempel, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The acoustic and dielectric properties of amorphous solids at low temperatures are governed by two level tunneling systems and can be described in similar ways. One difference is however, that electric fields couple only to tunneling systems carrying an electric dipole moment, whereas acoustic measurements couple to all tunneling systems. Thus, the two methods complement each other and can therefore lead to a better understanding of the underlying processes.

Low frequency measurements of the dielectric properties of the two multicomponent glasses N-KZFS11 and HY-1, containing significant amounts of tantalum and holmium respectively, have recently shown unexpected behavior, which cannot be understood in terms of the so called standard tunneling model. This behavior has been attributed to the very large nuclear electric quadrupole moments of ^{181}Ta and ^{165}Ho.

We present the first measurements of the acoustic properties of N-KZFS11 and HY-1 in the kHz range down to 10 mK. The results of these measurements underpin the observations seen in dielectric experiments and provide further evidence for a novel relaxation mechanism in such glasses.

DY 52.8 Thu 17:00 BH-N 128

Non-Universal Dielectric Properties of Glasses at Very Low Temperatures — •Annina Luck, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The universal behaviour of amorphous solids at low temperatures, governed by two level tunneling systems and described by the standard tunneling model, has long been a generally accepted fact. In the last years, however, measurements of dielectric two-pulse polarization echoes have revealed that nuclear electric quadrupole moments involved in atomic tunneling systems can cause specific material-dependent effects in magnetic fields.

We show measurements of dielectric properties of the two multicomponent glasses N-KZFS11 and HY-1, containing significant amounts of tantalum and holmium respectively. As ^{181}Ta and ^{165}Ho both carry very large nuclear electric quadrupole moments, these glasses are ideal candidates to determine the influence of these moments on the physical properties of glasses down to very low temperatures.

Our measurements not only show unique dielectric behaviour in both glasses, but also differ significantly from various predictions of the standard tunneling model.

DY 52.9 Thu 17:15 BH-N 128

Thermography on Luminescent Barium Borate Glass for White-LED Applications — •Florian Wagner[1], Peter Nolte[2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Mechanics of Materials IWM, Lübecker Ring 2, 59494 Soest

White light-emitting diodes (W-LEDs) represent one of the most promising lighting technologies for the future. Primarily used in many lighting applications is a blue LED combined with a yellow phosphor. The phosphor powder is usually embedded in an organic polymer and coated onto the LED chip. Heat-induced degradation of the organic encapsulate, however, results in an efficiency decrease and color temperature change. Luminescent glasses or glass ceramics are an interesting alternative due to their higher thermal and chemical stability. This work focuses on the thermal behaviour of luminescent barium borate glasses under intense excitation with ultraviolet/blue light. The glasses are doped with rare-earth ions for optical activation. Upon absorbing the ultaviolet/blue light, the rare-earth ions show their typical emission in the visible spectral range. Here, not all of the absorbed light is frequency-downshifted, but a significant part is released in the form of heat. Contact-free infrared thermography enables an analysis of the heat development in these materials. An algorithm based on the partial differential heat equation is developed to calculate the heat source density of the optical excitation from the surface temperature distribution.