

MM 11: Topical Session Glass Dynamics IV

Time: Monday 16:00–17:30

Location: H16

Topical Talk

MM 11.1 Mon 16:00 H16

Slow transport in densely packed random environments — •THOMAS FRANOSCH — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany — Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, D-91058 Erlangen, Germany

Conventionally the dynamics close to the glass transition slows down uniformly, deviations being often referred to as violations of the Stokes-Einstein relation. In strongly size disparate mixtures the violations may even include that only one component freezes whereas the other exhibits long-range transport often accompanied by subdiffusive motion. A minimal model explaining the observed anomalous transport is the Lorentz model where a single tracer particle meanders through a frozen array of randomly distributed obstacles. As the packing fraction of the obstacles is increased, the motion is more and more confined to narrow channels of void space accompanied with a drastic reduction of the diffusion coefficient. Contrary to the standard glass transition scenario this suppression of motion is connected to a divergent length scale characterizing the underlying geometric percolation transition of the void space. Relying on extensive computer simulation, we explain the emergence of anomalous transport, the divergence of the non-gaussian parameter, and elucidate the role of correlations in the obstacle distribution.

Topical Talk

MM 11.2 Mon 16:30 H16

A structural origin of cooperativity in supercooled liquids. — •EMANUELA DEL GADO — ETH Zürich, Switzerland

It is still debated whether and how the onset of cooperative dynamics in supercooled liquids approaching the glass transition can take place without any straightforward connection to structural changes. We have investigated the response to static deformation of the inherent structures (IS) of supercooled liquids, by using numerical simulations of model glass formers subject to deformations, combined with local energy minimization [1]. At low temperature, where the slow cooperative dynamics arise, non-affine rearrangements of the inherent structures allow to detect the presence of large correlated domains [2]. We propose that these non-affine domains are the IS counterpart of the cooperatively rearranging regions in the dynamics, and their presence supports the connections with elastic heterogeneity found in amorphous solids. Starting from these ideas, we quantitatively study the extent of spatial correlations of non-affine rearrangements in the IS and extract a static length-scale significantly growing in the temperature range where the dynamics become strongly cooperative [3]. Our analysis indicate a new, structural signature of glass transition.

[1] H. C. Oettinger, Phys. Rev. E 74, 011113 (2006).

[2] E. Del Gado, P. Ilg, M. Kroeger and H.C. Oettinger, Phys. Rev. Lett. 101, 095501 (2008).

[3] M. Mosayebi, P. Ilg, E. Del Gado and H.C. Oettinger, in preparation.

MM 11.3 Mon 17:00 H16

Thermodynamics and kinetics of glass transition during structural ordering of Fe50Co50 — •SHUAI WEI¹, ISABELLA GALLINO¹, RALF BUSCH¹, and AUSTEN ANGELL² — ¹Department of Materials Science and Engineering, Saarland University, 66123 Saarbrücken, Germany — ²Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85278, USA

The glass transition is not only the formation of an amorphous material from a supercooled liquid, but also, in general, the ergodicity-breaking of a system during a kinetic slow down process like cooling (i.e. freezing-in). Therefore, there are various kinds of glasses, conventional glasses (e.g. SiO₂), spin glasses and orientational glasses...

Here we report a glass-like transition event that occurs in a simple crystalline alloy Fe50Co50 during the order-disorder transition (lambda transition). By studying the thermodynamics and kinetics of this glass-like transition, we identify the transition as a glass transition with respect to ordering of this crystalline system. The structural relaxation times as a function of temperature are fitted with the Arrhenius law and the VFT equation. The results show that the kinetics of Fe50Co50 is simple Arrhenius. We also show that the enthalpy relaxation function evolving with time is non-exponential. By comparing the glass transition of Fe50Co50 with the strong glass-formers, BeF₂ and SiO₂, we found that they have great similarity in heat capacity behaviour and the change in entropy. Additionally, the study solves the old problem of the incomprehensible kinks in the tail of lambda transition peak in the heat capacity curves of of β -brass and Cu3Au.

MM 11.4 Mon 17:15 H16

Proton dynamics in sodium silicate melts studied with high temperature high pressure QENS — •FAN YANG¹, ANDREAS MEYER¹, TOBIAS UNRUH², and EUGENE MAMONTOV³ — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — ²Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), TU München, 85748 Garching, Germany — ³Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6475, USA

We apply quasielastic neutron scattering method under high temperature high pressure condition to investigate water dynamics in hydrous silicate melts. Neutron scattering offers the possibility to access pure proton dynamics via contrast variation by isotope substitution and to understand the water transport mechanisms in great detail. With the results from the time-of-flight spectrometer TOFTOF at FRM II in combination with the ones from the backscattering spectrometer BASIS at SNS, we are able to access a microscopic dynamic time window from 0.2 picosecond up to of about 800 picoseconds. Experiments on hydrous sodium silicate melts with 10 mol% (total) water concentration have been performed at 4 different temperatures under a constant pressure of 200 MPa. Our results show that the proton dynamics in hydrous silicate melts can be fitted into a glass-glass transition scenario under the frame work of the mode coupling theory.