CPP 12: Glasses II (joint session with DY)

Time: Tuesday 10:00–12:30 Location: MA 004

CPP 12.1 Tue 10:00 MA 004

The coupled energy landscape model — •Christian Rehwald and Andreas Heuer — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, 48149Münster

While the dynamics of small glass-forming systems can be described by properties of the underlying potential energy landscape (PEL), this concept breaks down in large systems. Here we present the "coupled energy landscape model" (CLM) which extends the PEL description to macroscopic system by introducing a coupling mechanism between the PEL of elementary systems (ES).

First we use the distance dependence of structural relaxations after an initial reorganization in an iso-configurational ensemble of a non-equilibrium configuration. The results indicate the existence of a causal connection between successive events, which can be identified as dynamical coupling between ES.

In a next step we use different observables to extract coupling mechanisms and their strength in the CLM from MD simulations (of a binary mixture of LJ particles): Finite size effects of τ_α and the non-exponentiality parameter β_{KWW} are proving to be an appropriate measure for comparing the two dynamics. The CLM combines advantages of recently discussed models for the glass transition like facilitated spin models and the mosaic approach and can be used to understand principles of glassy dynamics like increasing τ_α and emergence of the growing dynamical length scale χ_4.

CPP 12.2 Tue 10:15 MA 004

Glassy dynamics on the atomic scale measured with XPCS — •Manuel Ross[1], Michael Leitner[1,2], Markus Stana[1], and Bogdan Sepiol[1] — [1]Department of Physics, University of Vienna, 1090 Vienna, Austria — [2]Physics Department E13, Technical University of Munich, 85747 Garching, Germany

The world of solids can be divided into crystals and amorphous materials. One of physics' unsettled questions is the dynamic behavior of these amorphous materials, especially that of glasses. In our group, we developed a new method for observing dynamics on the atomic level [1]. Utilizing the most brilliant X-rays generated by high energy synchrotron sources and measuring in the diffuse regime of scattering, the principle of photon correlation spectroscopy can be extended to the sub-nanometer range. We currently apply our method to glasses in order to shed light on the processes which govern glassy dynamics. In particular, we study lead and silicate glasses, where the network is built of tetrahedral structures. I will present our recent results obtained from measurements at ESRF and PETRA III and the consequences for our view on the atomic dynamics of glasses.

[1] M. Leitner, B. Sepiol, L. M. Stadler, B. Pfau, and G. Vogl, Atomic diffusion studied with coherent X-rays, Nature Mat. 8, 717 (2009).

CPP 12.3 Tue 10:30 MA 004

Computer simulation of micro-rheology in glass-forming systems — David Winter[1] and •Juergen Horbach[2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [2]Institut für Theoretische Physik II, Heinrich Heine-Universität Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany

In the last ten years, micro-rheology has been established as a new tool to probe the non-linear response of soft-matter systems to external fields. In a micro-rheological experiment,single particles are pulled through a viscous medium by a constant or oscillatory force using, e.g., optical tweezers. In the work presented in this talk, the single-particle response to a constant external force of varying strength is investigated for a glass-forming Yukawa mixture using molecular dynamics computer simulation. Beyond linear response, a scaling regime is found where a force-temperature superposition principle of a Peclet number holds. In the latter regime, the diffusion dynamics perpendicular to the force can be mapped on the equilibrium dynamics in terms of an effective temperature whereas the diffusion coefficient parallel to the force does not exist. This behavior is associated with a hopping motion of the pulled particle from cage to cage and can be qualitatively understood by a simple trap model, as proposed by Bouchaud and coworkers.

CPP 12.4 Tue 10:45 MA 004

Statistical analysis of the non-linear dynamics of a supercooled model fluid under a microrheological perturbation — •Carsten Schroer[1,2] and Andreas Heuer[1,2] — [1]Institut für physikalische Chemie, Münster, Germany — [2]Graduate School of Chemistry, Münster, Germany

In our approach we regard the complex dynamics of glass-forming systems as a stochastic process on the potential energy landscape (PEL). Via computer simulations it is possible to map the continuous dynamics onto a hopping motion between the corresponding inherent structures of the system. We find mesoscopic regions (metabasins) in the PEL where the system is located for long times so that dynamics is mainly determined by the transitions between those metabasins. These discrete processes allow us to describe the dynamics in terms of a continuous time random walk.

This approach is of particular interest when including a microrheological perturbation via non-equilibrium molecular dynamic simulations. We report how linear and non-linear responses translate into the continuous time random walk properties of the system. Furthermore we show what consequences for the pathway of the system in its PEL arise by the application of a microrheological perturbation. We discuss these effects in terms of a rejuvenation scenario.

CPP 12.5 Tue 11:00 MA 004

Glass structure with well defined thermal history and glassy dynamic — •Christoph Scherer[1,2], Friederike Schmid[1], and Martin Letz[2] — [1]Institut fuer Physik, Johannes-Gutenberg Univ. Mainz, Staudingerweg 9, 55099 Mainz — [2]Schott AG, Hattenbergstr. 10, 55122 Mainz

Glasses have a huge range of applications, however, they are still theoretically not well understood. Also experimental access to the structure of glasses is limited. This motivates the study of glass systems by means of computer simulations. In this work a set of glass structures with well defined thermal history is generated on the computer. Each glass structure is created by gradually cooling down a set of 100-200 atoms by means of a molecular dynamics simulation as long as the system still can be equilibrated in reasonable simulation time. Afterwards, it is quenched down to room temperature and the resulting atom coordinates and velocities are stored. They are used as a starting point for a quantum-mechanical relaxation by means of density functional theory. Then the vibrational spectrum is determined and compared to experimental results. From the vibrational spectrum a set of thermodynamic quantities, as the temperature dependent specific heat, are obtained and compared to measured data. First successful tests on the model glass former SiO2 are presented.

CPP 12.6 Tue 11:15 MA 004

Microscopic picture of the beta-wing in simulated Ni0.5Zr0.5 melt — •Helmar Teichler — Inst. f. Materialphysik, Univ. Göttingen, Göttingen, Germany

The beta-wing is found in a large variety of liquids as an additional contribution to the susceptibility on the high frequency flank of the alpha peak. The underlying microscopic processes are not well understood so far. Regarding this, we have analyzed simulation data of a Ni0.5Zr0.5 model, using as main tool the fraction of un-displaced particles (FUDP). In the alpha and beta regime, the FUDP is a nearly linear mapping of the incoherent intermediate scattering function (ISF) (for suitably q) (H. Teichler, PRL, 107,067801 (2011)). Hence, the susceptibilities of FUDP and ISF display nearly identical alpha peak and beta-wing. The analysis unambiguously shows that this susceptibility is due to temporal accumulation of incoherent short-ranged displacement processes, where the stretched exponential behavior reflects "structure conserving correlations" in the accumulation process. Accordingly, the beta-wing reflects stronger structure restoring effects in the wing range than in the rest of the alpha regime.

CPP 12.7 Tue 11:30 MA 004

Glass form factors in confined geometry — •Simon Lang[1], Vitalie Botan[2], Martin Oettel[2], Rolf Schilling[2], and Thomas Franosch[1] — [1]Friedrich-Alexander Universität, Erlangen, Germany — [2]Johannes Gutenberg-Universität, Mainz, Germany

Supercooled liquids embedded in complex geometries exhibit an intriguing interplay between particle interaction and incommensurability

effects. Recently, the mode-coupling theory (MCT) of the glass transition was elaborated for a symmetric hard-wall confinement, where the glass-transition line reveals a striking re-entry phenomenon by varying the wall-to-wall separation [1]. A subtle point of the mathematical structure of these MCT equations is the emergence of two relaxation channels, which arise from a splitting of the current into a parallel and perpendicular direction with respect to the walls. Here, we present the glass form factors evaluated at the critical point for several distances. These arrested parts of the intermediate scattering function yield information about the structural arrangement of the particles in the confined glass state. We show, that the structure changes drastically upon varying the wall separation and the hallmarks of the phase diagram for confined liquids are reflected in the glass form factor. We demonstrate that the MCT equations for the glass form factor in confinement can be solved by a convergent iteration. From a generalized covariance property, the maximum principle for the glass form factors holds also for the MCT for confined liquids.

[1] S. Lang, V. Boţan, M. Oettel, D. Hajnal, T. Franosch, and R. Schilling, Phys. Rev. Lett.105 125701 (2010).

CPP 12.8 Tue 11:45 MA 004

Transient stresses and MSDs in sheared dispersions as described by mode-coupling theory (MCT) — •Christian Peter Amann and Matthias Fuchs — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Sheared viscoelastic media exhibit a stress overshoot between elastic and plastic regime, i.e. a maximum in the shear stress vs strain plot after switching on a constant shear rate. This maximum characterizes the transient evolution between equilibrium and steady state. A way to model such overshoots is the $F_{12}^{(\dot\gamma)}$ model, a schematic model in MCT to describe glass forming liquids. This approach is tested by comparing results with various rheological experiments. Flow curves, linear- and non-linear stress response, and stress-strain curves can be fitted consistently with the same model [1,2]. Within microscopic MCT the stress overshoot is identified as negative dip in the dynamic stress autocorrelation function [3].

This mechanism also causes super-diffusive colloid motion [3]. We connect shear stress and colloidal MSD via a generalized Stokes–Einstein relation and compare shear–stress and MSD simulations to define a characteristic strain determining maximum shear stress and onset of superdiffusion.

[1] M. Siebenbürger et al., *J. Rheol.* **53**, 707–726 (2009)
[2] J.M. Brader et al., *Phys. Rev. E* **82**, 061401 (2010)
[3] J. Zausch et al., *J. Phys.: Condens. Matter* **20**, 404210 (2008)

CPP 12.9 Tue 12:00 MA 004

Probing Spectral Diffusion Theory in Glasses Through Polarization Echo Measurements — •Gudrun Fickenscher, Christian Schötz, Paul Fassl, Masoomeh Bazrafshan, Manfred von Schickfus, Andreas Fleischmann, and Christian Enss — Kirchhoff Institute, Heidelberg University, Germany

Many low temperature properties of glasses can be well described by the standard tunnelling model. It assumes an ensemble of isolated tunnelling systems (TS) with a broad distribution in energy splitting and asymmetry. They can couple resonantly to electric fields and can therefore be probed by polarization echo measurements. When looking at dynamic properties of glasses, however, the influence of the TSs in the surrounding of the resonantly probed TSs has to be taken into account. Spectral diffusion theory* assumes that transitions in thermally excited TSs change the local fields at the positions of the resonant TSs, thus changing their energy splitting and phase. This affects the decay behaviour of the polarization echo amplitude with respect to the delay time.

We have performed different types of polarization echo measurements including 2-pulse echoes which show an almost pure T_2 decay and 3-pulse echoes which are more sensitive to T_1 processes. The setup allows for measurements with very long delay times of several milliseconds. We calculated the decay in echo amplitude within the framework of the spectral diffusion theory and compared the results.

* J.L. Black, B.I. Halperin, Phys. Rev. B **16** (1977), 2879.

CPP 12.10 Tue 12:15 MA 004

Dielectric polarization noise and permittivity - A fluctuation-dissipation analysis during the curing of an epoxy resin — Clemens Hassel, •Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Dielectric spectroscopy as a driven method combined with non-driven dielectric noise spectroscopy is a powerful experimental method for studying the fluctuation-dissipation theorem experimentally. We apply both methods during the curing process of the epoxy resin Epon 828 with n-butylamine. Setting the sample temperature properly allows controlling the time scale of curing. We measure in the temperature range between 293 K and 303 K at fixed temperatures. During curing the Epon-n-butylamine mixture undergoes a chemically induced glass transition. We analyze the validity of the fluctuation-dissipation theorem and calculate an effective temperature for this system.