CPP 41: Glasses and Glass Transition II (jointly with DY, DF)

Time: Thursday 10:45–13:00 Location: ZEU 114

Topical Talk CPP 41.1 Thu 10:45 ZEU 114

Local Anisotropy of Fluids, Glasses and Jammed Bead Packs — •Gerd Schroeder-Turk — Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr 7B, 91058 Erlangen

The local structure of particle ensembles is important for physical properties of normal or super-cooled fluids, jammed bead packs or structural glass phases. It is often characterized by order parameters such as q_4 or q_6, defined by spherical harmonics of particle neighborhoods. Here we show that a Minkowski tensor analysis of the particles' Voronoi cells provides shape indices that give a clear signature of various structural transitions in particle systems. In particular, all of the above mentioned systems consist of locally anisotropic environments. We show that the degree of cell anisotropy shows a clear signature of the jamming transition in bead packs, the transition to partially ordered states at the random close packing limit, and of the transitions from fluid to ordered phases in simple liquids. For jammed bead packs, these findings suggest an inherent geometrical reason why anisotropic shapes can fill space more efficiently than spheres.

[1] Schröder-Turk *et al*, Europhys. Lett., **90**(3), 34001 (2010)
[2] Kapfer *et al*, J. Stat. Mech. (2010) P11010

CPP 41.2 Thu 11:15 ZEU 114

In-situ characterization of vapor-deposited glasses of toluene by differential AC chip nanocalorimetry — •Mathias Ahrenberg[2], Heiko Huth[2], Katie Whitaker[1], Mark D. Ediger[1], and Christoph Schick[2] — [1]University of Wisconsin - Madison — [2]University of Rostock

We use ac nanocalorimetry to investigate extraordinarily stable glasses of toluene prepared by vapor deposition. For that purpose we have built a vapor deposition chamber that allows in-situ characterization of vapor-deposited organic glasses down to liquid nitrogen temperature. With highly sensitive nanocalorimeters in a differential setup, we are able to measure ng-samples over a frequency range from 0.1 Hz up to 8 kHz. The device was used to investigate the transformation of as-deposited stable toluene glasses into ordinary glasses. For films about 100 nm thick, the transformation was studied as a function of time at constant temperature above the common glass transition and as function of temperature at constant heating rate. The stability of the thin films was investigated as a function of substrate temperature and deposition rate.

CPP 41.3 Thu 11:30 ZEU 114

Structural relaxation times in high-density amorphous ice (HDA) — •Philip H. Handle[1], Markus Seidl[1], Erwin Mayer[2], and Thomas Loerting[1] — [1]Institute of Physical Chemistry, University of Innsbruck, Austria — [2]Institute of General, Inorganic & Theoretical Chemistry, University of Innsbruck, Austria

Solid water (H2O) exists in a variety of different forms. Besides common hexagonal Ice (Ih) today 15 different crystalline and three different amorphous forms are known. It is under discussion whether the amorphous forms are glassy (related to liquid water [1]) or nano-crystalline (related to ice). In case of high-density amorphous ice (HDA) this question has been addressed in some studies [2-4], yet remains controversial. In our work we measured structural relaxation times of HDA at elevated pressures (0.1 and 0.2 GPa) and different temperatures (125-135 K) on the basis of differential scanning calorimetry (DSC) at 1 bar. Our data suggest that at 135 K the structural relaxation time is only slightly higher than 100s, i.e., HDA is on the borderline to the glass transition.

[1] Poole, P. H.; et al.; Nature 360, 324-328 (1992). [2] Tse, J. S.; et al.; Nature 400, 647-649 (1999). [3] Mishima, O.; J. Chem. Phys. 115, 4199-4202 (2001). [4] Andersson, O.; Phys. Rev. Lett. 95, 205503-205507 (2005).

CPP 41.4 Thu 11:45 ZEU 114

Dynamics of glass forming liquids in soft confinement — •Emmanuel Gouirand[1], Thomas Blochowicz[1], Andreas Blank[1], Bernd Stühn[1], and Bernhard Frick[2] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut Laue-Langevin, Grenoble, France

In search of a characteristic length scale associated with cooperative dynamics at the glass transition, intensive effort has been devoted to investigating the influence of confinement on the dynamics of glass forming liquids. Nevertheless, no generally accepted picture exists so far because of the complex interplay of surface, pressure and finite size effects affecting the dynamics. We investigate the dynamics in confinements of different nature in order to be able to disentangle these various effects. Therefore, we apply photon correlation spectroscopy and quasi elastic neutron scattering on glass formers confined within microemulsion droplets, the structure of which proved to remain stable over the whole temperature range by means of small angle scattering. First, we report on the dynamics of glycerol confined in AOT micelles where the glass transition temperature (T_g) of the matrix is chosen to be smaller than T_g of the glycerol core (fast soft confinement). We find glycerol to relax faster than in bulk with an Arrhenius temperature dependence [1]. Then we compare the dynamics of toluene in Cremophor ELP micelles. Contrary to the former situation, here the matrix relaxes slower than the core and slows down the latter due to interfacial effects. Finally, below T_g of the matrix actual hard confinement of toluene within the droplets is realized.
[1] Blochowicz et al., CPL 475, 171-174 (2009)

CPP 41.5 Thu 12:00 ZEU 114

Crystallization and induced glass transition of n-alcohols in silicon-nanochannels — •Rolf Pelster, Rene Berwanger, Carsten Biehl, and Christoph Schuhmacher — FR 7.2 Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken, Germany

We have investigated the molecular dynamics of n-alcohols (C_4H_9OH - $C_{11}H_{23}OH$) confined in mesoporous silicon and silicon oxide with pore radii ranging from 3.5 to 7 nm. Using dielectric and infrared spectroscopy we show that the temperature of the liquid-solid phase transition and the structure of the solid phase depend on both the chain length and the radius of the pores:

Long-chain alcohols exhibit a crystalline structure at low temperatures. The confinement induces a lowering of the freezing temperature. The shorter the chain length or the smaller the pore radius, the lower the freezing temperature. Below the phase transition only the dynamics of amorphous wall layers are observable [1].

Short-chain alcohols behave differently. While bulk alcohols still freeze upon slow cooling, we observe a glass transition for the confined phase. The glass transition temperature is close to that reported for quenched bulk alcohols. We thus conclude that nano-confinement suppresses the crystallization process and induces a glass transition.

[1] R. Berwanger, Ch. Schumacher, P. Huber, and R. Pelster, Eur. Phys. J. Special Topics 189, 239-249 (2010)

CPP 41.6 Thu 12:15 ZEU 114

Glass Transition in Confined Geometry — •Simon Lang[1,2], Viatlie Botan[1], Martin Oettel[1], David Hajnal[1], Thomas Franosch[2], and Rolf Schilling[1] — [1]Johannes Gutenberg-Universität Mainz, Germany — [2]Universität Erlangen/Nürnberg, Germany

Confinement of a simple liquid is accompanied by introducing a further length scale in addition to the average distance of the particles. The interplay between them strongly influences the glass transition according to numerous significant experiments and simulations.

To achieve a theoretical description, we extend the microscopic mode-coupling theory to a liquid confined between two parallel flat hard walls [1]. The theory contains the standard mode-coupling equations in bulk and in two dimensions as limiting cases and requires as input solely the equilibrium density profile and the static structure factors of the fluid in confinement. We evaluate the phase diagram for a hard-sphere liquid as a function of the distance of the plates and obtain an oscillatory behavior of the glass transition line as a result of the structural changes related to layering. We detect a facilitation of the glass transition at half-integer values of the distance with respect to the hard-sphere diameter. In contrast, at commensurate packing particles can more easily slide along the walls and therefore the liquid phase remains favored for higher packing fractions.
[1] S. Lang, V. Botan, M. Oettel, D. Hajnal, T. Franosch, and R. Schilling, Phys. Rev. Lett. 105 125701 (2010)

Topical Talk CPP 41.7 Thu 12:30 ZEU 114

Concentration fluctuations and intrinsic confinement effects in binary glass forming liquids: Insights from neutron scattering and X-ray photon correlation spectroscopy

— •Thomas Blochowicz[1], Sebastian Schramm[1], Emmanuel Gouirand[1], Philipp Gutfreund[2], Bernd Stühn[1], Bernhard Frick[2], and Yuriy Chushkin[3] — [1]TU-Darmstadt, Darmstadt, Germany — [2]ILL, Grenoble, France — [3]ESRF, Grenoble, France

We investigate the dynamics in a series of binary glass forming liquids using dielectric spectroscopy (DS) in combination with quasielastic neutron scattering, dynamic light scattering and X-ray photon correlation spectroscopy (XPCS). It turns out that, although macroscopically the systems are fully miscible in the whole temperature range, two glass transitions can be clearly distinguished due to the high T_g contrast of the components. By means of DS the corresponding relaxation processes are identified, and it turns out that contrary to expectation the small molecules take part in both glass transitions, which suggests that two dynamical species can be distinguished among the small molecules. Moreover, the relaxation connected with the lower glass transition shows properties typical of dynamics in confinement like an Arrhenius-type temperature dependence and a broad distribution of relaxation times. On the other hand it is revealed by XPCS that the concentration fluctuations exhibit a significantly weaker temperature dependence than the α-relaxation and show a crossover from a diffusive to a so-called ballistic wave vector dependence and from stretched to compressed relaxation functions around the upper T_g.