CPP 22: Poster: Glass Transition and Dynamics of Liquids

Time: Tuesday 18:00–20:00 Location: P2

CPP 22.1 Tue 18:00 P2

Elastic Properties of Glasses — •Christian L. Klix, Florian Ebert, Georg Maret, and Peter Keim — University of Konstanz, D-78457 Konstanz, Germany

In this contribution, we present experimental results on the elastic properties of a two dimensional colloidal glass former. Given that glasses are solids, they exhibit a mechanical behaviour similar to crystals, i.e. they possess a finite shear modulus μ. We first extract the dispersion relation of the system where data hinting at structural change in the glassy state is found. Next, this dispersion relation is used to derive the moduli from modes in the long wavelength limit which are thermally excited [1]. We consider finite size and time effects and find the expected frequency dependence of the shear modulus μ. By cooling the system, the significant increase of μ lets us determine the glass transition temperature T_g precisely.

[1] H. H. Von Grünberg, P. Keim, and G. Maret, Phys. Rev. Lett. **93**, 255703 (2004)

CPP 22.2 Tue 18:00 P2

Low-Temperature Dynamics in Amorphous Polymers and Low-Molecular-Weight Glasses — Study with Single-Molecule Spectroscopy — Ivan Yu. Eremchev[1], Yury G. Vainer[1], Andrei V. Naumov[1], and •Lothar Kador[2] — [1]Molecular Spectroscopy Department, Institute for Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow reg., 142190, Russia — [2]University of Bayreuth, Institute of Physics and Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth, Germany

The dynamics in several low-molecular-weight glasses and in amorphous polyisobutylene of different molecular weights is investigated with single-molecule spectroscopy at temperatures of 4.5 and 7 K. Surprisingly, only the polymers with long chain lengths follow the prediction of the standard tunneling model and feature spectral jumps of the single-molecule lines between a small number of well-defined frequency positions corresponding to the coupling to few isolated tunneling systems. Glasses consisting of smaller molecules and oligomers show much richer dynamics: In most of them the spectral diffusion is so fast that single-molecule spectra can hardly or not at all be recorded and only irregular fluorescence flares are detected. Hence, the low-temperature dynamics of disordered solids is not universal but depends on the structure and chemical composition of the material. In polyisobutylene, the transition from small-molecule-like to polymer-like behavior occurs at chain lengths of a few hundred repeat units.

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Shear relaxation of simulated glass-forming polymer melts — •Stephan Frey[1], Hendrik Meyer[1], Joerg Baschnagel[1], and Matthias Fuchs[2] — [1]Institut Charles Sadron, F-67034 Strasbourg, France — [2]University of Konstanz, D-78457 Konstanz, Germany

Approaching the glass transition polymer melts show a remarkable increase of their viscosity by many orders of magnitude. The aim of this study is to gain a deeper insight into the processes which are involved in this phenomenon. We simulate polymer melts using a generic bead-spring model in which polymers are modeled as flexible chains. During long simulation runs the polymer melt is cooled down towards the glass transition temperature. The present work builds upon previous work which was focussed on the scattering function and related quantities. Here we concentrate on current correlation functions and connected quantities which are analyzed as a function of temperature, chain length and system size.

CPP 22.4 Tue 18:00 P2

Molecular relaxation processes in a MOF-5 structure revealed by broadband dielectric spectroscopy: signature of phenylene ring fluctuations — Stefan Frunza[1], •Andreas Schönhals[2], Ligia Frunza[1], Paul Ganea[1], Hendrik Kosslick[3], Jörg Harloff[4], and Axel Schulz[3] — [1]National Institute of Materials Physics, R-077125 Magurele, Romania — [2]BAM Federal Institute for Materials Research and Testing, D-12205 Berlin, Germany — [3]Leibnitz Institute for Catalysis at the University of Rostock, D-18059 Rostock, Germany — [4]University of Rostock, Institute of Chemistry, D-18059 Rostock, Germany

The molecular mobility of a MOF-5 metal-organic framework was investigated by broadband dielectric spectroscopy. Three relaxation processes were revealed. The temperature dependence of their relaxation rates follows an Arrhenius law. The process observed at lower temperatures is attributed to bending fluctuations of the edges of the cages involving the Zn-O clusters. The processes (*region II*) at higher temperatures were assigned to fluctuations of phenyl rings in agreement with the NMR data found by Gould et al. [J. Am. Chem. Soc. 2008, 130, 3246]. The carboxylate groups might be also involved. The rotational fluctuations of the phenyl rings leading to the low frequency part of relaxation region II might be hindered either by some solvent molecules entrapped in the cages or by an interpenetrated structure and have a broad distribution of activation energies. The high frequency part of region II corresponds nearly to a Debye-like process: This is explained by a well-defined structure of empty pores.

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Molecular dynamics of glass forming liquids under geometrical nano-confinement — •Wycliffe Kipnusu[1], Ciprian Iacob[1], Joshua Sangoro[1], Roger Gläser[2], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, University of Leipzig, Leipzig, Germany — [2]Institute of Chemical Technology, University of Leipzig, Leipzig, Germany

Translational and rotational dynamics in glass forming liquids confined in porous silica membranes having parallel cylindrical pores with diameters ranging between 5-12nm is studied by Broadband Dielectric Spectroscopy (BDS). Molecular dynamics, as reflected on the microscopic scale by the rotational and translation diffusion, exhibit deviations from the bulk behaviour when glass forming liquids are under mesoscopic confinement. The deviation is a result of interplay between surface effects due to interaction of the molecules with the pore walls and confinement effects pressumably caused by a change in packing density of the constrained molecules.

References:

[1]C. Iacob et al., Phys.Chem.Chem.Phys.11, 913-916, (2010).

[2]J. Sangoro et al., Phys.Chem.Chem.Phys. 12, 13798-13803, (2009).

CPP 22.6 Tue 18:00 P2

Dielectric relaxation of a nematic liquid crystal dispersed in a polar or non-polar polymer matrix — Lakshmi Meena Ganesan, •Lars Holländer, Werner Wirges, Peter Frübing, and Reimund Gerhard — Universität Potsdam

Polymer-dispersed liquid-crystal (PDLC) films were prepared from a nematic liquid crystal (LC) and polar poly(vinylidene fluoride-trifluoroethylene) (P(VDF-TrFE)) or non-polar poly(methyl methacrylate) (PMMA) as polymer matrix materials. During the preparation process, micrometer-sized droplets of LC are formed inside the polymer matrices.

The influence of the polymer matrix on the dielectric behavior of the LC was investigated by means of dielectric relaxation spectroscopy. From activation-energy calculations, it is assumed that the LC in the center of the droplets behaves like bulk material. Nevertheless, the angular motions of the dipole moments of the nematogen are slowed down in PDLC films by interfacial effects. This hindrance in motion is more pronounced in samples of polar P(VDF-TrFE) than in samples of non-polar PMMA and indicates a stronger interaction between the liquid-crystal molecules and the polar polymer molecules.

CPP 22.7 Tue 18:00 P2

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

We have investigated the molecular dynamics of n-butanol, C_4H_9OH, confined in mesoporous silicon oxide with a mean pore radius of 7 nm. In contrast to the bulk material, confined butanol does not crystallize upon slow cooling. Using dielectric spectroscopy we observe a glass transition and determine the glass transition temperature T_g. Upon slow heating we observe indications for a partial crystallization in the temperature range above 125 K. We compare these results to measurements on quenched bulk butanol showing the formation of a metastable glacial state as a result of a frustrated crystallization process [1,2].

[1] I. M. Shmyt'ko. R. J. Jiménez-Riobóo, M. Hassaine and A. A. Ramos, J. Phys.: Condens. Matter 22, 195102 (2010)

[2] M. Hassaine et al, J. Chem. Phys. 131, 174508 (2009)

CPP 22.8 Tue 18:00 P2

Investigation of discotic liquid crystals — •Christina Krause, Huajie Yin, and Andreas Schönhals — BAM, Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Broadband Dielectric Spectroscopy is applied in a broad frequency ($10^{-1} - 10^9$ Hz) and temperature range (173-283 K) to study the discotic liquid crystal Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther, 2,3,6,7,10,11 Hexakis(pentyloxy)triphenylene and 2,3,6,7,10,11-Hexakis(hexyloxy)triphenylene in the bulk state. The temperature dependence of the relaxation rates of Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther and 2,3,6,7,10,11-Hexakis(hexyloxy)triphenylene in the lower temperature range might be described by the Vogel-Fulcher-Tamann equation. For 2,3,6,7,10,11-Hexakis(pentyloxy)triphenylene the relaxation process in the lower temperature range shows an Arrhenius-type temperature dependence. To obtain an extensive understanding of the underlying processes Differential Scanning Calorimetry and Alternating Chip Calorimetry are performed. Investigations of Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther confined to porous silicon membranes and similar measurements of other discotic liquid crystals will be carried out in the future.

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Perfluorinated surfactants as model charged systems for understanding the effect of confinement on proton transport and water mobility in fuel cell membranes. A study by QENS — Sandrine Lyonnard[1], Quentin Berrod[1], •Beate-Annette Brüning[1], Gerard Gebel[1], Armel Guillermo[1], Hossein Ftouni[1], Jacques Ollivier[2], and Bernhard Frick[2] — [1]CEA, INAC/SPrAM/PCI, UMR 5819, 17 Av. des Martyrs, 38000 Grenoble, France — [2]Institut Laue-Langevin,6 rue Jules Horowitz,38042 Grenoble,France

We have investigated the dynamical properties of water confined in mesomorphous phases of perfluorinated sulfonic surfactants [1]. These systems mimic the physico-chemical properties of the perfluorinated Nafion membranes which are used as electrolyte in fuel cells. As the surfactants offer the advantage to self-assemble in well defined organized phases (e. g. hexagonal, lamellar), they are used as model charged systems to understand the structure transport relationship in complex real materials. Geometry and typical confinement size can be tuned through water concentration and temperature. A QENS study on hexagonal and lamellar phases was performed on both time-of-flight and backscattering spectrometers, covering a dynamic range from pico- to nanoseconds. Analysis of the data with localized translational diffusion models shows the existence of a strong confinement effect that depends on geometry. Typical confinement sizes and diffusion coefficients are obtained and compared to Nafion.

[1] S. Lyonnard et al., Eur. Phys. J ST 189, 205-216 (2010).