

DF 6: Glasses I (joint session DF/DY)

Time: Tuesday 9:30–12:15

Location: EB 407

Invited Talk DF 6.1 Tue 9:30 EB 407

Glass freezing in confined geometries studied by DMA — ●WILFRIED SCHRANZ, JOHANNES KOPPENSTEINER, and MADALINA-ROXANA PUICA — Faculty of Physics, University of Vienna, Boltzmannngasse 5, A-1090 Wien, Austria

Dynamics in confined surroundings appears in many fields, i.e. in chemistry, physics, biology, material science, etc. Using a dynamic mechanical analyser (DMA) we measured [1] the low frequency elastic response of the glass former salol confined in silica based nanoporous media of various pore sizes (2.5nm to 7.5 nm). In addition to the glass transition of the bulk material of salol we find a second freezing process, showing up in the real and imaginary parts of the complex elastic response. This is explained by a radial distribution of Vogel-Fulcher temperatures inside the pores, an assumption which is consistent with recent computer simulations [2] showing an increase of the molecular relaxation time with decreasing distance from rough pore surfaces. The observed glass transition temperatures decrease with decreasing pore size. The mechanism of the glass transition reduction will be discussed. Acknowledgements: Support by the Austrian FWF (P19284-N20) and the University of Vienna (IK 1022-N) is gratefully acknowledged.

[1] W. Schranz, M.R. Puica, H. Kabelka and A.V. Kityk. Europhys. Lett. 79, 36003 (2007) [2] P. Scheidler, W. Kob and K. Binder, Europhys. Lett. 59, 701 (2002).

DF 6.2 Tue 10:00 EB 407

Confined glass formers in nanoporous materials studied by ^{31}P NMR — ●SABINE GRADMANN¹, GILBERTE DOSSEH², CHRISTIANE ALBA SIMIONESCO², and ERNST RÖSSLER¹ — ¹Experimentalphysik II, Universität Bayreuth, 95440 Bayreuth, Germany — ²Laboratoire de Chimie Physique, CNRS-UMR 8000, Bâtiment 349, Université de Paris-Sud, 91405 Orsay, France

We investigate the dynamics of the glass former m-tricresylphosphate (mTCP) confined in the nanoporous matrices CPG, SBA15, MCM41 with different pore sizes, varying in diameter from 4nm up to 300nm, within a temperature range above the glass transition temperature (from 210K up to 370K). The performed ^{31}P NMR experiments demonstrate a great change in the relaxation times (T_1 and T_2) reflecting a significant slowing down of the dynamics for small pore systems in comparison with the bulk. Additionally, a detailed analysis of 1D spectra reveals pronounced dynamic heterogeneities, which we describe by a distribution of correlation times. The width of the latter decreases gradually while approaching the bulk limit. Furthermore, exploiting the large dynamic window of ^{31}P NMR, 2D exchange NMR is applied in order to establish whether the dynamic heterogeneities are of static or transient nature.

DF 6.3 Tue 10:15 EB 407

On the nature of the high-frequency relaxation in a molecular glass former: A joint study of glycerol by field cycling NMR, dielectric spectroscopy and light scattering — ●CATALIN GAINARU¹, OLIVER LIPS², ANNA TROSHAGINA¹, ROBERT KAHLAU¹, ALEXANDER BRODIN¹, FRANZ FUJARA², and ERNST A. RÖSSLER¹ — ¹Experimentalphysik II, Universität Bayreuth, D-95444 Bayreuth — ²Inst. f. Festkörperphysik, TU Darmstadt, Hochschulstraße 6, D-64289 Darmstadt

Recently we introduced a new approach to disentangle α -peak and excess wing (EW) contributions in the dielectric spectra of glass formers, assuming that the α -process obeys frequency-temperature superposition (FTS) in the full temperature range above the glass transition temperature T_g . Based on this scenario, a comparison between the orientational correlation functions of rank $l = 1$ (probed by dielectric spectroscopy – DS) and $l = 2$ (probed for the first time over a broad frequency range by field cycling NMR and light scattering – LS) is carried out. For the glass former glycerol DS, NMR and LS spectra are scaled according to FTS over 15 decades in frequency. Significant differences in the spectral shape of the susceptibilities of different ranks are recognized on both sides of the relaxation peak, while the time constants turn out to be the same. Regarding the systematic differences observed at high frequencies, they are explained by assuming that the fast dynamics (EW) proceeds via small angles. Below T_g , NMR and DS reflect the same dynamics down to cryogenic temperatures.

DF 6.4 Tue 10:30 EB 407

Dielectric polarization noise near the glass transition — ●SANDRA JENEWEIN, ANDREAS FLEISCHMANN, GERNOT KASPER, ANDREAS REISER, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Dielectric polarization noise can reveal fundamental information on relaxation processes in glass forming liquids or glasses. We measured the voltage and current noise spectral density in the organic glass former tri-propylene glycol in the vicinity of the glass transition. A home built electrometer amplifier was used to measure the voltage fluctuations of a capacitor filled with the sample. Using a custom built current-to-voltage converter we measured the current fluctuations of the sample. From the noise spectra we determined the dynamic glass transition. Using the fluctuation-dissipation theorem a comparison to frequency domain dielectric spectroscopy will be given.

DF 6.5 Tue 10:45 EB 407

Glassy dynamics in the mono-, di- and trimer of glass-forming propylene glycol — ●MELANIE KÖHLER, ROBERT WEHN, PETER LUNKENHEIMER, and ALOIS LOIDL — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg

We report broadband dielectric spectra on glass-forming propylene glycol and its di- and trimer. Aside of the α -relaxation, we focus on the dynamics at higher frequencies, which is believed to play an important role for the glass transition. While the monomer of propylene glycol has a well-developed excess wing, a characteristic spectral feature of glassy dynamics beyond the α -relaxation [1], the di- and trimers show a Johari-Goldstein β -relaxation [2]. Interestingly, as revealed by long-time aging experiments performed in our group [1], the excess wing in propylene glycol also can be described as signature of a β -relaxation. The data is analysed in the framework of different models, as the coupling model and the minimal model [3, 4]. In addition we treat the relation between the Cole-Cole peak, recently suggested within an extended version of mode coupling theory [5], and the spectral properties of the experimentally detected β -relaxation in these glass formers. Also first results in the region beyond GHz frequencies, where additional fast processes are expected, are provided. [1] K.L. Ngai *et al.*, J. Chem. Phys. 115, 1405 (2001). [2] K. Grzybowska *et al.*, J. Chem. Phys. 125, 044904 (2006). [3] K. L. Ngai, Comments Solid State Phys. 9, 127 (1979). [4] J. C. Dyre, N. B. Olsen, Phys. Rev. Lett. 91, 155703 (2003). [5] W. Götze and M. Sperl, Phys. Rev. Lett. 92, 105701 (2004).

DF 6.6 Tue 11:00 EB 407

The high frequency wing of the α -process as probed by depolarized light scattering — ●NIKOLAUS PETZOLD, ALEXANDER BRODIN, and E. A. RÖSSLER — Universität Bayreuth

We show that the "intermediate power law" recently observed in optical Kerr effect (OKE) measurements is equivalent with the excess wing from frequency-domain data long since known from dielectric spectroscopy (DS), and is an equally common feature in depolarised light scattering (DLS). From the OKE representation we find that the wing from OKE and DS data has a temperature independent exponent γ . Based on this behavior, we build a mastercurve from the literature OKE data and transform it into DLS representation. The mastercurve obtained that way fits nicely our DLS data. We are able to obtain a model independent crossover temperature for several liquids (benzophenone BZP, propylene carbonate (PC), glycerol (GY), propylene glycol (PG), ortho-terphenyl (OTP), decahydroisoquinolin (DHIQ)), at which temperature the onset of the wing first appears and which corresponds to a characteristic relaxation time of $\tau_x \approx 10\text{ns}$. In the high temperature range, where no wing is observable, the apparent width of the α -peak correlates with the relaxation strength of the fast dynamics and anticorrelates with fragility opposite to common wisdom.

DF 6.7 Tue 11:15 EB 407

Secondary relaxations in molecular glasses and polymers studied by 2D ^2H NMR — ●BJÖRN MICKO¹, DIETER BINGEMANN², and ERNST RÖSSLER¹ — ¹Experimentalphysik II, Universität Bayreuth, 95440 Bayreuth, Germany — ²Department of

Chemistry, Williams College, Williamstown, MA 01267, USA

We present a two-dimensional (2D) ^2H exchange NMR study, attempting to clarify the geometry of the molecular motion involved in the secondary relaxation (β -process) of three glass formers: PMMA, polybutadiene and a mixture of decaline and chlorobenzene. Stimulated echo measurements of the orientational correlation function circumscribe the temperature range, in which the β -process is expected to dominate the spectra. In this range we will show by comparison with the spectra of *o*-terphenyl, which does not show a pronounced β -process, that the β -process is also clearly observable in the 2D NMR spectra below and somewhat above T_g , until upon further heating the structural relaxation (α -process) enters the time window of the experiment and gives rise to a convergence of the spectra. Whilst the time constants for the studied systems (obtained from dielectric spectroscopy) are very similar on the reduced temperature scale T_g/T , the dielectric relaxation strength differs for each system. In contrast the 2D NMR spectra turn out to be practically identical on the T_g/T scale - which implies strong similarities concerning time scale and underlying geometry of the motion. To get further insight on the reorientation angles involved, simple motional models will be compared against the spectra.

DF 6.8 Tue 11:30 EB 407

Raman scattering in glasses and the boson peak — ●BERNHARD SCHMID¹ and WALTER SCHIRMACHER² — ¹FB Physik, Univ. Mainz — ²Phys.-Dept. TU München

Vibrational spectra of glasses as measured e.g. by inelastic neutron scattering exhibit at low frequencies ($\sim 1\text{THz}$) an enhancement over Debye's ω^2 law ("boson peak"). Using a theory of light scattering from disordered materials developed recently [1,2], we show that the anomalous low-frequency Raman spectra observed in this frequency regime are *not* proportional to the density of states (as was widely believed) but are related to the disorder-induced self-energy function. The latter, in turn, can be related to the width of the Brillouin line in the same frequency regime.

[1] B. Schmid, Diploma thesis, TU München, 2007

[2] B. Schmid and W. Schirmacher, to be published

DF 6.9 Tue 11:45 EB 407

Fractional approaches in dielectric broadband spectroscopy — ●SIMON CANDELARES¹ and RUDOLF HILFER^{1,2} — ¹ICP, Universität Stuttgart, 70569 Stuttgart, Germany — ²Institut für Physik, Universität Mainz, 55099 Mainz, Germany

A fractional approach is used to describe data from dielectric spectroscopy for several glassy materials. Using composite fractional time evolution propagators [1] a modified law for relaxation in glasses [2] is found that describes the experimental data for broadband dielectric spectroscopy [3]. Properties and solutions of some particular fractional differential equations (fDEQs) are investigated both for rational and irrational order. The laws of Debye, Kohlrausch, Cole-Cole, Cole-Davidson and Havriliak-Negami are compared with this new approach in frequency and time space.

[1] R. Hilfer; Time, Quantum and Information, L.Castell and O.Ischebeck (Eds.); Springer-Verlag Berlin 2003 p.235

[2] R. Hilfer Chemical Physics, **284**, 399 (2002)

[3] U. Schneider et al., Phys. Rev. E, **59**, 6924 (1999)

DF 6.10 Tue 12:00 EB 407

Collective atomic dynamics and relaxation processes in Al_2O_3 melt — ●SANDRO JAHN¹ and PAUL A. MADDEN² — ¹GeoForschungsZentrum Potsdam, Telegrafenberg, 14473 Potsdam — ²Chemistry Department, University of Edinburgh, Edinburgh EH9 3JJ, UK

The atomic dynamics of Al_2O_3 melt are studied by molecular dynamics simulation. The particle interactions are described by an advanced ionic interaction model that includes polarization effects and ionic shape deformations. The model has been shown to reproduce accurately the static structure factors $S(Q)$ from neutron and x-ray diffraction and the dynamic structure factor $S(Q, \omega)$ from inelastic x-ray scattering. Analysis of the partial dynamic structure factors show inelastic features in the spectra up to momentum transfers, Q , close to the principal peaks of partial static structure factors. The broadening of the Brillouin line widths is discussed in terms of a frequency dependent viscosity $\eta(\omega)$.