DY 11: Glasses I (joint session DF/DY)

Time: Tuesday 9:30–12:15   Location: EB 407

Invited Talk   DY 11.1   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, Boltz-
manngasse 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 pro-
cess, 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. Euro-
phys. Lett. 79, 36003 (2007) [2] P. Scheidler, W. Kob and K. Binder,
Europhys. Lett. 59, 701 (2002).

DY 11.2   Tue 10:00   EB 407

Confined glass formers in nanoporous materials studied by
^{31}**P NMR —** •Sabine Gradmann[1], Gilberte Dosseh[2], Christiane
Alba Simionesco[2], and Ernst Rössler[1] — [1]Experimentalphysik
II, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Laboratoire
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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 210 K up to 370 K). The performed ^{31}P NMR experiments
demonstrate a great change in the relaxation times (T1 and T2) reflec-
ting 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.

DY 11.3   Tue 10:15   EB 407

**On the nature of the high-frequency relaxation in a molec-
ular glass former: A joint study of glycerol by field cycling
NMR, dielectric spectroscopy and light scattering —** •Catalin
Gainaru[1], Oliver Lips[2], Anna Troshagina[1], Robert Kahlau[1],
Alexander Brodin[1], Franz Fujara[2], and Ernst A. Rössler[1] —
[1]Experimentalphysik II, Universität Bayreuth, D-95444 Bayreuth —
[2]Inst. f. Festkörperphysik, TU Darmstadt, Hochschulstraße 6, D-
64289 Darmstadt

Recently we introduced a new approach to disentangle α-peak and ex-
cess wing (EW) contributions in the dielectric spectra of glass formers,
assuming that the α-process obeys frequency-temperature superposi-
tion (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 con-
stants 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.

DY 11.4   Tue 10:30   EB 407

Dielectric polarization noise near the glass transition —
•Sandra Jenewein, Andreas Fleischmann, Gernot Kasper, An-
dreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik,
Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Dielectric polarization noise can reveal fundamental information on re-
laxation 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.

DY 11.5   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 gly-
col 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 cou-
pling model and the minimal model [3, 4]. In addition we treat the
relation between the Cole-Cole peak, recently suggested within an ex-
tended 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).

DY 11.6   Tue 11:00   EB 407

**The high frequency wing of the α-process as probed by de-
polarized light scattering —** •Nikolaus Petzold, Alexander
Brodin, and E. A. Rössler — Universität Bayreuth

We show that the "intermediate power law"recently observed in op-
tical 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 expo-
nent 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 liq-
uids (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 $\tau_x \approx$ 10ns. In
the high temperature range, where no wing is observable, the appar-
ent width of the α-peak correlates with the relaxation strength of the
fast dynamics and anticorrelates with fragility opposite to common
wisdom.

DY 11.7   Tue 11:15   EB 407

**Secondary relaxations in molecular glasses and poly-
mers studied by 2D ^{2}H NMR —** •Björn Micko[1], Dieter
Bingemann[2], and Ernst Rössler[1] — [1]Experimentalphysik II, Uni-
versität Bayreuth, 95440 Bayreuth, Germany — [2]Department of

Chemistry, Williams College, Williamstown, MA 01267, USA

We present a two-dimensional (2D) ^{2}H 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 spectrocopy) 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.

DY 11.8   Tue 11:30   EB 407

Raman scattering in glasses and the boson peak — •Bernhard Schmid[1] and Walter Schirmacher[2] — [1]FB Physik, Univ. Mainz — [2]Phys.-Dept. TU München

Vibrational spectra of glasses as measured e.g. by inelastic neutron scattering exhibit at low frequencies ($\sim$ 1THz) 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

DY 11.9   Tue 11:45   EB 407

Fractional approaches in dielectric broadband spectroscopy — •Simon Candelaresi[1] and Rudolf Hilfer[1,2] — [1]ICP, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Institut 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)

DY 11.10   Tue 12:00   EB 407

Collective atomic dynamics and relaxation processes in Al_2O_3 melt — •Sandro Jahn[1] and Paul A. Madden[2] — [1]GeoForschungsZentrum Potsdam, Telegrafenberg, 14473 Potsdam — [2]Chemistry 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 $\eta(\omega)$.