DY 13: Glass I (joint session with DF)

Time: Tuesday 10:00–13:00 Location: H23

DY 13.1 Tue 10:00 H23

Connection of the slow β-relaxation and physical aging in metallic glasses — •Jörg Hachenberg, Dennis Bedorf, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Metallic glasses are commonly used as model systems for glassy dynamics. This is due to the fact that their interactions can be simplified as such of hard spheres. Special attention has been attracted by recent experimental studies [1] and computer simulations [2] revealing the existence of a secondary, slow β-relaxation as a universal feature of the glass transition. Here, heat rate dependant mechanical spectroscopy is used to investigate the connection between this β-relaxation and physical aging, commonly described as a change in fictive temperature. The close dependence of both phenomena can be interpreted as a single relaxation showing up on two timescales (heating rate resp. spectroscopy frequency). It is proposed that both phenomena share a common origin.

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[1] J. Hachenberg, K. Samwer, J. Non-Cryst. Sol. 352, 5110 (2006)
[2] H. Teichler, Phys. Rev. E 71, 031505 (2005)

DY 13.2 Tue 10:15 H23

Fast β-relaxation of Na in Na_2O-xB_2O_3 melts — •Florian Kargl[1], Andreas Meyer[2], and Michael Marek Koza[3] — [1]Physik Department E13, TU München, 85748 Garching, Present Address: Department of Applied Physics, Chalmers University of Technology, 41296 Göteborg, Schweden — [2]Physik Department E13, TU München, 85748 Garching, Permanent Address: Institut für Raumsimulation, DLR, 51147 Köln — [3]Institut Laue-Langevin, 38042 Grenoble, France

We report on a fast β-relaxation process in a network-glass forming system that is up to the melt a fast-ion conductor. The process is evidenced by means of quasielastic neutron scattering [1]. The data are analysed in the framework of the mode-coupling theory (MCT) of the liquid to glass transition [2]. It is shown that this fast β-relaxation process, that can consistently be described within the framework of this theory, prepares the α-relaxation of the fast diffusing Na ions. We discuss the q- and T-dependence of the relevant parameters of the β-scaling law of the MCT and its dependence on Na concentration.
[1] F. Kargl, A. Meyer, M. M. Koza (submitted).
[2] W. Götze, J. Phys.: Condens. Matter **2**, 8485 (1990).

DY 13.3 Tue 10:30 H23

Microscopic mechanism of the β-process in metallic glass formers: molecular dynamics results for NiZr — •Helmar Teichler — Inst. f. Materials Physics, University of Göttingen

For glass formers around and below the dynamical critical temperature Tc of mode coupling theory (MCT), the fluctuation spectrum shows the β-regime in the time domain as precursor of the final α-decay. Recently, the β-regime has re-attracted much interest due to observation of the β-excess wing in spectroscopic data of a metallic glass by Rösner, Samwer, and Lunkenheimer (Europhys. Lett. 92, 105701(2004)) and the evaluation of the interconnection between Cole-Cole peak and spectral properties of the β-regime in the MCT by Sperl (PRE, 74, 011503(2006)). Here we address the question of the microscopic mechanisms that take place in the corresponding frequency regime in metallic glasses. Regarding this, molecular dynamics simulation data of vitrifying Ni0.5Zr0.5 melts are investigated by studying their inherent structure dynamics in order to eliminate the masking, predominant effect of thermal single-particle vibrations. Analysis of the remaining dynamics by nearest neighbour correlation functions, aimed at identifying topological fluctuations of the system, yields reversible over-barrier transitions of correlated chains of atoms as source of a β-peak between single-particle vibrations and the α-decay.

DY 13.4 Tue 10:45 H23

Liquid-to-glass transition of bulk-glass forming Cu60Ti20Zr20 alloy by molecular dynamics simulations — •Xiujun Han[1,2] and Helmar Teichler[1] — [1]Inst. f. Materials Physics, University of Göttingen — [2]IFF, Forschungszentrum Jülich

The present work reports results from molecular dynamics studies about microscopic structure and dynamics of the ternary, bulk metallic glass forming Cu60Ti20Zr20. In detail we consider nearest neighbour numbers, specific heat, simulated glass temperature, diffusion coefficients, and the incoherent intermediate scattering function (ISF). The applied atomic model reproduces well experimental X-ray data of total radial distribution function. It provides for Cu60Ti20Zr20 a structure with marked intermediate range order. The incoherent ISFs are analyzed within an extension of the mode coupling theory (MCT), where the memory kernel is evaluated from Laplace transform of the ISF. The dynamics of the system fulfils in most respects the predictions of the MCT, up to a suppression of the algebraic t^{-a}-decay in the early β-range, which is traced back to effects of single particle vibrations in the effective memory kernel that are not fully included in the MCT. As by-product, our investigation provides a method to re-construct, around the critical temperature, major parts of the memory kernel from λ and the plateau-value of the ISF.

DY 13.5 Tue 11:00 H23

Neutron scattering on levitated metallic droplets — •Andreas Meyer[1], Dirk Holland-Moritz[1], Sebastian Stueber[2], Thomas Hansen[3], and Tobias Unruh[4] — [1]Institut für Materialphysik im Weltraum, DLR Köln — [2]Physik Department E13, TU München — [3]ILL, Grenoble — [4]FRM-II, TU München

We report on first quasielastic neutron scattering experiments on metallic droplets using an electromagnetic levitation device on the neutron time of flight spectrometer ToF-ToF of the FRM-II. With this containerless processing undercoolings of the liquids up to 230K below the melting point were achieved. In binary ZrNi and ternary ZrNiAl glass forming melts the undercooling leads to a slowing down of the atomic mobility. The relation to the atomic dynamics in bulk glass forming metallic alloys in a Zr base will be discussed. We measured static structure factors of these systems on the neutron diffractometer D20 of the ILL. By isotopic substitution partial structure factors are accessible in liquid ZrNi. The partial structure factors also serve as an input for numerical mode coupling calculations.

15 min. break.

DY 13.6 Tue 11:30 H23

Understanding the fragility of supercooled liquids in terms of the properties of the potential energy landscape — •Andreas Heuer — Inst. f. Phys. Chemie, Corrensstr. 30, 48149 Münster

According to the Angell representation supercooled liquids are classified according to their fragility, i.e. the degree of non-Arrhenius behavior. Although in recent years fragility has been empirically correlated with different properties such as, e.g., mechanical behavior no microscopic understanding of the fragility exists. We report computer simulations of different glass-forming systems (silica, binary Lennard-Jones) where a detailed characterization of the potential energy landscape has been achieved. A crucial parameter is the crossover energy scale above which the local dynamics is fluid-like and below which it becomes activated. For these systems the macroscopic diffusion constant can be analytically expressed in terms of landscape parameters, reflecting its thermodynamic properties and its local dynamics. In this way we can show that the fragility strongly depends on the crossover energy scale and that for fragile systems the crossover to activated behavior only starts for very low-energy configurations. This result is interpreted in qualitative terms.

DY 13.7 Tue 11:45 H23

Molecular dynamics of a bioprotective fluid confined to nanopores — •Nicolas Ubrig[1], Rémi Busselez[2], René Berwanger[1], Denis Morineau[2], and Rolf Pelster[1] — [1]Fachrichtung 7.2, Experimentalphysik, Universität des Saarlandes, Postfach 151150, 66 041 Saarbrücken, Germany — [2]GMCM, campus de Beaulieu, 35042 Rennes Cedex, France

We study structure and molecular dynamics of a bioprotective fluid. This is a solution of glycerol and trehalose , the glass transition of which depends on the mixing ratio. The fluid is confined in parallel rodlike nanopores of a silicon matrix. Different techniques such as temperature dependent NMR, Raman-, infrared- and dielectric spectroscopy are applied in order to detect confinement-induced deviations

from the bulk behavior.

DY 13.8 Tue 12:00 H23

Continuous Time Random Walk Description of the Dynamics of a Model Glass Former — •OLIVER RUBNER and ANDREAS HEUER — Institut für Physikalische Chemie, Universität Münster

In this work we present an analysis of data obtained by simulations on a 65 particle binary Lennard-Jones Mixture (BMLJ65). We show that the dynamics of this system can be interpreted on the grounds of a Continuous Time Random Walk (CTRW) description. The basic assumptions of the CTRW model are well fulfilled and thus the picture of spatially and temporally independent jump processes between metabasins is supported.

Given the waiting time distribution of the jumps, it is then possible to deduce analytically some of the properties of the incoherent scattering function F(q,t). These predictions are compared to the numerical data and show very good agreement which supports strongly the notion of the BMLJ65-dynamics as a CTRW-process.

DY 13.9 Tue 12:15 H23

Complex Dynamics in a Binary Glass Former investigated by Dielectric Spectroscopy — •PHILIPP GUTFREUND, THOMAS BLOCHOWICZ, and BERND STÜHN — TU Darmstadt

Previous work on binary glass forming mixtures showed pronounced dynamic heterogeneities and a broad distribution of relaxation times of the smaller molecules in the mixture and in some cases even a distinct secondary relaxation peak was observed. It was also demonstrated that an additional power law contribution at the high frequency side of the main relaxation peak in neat glass-formers, called excess wing, can be separated as a distinct secondary relaxation peak if the molecule is contained in a slower matrix.

In the present work a mixture of Methyl-Tetrahydrofuran (M-THF) in Tristyrene was investigated by dielectric spectroscopy. The dielectric spectra are dominated by the smaller M-THF molecules due to the much stronger dipole moment. Calorimetry measurements show full miscibility in the whole concentration and temperature range. Pure M-THF is known to show a pronounced high frequency wing and a small secondary relaxation process, it is shown that in the mixtures several other processes emerge. The fastest of these processes seems to show certain typical signs of liquid dynamics far below T_G of the mixture. The fact of coexisting glassy and liquid states in a binary mixture below T_G was already shown in NMR measurements [1] and was previously anticipated by theoretical considerations [2].

[1] T. Blochowicz et al., J. Phys. Chem. B 103 (1999) 4032
[2] J. Bosse and Y. Kaneko, Phys. Rev. Lett. 74 (1995) 4023

DY 13.10 Tue 12:30 H23

Ab-inito calculations of atomic cluster configurations for ion conducting glasses — •CHRISTIAN MÜLLER and PHILIPP MAASS — Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany

Ab-inito quantum mechanical simulations of atomic configurations are carried out in order to explore structural properties of ion conducting glasses and in order to develop effective pair potentials for molecular dynamics simulations. Such potentials are of crucial importance for the modelling of ionic transport properties, which require a realistic identification of ion-sites and diffusion pathways [1]. In previous work mostly small structural units of a glass with high symmetry were considered. The computational power nowadays allows one to simulate much larger clusters, and to take into account the medium range order by means of Hartree Fock and density functional theory calculations. We present calculations for lithium borate and lithium sulphate glasses. In particular a comparison of calculated and experimental infra-red and Raman spectra is shown, which allows to judge the quality of the energy-optimized disordered cluster configurations.

[1] C. Müller, E. Zienicke, St. Adams, J. Habasaki, P. Maass, Phys. Rev. B, in press; condmat/0607523

DY 13.11 Tue 12:45 H23

Evaluation of effective one-particle potentials for the identification of ion conduction pathways in glasses — •EGBERT ZIENICKE, CHRISTIAN MÜLLER, and PHILIPP MAASS — Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany

The energetic characteristics of sites and the topology of diffusion pathways of mobile ions in network glasses play a key role for the understanding ion transport in vitreous electrolytes [1], which are used in many different technological applications. In molecular dynamics simulations of such systems the sites and diffusion pathways can be identified from the local number density of mobile ions determined from their motion [2,3]. Here we study the possibility of determining them from the time-averaged immobile network structure by applying an effective one-particle potential. To this end we compare the results of such analysis with those obtained from molecular dynamics simulations of lithium silicate glasses at various temperatures and compositions. In addition a comparison is made to results obtained from a bond valence analysis [3].

[1] W. Dieterich, P. Maass, Chem. Phys. **284**, 439 (2002).
[2] H. Lammert, M. Kunow, A. Heuer, Phys. Rev. Lett. **90**, 215901 (2003).
[3] C. Müller, E. Zienicke, St. Adams, J. Habasaki, P. Maass, Phys. Rev. B, in press; condmat/0607523.