

CPP 4: Glasses and Glass Transition (joint session CPP/DY)

Time: Monday 9:30–11:15

Location: ZEU 255

Invited Talk

CPP 4.1 Mon 9:30 ZEU 255
Shear-stress fluctuations and relaxation in glassy liquids
 — LIUDMYLA KLOCHKO, IVAN KRIUCHEVSKYI, JOACHIM WITTMER, ALEXANDER SEMENOV, HENDRIK MEYER, and ●JÖRG BASCHNAGEL
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By means of molecular dynamics simulations we study the shear modulus μ and shear stress relaxation function $G(t)$ of a short-chain glass-forming liquid. We determine μ via the shear-stress fluctuation formalism as a function of temperature T and sampling time Δt . When cooling the system below the glass transition temperature T_g the shear modulus has a finite, T -dependent, value which depends on Δt . We show that this sampling time dependence can be traced back to the relaxation of $G(t)$, thereby establishing a relation between two often employed means—i.e. shear stress fluctuation formalism and $G(t)$ —to characterize the shear response of glassy systems. We repeat the analysis for 100 independent configurations (samples) and find that the glass transition is accompanied by strong sample-to-sample fluctuations, implying that the standard deviation $\delta\mu$ of the (ensemble-averaged) modulus displays a peak near T_g and is of the same order of magnitude as μ itself. We propose a theory which explains this behavior.

CPP 4.2 Mon 10:00 ZEU 255

Molecular dynamics study of 1,4-polybutadiene supported film — ●FEDIR DEMYDIUK¹, HENDRIK MEYER¹, JOERG BASCHNAGEL¹, MATHIEU SOLAR¹, and WOLFGANG PAUL² — ¹Institute Charles Sadron, University of Strasbourg, UPR22 CNRS, 67034 Strasbourg, France — ²Institut für Physik, University of Halle, 06120 Halle (Saale), Germany

Our work is dedicated to studying the influence of realistic intrachain constraints imposed due to the presence of torsional barriers on the glass transition in thin polymer films of supported geometry by means of classical molecular dynamics simulations. In order to do so, we use the well-established united-atom model of 1,4-polybutadiene, that has been developed by W. Paul and coworkers (G. D. Smith and W. Paul, *J. Phys. Chem. A*, 102, 1200 (1998)) and studied in confined systems (M. Solar, K. Binder and W. Paul, *J. Chem. Phys.*, 146, 203308 (2017)). In our case, the model had to be adapted for usage in systems with free surface.

Focusing on dynamics of united atoms and shear-stress relaxation, we first discuss our results for bulk polybutadiene and then present first extensions of bulk simulations to supported films. First analysis of the supported films shows that dynamics is enhanced at the free surface and slowed down at the substrate.

CPP 4.3 Mon 10:15 ZEU 255

Dynamics of an arrested phase transition in a protein system — ●ANITA GIRELLI¹, HENDRIK RAHMANN², NAFISA BEGAM¹, ANASTASIA RAGULSKAYA¹, FABIAN WESTERMEIER³, FAJUN ZHANG¹, CHRISTIAN GUTT², and FRANK SCHREIBER¹ — ¹Universität Tübingen, Germany — ²Universität Siegen, Germany — ³DESY, Germany

The interest in phase transitions in biological systems has attracted much effort because of their numerous applications and its role as a mechanism underlying intracellular organization [1]. In this study the development of the spinodal decomposition near the gel/glass transition in a globular protein system was studied using X-Ray Photon Correlation Spectroscopy (XPCS) in the ultra small angle X-Ray scattering (USAXS) regime. The dynamics was probed at different quench depth, exhibiting two regimes: the first regime shows a single exponential decay of the correlation function, and the corresponding decorrelation time increases exponentially with waiting time t_w . In the second regime, a second relaxation channel appears and the associated nonergodicity parameter increases with t_w until it becomes the dominating decay. The corresponding decorrelation time increases as a power law in t_w . The dynamics was compared to simulations, which were performed by solving numerically the Cahn-Hilliard equation coupled with a gel transition. The effect of nanoscale arrested dynamics can be seen on the microscopic dynamics. Aging with quench depth dependence is visible and can be connected to real space parameters such as final concentration and mobility.

[1] Berry et al., *Rep. Prog. Phys.*, **81**, 046601, 2018

CPP 4.4 Mon 10:30 ZEU 255

molecular dynamics of glassy polynorbornenes bearing flexible side substituents: nanophase separation and glass transition — ●MOHAMED AEJAZ KOLMANGADI¹, PAULINA SZYMONIAK¹, GLEN JACOB SMALES¹, BRIAN PAUW¹, MAXIM BERMESHEV², MARTIN BÖHNING¹, and ANDREAS SCHÖNHALS¹ — ¹Bundesanstalt für Materialforschung und prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — ²A.V. Topchiev Institute of Petrochemical Synthesis of Russian Academy of Science, Leninskii prospect, 29, 119991 Moscow, Russia

Polynorbornenes are latest among the high-performance polymers in the field of membrane gas separation. Not much has been studied regarding their molecular dynamics till now. In the present work, we report dielectric and calorimetric investigations of series of polynorbornenes with rigid main backbone and flexible (AlkO)3Si side groups with different length (Al = Propyl, Butyl, Octyl, Decyl). Two dielectrically active α and β relaxations observed are assigned to localized fluctuations and segmental relaxation of the flexible side groups of the polymer. A nanophase separation between the main and side chain parts is concluded from the presence of two dynamic glass transitions of the polymer, is confirmed by means of small and wide-angle X-ray scattering. Furthermore, for the first time, the glass transition temperatures of these polymers which are beyond or near to their degradation temperature are determined using Fast Scanning calorimetry employing high heating and cooling rates. The glass transition temperatures of the polymers decrease with increasing length of the alkyl side chain.

CPP 4.5 Mon 10:45 ZEU 255

Controlled crystallisation of luminescent borate-based glasses — ●MARC BÜRGER¹, A. CHARLOTTE RIMBACH¹, and STEFAN SCHWEIZER^{1,2} — ¹Faculty of Electrical Engineering, South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — ²Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Lübecker Ring 2, 59494 Soest

Luminescent borate glasses and glass ceramics offer a broad spectrum of optical applications. Here, the optical properties of the glass as well as the glass ceramic strongly depend on their composition and the production process. In this work, two different glass systems and their crystallization processes therein are analysed: (i) Lithium borate glass comprised of $\text{Li}_2\text{O-Al}_2\text{O}_3\text{-B}_2\text{O}_3$ and (ii) barium borate glass with $\text{BaO-B}_2\text{O}_3$. For optical activation, the lanthanide ion Dy^{3+} is added in the form of Dy_2O_3 to enable for a bright green-yellowish luminescence. To initiate the crystallization process in the glass, the samples are thermally-processed at a temperature above the glass transition temperature. The number and size as well as the phase of the grown crystallites depend significantly on annealing temperature and time as well as the heating rate. The crystallite growth is investigated and analysed in detail by differential scanning calorimetry and *in situ* x-ray diffractometry. In addition, the samples are optically characterized for transmittance, reflectance and scattering.

CPP 4.6 Mon 11:00 ZEU 255

X-ray computed tomography of glass foams with controlled bi-modal pore size distribution — ●CRISTINE S. DE OLIVEIRA¹, RICHARD KOHNS², FELIX MEYERHOEFER², MATTHIAS NEUMANN³, DIRK ENKE², VOLKER SCHMIDT³, RALF B. WEHRSPHON¹, and JULIANA MARTINS DE S. E SILVA¹ — ¹Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — ²Institut für Technische Chemie, Universität Leipzig, Germany — ³Institut für Stochastik, Universität Ulm, Germany

Glass foams are materials consisting of a light-weight porous glass structure of special importance in the fields of civil engineering and bio-implants. Typically, their synthesis involves the thermal foaming of a powder mixture of glass with a foaming agent that decomposes at the foaming temperature, resulting in a solid glass skeleton permeated by empty pores. In our work, we synthesized a series of glass foams followed by a phase-separation procedure and acid leaching. We used a powdered mixture of silica-based glasses, MnO_2 and C which we submitted to a foaming process at 815 °C. Afterwards, the material was left to cool inside the oven to temperatures around 500 °C and maintained at a constant temperature for phase separation. We then

acid leached, washed and dried the samples. Based on the results obtained using X-ray CT at the micro and nanometer scales we observed

that slight changes in the preparation procedure resulted in foams with different porosity, pore sizes, pore volumes and sphericity.