

CPP 27: Poster: Soft Matter Dynamics / Glasses

Time: Tuesday 18:15–21:00

Location: Poster B2

CPP 27.1 Tue 18:15 Poster B2

Fragile-to-strong transition in liquid silica — ●JULIAN GESKE, BARBARA DROSSEL, and MICHAEL VOGEL — Institut für Festkörperphysik, Technische Universität Darmstadt

We investigate anomalies in liquid silica with molecular dynamics simulations and present evidence for a fragile-to-strong transition at around 3000K. To this purpose, we studied the structure and dynamical properties of silica over a wide temperature range, finding three indicators of the fragile-to-strong transition. First, there is a density minimum at around 3000K and a density maximum at 3400K. Second, the local structure characterized by the tetrahedral order parameter changes dramatically around 3000K and changes from a higher-ordered, lower-density phase to a less ordered, higher-density phase. Third, the correlation time τ changes from an Arrhenius behaviour below 3000K to a Vogel-Fulcher behaviour at higher temperatures.

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Molecular Mobility and Gas Transport Properties of PIM-1 and Nano composites based on PIM-1 and PhenethylPOSS — NORA KONNERTZ, YI DING, MARTIN BÖHNING, and ●ANDREAS SCHÖNHALS — Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin

Polymers with intrinsic microporosity are of highly interest in the field of gas separation membranes. Especially the first synthesized PIM-1 shows extraordinary permeabilities and selectivities. Unfortunately, PIM-1 tends to physical aging and loses its good properties. Physical aging is related to the molecular mobility of PIM-1 which was here investigated by broadband dielectric spectroscopy (BDS). Besides the studies on pure PIM-1 a polyhedral oligomeric silsesquioxane with phenethyl substituents (PhenethylPOSS) was used as nanofiller (0 - 40 wt-%) in the PIM-1 matrix to improve the gas transport properties and prevent physical aging. The molecular mobility of the solution casted nano composite films was analyzed by BDS as well. Furthermore, gas transport properties were determined with the time lag method (0 - 20 bar) in a temperature range of 35°C to 65°C with N₂, O₂, CH₄ and CO₂.

CPP 27.3 Tue 18:15 Poster B2

Dynamical coexistence in polydisperse hard spheres — ●MATTEO CAMPO and THOMAS SPECK — Institut für Physik, JGU Mainz, Germany

We investigate the slow dynamics of a model glass former, the polydisperse hard-sphere liquid, using a combination of molecular dynamics and importance sampling in the trajectory ensemble. According to dynamical facilitation theory, the glass transition takes place as a consequence of dynamical heterogeneity which develops as the liquid is quenched. We characterize dynamical heterogeneity by a parameter, the mobility, which quantifies how far particles move in the supercooled liquid. By studying trajectories longer than the structural relaxation time, we observe exponential tails in the probability distribution of mobility, which indicate phase coexistence of normal and exceptionally slow trajectories.

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Time needed to form stable glasses is comparable to β -relaxation time — ●YEONG ZEN CHUA, MATHIAS AHRENBERG, and CHRISTOPH SCHICK — Institute of Physics, University of Rostock, Rostock 18051 Germany

Glasses produced by physical vapor deposition (PVD) exhibit different properties, depending on the deposition conditions. Consistent with previous works, glasses of ethylcyclohexane (ECH) vapor-deposited at temperature of about 0.85 of glass transition temperature, T_g observed to be the most stable glasses with low enthalpy, low heat capacity, high kinetic stability and high density. Isothermal transformation of the as-deposited glasses into the supercooled state is investigated for the deposition rate dependency, covering four orders of magnitude, at different substrate temperatures. The kinetic stability of the glasses (transformation time at 103 K) shows strong deposition rate dependency for lower substrate temperatures. The data provide an estimate for the substrate temperature dependent free surface residence time needed for the molecules in the assumed mobile surface layer to promote stable glass formation. Stable glasses are formed if this time is

of the order of the β -relaxation time, many orders of magnitude faster than the α -relaxation at the substrate temperature. Stable glasses are observed even for substrate temperatures below the Vogel and the Kauzmann temperatures, indicating a full decoupling of the process of stable glass formation from the α -relaxation.

CPP 27.5 Tue 18:15 Poster B2

Diffusion of PMMA: microgels and linear polymer — ●BASTIAN PUR¹, WERNER KÖHLER¹, KLAUS HUBER² und MARTIN SCHNEIDER² — ¹Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — ²Physikalische Chemie, Universität Paderborn, 33098 Paderborn, Germany

In present theories for polymer thermophoresis in dilute solutions there are two theoretical models under discussion: draining coil and nondraining coil, corresponding to the Rouse and the Zimm picture, respectively. In order to discriminate between these models we have started a comparative investigation of a linear chain polymer and cross-linked microgels. The linear polymer sample used is poly(methylmethacrylate) (PMMA) and the micro-gel samples are PMMA cross-linked with different amounts of ethylen-di-methacrylate (EGMA). In either case toluene is used as solvent. By means of transient holographic grating technique we obtained the thermal diffusion coefficient D_T , the Fickian diffusion coefficient D and the Soret coefficient S_T as functions of the polymer concentration c . We have found out that for $c \rightarrow 0$ the thermophoretic mobility of the linear polymer and the microgel with 3.5% EGMA are identical within experimental accuracy. In addition we performed dynamic light scattering experiments to characterize the different microgel samples. Thereby we obtained that the diffusion coefficient is independent of the amount of cross-linker and so are (by using Stokes-Einstein equation) the hydrodynamic radii of the microgels.

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Diffusion of PMMA: microgels and linear polymer — ●BASTIAN PUR¹, WERNER KÖHLER¹, KLAUS HUBER² und MARTIN SCHNEIDER² — ¹Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — ²Physikalische Chemie, Universität Paderborn, 33098 Paderborn, Germany

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CPP 27.7 Tue 18:15 Poster B2

Extracting material net properties of monomolecular coverages with nano-structured electrode arrangements — ●MARTIN TRESS^{1,2}, NILS NEIBAUER², RENE WINKLER³, PETRA UHLMANN³, EMMANUEL MAPESA², MANFRED REICHE⁴, and FRIEDRICH KREMER² — ¹Max Planck Institute for Polymer Research, Mainz — ²University of Leipzig — ³Leibniz-Institut für Polymerforschung Dresden e.V. — ⁴Max Planck Institute of Microstructure Physics, Halle (Saale)

Recently, Broadband Dielectric Spectroscopy (BDS) has been combined with a nano-structured electrode arrangement to investigate glassy dynamics in monomolecular layers and isolated polymer chains [1]. Thereby, insulating nano-structures serve as spacers between the silicon electrodes enabling an electrode separation of only 40 nm. Since

this is still larger than the height of the actual sample material, a major fraction of the capacitor volume is empty. Consequently, the measured signal is an average of several contributions, including the dielectric properties of the sample itself, the spacer material and the gap between the electrodes. Due to the particular geometry, the composition of these contributions is not straight-forward. To unravel the individual dielectric functions of all components an equivalent circuit model is employed. Using BDS spectra of poly(2-vinylpyridine) (P2VP) brushes and condensed isolated P2VP chains as examples it is demonstrated how to unravel molecular relaxations, polarization effects and charge transport as well as the extraction of their net properties.

[1] M. Tress et al. Science 341 (2013) 1371

CPP 27.8 Tue 18:15 Poster B2

Molecular Dynamic Simulation and forcefield creation of Poly(3-hexylthiophene) for aggregation investigations —

•MARIE KATHRIN TRITSCHER and STEPHAN GEKLE — Universität Bayreuth

Poly(3-hexylthiophene) is a widely investigated polymer for light harvesting devices as it possesses comparably good performances due to its high charge carrier mobility.

Using molecular dynamics simulation we show that there is a temperature dependent aggregation between different polymer chains in agreement with corresponding spectroscopic experiments.

Additionally investigations of the ordering and the packing behaviour of the chains are performed in atomistic and coarse grained representations of the system.