CPP 19: Glasses and Glass Transition 1 (joint session DY/CPP)

Time: Wednesday 9:30–10:30 Location: DYc

CPP 19.1 Wed 9:30 DYc

Molecular dynamics study of 1,4-polybutadiene supported films — •Fedir Demydiuk[1], Hendrik Meyer[1], Joerg Baschnagel[1], Mathieu Solar[1], and Wolfgang Paul[2] — [1]Institute Charles Sadron, University of Strasbourg, UPR22 CNRS 67034 Strasbourg, France — [2]Institut 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 19.2 Wed 9:50 DYc

Glassy dynamics, glass transition and electrical conductivity of Guanidinium based ILCs: Influence of the cation headgroup configuration — •Mohamed A Kolmangadi, Arda Yildirim, and Andreas Schönhals — Bundesantalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Molecular mobility and conductivity of four bent shaped tetramethylated guanidinium based ionic liquid crystals (ILCs) with varying head group configuration (cyclic or acyclic) and alkyl chain length is investigated by a combination of broadband dielectric spectroscopy (BDS) and specific heat spectroscopy (SHS). BDS investigation reveals two relaxation processes: a localized γ process and α1 process corresponding to the glassy dynamics. SHS investigations show one calorimetrically active α2 relaxation process also corresponding to the glassy dynamics of the system. The temperature dependencies of the relaxation rates of two different glassy dynamics are similar for the cyclic ILC while for the acyclic counterpart they are different. Possible molecular assignments for the α1 and α2 relaxation are discussed in detail. Alongside relaxation processes, a significant conductivity contribution was observed for all ILCs, where the absolute value of DC conductivity increases by 4 orders of magnitude at the transition from the crystalline to the hexagonal columnar phase. The increase is traced to the change in the underlying conduction mechanism from the delocalized electrical conduction in the Cry phase to ionic conduction in the quasi 1D ion columns formed in the hexagonal columnar mesophase.

CPP 19.3 Wed 10:10 DYc

A new approach to probe the plastic rearrangements inside a shear band. — •Moumita Maiti and Andreas Heuer — University of Münster, Münster, Germany

We follow a single particle trajectory of a system subjected to a uniform shear by calculating it's instantaneous displacement with time. There are intermittent hops in the trajectory, which are treated as plastic events, and the particles which have performed hops, are called active. In the steady state, the number of events per particle of the whole system increases initially by increasing system size, and by further increment the number almost saturates. The onset of saturation is the onset of shear banding. Interestingly, above the onset, we observe a system size scaling in the number of plastic events only inside the shear band. The scaling is explained from the intervals between two consecutive hops of a particle, which decreases on an average with increasing size. We further show that there is a stronger coupling between active particles with increasing system size which helps to understand the smaller value of the intervals, so our approach captures the collective nature of plastic events. Additionally, we observe a system spanning avalanches for these sizes which exhibit shear banding, and the distribution of avalanche sizes have a different exponent from the mean field theory.