Kremer-Grest models for commodity polymer melts: Linking theory, experiment and simulation at the Kuhn scale

Ralf Everaers

The Kremer-Grest (KG) polymer model is a standard model for studying generic polymer properties in Molecular Dynamics simulations. It owes its popularity to its simplicity and computational efficiency, rather than its ability to represent specific polymers species and conditions. In the first part of the talk, I will present results of our efforts to determine the characteristic time and length scales of KG melts as a function of an additional parameter characterising a wormlike bending stiffness, which as introduced by Faller and Muller-Plathe. Then I will introduce a one-parameter KG "force field'' and provide mapping relations from KG to SI units for a wide range of commodity polymers. The connection between the experimental and the KG melts is made at the Kuhn scale, i.e. at the crossover from chemistry-specific small scale to the universal large scale behavior. We expect Kuhn scale-mapped KG models to faithfully represent universal properties dominated by the large scale conformational statistics and dynamics of flexible polymers. While it is sufficient to reproduce the number of entanglements per chain, Z, to account for linear viscoelastic behavior, our models also the number of Kuhn segments per entanglement length, N_{eK}. As a consequence, they account for the maximal chain extension, $\sim\sqrt{N_{eK}}$, under strong deformations. Furthermore, we speculate, that they ought to exhibit friction reduction in fast elongational flows, in so far as the effect can be attributed to the alignment of the Kuhn segments to the stretching direction.