Multi-chain slip-spring simulations for entangled polymer dynamics

Y. Masubuchi and T. Uneyama

Dept. Mat. Phys., Nagoya University, Nagoya 4648603, Japan (mas@mp.pse.nagoya-u.ac.jp)

The multi-chain slip-spring (MCSS) model[1–4] is an extension of the single-chain version proposed by Likhtman[5], mimicking entanglement between polymers by virtual springs on Rouse chains. The significant difference from the single-chain model is the weak repulsive interaction between Rouse beads to compensate for artificial attraction due to the virtual springs. We have derived kinetic equations for the Rouse beads and the virtual springs considering detailed balance from the free energy that includes the inter-bead interaction. Simulations with these equations have reproduced entangled/unentangled polymer dynamics fully consistent with the bead-spring simulation and the multi-chain slip-link simulation for diffusion and linear relaxation modulus[6]. Inheriting the scale-free nature of Rouse chains, MCSS models with different slip-spring densities, Rouse bead densities, and virtual spring intensities are equivalent to each other, as shown in Fig. 1, with conversion parameters for length, time, and modulus[7,8]. The model has been extended to branch polymers, and the model prediction is consistent with experimental data for star-branched polystyrene, polyisoprene, and H-branched polystyrene[9]. Taking advantage of multi-chain modeling, we have examined the effect of entanglement on gelation[10]. We have confirmed that the MCSS simulation is fair also under mild shear[11].

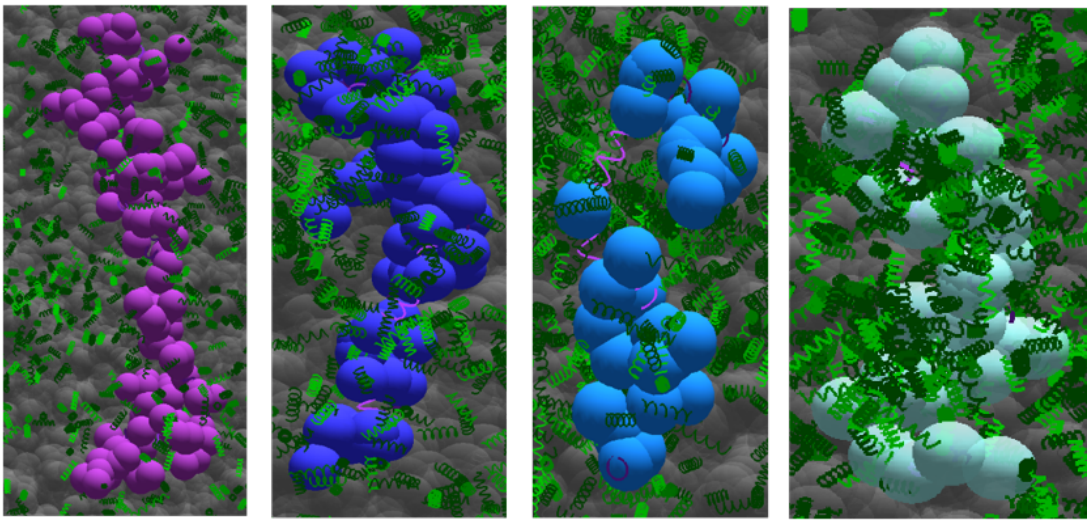

Figure 1: Equivalent MCSS models with different virtual spring densities

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