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Dynamics of entangled polymers in the presence of obstacles
NIGEL CLARKE, University of Sheffield, KAREN WINEY, RUSSELL COMPOSTO, University of Pennsylvania — We have observed that, for a wide range of spherical nanoparticles, the polymer diffusion coefficient relative to the pure melt value as a function of the interparticle distance relative to the chain radius of gyration collapses onto a master curve. In order to gain insight into the molecular basis for this behaviour, we use the Evans-Edwards Monte Carlo model for reptation dynamics in which the chains are coarse-grained such that each bead within the simulation represents one entanglement segment. We investigate the long time diffusion behaviour when the chains are constrained by a lattice structure with regularly spaced holes each the size of an entanglement spacing. We find that as the dimensions of the lattice decreases, the power law for the scaling of the diffusion coefficient with molecular weight changes from the well known result for melt diffusion of entangled chains of approximately -2 to approximately -3. We present a simple physical model that captures this result.

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