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Dynamics in Polymer Nanocomposites[1]

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Since nanoparticles are increasingly being added to polymers to impart mechanical and functional properties, we are exploring how nanoparticles impact polymer dynamics with a focus on the diffusion coefficients. In high molecular weight polymer melts, chain diffusion is well described by the reptation model. Motion proceeds as a snake-like diffusion of the chain as a whole, along the contour of a tube that mimics the role of physical entanglements, or topological constraints, with other chains. In polymer nanocomposites there are additional constraints due to the dispersed nanoparticles in the polymer matrix. Chain motion can be altered by nanoparticle size, shape , aspect ratio, surface area, loading and the nature of the interactions between the nanoparticles and the polymer matrix. We have observed a minimum in the diffusion coefficient as a function of nanoparticle concentration when the nanoparticles are rod-like and a collapse of the diffusion coefficient onto a master curve when the nanoparticles are spherical. We are simulating the dynamics using molecular and dissipative particle simulations in order to provide physical insight into the local structure and dynamics, and have also carried out highly coarse grained Monte Carlo simulations of entangled polymers to explore how reptation is affected by the presence of larger scale obstacles.

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