

207g A Coarse-Grained Simulation of Rheology of Polymer Nanocomposites

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We use a coarse-grained simulation approach to address the dynamical properties of nanoparticles in polymeric fluids. We have studied influence of polymer-particle friction, polymer-particle interactions and particle concentration upon polymer matrix relaxation dynamics, particle diffusion and rheology of the composite. Our results suggest nontrivial impact of the polymer relaxations upon the particle dynamics. Moreover, we elucidate the manner in which polymer conformations and structure around the particle significantly impact upon the properties of the nanocomposite. We also specifically address the rheological and mechanical effects arising from the interplay between particle jamming and transient network phenomena. Our results provide insights into the microscopic/molecular origins of polymer nanocomposite rheology and properties and the influence of various physical parameters governing them.