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Diffusivity and Transient Localization of Filler Particles in Polymer Melts and Crosslinked Systems ZACHARY E. DELL, KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign — Building on recent progress in describing the microscopic equilibrium structure of polymer nanocomposites (PRISM theory), as well as the naïve mode coupling and nonlinear Langevin equation approaches for predicting localization and activated barrier hopping, we have initiated the study of dynamical phenomena in nanocomposites at finite filler loading. A colloidal suspension perspective is adopted whereby the polymer dynamics are assumed to remain unperturbed by fillers. Both entangled polymer melts and crosslinked systems are studied. The long time behavior of a tagged nanoparticle (localization and diffusivity) is calculated for various melt (tube diameter, polymer radius of gyration) and nanoparticle (filler size and volume fraction, polymer-filler attraction strength) parameters. For transiently localized particles, a dynamic free energy is constructed and employed to compute the nanoparticle localization length, mean barrier hopping time, and self-diffusion constant. The influence of filler-filler interactions on the Stokes-Einstein violation phenomenon in entangled melts is established. In addition, the influence of nanocomposite statistical structure (e.g., in the depletion, steric stabilization, or bridging regimes) on slow dynamics and localization is investigated.

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