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Microscopic Theory of Nanoparticle Diffusivity in Entangled and Unentangled Polymer Melts UMI YAMAMOTO, KENNETH SCHWEIZER, University of Illinois, Urbana-Champaign

— We present a statistical dynamical theory at the level of forces for the violation of the Stokes-Einstein (SE) diffusion law of a spherical nanoparticle in entangled and unentangled polymer melts. Based on a combination of mode-coupling and polymer physics ideas, the non-hydrodynamic friction coefficient is related to microscopic structure and the length-scale-dependent polymer melt collective density fluctuation dynamics. When local packing correlations are neglected, analytic expressions are derived for the non-hydrodynamic diffusivity as a function of particle size, polymer radius-of-gyration, tube diameter, degree of entanglement and temperature; local packing effects are numerically investigated under athermal and attractive conditions. The conditions for the recovery of the SE law are qualitatively distinct for unentangled and entangled melts, and entanglement effects are the origin of large SE violations consistent with recent experiments. The influences of melt packing fraction and interfacial attraction strength are also qualitatively different depending on whether the polymers are entangled or not. The anomalous time-dependence of the nanoparticle mean square displacement is studied using a self-consistent Generalized Langevin Equation approach.

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