

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Nanoparticle diffusion in dense polymer melts JAGANNATHAN T. KALATHI, SANAT K. KUMAR, Columbia University, GARY S. GREEST, Sandia National Laboratories — The diffusion of nanoparticles in melts and solutions of polymers facilitates understanding of the viscoelastic behavior of the respective polymers and their composites. It also plays a vital role in determining the equilibrium structure and morphology of polymer nanocomposites and hence, their mechanical properties. In this work, we present the diffusion coefficients of non-sticky smooth spherical particles of different sizes (1-10 σ) in an athermal mixture of particles and polymers of different chain lengths ($N = 20$ to 400) using molecular dynamics simulations. The diffusion of nanoparticles of size comparable to the polymer segment size (σ) is independent of chain length and hence, nanoparticles apparently feel only the local viscosity, as predicted by scaling theories. When the nanoparticle becomes larger than a segment (or alternately the correlation length in the melt), then, the diffusion coefficient decreases. This is due to the fact that the mobility of the particles is retarded either by a chain section of size equivalent to the particle size or by entanglement mesh size depending on the nanoparticle size. We also elucidate the role of chain entanglements on diffusion of nanoparticles.

Jagannathan T. Kalathi
Columbia University

Date submitted: 17 Dec 2012

Electronic form version 1.4