Nanoparticle Motion in Entangled Melts of Linear and Non-Concatenated Ring Polymers MICHAEL RUBINSTEIN, TING GE, University of North Carolina, JAGANNATHAN KALATHI, National Institute of Technology Karnataka, India, JONATHAN HALVERSON, Max Planck Institute for Polymer Research, Germany, GARY GREST, Sandia National Laboratories — The motion of nanoparticles (NPs) in entangled melts of linear polymers and non-concatenated ring polymers are compared by large-scale molecular dynamics simulations. The comparison provides a paradigm for the effects of polymer architecture on the dynamical coupling between NPs and polymers in nanocomposites. Strongly suppressed motion of NPs with diameter d larger than the entanglement spacing a is observed in a melt of linear polymers before the onset of Fickian NP diffusion. This strong suppression of NP motion occurs progressively as d exceeds a, and is related to the hopping diffusion of NPs in the entanglement network. In contrast to the NP motion in linear polymers, the motion of NPs with $d > a$ in ring polymers is not as strongly suppressed prior to Fickian diffusion. The diffusion coefficient D decreases with increasing d much slower in entangled rings than in entangled linear chains. NP motion in entangled non-concatenated ring polymers is understood through a scaling analysis of the coupling between NP motion and the self-similar entangled dynamics of ring polymers.

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