Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Chain-Scale Polymer Dynamics Through Homogeneously Confining Nanoparticles ERIC BAILEY, HUIKUAN CHAO, ROBERT A. RIGGLEMAN, KAREN I. WINEY, Univ of Pennsylvania — The addition of nanoparticles (NPs) to a polymer matrix can significantly enhance polymer mechanical and functional properties. Recent tracer diffusion experiments in nanocomposites show that polymer diffusion is significantly reduced relative to the bulk. In fact, a master curve was developed by plotting diffusion coefficients normalized by that of the bulk polymer against the confinement parameter, ID/2Rg, where ID is the interparticle distance and Rg is the tracer size. To further study the role of confinement, coarse-grained MD simulations are used to systematically study the independent effect of ID and Rg on chain-scale dynamics. A uniquely constructed simulation box with a monolayer of hexagonally packed NPs creates regions of homogeneously confined polymer and pristine bulk polymer. This reveals the magnitude and length scale of NP-induced perturbations for several values of ID/2Rg. Displacement distributions show significant asymmetries in polymer motion near NPs and localized diffusion coefficients show more than a 25% reduction in diffusion coefficient. Surprisingly, chain dynamics are perturbed several times Rg from the NP region. These MD simulations are then compared to calculations on a minimal model in the same simulation environment.

Eric Bailey
Univ of Pennsylvania

Date submitted: 11 Nov 2016 Electronic form version 1.4