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Polymer Diffusion in the Presence of Nanoparticles

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The center-of-mass diffusion of polymers within a polymer melt proceeds by the mechanism of reptation wherein the polymer is confined to a tube that is defined by neighboring entanglements and moves along its contour. Polymer diffusion is perturbed when the melt contains nanoparticles that are comparable in size to the radius of gyration (Rg) of the polymers. Within this talk, we will present tracer diffusion coefficients (D) results for three types of nanocomposite: spherical nanoparticles with surface functionalization, spherical nanoparticles with brushes, and cylindrical nanoparticles (aspect ratio = 5 to 50). When functionalized spherical nanoparticles have neutral or attractive interactions with the polymer matrix, a monotonic decrease in the diffusion coefficient is observed across a wide range of polymer molecular weight, nanoparticle size, and nanoparticle concentration. These data collapse onto a master curve when plotted as D normalized by the diffusion coefficient into a neat homopolymer (D/Do) versus our confinement parameter defined as the interparticle distance divided by 2Rg (ID/2Rg). Polymer diffusion in systems with grafted spherical nanoparticles exhibit the same D/Do versus ID/2Rg, when ID accounts for the extent to which the tracer polymer penetrates the polymer brush. For various cylindrical nanoparticles D/Do versus nanoparticle concentration exhibits a minimum when 2Rg is both larger than the nanoparticle diameter and smaller than the nanoparticle length. Complimentary molecular dynamics simulations and neutron scattering results will also be presented.