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Simulations of Polymer Grafted Nanoparticles in a Polymer Matrix

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We have performed molecular dynamics (MD) simulations of polymer-grafted nanoparticles in a polymer melt. The model is a coarse-grained representation of spherical nanoparticles with a grafted poly(methyl methacrylate)-like bead-spring polymer in a matrix of the same polymer. Simulations were performed on both a single polymer-grafted nanoparticle as well as for a pair of polymer-grafted nanoparticles. The nanoparticle has a diameter of 5 nm. We have investigated the role of the molecular weight of the grafted and matrix polymer on both brush structure and nanoparticle-nanoparticle interactions. We find that brush density profile is independent of matrix molecular weight. Furthermore, the matrix chains penetrate almost to the particle surface, and there is no extended region with zero or near-zero matrix chain density. Hence, the highly curved brush does not exhibit "dry brush" behavior that would be expected at this investigated grafting density. We observe a repulsive interaction between the nanoparticles that sets in at a separation consistent with the polymer brush height. The combined brush-brush plus matrix effect on the nanoparticle-nanoparticle interactions is repulsive at all separations. Our simulations profile reveals no matrix-induced attraction between nanoparticles that is anticipated when the brush are truly "dry", i.e., largely non-penetrable by the matrix. Such behavior would be expected for larger particles where the surface curvature effects on brush structure and brush-melt interactions are less important. However, for small nanoparticles, our simulations reveal that surface curvature effects are very important in determining the structure of the grafted polymer as well as nanoparticle-nanoparticle interactions.