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Evaporation-induced Nanoparticle Self-Assembly in a Polymer Matrix

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A critical challenge in many applications of polymer nanocomposites is to control the dispersion of nanoparticles in a polymer matrix. We employ large-scale molecular dynamics simulations to study the assembly of nanoparticles as the solvent evaporates from a polymer solution containing nanoparticles. Results show that the organization of nanoparticles can be controlled by varying the strength of the polymer-nanoparticle interactions. When the nanoparticles and polymers strongly attract, as the solvent evaporates, a concentrated polymer film forms at the surface and entraps a layer of nanoparticles, which assemble into a close-packed hexagonal lattice. This dense film of polymers and nanoparticles dramatically reduce the rate of evaporation as the solvent has to transverse the film to reach the surface. If the nanoparticle-polymer interactions are weak, then as the solvent evaporates, the surface layer is almost entirely made of polymers. The nanoparticles are largely excluded from the surface and dispersed randomly in the region below the surface layer. In this case the slowing-down of the evaporation by the surface layer is less dramatic. Also of interest is the case of a nanoparticle solution in contact with polymers that are end grafted to a flat surface to form a polymer brush. For a relatively weak nanoparticle-brush attraction, after evaporation of the solvent the nanoparticles straddle the brush surface and form an ordered lattice. For a strong nanoparticle-polymer attraction, however, the nanoparticles are engulfed inside the brush and the packing quality diminishes because the lateral diffusion of the nanoparticles is suppressed. To better understand the nanoparticle-brush interactions, our calculations to quantify the free energy penalty of inserting a nanoparticle into a polymer brush will also be discussed.