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Nanoparticle distribution in complex block-copolymer morphologies YONGJOO KIM, HSIEH CHEN, ALFREDO ALEXANDER-KATZ, MIT —

We present our work on the distribution of nanoparticles (NPs) having various shapes (sphere, rod or disk) in different types of directed-self-assembled block-copolymer (BCP) morphologies using hybrid particle-field simulations. The BCP patterns are first obtained by modeling a nanoscale template consisting of ordered posts that are attracted to one of the blocks of BCPs. Once a desired pattern is obtained, we run simulations using the pattern as the initial condition while also including nanoparticles with different shapes, sizes and positions. By calculating the mean-field free energy of the entire system, we study the role that chain stretching and nanoparticle shape and size play in the equilibrium location of the NPs in the BCP matrix. Our results can have important implications in directing the self-assembly of multi-component hierarchical materials.

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