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**Modeling nanoparticle aggregation in nanocomposites** TANYA CHANTAWANSRI, Army Research Laboratory, LEE TRASK, ERIC COCHRAN, Iowa State University, JAN ANDZELM, Army Research Laboratory — A hybrid self-consistent field theory model (H-SCFT) was utilized to model the morphology of nanocomposites composed of cylinder forming ABA triblock copolymer and large nanoparticles (radius on the order of 10 nm). In this system, the size of the nanoparticles is comparable to the cylindrical domains such that nanoparticle segregation into this otherwise compatible phase would cause a significant loss in conformational entropy. To reduce this loss, the nanoparticles could instead macrophase separate out to form aggregates. To capture this particle aggregation in the H-SCFT model, we incorporated a Lennard-Jones potential into the framework. The incorporation of this interaction into the model can significantly alter the observed phase morphology since aggregation can prevent the nanoparticles from swelling and distorting the compatible block copolymer domain. We will demonstrate how the morphology of this nanocomposite varies as a function nanoparticle volume fraction and functionalization. Results will be compared to experimental findings when available.

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