Assembly of diblock copolymer grafted nanoparticles in a homopolymer blend matrix

CARA ESTRIDGE, ARTHI JAYARAMAN, University of Colorado — Hybrid materials comprised of nanoscale fillers embedded in a polymer matrix, also termed polymer nanocomposites, are used in many applications, such as photovoltaics, photonics, automobile parts, where their macroscopic properties are governed by the nanocomposite morphology. The structure and composite morphology is controlled by the interactions of the nanoscale fillers and the polymer matrix. In this talk we show using molecular simulations that functionalization of the nanoparticle surface with AB diblock copolymer grafts is a way to tune the interactions between the grafted particle and the A and B homopolymer blend matrix. Specifically, our work demonstrates that by tailoring the copolymer composition and the copolymer grafting density one can tune the location of the copolymer grafted particles in the matrix, (e.g. within a domain versus interface of two domains). Additionally, in the case where the grafted particles locate themselves at the interface between the two domains, the interfacial tension is reduced below that possible with bare ungrafted particles at the interface.

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Date submitted: 12 Nov 2013

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