

Abstract Submitted
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Copolymer mediated interactions in dense nanocomposites: role of chemical heterogeneity and sequence DEBAPRIYA BANERJEE, KENNETH S. SCHWEIZER, UIUC — Microscopic PRISM integral equation theory is applied to study the structure and dispersion of nanospheres in AB copolymer melts as a function of architecture and chemical heterogeneity of the interfacial attractions spanning the depletion, stabilization and bridging regimes. For a random copolymer (RCP) with coexisting weak and strong monomer-particle attractions, the nanoparticle potential-of-mean-force (PMF) at intermediate copolymer compositions varies non-monotonically between the two homopolymer limits. Non-adsorbing monomers are generically found to be crucial for achieving good filler dispersion in RCP melts. For 50/50 multiblock melts the role of block length, R , has been studied over a wide range ($R=1,2,5,10,25,50$). Filler miscibility dramatically increases when one of the monomers is weakly adsorbing (depletion). Dispersion is also improved for some block lengths when one of the monomers strongly adsorbs (bridging) due to the emergence of a long-ranged repulsive barrier in the PMF just beyond a local non-contact minimum, resulting in a positive second virial coefficient. Strikingly, better stability is predicted as the particle-to-monomer diameter ratio increases from 2 to 10, contrary to the behavior in homopolymer or RCP melts.

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