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Effective Interactions, Structure and Phase Behavior of Polymer Nanocomposites with Nonspherical Fillers LISA M. HALL, KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign — The Polymer Reference Interaction Site Model is applied to study polymer-mediated inter-nanoparticle interactions, fluid structure, and miscibility of nonspherical filler particles in a melt of adsorbing freely-jointed chains. The behavior of hard rod, disk, and cube-like nanoparticles are compared. The depletion contact aggregation, dispersed, and polymer bridging mediated nanoparticle network states of organization are sensitive to filler shape. A detailed study of thin rod fillers, including the rod-rod potential of mean force and second virial coefficient, B_2, as a function of polymer-rod and rod-rod attraction strengths, has also been performed. A primary goal is to identify design rules for dispersing nanotubes in polymer melts. Shortening the spatial range of rod-rod attraction compared to polymer-rod attraction increases miscibility. The transition from positive to negative B_2 at low polymer-rod interfacial attraction (entropic depletion) occurs more readily (at higher attraction strength) as rod-rod attraction is increased. However, the transition to negative B_2 at high polymer-rod attraction strength, driven by polymer-induced enthalpic bridging of rods, is relatively invariant to inter-rod attraction strength. Increasing rod length reduces the stabilizing consequences of polymer adsorption and the attendant steric repulsion.

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