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Structure and Assembly of Dense Solutions and Melts of Polymer Tethered Nanoparticles ARTHI JAYARAMAN, KENNETH S. SCHWEIZER, University of Illinois, Urbana-Champaign — We generalize the microscopic Polymer Reference Interaction Site Model theory to study intermolecular pair correlation functions and collective structure factors of dense solutions and melts of polymer-tethered spherical nanoparticles. The complex interplay of entropy (translational, conformational and packing) and enthalpy (particle-particle attraction) leads to different structural arrangements with distinctive scattering signatures. Strong concentration fluctuations indicative of aggregate formation and/or a tendency for microphase separation occur as the total packing fraction and/or particle-particle attraction strength increase. A microphase spinodal curve is estimated by extrapolation of the inverse of the amplitude of the small angle scattering peak. For nanoparticles, twice the diameter of monomers, carrying a single tether the microphase spinodal temperature grows roughly as a power law function of packing fraction with an exponent much less than unity. Increasing the nanoparticle diameter lowers the microphase spinodal temperature and results in a qualitative change of its packing fraction dependence. The effect of nanoparticle size, number and length of tethers, position of the grafting sites, total packing fraction, and particle-particle attraction strength on the structure, scattering patterns and tendency for microphase ordering has been studied in detail.

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