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Statistical Mechanical Theory of Phase Separation and Structure in Dense Polymer-Particle Mixtures LISA HALL, KEN SCHWEIZER, University of Illinois — Microscopic liquid state theory has been applied to investigate phase separation and structure of dense mixtures of hard spherical particles and flexible polymer chains in the presence of interfacial attractive interactions. The entire range of filler loading, from the dilute particle regime to the colloid science relevant case of ultra-high particle volume fraction with dilute polymer additives, has been studied for the first time. Many body effects can result in large quantitative, or even qualitative, changes of spinodal demixing boundaries compared to a low order virial treatment. In the temperature-particle volume fraction representation both upper and lower critical temperatures are present, separated by a miscibility window. Entropic effects dominate for weak interfacial attractions (high temperature) resulting in depletion phase separation with a critical point at roughly 10% filler loading. At relatively high interfacial cohesion (low temperature) a network bridging transition occurs characterized by a highly asymmetric spinodal boundary which depends sensitively on attraction spatial range. Deep contact or bridging minima in the particle potential of mean force can occur, which raises the possibility that kinetic gelation or aggregation pre-empts equilibrium phase separation. The evolution of the real space correlations and scattering structure factors as phase separation is approached has been studied in detail.

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