Fluid–Fluid Interface in a Model Colloid–Polymer Mixture: Application of a Grand Canonical Monte Carlo Method

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Mixtures of colloids and non-adsorbing polymers exhibit a fluid–fluid unmixing transition that is of purely entropic origin. It stems from a depletion effect that leads to an effective attraction between colloidal particles. A simple model that captures this phenomenon is the model of Asakura and Oosawa (AO). Here colloidal particles and polymers are treated as spheres with respective radii R_c and R_p. Hard sphere interactions are assumed between colloid–colloid and colloid–polymer pairs, while polymer–polymer pairs can interpenetrate freely.

We present a grand canonical Monte Carlo method that is well–suited to simulate asymmetric binary mixtures. This method is used to study the AO model with a polymer–to–colloid size ratio $q = R_p/R_c = 0.8$. We determine the phase diagram of the fluid–fluid unmixing transition and the interfacial tension, both at high polymer density and close to the critical point. A finite–size scaling analysis leads to an accurate estimate of the critical point. The results are compared to predictions of a recent density functional theory by Schmidt *et al.* [*Phys. Rev. Lett.* **85**, 1934 (2000)]. Whereas the latter DFT yields mean field critical behavior, the simulation shows that the critical behavior of the AO model belongs to the 3D Ising universality class. We also study density profiles in the two–phase region of the fluid–fluid unmixing transition. The interfacial width is subject to strong finite–size effects which are not due to the proximity of the critical point. We show that they stem from the presence of capillary waves and we test the scaling laws that are expected from capillary wave theory.