The phase behavior of two-dimensional symmetrical mixtures

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Using Monte Carlo simulation methods in the grand canonical and semi-grand canonical ensembles, we study the phase behavior of two-dimensional symmetrical binary mixtures of Lennard-Jones particles. We discuss the interplay between the demixing transition in a liquid and the freezing in detail. It is demonstrated, that different scenarios involving demixing and freezing transitions are possible. In one class of systems, the λ-line representing a continuous demixing transition in a liquid phase starts at the liquid side of either the vapor-liquid or liquid-solid coexistence. The second class involves the systems in which the λ-line begins at the liquid side of the vapor-liquid coexistence, in the lower critical end point, and then terminates at the liquid side of the liquid-solid coexistence, in the upper critical end point. It is also shown that in such systems the solid phase may undergo a demixing transition at the temperature above the upper critical end point.

Moreover, we discuss the formation of thin solid films on strongly attractive substrate at low temperatures. Under such conditions the film grows in a layer-by-layer fashion. It is shown that the demixing transition as well as the structure of thin films is considerably different than observed in bulk systems. In particular, we show that the film may exhibit different stacking of layers formed by pure compomenets, depending on the parameters representing the interaction between unlike particles.