Complex Phase Behavior and Liquid-Liquid Phase Transition in the System of Particles with Repulsive Shoulder Potential

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It is well known that some liquids (for example, water, silica, silicon, carbon, phosphorus, and some biological systems) show an anomalous behavior in the vicinity of their freezing lines. As it was discussed in many works (see, for example, the review [1]) the presence of two length scales in the core-softening potential may be the origin of anomalous behavior because in this case a system of particles behaves, in many respects, as a mixture of two species of different sizes [2]. This leads to the existence of two competing local structures. The evolution of these structures under changing the thermodynamic conditions can result in the anomalous behavior.

In the present talk we report a detailed simulation study of the phase behavior of core softened systems with and without attractive well [2-4]. Different repulsive shoulder widths and attractive well depths are considered which allow monitoring the influence of repulsive and attractive forces on the phase diagram of the system. Thermodynamic anomalies in the systems are also studied. The possible liquid-liquid phase transition is also discussed.

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