Anomalous Behavior of Core-Softened Systems

V. N. Ryzhov, Yu. D. Fomin, and E. N. Tsiok

Institute for High Pressure Physics, Russian Academy of Sciences, 142190 Kaluzhskoe sh. 14, Troitsk, Moscow Region, Russia
E–mail: ryzhov@hppi.troitsk.ru

In the present talk we report a computer simulation study of the phase diagram and anomalous behavior of the core-softened system [1-4]. 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. The water phase diagrams have regions where a thermal expansion coefficient is negative (density anomaly), self-diffusivity increases upon compression (diffusion anomaly), and the structural order of the system decreases with increasing pressure (structural anomaly). This kind of behavior may be described by the core-softening potential with two length scales [1-4]. In those thermodynamic regimes where the two length scales are both partially effective, a system of particles behaves, in many respects, as a mixture of two species of different sizes [1-4]. This leads to the existence of two competing local structures. The evolution of these structures under changing the thermodynamic conditions can result in the maxima on the melting line, structural phase transitions and anomalous behavior in liquid phase. The relation of the anomalous behavior to the possible liquid-liquid phase transition is also discussed.

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