

Inversion of Sequence of Diffusion and Density Anomalies in Core-Softened Systems

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

Institute for High Pressure Physics, Russian Academy of Sciences, Kaluzhskoe shosse 14, Troitsk 142190, Moscow Region, Russia, E-mail: fomin314@gmail.com

In this paper we present a simulation study of water-like anomalies in smooth repulsive shoulder system introduced in our previous publications [1, 2]. We investigate the anomalous regions for systems with the same functional form of the potential but with different parameters. Using the thermodynamic arguments and the computer simulations, we show that while the density anomaly is always inside the structural anomaly region, the location of the diffusion anomaly depends on the parameters of the potential. In particular, for small values of the repulsive shoulder width one has the order of the anomalies which is similar to that found in water: the density anomaly region is inside the diffusion anomaly domain, and both of these anomalous regions are inside a broader structurally anomalous region. However, with increase of the repulsive shoulder width the location of the diffusion anomaly in the density-temperature plane moves inside of the density anomaly region and disappears under the melting line [3].

Our results spread light on the anomalous behavior in real substances like, for example, water and liquid silica.

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References

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