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Thermodynamic Perturbation Theory for Solid-Liquid Phase Transition of Lennard-Jones Model

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Abstract: Both a free volume approach for Helmholtz free energy and a theoretically-based fitted formula for radial distribution function (rdf) of hard sphere solid are employed to describe the Helmholtz free energy of Lennard-Jones solid in the framework of the first order thermodynamic perturbation theory, which also is employed for the uniform Lennard-Jones fluid. The dividing of the Lennard-Jones potential follows from the WCA prescription, but the specification of the equivalent hard sphere diameter is determined by a simple iteration procedure devised originally for liquid state, but extended to solid state in the present study. Two hundred shells are used in the rdf to get an accurate perturbation term. The present approach is very accurate for the description of excess Helmholtz free energy of LJ solid, but shows some deviation from the simulation for excess Helmholtz free energy of uniform LJ fluid when the reduced temperature kT/ε is higher than 5. The present approach is satisfactory for description of solid-liquid phase transition of the Lennard-Jones model.

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Key words: thermodynamic perturbation theory, solid-liquid transition

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