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Thermodynamic properties of diamond and wurtzite model fluids from computer simulation and thermodynamic perturbation theory

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Abstract Monte Carlo *NVT* simulations have been performed to obtain the thermodynamic and structural properties and perturbation coefficients up to third order in the inverse temperature expansion of the Helmholtz free energy of fluids with potential models proposed in the literature for diamond and wurtzite lattices. These data are used to analyze performance of a coupling parameter series expansion (*CPSE*). The main findings are summarized as follows, (1) The *CPSE* provides accurate predictions of the first three coefficient in the inverse temperature expansion of Helmholtz free energy for the potential models considered and the thermodynamic properties of these fluids are predicted more accurately when the *CPSE* is truncated at second or third order. (2) The Barker-Henderson (*BH*) recipe is appropriate for determining the effective hard sphere diameter for strongly repulsive potential cores, but its performance worsens with increasing the softness of the potential core. (3) For some thermodynamic properties the first-order *CPSE* works better for the diamond potential, whose tail is dominated by repulsive interactions, than for the potential, whose tail is dominated by attractive interactions. However, the first-order *CPSE* provides unsatisfactory results for the excess internal energy and constant-volume excess heat capacity for the two potential models.

Keywords: Diamond potential; wurtzite potential; thermodynamic properties; coupling parameter series expansion

I Introduction

Anisotropic interactions are responsible for many interesting features of fluids and solids. Thus, for example, the anomalous thermodynamic properties of water can be attributed to competing interactions between nearest and non-nearest neighbors. The latter gives rise to