The entropies and structure factors of liquid simple metals

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Abstract

Some results of a systematic study of the entropies and structure factors of fourteen liquid simple metals are presented. The ab initio model potentials of Shaw (1968) and the dielectric function of Vashista and Singwi (1972) have been used to construct effective pairwise interatomic potentials for these liquid metals. These pairwise potentials have then been employed in both the Weeks-Chandler-Anderson (WCA) and the variational thermodynamic perturbation theories to determine appropriate effective hard-sphere diameters. The authors examine in detail the short-range repulsive part of the pairwise potential in several liquid metals and show, within the WCA theory, how the softness of this influences the form of the liquid structure factor. The calculation is briefly discussed of the compressibility from the long-wavelength limit of the structure factor.