Thermodynamic properties of liquid metals

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Abstract

The ability of the model potentials to yield accurate thermodynamic properties of liquid metals is tested. The pressure and bulk moduli calculated by the homogeneous deformation (HD) method depend on the electron density derivative of the self-energy. The latter is determined predominantly by the choice and specification of the bare ion form factor for $q>2k_F$. Most of the empirical model potential in the literature have been tested to give a good description only in the region $0<or=q<or=2k_F$. The bare ion form factors widely differ from one another for $q>2k_f$ and are not tested to give a good description in this range. Therefore no meaningful calculation of the pressure and bulk moduli of liquid metals can be made at present using the HD method.