Pair potentials and structure factors of liquid alkali metals

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Abstract

Measured structure factors of liquid alkali metals are examined in the framework of screened pair potential theory. Information on the main attractive well in the effective pair potential is obtained from the structural data by an approximate method stemming from an optimized random-phase treatment of the indirect ion-ion attraction. The results are compared with a variety of theoretical pair potentials in the cases of sodium and potassium, after a test of the method against computer simulation data on a model for rubidium. Results for the other alkali metals are also given and discussed. The small-angle scattering region is then examined in considerable detail, with special attention to the possibility of a linear term in a series expansion of the structure factor at very small momentum transfer. Although sensitivity to both the bare electron-ion coupling and the local field factor in the screening function is demonstrated and analysed, no linear term of the magnitude reported in recent X-ray diffraction experiments is found in the present theoretical framework.

Author keywords

Studies of specific liquid structures