Effective pair potentials of molten CuI estimated from the experimental partial structure factors

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Introduction

A clear understanding of the physical properties of molten salts is known to depend upon their structure and pair potential at a microscopic level. It is also well recognized that the effective pair potentials estimated from the experimental structural data are quite useful, because they are considered to include, more or less, the particular features of liquid of interest. The main purpose of this work is to estimate the effective pair potentials of molten salt of CuI from the experimental partial structure factors[1] estimated from anomalous X-ray scattering (AXS) measurements by applying the modified hypernetted-chain equation.

Experimental

The AXS measurements for molten CuI were carried out with synchrotron radiation at BL-7C with incident energies of 8.6803, and 8.9553keV, which are 300eV and 25eV below Cu K absorption edges. Scattered intensities were collected using symmetrical transmission geometry with a devised silica glass cell.

Results and Discussion

The resultant effective pair potentials of molten CuI are shown in **Fig. 1** together with the model potentials. Calculated pair distribution functions from MC simulations using the potential presently obtained or model potential[2] are shown in **Fig. 2** together with experimental one. The following remarks could be given from these results. (a) The experimental pair distribution functions of Cu-Cu pair are well reproduced by MC simulation using the pair potentials presently obtained. The distribution functions indicate the characteristic like-ion penetration into the first unlike-ion coordination shell when compared with the model potential case. The present results of the Cu-Cu pair potential of molten CuI suggest more freely movement of Cu ions. (b) The present results of the Cu-I pair potentials show that there are negative deviations from the model potentials (Coulombic form) in the range from 0.4 to 0.9 nm. The deviation of the Cu-I pair potential from the Coulombic form is considered to be essential for the understanding of the density fluctuation of Cu ions by keeping the charge neutrality in Coulomb liquids. (c) The present results of the I-I pair potential are, in the authors' view, relatively close to the model potentials, this contrasts to the Cu-Cu and Cu-I cases. As a result, fairly good agreement is observed for the partial structure factors simulated using these two potentials.

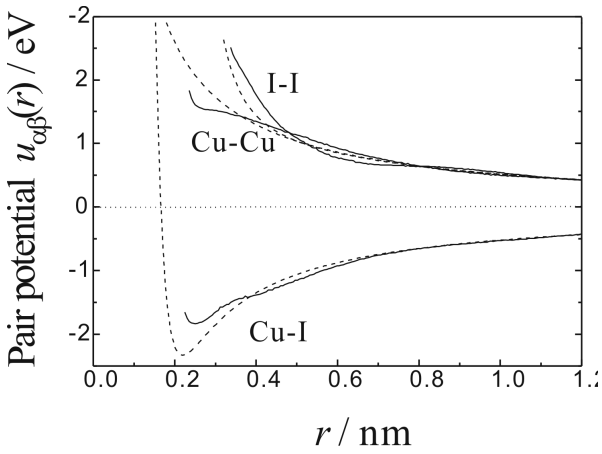

Fig. 1Effective pair potentials of molten CuI (solid line) estimated from the experimental partial structure factors in comparison with model potential (dotted line).

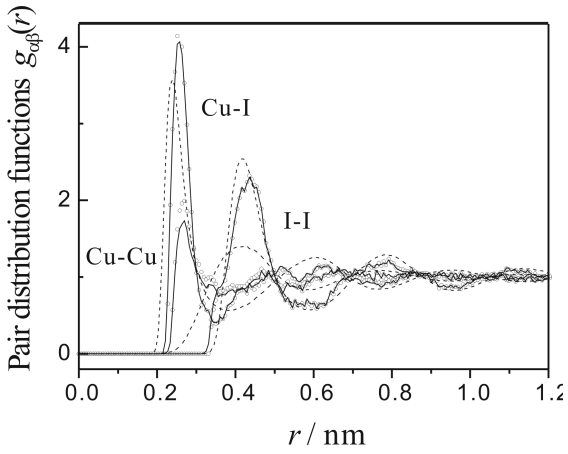

Fig. 2 Experimental PDF of molten CuI (open circles), in comparison with those of MC simulation with the effective pair potentials (solid line) and model potentials (dotted line).

References

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