Effective Pair Potentials of Molten RbBr 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 heavily 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 RbBr 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 were carried out at beam line 7C. The measurements were in the asymmetrical reflection mode for molten RbBr with a beam direction changing mirror system. The high temperature chamber is mounted on the center of the diffractometer. The molten sample was prepared from high purity RbBr and it was heated up to temperature of 960 K in a rectangular platinum crucible under a high-purified N_2 atmosphere.

Results and Discussion

The resultant effective pair potentials of molten RbBr are shown in **Fig.1** together with the model potentials for comparison. The present results are found to agree well with the model potential[2], although there are small differences in detail. **Fig. 2** shows the experimental pair distribution functions together with those of simulated results using both potentials for molten RbBr. The present authors maintain the view that the agreement between the simulated results using potentials presently determined and the experimental data is good by reducing discrepancies detected in the first peak region of the pair distribution functions in the model potential case, particularly for the Rb-Br pair. This may be attributed to the difference in the depth of the Rb-Br pair potential of molten RbBr as seen in **Fig.1**. From the results for partial pair distribution functions of molten RbBr in **Fig. 2**, it can be found that $g_{RbRb}(Q)$ and $g_{BrBr}(Q)$ are approximately in anti-phase to $g_{RbBr}(Q)$. This indicates well-defined charge (chemical) ordering. Considering some observed structural results, it is suggested that the symmetrical first coordination shell of Rb-Br pair can be described by the octahedral configuration, as it is in the crystalline state. These structural features are quite similar to the simple molten salt case of alkali chlorides.
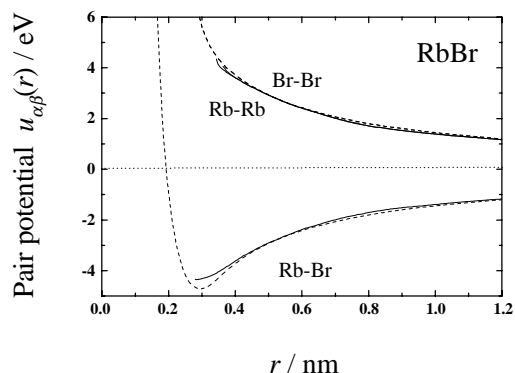

Fig. 1 Effective pair potentials of molten RbBr (solid line) estimated from the experimental partial structure factors in comparison with model potential (dotted line).
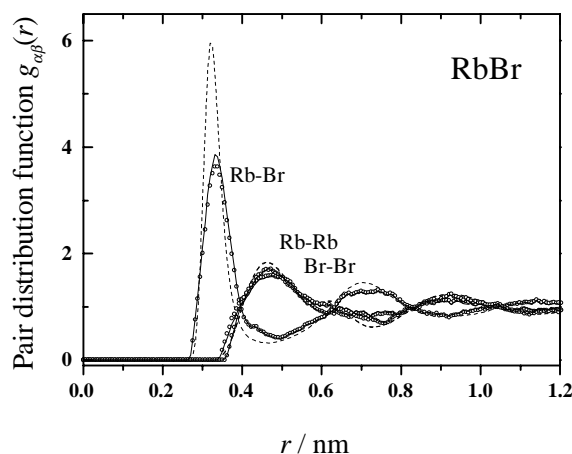

Fig. 2 Experimental pair distribution function of molten RbBr (open circles), in comparison with those of Monte Carlo simulation with the effective pair potentials (solid line) and model potentials (dotted line).

References

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