Effective Pair Potentials of Molten AgBr Estimated from the Experimental Partial Structure Factors

Pavlin D. MITEV[1], Masatoshi SAITO*[2], Kazumasa SUGIYAMA[3] and Yoshio WASEDA[1]
[1]IMRAM, Tohoku University, Sendai 980-8577, Japan
[2]Sch. of Health Sciences, Fac. of Medicine, Niigata Univ., Niigata 951-8518, Japan
[3]Dep. of Earth and Planetary Science, The University of Tokyo, Tokyo 113-0033, Japan

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 AgBr 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 AgBr were carried out in the asymmetrical reflection mode at a beam line 7C with incident energies of 13.170 and 13.445 keV, which are 300 and 25eV below the Br *K* absorption edge.

Results and Discussion

The resultant effective pair potentials of molten AgBr 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 function of Ag-Br pair is found to be well reproduced by MC simulation using the pair potential presently obtained. On the contrary, the simulated results using the model potential clearly differ from the experimental data. A significant difference was found in the interatomic distance for the nearest neighbor Ag-Br pairs. This could be attributed to the difference detected in the position of the minimum for the pair potential. (b) The present potential for Br-Br pair in molten AgBr shows an oscillatory behavior against the model potential. Such profile of Br-Br pair is rather similar to that in molten alkali halide cases. This may correspond to the common structural feature described by disordered close packing of Br ions. (c) The resultant effective pair potential of Ag-Ag pair successfully reproduced the experimental pair distribution function, while the simulated result using the model potential differs from the experimental data again. This may be attributed to slightly positive deviation from the model potential in the range from 0.37 to 0.52 nm. This small difference in the potential could be related with the particular feature of molten AgBr.

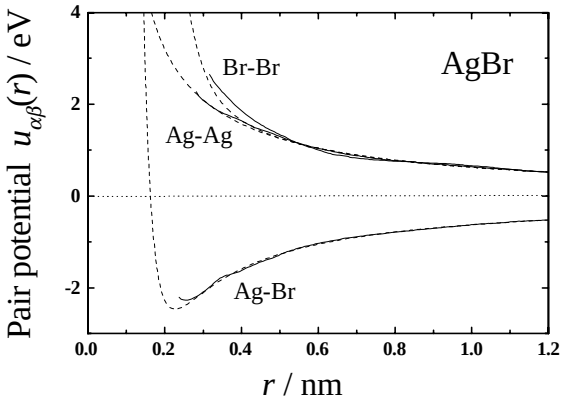

Fig. 1Effective pair potentials of molten AgBr (solid line) estimated from the experimental partial structure factors in comparison with model potential (dotted line).

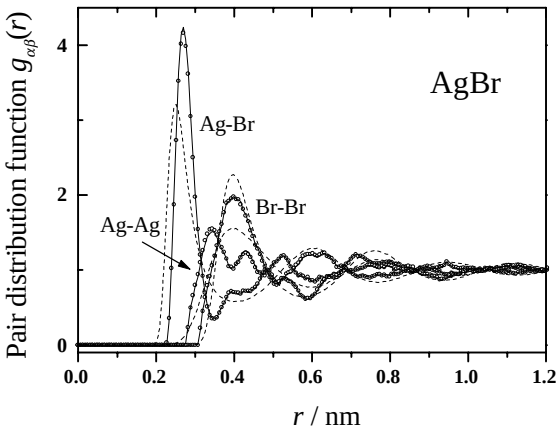

Fig. 2 Experimental PDF of molten AgBr (open circles), in comparison with those of MC simulation with the effective pair potentials (solid line) and model potentials (dotted line).

References

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* masaito@clg.niigata-u.ac.jp