Structural modelling of molten noble metal halides using RMC technique

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AgI and CuI are well known as superionic conductor in a high-temperature solid phase, where Ag or Cu ions migrate like liquid through the sites in the sublattice of immobile iodine ions. This may result from intermediate property of cation-anion bond between ionic and covalent one[1]. Recent *ab initio* MD simulation indicates that the covalent character of cation-anion bond remains in molten phase and moreover there is a little covalent character even in cation-cation[2] pairs. For molten AgCl, AgI and CuI, we have carried out high-energy X-ray diffraction using BL04B2 beamline at SPring-8, Hyogo, Japan and neutron diffraction measurements are carried out using HIT-II spectrometer at the Neutron Science Laboratory, KENS in KEK, Tsukuba, Japan and HERMES spectrometer at the JRR-3 in JAEA, Tokai, Japan.

The Reverse Monte Carlo simulation has been performed to visualize atomic distributions of these matters. The number of particles was 5000 in each matter and width of cubic-box for molten AgCl, AgI, CuI were 50.9(A), 57.0(A), 56.2(A), respectively. As a result, molten AgI and CuI[3] exhibit compositional fluctuations. This may be consistent with the existence of a little covalency in cation-cation bond. On the other hand, Ag ions in molten AgCl tend to distribute at random like gas. Adding to this property, Trullas et al. suggested that the polarization effect of Cl ions[4] causes the complicated shape of the first peak in a total structure factor for molten AgCl. We will discuss structural details for molten silver and cuprous halides.

References

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