Comparison in the partial structures between molten AgCl and superionic melts of AgI and CuI

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The structure of molten noble metal halides have been attracted many researchers since Mika and Page found the featureless gas-like structure factor of cation-cation correlation for molten CuCl by isotope enrichment technique on neutron diffraction [1]. For molten AgCl, Derrien and Dupuy [2] proposed a strongly structured distribution of Ag-Ag correlation, different from the featureless structure of Cu-Cu, from their results of neutron. Inui et al. [3] discussed on the local structure of molten AgCl by comparing with the relating molten salts such as AgBr and AgI from their experimental total structure by neutron diffraction. They suggested tetrahedral local structure for every molten silver halide and ionic character for AgCl and AgBr compared with AgI from the temperature dependence of the structure.

On the other hand, it is reported that the Cu-Cu partial correlation in the superionic melts of CuI penetrates significantly into the first coordination shell of Cu-I correlation [4,5] , which is the feature different from the structureless profile of Cu-Cu correlation in molten CuCl or CuBr [1,6,7].

What is difference between non-superionic melts and superionic-melt ? To answer this question, neutron diffraction (ND) with time-of-fight method and high energy X-ray diffraction measurements (HEXRD) for molten AgCl, AgI and CuI have been performed. In this presentation, we will discuss in detail the partial structures deduced from ND and HEXRD by applying the Reverse Monte Carlo simulation.

References

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