

Dynamic Correlation Functions of CuI Superionic Melt

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CuI is a superionic conductor where the mobile Cu ions migrate between interstitial sites in the sublattice of immobile halogen ions [1]. Even in the molten state, the distribution of Cu ions exhibits large fluctuations and when we see only Cu ions, they look form one dimensional streams, which strongly suggests cooperative motion of successive Cu ions [2,3].

To study ion dynamics in molten CuI, quasielastic neutron scattering was carried out at AMATERAS cold disk chopper neutron spectrometer in MLF, J-PARC. From molecular dynamics (MD) simulation using Vashishta Rahman potential with polarizable ion model which reproduces a reasonable static structure of molten CuI [4], we deduced dynamical correlation functions such as intermediate scattering function, $F(Q,t)$, van Hove function, $G(r,t)$, and so on. In this presentation, The experimentally-obtained total dynamical correlation function is interpreted from the MD partials of Cu-Cu, Cu-I and I-I. From the MD, Cu ions shows about 8 times larger diffusion constant as I ions, which means that superionic behavior of Cu ions exists even in molten phase.

References

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