【別紙２】

論文名：Thermal Conductivity of Molten Alkali Halides: Ionic Mass Dependence（要約）

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In order to clarify the true ionic mass and number density dependence of the thermal conductivity of molten alkali halides, that is, to obtain the relation of $\lambda(m)$ under constant N/V and $\lambda(N/V)$ under constant m, where m is the average ionic mass between anion and cation and N/V the number density, we have performed the equilibrium MD simulations of molten LiI at 1000 K within the framework of Fumi-Tosi potential models, and calculated the thermal conductivity by using the Green-Kubo formula as a function of ionic mass under constant number density. In these calculations, the same potentials for LiI, number density, and temperature were used except for artificially changed ionic masses of cation and anion. As a result, it turned out that the thermal conductivity has the ionic mass dependence of $m^{-1/2}$ in molten LiI. We have divided by $m^{-1/2}$ all the calculated thermal conductivities of a series of molten alkali halides so that we have found that the normalized thermal conductivities which means $\lambda(N/V)$ shows a linear relationship with $(N/V)^{2/3}$. Then, we have plotted all the calculated thermal conductivities of a series of molten alkali halides vs. $m^{-1/2}(N/V)^{2/3}$ so that we have found a linear relationship in the plot. This means that the thermal conductivity can be expressed as $m^{-1/2}(N/V)^{2/3}$ and there is no significant coupling between m and N/V. Therefore, we have concluded that the thermal conductivity scales with $m^{-1/2}(N/V)^{2/3}$.

In order to examine the collective excitations in molten alkali halides, we have evaluated the dynamic structure factor for molten LiI with artificially varied ionic masses by using the MD method. On the basis of the obtained dynamic structure factor of charge density, the dispersion curve was derived from the peak frequency of collective excitation. The peak frequency at zero wavevector and the modulus of group velocity were estimated from the dispersion curves, as a function of ionic mass. The peak frequency at zero wavevector shows that the optic mode can be thermally excited for all the molten alkali halides. This suggests the ideas that the charge-density modes may dominate the thermal transport in these systems, and that insensitivity of the thermal conductivity of molten alkali halides to details of interionic potentials can be attributed to the behavior. The obtained modulus of group velocity was roughly proportional to $m^{-1/2}$. This suggests that it can replace the mass term partially in expression of thermal conductivity.

In order to explore the suitable definition of the average of ionic masses for the expressions of the thermal conductivity of molten alkali halides, we have examined the effect of the difference of ionic masses between cation and anion on the thermal conductivity from the viewpoint of definition of average of ionic masses such as arithmetic, geometric, etc. In this work, we have explored two kinds of expressions of the thermal conductivity for molten alkali halides. One is the scaling

equation, $\lambda \propto m^{-1/2}(N/V)^{2/3}$ which was obtained from the present MD simulation. The other is the equation obtained by applying the corresponding-states (CS) analysis to all the calculated thermal conductivities by the MD simulation. Among some representative definitions, it turned out that the simple arithmetic average is best for the equations. As an estimation method of the thermal conductivity, it was shown that both the equations have comparable precision. It was indicated that considering the difference in ionic masses between anion and cation is important for building more precise correlation in the CS analysis.