Numerical and theoretical investigations of peculiar phenomena in microclusters

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In the thesis the two different phenomena peculiar to nano scale systems such as microclusters are investigated. One is the inhomogeneous distribution of temperature in microclusters and an-other one is the rapid diffusion phenomenon peculiar to nano-scale microclusters.

In the first part, we investigate the inhomogeneous distribution of local kinetic temperature in microclusters, which is discovered numerically in microcanonical dynamical simulation of micro-clusters. The essential origin of the inhomogeneity is due to the conservation of total translational and angular momentum. Statistical mechanical analysis based upon a microcanonical measure taking into account of the additional conserved quantities gives general formula for the statistical average of local kinetic temperature. The local Maxwell-Boltzmann distribution characterized by the local kinetic temperature is also derived. These results agree very well with the numerical re-sults. Finally, we propose an intuitive interpretation for the inhomogeneity of the local kinetic temperature distributions.

In the second part, we investigate rapid diffusion phenomenon which is peculiar to metal and alkali halide microclusters. Molecular dynamics simulations for three dimensional cluster models (many-body Gupta and two-body Morse type potentials are used for metal clusters and Coulomb plus Born-Mayer type potential is used for binary alkali halide clusters) show that components of the cluster mix with each other spontaneously without melting. In particular, investigations for alkali halide clusters reveal that necessary time for the diffusion of the clusters has size and Ar-rhenius-type temperature dependence. Finally, it is revealed that the mixing mechanism of alkali halide cluster is quite different from the mixing process of metal clusters; the rapid diffusion of atoms into metal clusters is caused by atomic convection, while the rapid diffusion in alkali halide clusters is dominated by the vacancy-induced diffusion mechanism known as the mechanism in bulk solids.