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分子動力学計算によるレナードジョーンズ型分子のガスから固体への核生成と結晶化過程

Molecular-dynamics simulations of nucleation and crystallization from vapor to solid with Lennard-Jones-type molecules

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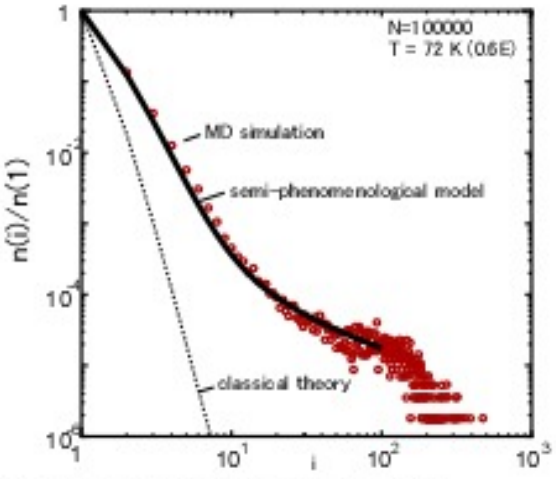

Fig.1 Size distribution of clusters in nucleation phase. Red circles show the result of MD simulation (N=100000,T=0.6E). Size distributions obtained by semi-phenomenological model and classical theory are also plotted by the solid line and dotted line, respectively.

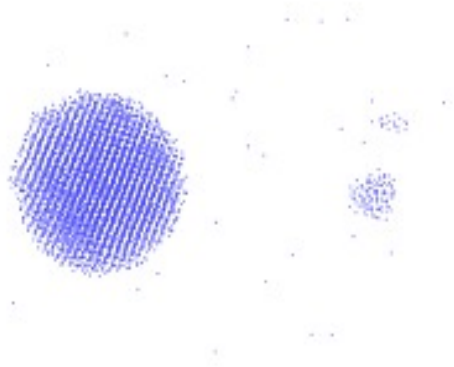

Fig.2 Snapshot of clusters obtained by MD simulations (T=0.4E)。Crystallization of cluster occurs during the cluster growth.

We performed molecular-dynamics (MD) simulations of nucleation from vapor to solid with 100000 Lennard-Jones-type molecules. Simulations were done for various of supersatuation ratios from 20 to $10^8$and temperature of 0.2-0.6 E, where E (= 119.8 K for argon) is a potential parameter of Lennard-Jones-type molecules. We compared size distribution of clusters in the MD simulations with those in theoretical models since the number density of critical clusters governs the nucleation rate. We found that the semi-phenommenological model using the saturated pressure and surface energy of supercooled liquid achieves excellent agreements in size distributions of clusters with all MD simulations we done. Our results strongly suggest the

nucleation occurs in liquid phase even though the temperature is much less than the triple point (T =0.67 E), as long as the nucleus is small. We also found that crystallization of clusters occurs during the cluster growth.

キーワード:結晶化,核生成,分子動力学計算

Keywords: crystallization, nucleation, molecular dynamics simulation