

# Homogeneous nucleation process of water by molecular dynamics simulations

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Nucleation process is one of important processes related to the origin of planetary materials. In this study, we performed molecular dynamics (MD) simulations of homogeneous nucleation from vapor to liquid of water molecules. Tanaka et al. (2005, *J.Chem.Phys.*, submitted) performed MD simulations for Lennard-Jones type molecules and compared the size distribution of clusters in MD simulations with those in the theoretical models. As the same method in Tanaka et al. (2005), we compared the size distribution of clusters in MD simulations for water molecules with those in the theoretical models.

In the MD simulations we used an atom-atom potential model, KAWAMURA model, which improved the KKY potential model (Kumagai et al. 1994, *Mol.Simul.* 12, 177). The potential model has two-body interactions for all atom pairs (i.e., O-O, O-H, and H-H) and three-body force for the H-O-H system. In our MD simulations, we used NVT (constant volume and temperature) ensembles. The temperature is a parameter and regulated to be constant by the simple velocity scaling.

We started the simulation under the initial condition that the monomers are located randomly and the supersaturation ratio of the system is set to be greater than unity. The simulation contains 2400 hydrogen atoms and 1200 oxygen atoms, i.e., 1200 water molecules. The computational area is a cube with a side  $L$  of 130-170 angstrom. We performed an MD simulation in the case of  $T= 400-430\text{K}$ . At the initial state, the monomers are distributed uniformly. In the simulation, clusters are formed and some of them grow into large ones.

Since the number density of critical clusters governs the nucleation rate, we compared the size distribution of clusters in MD simulations with those in the theoretical models. In the course of nucleation, the number of the nucleated stable clusters increases and that of monomers decreases. We also compared time evolution of the numbers of the monomers and the nucleated stable clusters in MD simulations with the theoretical models. The results show that the classical theory overestimates the number density of the clusters about one order of magnitude. This means the classical theory also overestimates the nucleation rate. The semi-phenomenological model (Dillmann and Meier 1991, *J.Chem.Phys.* 94. 3872). predicts correctly the size distributions of the clusters with the MD simulations we done. The results suggest the validity of the semi-phenomenological model for water condensation.