Homogeneous nucleation of iron from saturated vapor by molecular dynamics simulation

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Condensation process from vapor to liquid (or solid) via homogeneous nucleation is a fundamental process and plays an important role in many areas of science and technology. Despite the familiarity of the process, serious unreliability remains in model predictions for nucleation rates. Molecular dynamics (MD) simulations are able to directly resolve details of the nucleation process and provide useful test cases for nucleation models. There were a lot of previous studies with MD simulations for the investigation of nucleation in a supersaturated vapor, but only limited type of substances such as rare gas and water have been examined. In this study, we performed the MD simulations of homogeneous nucleation process from a saturated vapor composed of iron atoms. There was an example of MD simulation for iron (Lummen&Kraska2005), but there was no detail comparison with the theory because of the small system with 343-1,331 atoms. In this study, we performed the MD simulations of homogeneous nucleation process from a vapor with 1,000-100,000 iron atoms. The simulations were performed with the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code developed at Sandia National Laboratories. We used the embedded atom method (EAM) for modeling the force field acting between the iron atoms (Mendelev et al. 2003). We reproduced the homogeneous nucleation process with the nucleation rate of orders of magnitude lower than the previous study. Comparing the results of our MD simulations with theoretical models requires knowledge of the thermodynamic properties, especially the surface tension and equilibrium vapor pressure. To estimate the quantities we performed a series of equilibrium MD simulations of liquid-vapor systems consisting of a liquid slab with vapor at fixed temperature (NVT) and with periodic boundaries. In the MD simulations, the values of the critical nucleus were almost unity because of high supersaturation ratio, while the nucleation rates were several orders of magnitude lower than the gas kinetic collision limit for nucleation rates. The results may indicate a difficulty of dimerization in the nucleation process.

Keywords: Nucleation, iron, Molecular dynamics simulation

