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Nucleation process from vapor due to molecular dynamics simulations: effect of the sticking probability

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In the previous studies (Tanaka et al. 2005, 2011), we performed molecular dynamics (MD) simulations of nucleation from vapor of Lennard-Jones (L-J) type molecules and found that the semi-phenomenological (SP) model reproduces very well the nucleation rates obtained from the MD simulations. In this study, we performed MD simulations of nucleation from vapor for systems of 4000 water molecules to test nucleation theories. Simulations were done for wide ranges of the initial supersaturation ratio (S=4-400) and temperature (T =250-375 K). Through comparison with the nucleation rates and the cluster size distributions obtained from our MD simulations, we investigated the validity of the SP model. Our results show that the semi-phenomenological model reproduces well the size distributions of the clusters and the nucleation rates. Furthermore, the sticking probability of vapor molecules onto clusters was examined in MD simulations, by observing the growth rate of stable clusters larger than the critical size. In all runs in the present study, the values of the sticking probability are larger than 0.1. Our results show that the obtained sticking probability depends on the supersaturation ratio.

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