

PPS025-08

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Molecular dynamics simulation of nucleation from vapor

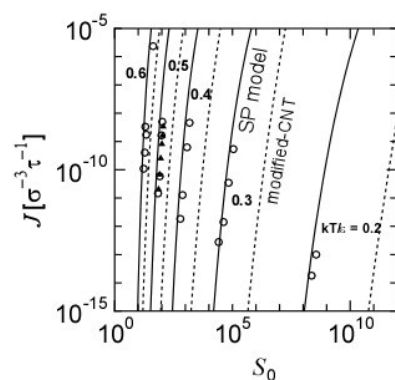
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We performed molecular dynamics (MD) simulations of nucleation from vapor at temperatures below the triple point for systems of 10^4 - 10^5 Lennard-Jones (L-J) type molecules in order to test nucleation theories at relatively low temperatures. Simulations are done for wide ranges of the initial supersaturation ratio ($S_0 = 10$ - 10^8) and the temperature ($T = 24$ - 72 K for argon). Clusters are nucleated as supercooled liquid droplets because of their small size. Crystallization of the supercooled liquid nuclei is observed after the slow down of their growth. The classical nucleation theory (CNT) extremely underestimates the nucleation rates (or the number density of critical clusters) at the low-T region. It is found that the semi-phenomenological (SP) model[1], which corrects the CNT-prediction of the formation energy of clusters using the second virial coefficient of vapor, reproduces the nucleation rate and the cluster size distributions with a good accuracy in the low-T region as well as in the higher-T cases in our previous study[2]. The sticking probability of vapor molecules onto the clusters are also obtained in our MD simulations. By using the obtained values of the sticking probability in the SP model, we can further refine the accuracy of the SP model.

[1]A.Dillmann,G.E.A.Meier,J.Chem.Phys.,94,3872(1991)

[2]K.K.Tanaka,K.Kawamura,H.Tanaka,K.Nakazawa,J.Chem.Phys. 122,184514 (2005)



Keywords: nucleation, condensation, MD simulation