Numerical Investigation of Temperature Effects on Nucleation Rate

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This work employs molecular dynamics simulations to investigate both isothermal and non-isothermal vapor–liquid nucleation kinetics in a system of particles interacting via the Lennard-Jones potential. For the first time, the temperature size distribution has been determined. Starting at the monomer temperature as a reference, it goes down slightly, but as the cluster size approaches the critical one, the temperature reaches its value of monomers, then starts to gain faster. The temperature distribution over cluster sizes defines the distribution of their number densities and thereby controls the vapor nonideality, which in turn can strongly affect the nucleation rate. It has been shown in [1] that taking into account vapor nonideality results in a significant difference in the nucleation rates. Thus, knowledge of cluster temperature is crucial for analytical models to accurately determine vapor supersaturation and the actual nonisothermal nucleation rate. A special simulation method was used, in which all clusters that had grown to a sufficiently large size were removed from the system, and the particles that formed them were returned to the system in the form of monomers. Nucleation rates and critical cluster sizes for both isothermal and nonisothermal cases have been determined over a broad range of supersaturations. The results obtained for nonisothermal nucleation rates show satisfactory agreement with the theoretical model [2], which preditcts a decrease in the nucleation rate for nonisothermal case.

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[2] Zhukhovitskii D I 2024 *J. Chem. Phys.* **160**(19) 194505–1–194505–20