Optimized Particle-Based Computational Simulation Method for Studying Bubble Nucleation

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We present an optimized particle-based computational method for studying kinetics, computing nucleation rate, and analyzing mechanism of both homogeneous and heterogeneous bubble nucleation. As a rare event, bubble nucleation is difficult to study with traditional computational method: a rare event is hard to happen due to the free-energy barrier; but once it happens, the process is fast. We incorporated the forward flux sampling technique into molecular dynamics simulations, where the forward flux sampling allows us to track the pathways and flux of a rare phase-transition process between the liquid and the vapor in phase space, while the molecular dynamics simulations allow us to study the kinetics of bubble nucleation. We systematically optimized the added stochasticity, the order parameter of bubble nuclei, the superheated thermodynamic condition, the set of interfaces of forward flux sampling, and the fundamental wall-liquid interactions for heterogeneous bubble nucleation. The optimized forward-flux-sampling molecular dynamics is proved to be a powerful simulation method in computing nucleation rate and in analyzing kinetics of nuclei formation and growth. It is found that classical nucleation theory underestimates the nucleation rate for both homogeneous and heterogeneous bubble nucleation due to its overlook of the facts that kinetic fluctuations of bubble nuclei correlate strongly with bubble formation and subsequent growth.