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Direct molecular dynamics simulations of homogeneous bubble nucleation and improvements of classical theory

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Bubble nucleation in liquid is a liquid-to-vapor transition phenomenon and plays an important role in vulcanism. Studies of homogeneous liquid-vapour nucleation typically use the classical formula (CNT) for the bubble nucleation rate. However, the applicability of the CNT is not well understood.

Numerical techniques such as molecular dynamics and Monte-Carlo simulations are powerful methods to resolve details of the nucleation process and provide useful test cases for nucleation models. Typically, these simulations show large deviations from the CNT predictions. Most of the simulations for bubble nucleation in the literature use around 10^5 or fewer atoms, making it difficult to measure nucleation rates directly.

Recently, we presented large-scale, micro-canonical molecular dynamics simulations of homogeneous bubble nucleation with $5 * 10^8$ Lennard-Jones atoms, and succeeded to directly measure nucleation rates in the range of $10^{21-25}\mathrm{cm}^{-3}\mathrm{s}^{-1}$ for argon by resolving bubble nucleation events in the steady state nucleation phase [1,2]. The unprecedented size of the simulated volumes allows us to resolve the nucleation and growth of many bubbles per run in simple direct micro-canonical (NVE) simulations while the ambient pressure and temperature remain almost perfectly constant.

We find bubble nucleation rates which are lower than in most of the previous, smaller simulations. It is widely believed that classical nucleation theory (CNT) generally underestimates bubble nucleation rates by very large factors. However, our measured rates are within two orders of magnitude of CNT predictions - only at very low temperatures the CNT underestimates the nucleation rate significantly.

We also derive an improved classical formula for the homogeneous bubble nucleation rate, where we revise the prefactor in the nucleation rate and compare it with the widely used classical nucleation theory (CNT) [3]. Our large-scale molecular dynamics simulations and laboratory experiments for argon bubble nucleation enable us to precisely test our theoretical models. The improved formula including the Tolman correction with a small positive Tolman length leads to good agreement with both MD simulations and laboratory experiments.

[1] J. Diemand, R. Angelil, K. K. Tanaka, and H. Tanaka, Pys. Rev E 90, 052407 (2014)
[2] R. Angelil, J. Diemand, K. K. Tanaka, and H. Tanaka, Pys. Rev E 90, 063301 (2014)
[3] K. K. Tanaka, H. Tanaka, R. Angelil, and J. Diemand, submitted

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