Nano bubble—Size dependence of surface tension and inside pressure

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Abstract

The Young–Laplace (Y–L) equation describes the difference between inside pressure and outside pressure of a spherical bubble due to surface tension. The Y–L equation is simply deduced from mechanical stability of a bubble, but it is still controversial whether the Y–L equation can be used for tiny bubbles, such as a “nano bubble”, because the pressure difference divergently increases as the bubble radius \( R \) decreases. We investigated a spherical vapor bubble in Lennard-Jones liquid with molecular dynamics simulation, mainly looking into its mechanical stabilities. We generated a tiny bubble of various sizes \( (R \simeq 1.7-5 \text{ nm in argon unit}) \) under equilibrium conditions by changing the simulation cell size and the number of molecules. The liquid pressure was evaluated with the virial expression, which was negative in general and was found to be strongly dependent on \( R \). The vapor pressure was estimated from the vapor density via an empirical equation of state. The vapor pressure was found to be independent of \( R \) and very close to the vapor pressure at bulk liquid–vapor equilibrium. Then we assumed the Y–L equation to calculate the surface tension of the bubble, which turned out to be also independent of \( R \). Thus we confirm that the Y–L equation is valid even for nano-scale bubbles.

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