

Large-scale simulation on the formation and behavior of nanobubbles

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Abstract

In recent years, it has been found that nano-scale gas bubbles, called “nanobubbles”, possess noble properties that are not observed in ordinary bubbles. In particular, while ordinary bubbles quickly rise to the surface and collapse, nanobubbles remain suspended in liquid for a longer period of time and have the ability to change the normal characteristics of water. These properties, however, have not been convincingly explained yet. In the present study, we have focused on the mechanism for the stability of nanobubbles in water. In order to investigate the interface between the nanobubble surface and the surrounding water, we have performed classical molecular dynamics simulation on the atomic level.

Our simulation results indicate that the polarization is caused by oriented water molecules near the liquid/bubble interface. Then, taking this polarization into account, we clarified the conditions for the nanobubbles to remain stable in water by use of the Young-Laplace equation. As a result, we reached the conclusion that the gas pressure of about one atmosphere higher than the water pressure is appropriate for the nanobubbles, with its radius of about 100 nm, to remain stable in water.

Keywords: nanobubble, classical molecular dynamics simulation, Young-Laplace equation, polarization