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Proceedings of Symposium on Ultrasonic Electronics, Vol. 37 (2016)

16-18 November, 2016

Numerical Simulations of Extreme Conditions in a Dissolving Ultrafine Bubble in the Absence of Ultrasound

超音波が無い場合のウルトラファインバブルの溶解消滅における極限場

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1. Introduction

Most of microbubble and nanobubble (fine bubble) generators utilizes acoustic or hydrodynamic cavitation [1]. During the generation, liquid water becomes milky due to the presence of huge amount of bubbles. After stopping the generation, most bubbles move upward by buoyancy, and disappear at the liquid surface. Some nanobubbles (ultrafine bubbles) would be stablizied against dissolution in the liquid by the adsorption of hydrophobic impurities on the bubble surface [2]. Ultrafine bubbles less than 1 μm in diameter would stay in the liquid as buoyancy is negligible compared to the random thermal force causing the Brownian motion. Some other bubbles would dissolve into the liquid, and finally disappear by the complete dissolution.

It is widely known that in acoustic and hydrodynamic cavitation a bubble undergoes violent collapse called Rayleigh collapse. The reason for the violent collapse is the spherical geometry of the collapse and the inertia of the surrounding liquid [3]. For the Rayleigh collapse, expansion of a bubble due to lowering of the pressure in the surrounding liquid by the pressure oscillation of ultrasound or by some hydrodynamic motion is required. As a result of the violent collapse, the temperature and pressure inside a bubble increase significantly at the final moment of the collapse due to quasi-adiabatic compression of a bubble, where “quasi” means that appreciable thermal conduction takes place between the bubble interior and the surrounding liquid. At the final moment of the violent collapse, faint light is emitted, which is called sonoluminescence. Many of water vapor is dissociated inside a heated bubble, and OH radicals are created. Such chemical reactions are called sonochemical reactions.

On the other hand, simple dissolution of a bubble into liquid in the absence of ultrasound has been regarded as quasi-static with the bubble temperature and the liquid pressure kept nearly constant as assumed in the Epstein-Plesset theory of bubble dissolution [3, 4]. On the other hand, some researchers have experimentally suggested that OH radicals could be produced by simple dissolution of bubbles into the liquid [5]. In the present study, we have performed numerical simulations of simple dissolution of a bubble into the liquid in the absence of ultrasound taking into account the inertia of the surrounding liquid for the first time.

2. Model

The model used in the present numerical simulations is described in Ref. [6]. The following effects are taken into account; bubble dynamics (the inertia of the surrounding liquid), thermal conduction both inside and outside a bubble, the gas diffusion from the bubble interior to the surrounding liquid, non-equilibrium evaporation and condensation of water vapor at the bubble wall, temporal variation of the liquid temperature at the bubble wall, the temperature dependence of gas solubility and the diffusion coefficients, the dependence of surface tension on the bubble radius by Tolman equation, and temperature dependence of molar heat of gases. A bubble is assumed to disappear when the number of molecules inside a bubble becomes less than 1.

3. Results and Discussions

Dissolution of an air bubble into water saturated with air is numerically simulated. The initial bubble radius is 100 nm. During the bubble dissolution, a bubble passes any small size. Thus the presence of stable ultrafine bubble is not assumed here.

According to the simulation, the time for the complete dissolution is 75.4 μs which is slightly shorter than that estimated by the Epstein-Plesset theory (77.8 μs) due to the bubble dynamics (Fig. 1).

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Surprisingly, the temperature and pressure inside a bubble increase to about 3000 K and 5 GPa, respectively at the final moment (Fig. 2). At the final 2.3 ns, the bubble content is only N_2 because the solubility of N_2 is the lowest among the gas species. The liquid temperature increases to 85 °C, which is insufficient for the formation of OH radicals. The dissociation of N_2 molecules is also negligible because the probability is only on the order of 10^{-15}.

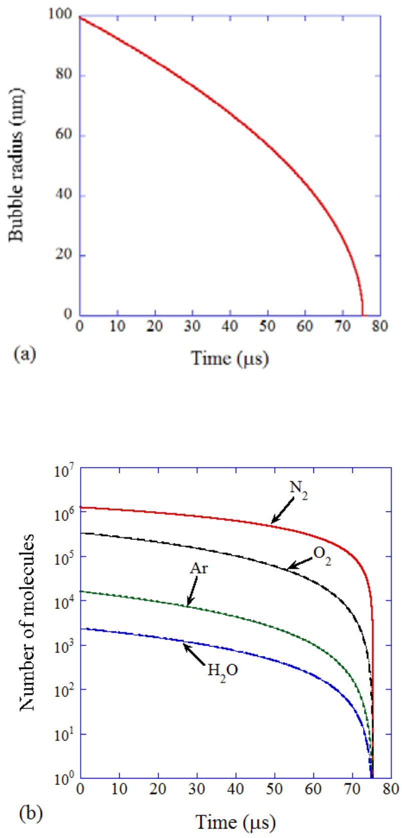

Fig. 1 The result of numerical simulation. (a) The bubble radius. (b) The number of molecules inside a bubble. Reprinted with permission from K.Yasui et al., Phys.Rev.E 94, 013106 (2016), Copyright (2016) by the American Physical Society.

4. Conclusion

Numerical simulations of dissolution of an air ultrafine bubble have shown that the temperature and pressure inside a bubble increase to 3000 K and 5 GPa, respectively at the final moment of complete dissolution.

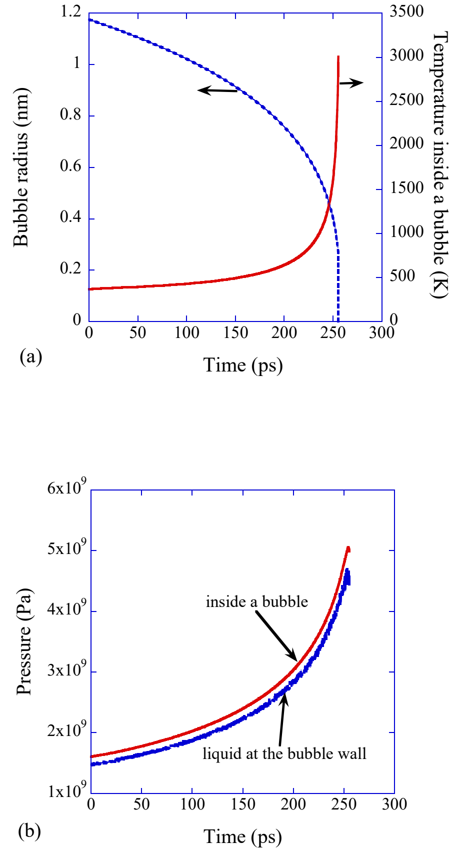

Fig. 2 The result of numerical simulation for the final 255 ps. (a) The bubble radius and temperature. (b) The pressure inside a bubble and the liquid pressure at the bubble wall. Reprinted with permission from K.Yasui et al., Phys.Rev.E 94, 013106 (2016), Copyright (2016) by the American Physical Society.

Acknowledgment

This work was partly supported by METI, Japan, as part of the international standardization project for fine bubbles.

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