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MOLECULAR DYNAMICS SIMULATION OF NANOBUBBLES

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ABSTRACT

Some results have been reported recently related to the bubble formation with Molecular Dynamics (MD) simulation method. Some of them conduct the MD simulations of the bubble nucleation including impurity molecules with L-J potential[1,2]. In the present study, we investigate the stability of the nanometer size bubble in water, using molecular dynamics (MD) simulation method. MD simulation of an aqueous surfactant system: water liquid and alcohols below the liquid saturation density is carried out to investigate the stability of "nanobubbles" and the structure of the gas-liquid interface. To analyze the effect of surfactant structure, volume, and polarization on the stability of bubble nuclei, we use water by SPC/E model as the solvent molecules and 1-propanol, 1-pentanol, 1-heptanol as the surfactant molecules.

Fig.1 shows the numerical result of instantaneous behavior of nanobubbles under the presence of surfactant in water. The calculation system is the cubic cell which has a side length of 25.057[Å], and a three-dimensional periodic boundary condition is applied. To include the intramolecular motion, AMBER force field [3] is adopted as a potential function. The momentum equations are integrated by velocity-Verlet argorithm [4]. Further, the time integration is extended to the Multi Time Scale algorithm by r-RESPA method[5]. As the surfactant molecules, to evaluate the influence of the hydrophobic effect of surfactants on the stability of bubble nuclei, we adopt 1-propanol (C_3H_7OH), 1-pentanol ($C_5H_{11}OH$), and 1-heptanol ($C_7H_{15}OH$), and to investigate the influence of the polarization of hydrophilic groups (-OH), "pseudo" 1-pentanol of which charge is cancelled away is also calculated.

As a result, it was found that from the MD simulation at the condition that the bubble nuclei could not exist stably in pure water, a stable bubble is formed in aqueous surfactant system and hydroxyl groups of surfactants tend to point to the liquid phase at the gas-liquid interface. It is also shown that the longer hydrophobic chains the surfactants have, the more stably the bubble nuclei can exist.

References

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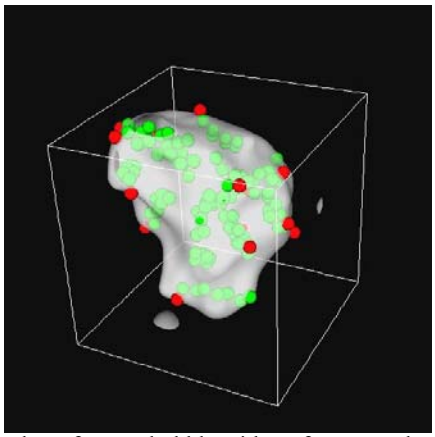

Fig.1 Snapshot of a nanobubble with surfactant molecules