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An investigation of nucleation-growth of bubbles using molecular dynamics simulation TAIGA KOMATSU, The University of Tokyo, SHINICHI TSUDA, Shinshu University, SHU TAKAGI, YOICHIRO MATSUMOTO, The University of Tokyo — Microscopic phase transition phenomena have been applied in medical or industrial area recently. However, the behavior of bubble nucleation in nano-scale has not been clarified yet. In this study, a bubble nucleation-growth process was investigated in a decompressed Lennard-Jones fluid using an NVT ensemble molecular dynamics simulation. As a result, as was reported in the NVE ensemble, a competitive growth similar to Ostwald ripening was also observed. On the other hand, more bubble nuclei were formed than those in the NVE ensemble, and the growing/shrinking speed of each bubble nucleus became slower. It was confirmed that the temperature rises in NVE ensemble when bubble nuclei are generated while it does not rise in NVT. Therefore, the pressure is lower in NVT and this pressure difference causes the results mentioned above. The growth exponent for the mean radius of bubble nuclei was also evaluated, and it was confirmed that the value of the exponent became smaller than that in the NVE ensemble, at least in the present time scale. However, since the competitive growth is similar to the result of the NVE simulation, the exponent value could be equal to that of the NVE by investigating the longer time behavior.

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