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Title: Molecular Dynamics Simulations on Thermal Fluctuation of Metastable Liquids

Abstract

Thermal fluctuations in a metastable liquid prior to and post bubble nucleation was analyzed to understand how the motion of a solid impurity inside the liquid will affect the bubble nucleation rate. A constant particle number, temperature, and volume ensemble was used to simulate metastable liquid argon by molecular dynamics. The impurity had metallic Lennard-Jones parameters and a comparison between a system having a freely moving impurity and fixed impurity was conducted. The figure shows an example of the system. The fixed system produced a relatively higher nucleation rate because the movement of the impurity could not hinder void growth in the liquid ambient. The nucleation rate was calculated using the Yasuoka-Matsumoto method [1]. Different sizes and shapes of the seed were examined [2].

References

1. Yasuoka K. and Matsumoto M. Journal of Chemical Physics. 1998. V. 109. pp. 8451-8462.
2. Suh D., Nakamura M. and Yasuoka, K. Journal of Physics: Conference Series. 2015. V. 656. pp. 012037.