

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Homogeneous bubble nucleation in liquids: a molecular dynamics study ZUN-JING WANG, Carnegie Mellon University, CHANTAL VALERIANI, University of Edinburgh, DAAN FRENKEL, University of Cambridge — We have studied homogenous bubble nucleation in a Lennard-Jones fluid by performing Molecular Dynamics simulation coupled with Forward-Flux Sampling (MD-FFS). The MD-FFS estimate of bubble-nucleation rate is higher than predicted on the basis of Classical Nucleation Theory (CNT). Although this discrepancy is consistent with earlier findings, our simulations show that bubble nuclei are compact rather than ramified as had been suggested by Shen and Debenedetti (J. Chem. Phys. 1999, 111:3581). We find bubble nucleation starts with local spots much hotter than superheated environment, and the local temperature correlates strongly with subsequent bubble formation - this mechanism is not taken into account in CNT.

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Date submitted: 19 Nov 2008

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