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Nucleation of Ice

VALERIA MOLINERO, University of Utah

The freezing of water into ice is a ubiquitous transformation in nature, yet the microscopic mechanism of homogeneous nucleation of ice has not yet been elucidated. One of the reasons is that nucleation happens in time scales that are too fast for an experimental characterization and two slow for a systematic study with atomistic simulations. In this work we use coarse-grained molecular dynamics simulations with the monatomic model of water mW[1] to shed light into the mechanism of homogeneous nucleation of ice and its relationship to the thermodynamics of supercooled water. Cooling of bulk water produces either crystalline ice or low- density amorphous ice (LDA) depending on the quenching rate. We find that ice crystallization occurs faster at temperatures close to the liquid-liquid transition, defined as the point of maximum inflection of the density with respect to the temperature. At the liquid-liquid transition, the time scale of nucleation becomes comparable to the time scale of relaxation within the liquid phase, determining –effectively- the end of the metastable liquid state. Our results imply that no ultraviscous liquid water can exist at temperatures just above the much disputed glass transition of water. We discuss how the scenario is changed when water is in confinement, and the relationship of the mechanism of ice nucleation to that of other liquids that present the same phase behavior, silicon [2] and germanium [3].

[1] Molinero, V. & Moore, E. B. Water modeled as an intermediate element between carbon and silicon. Journal of Physical Chemistry B (2008). Online at http://pubs.acs.org/cgi- bin/abstract.cgi/jpcbfk/asap/abs/jp805227c.html
[2] Molinero, V., Sastry, S. & Angell, C. A. Tuning of tetrahedrality in a silicon potential yields a series of monatomic (metal-like) glass formers of very high fragility. Physical Review Letters 97, 075701 (2006).