The Water Supercooled Regime and Ice Critical Nucleus Size

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The supercooled regime of water at ambient pressure is experimentally defined as the temperature range between melting and spontaneous crystallization. By performing a series of simulations with different initial conditions, we have quantitatively established the relation between the critical nucleus size and degree of supercooling. The results, which are well described by the Gibbs-Thomson equation, show that ice embryos containing hundreds or thousands of molecules are needed for the system to crystallize macroscopically. Our findings explain the relative ease with which water droplets can be supercooled in controlled experiments. Nevertheless, even at very low temperature no spontaneous crystallization is observed using several atomistic models, contrasting with the experimental observations. Our simulations of supercooled water suggest, as previously found by several authors, the existence of a liquid-liquid phase transition in the metastable regime that is accompanied by an important kinetic slowdown. These results, as they are not fully consistent with experiments, could be regarded as an indication of a failure of the current atomistic models to describe supercooled water.