Ice nucleation far from equilibrium

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The metastability and kinetics of non-equilibrium phase transformations in water present one of the greatest mysteries of condensed matter physics and chemistry. Owing to its unique inter- and intra-molecular interactions, water is likely the most polymorphic material in existence -- having over 17 ice phases, most of which are accessible only at high pressure. Developing an understanding of the nucleation of ice at high pressure has direct implications for the origins of life on extrasolar "super-earths", ocean worlds that have been detected by the Kepler telescope.

Over the years, experiments that solidify water into the high-pressure ice VII phase have presented seemingly contradictory results regarding the nucleation of ice far from equilibrium. Here we show that, under these extreme conditions, classical nucleation theory can successfully describe these freezing experiments but only if amended to include new aspects that are unique to the non-equilibrium state -- transient nucleation and thermal disequilibrium between ice and liquid -- and that by doing so we are able to reconcile the apparent discrepancies between various nucleation experiments.

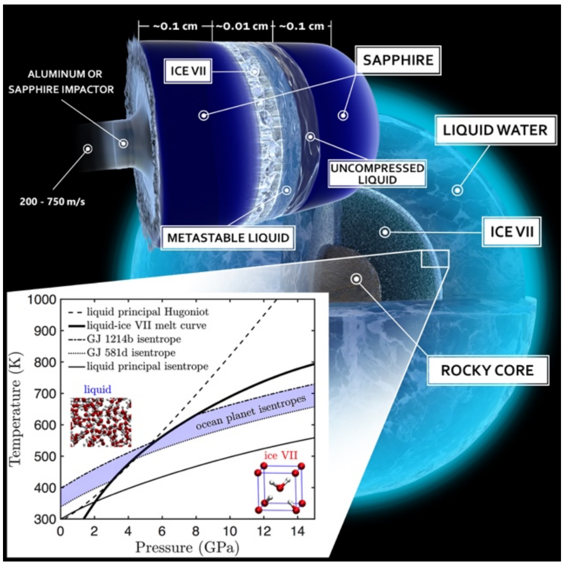

Figure 1. Isentropic compression experiments allow liquid water to be driven to an extremely undercooled state and nucleate a high-pressure polymorph known as ice VII. Theoretical work at LLNL has revealed the detailed of the nucleation and growth kinetics of this solidification process. This unique phase of ice is believed to exist near the core of “ocean world” planets recently detected by observation.

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