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Numerical modeling of the phase transition kinetics for the submicrosecond solidification of water under dynamic compression[1] DANE STERBENTZ, University of California, Davis, PHILIP MYINT, Lawrence Livermore National Laboratory, JEAN-PIERRE DELPLANQUE, University of California, Davis, JONATHAN BELOF, Lawrence Livermore National Laboratory — Several landmark experimental studies on the solidification of liquid water to the high-pressure ice VII phase under multiple-shock and ramp dynamic compression have been carried out over the past two decades, yet modeling this rapid phase transition has proven challenging. The application of classical nucleation theory (CNT)-based approaches to rapid phase transition kinetics occurring under extreme temperatures and pressures presents a variety of new opportunities for predictive computational modeling. This work attempts to model the liquid water—ice VII phase transformation using a numerical discretization scheme to solve the Zel'dovich—Frenkel partial differential equation, a fundamental CNT-based kinetic equation describing the statistical time-dependent behavior of solid cluster formation. One major result of this research is that the Zel'dovich—Frenkel equation is able to model—without the need for empirical scaling parameters—the duration of the lag time prior to the onset of the phase transformation.

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