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Atomistic simulation approach to constructing models of phase transition kinetics for hydrocodes¹

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Phase transformations under dynamic compression, of great interest due to their importance in interpreting high pressure experiments relevant to planetary physics, present several unique challenges to existing theoretical and computational methodologies. The wide disparity between the length and time scales of atomistic simulation (molecular dynamics) in comparison with the scale of experimental measurements results in a mismatch of theories: accurate models of phase kinetics are required at the hydrodynamic scale for experimental analysis, but our direct knowledge of the phase transition process is limited to the atomistic regime. Focusing on compressive solidification of water and copper, we will highlight atomistic methods for closing a kinetic theory derived from a classical nucleation approach. New techniques, based on the Gibbs-Thomson condition and free energy sampling, for the determination of the nucleation free energy barriers and growth rates at high pressure, will be presented. In addition to these quantities, it has been found that, for dynamic solidification, the nucleation kinetic prefactor and transient induction time play a crucial role in explaining the homogeneous nucleation behavior of water at high pressure. We will also highlight how classical nucleation theory predicts a cross-over from a heterogeneous to homogeneous nucleation mode depending upon the magnitude of the driving force (*i.e.*, shock strength).

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