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Toward a Multi-scale Phase Transition Kinetics Methodology: From Non-Equilibrium Statistical Mechanics to Hydrodynamics[1]

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— Shock and ramp compression experiments are allowing us to probe condensed matter under extreme conditions where phase transitions and other non-equilibrium aspects can now be directly observed, but first principles simulation of kinetics remains a challenge. A multi-scale approach is presented here, with non-equilibrium statistical mechanical quantities calculated by molecular dynamics (MD) and then leveraged to inform a classical nucleation and growth kinetics model at the hydrodynamic scale. Of central interest is the free energy barrier for the formation of a critical nucleus, with direct NEMD presenting the challenge of relatively long timescales necessary to resolve nucleation. Rather than attempt to resolve the time-dependent nucleation sequence directly, the methodology derived here is built upon the non-equilibrium work theorem [Jarzynski, *Phys. Rev. Lett.*, 78:2690 (1997)] in order to bias the formation of a critical nucleus and thus construct the nucleation and growth rates. Having determined these kinetic terms from MD, a hydrodynamics implementation of Kolmogorov-Johnson-Mehl-Avrami (KJMA) kinetics and metastabilty is applied to the dynamic compressive freezing of water and compared with recent ramp compression experiments [Dolan *et al., Nature* (2007)]

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