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Limits of metastability in shock-induced phase transitions[1]

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In dynamic compression, kinetic effects may delay a phase transition and under extreme strain rates of deformation, the parent phase can be loaded into metastable states from which the transition takes place, beyond the equilibrium phase boundary. Large-scale atomistic simulations coupled with first-principles calculations can provide valuable insights in the study of phase changes under extreme conditions, such as those produced by strong shock waves. The size scale of systems that can be studied via atomistic simulations are now sufficient to study large defective or multiphase structures, and the time-scales sampled in non-equilibrium molecular dynamics (NEMD) are currently in the nanoseconds, a time scale accessible in high-energy laser driven shock experiments. Atomistic simulations of shocked single crystals, show that sub-nanoseconds rise times and strain rates $> 10^9 s^{-1}$ can lead to deformation paths and transformation mechanisms different from homogeneous nucleation or thermally activated processes. We present a formulation of the limits of metastability of elastic-plastic and structural transitions in single crystals, including amorphization, under high strain-rates of deformation, based on large-scale atomistic simulations and ab-initio calculations.

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