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Coupling between plasticity and phase transition in single crystal iron at ultra-high strain rate NOUROU AMADOU, Dept de Physique, Univ Abdou Moumouni de Niamey, THIBAUT DE RESSEGUIER, ANDRE DRAGON, Institut P'. CNRS. ENSMA. Université de Poitiers, Poitiers, France — Solid materials behavior under ultra-high strain rate loading such as shock compression may involve various processes including plastic deformation, structural phase transformations, fracture, melting, etc., whose kinetics and coupling are complex functions of strain rate, initial conditions and microstructure. Here, we present molecular dynamics simulations of the dynamic response of single-crystal iron to either ramp or shock compression, at strain rates on the order of $10^9 s^{-1}$, where we focus on the coupling between plastic deformation and the bcc-hcp phase transition. Defect-free crystal at 50 K initial temperature was found to yield via twinning when compressed along the [001] direction. Then, the onset of the bcc-hcp transformation was shown to be tightly dependent on the plasticity history through a shear-stiffening effect, which in some conditions inhibits the nucleation of the hcp phase [N. Amadou et al., Phys. Rev. B 98, 024104, 2018]. Yet, changing the initial temperature, direction of load application versus crystal orientation, or introducing lattice defects lead to very different behavior, including dislocation-mediated plasticity.

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