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Ab Initio investigation of the shock-induced cd to beta-tin phase transition in single-crystal silicon GABRIELE MOGNI, ANDREW HIGGINBOTHAM, JUSTIN WARK, University of Oxford, UK, KATALIN GAAL-NAGY, Universitat Regensburg, Germany — An understanding of the mechanisms behind the relief of shear stress in shocked single-crystal silicon and germanium remains elusive. Silicon undergoes a first-order pressure-induced polymorphic phase transition from its ambient pressure cubic-diamond (cd) crystal structure to its first high-pressure stable phase, beta-tin, at about 120 kbar under hydrostatic compression. This phase transition was first the subject of an experimental investigation under shock-wave loading by Gust and Royce (J. Appl. Phys.: 42, 5 (1971)), who interpreted the wave profile measurements as an HEL at 92 kbar and consequent onset of 3D plastic deformation and a subsequent phase transition. By investigating the lowering of the transition pressure and enthalpy barrier as a function of increasing uniaxial shear stress via ab-initio DFT simulations, we predict a significant lowering of the transition stress, down to values close to those associated with the HEL itself. This raises the question as to whether the onset of inelastic response at the HEL is in fact the onset of a phase transition. Our plans for the future involve substantiating these findings in laser-based shock-wave experiments.

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