

Abstract Submitted
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Atomistic simulation of Shock Induced Structural Phase Transition of Single Crystal Copper NILANJAN MITRA, ANUPAM NEOGI, Indian Institute of Technology Kharagpur — It is well known that pure Single crystal copper subjected to shock wave loading of different intensities results in development of different types of plasticity mechanisms. Beyond that regime of shock wave intensity it has also been shown in several literature that single crystal Cu shows melting. A regime of shock loading has been identified in this research in which single crystal Cu undergoes a structural phase transition. Identification of this structural phase transition mechanism as well as the resulting phase has not only been done using radial distribution functions and structure factor but also with virtual X-Ray diffraction. Phonon dispersion at these high temperatures and pressures have also been investigated. The effect of crystallographic orientation and initial temperature of the sample has been investigated in this simulation study.

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