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Molecular dynamics simulation of shock compression of silicon

MIKHAIL LADANOV, University of South Florida, IVAN OLEYNIK, University of South Florida, SERGEY ZYBIN, California Institute of Technology, MARK ELERT, U.S. Naval Academy, CARTER WHITE, Naval Research Laboratory — Shock compression of condensed matter is a fascinating scientific field that provides an excellent opportunity to probe the fundamental physics and chemistry of matter at extreme pressures and temperatures. In spite of substantial theoretical and experimental efforts, a full understanding of shock-induced elastic and plastic responses and polymorphic phase transitions is still far from complete. These phenomena often occur at the nanometer size and picosecond time scales, which makes molecular dynamics simulations an ideal tool for exploring nanoscale mechanisms of shock induced processes such as chemical reactions and phase transitions. We report the results of a molecular dynamics simulation of shock wave propagation in silicon in the [100], [110], and [111] directions obtained using a classical interatomic potential. Several regimes of materials response are classified as a function of shock wave intensity and crystalline orientation of shock wave propagation using calculated shock Hugoniot. The shock induced chemistry and shock wave splitting are discussed in relation to recent experimental results [1] that indicate an anomalous elastic response of the lattice at high compression ratios. [1] A. Loveridge-Smith, Phys. Rev. Let. **86**, 2349 (2001).

Ivan Oleynik
University of South Florida

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