Elastic-plastic response and polymorphic phase transition in shock-compressed diamond

YOU LIN, ROMAIN PERRIOT, VASILY ZHAKHOVSKY, Department of Physics, University of South Florida, XIANG GU, Department of Applied Physics, Aalto University, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, Department of Physics, University of South Florida — Shock wave propagation in diamond along the \(\{110\}\) crystallographic direction was simulated by molecular dynamics (MD) using the reactive empirical bond order (REBO) potential. In addition to known regimes of shock wave propagation, such as single elastic, split elastic-plastic, and single plastic shock wave, two new regimes were observed: 1) a split elastic-elastic shock wave associated with a polymorphic phase transition; 2) a single two-zone elastic-plastic shock wave with the leading elastic zone followed by the plastic zone. In the case of the split elastic-elastic shock wave, the onset of phase transition occurs at a pressure below the Hugoniot elastic limit (HEL); therefore, the solid-solid transformation takes place in the uniaxially compressed material in the absence of plasticity. Within the single two-zone elastic-plastic shock wave, the material in the elastic zone is in a metastable state at a pressure exceeding the HEL. The metastable elastic state decays into the plastic state within the plastic zone, both elastic and plastic fronts moving with the same speed.

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