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Shock-induced phase transition in diamond YOU LIN, ROMAIN PERRIOTT, VASILY ZHAKHOVSKY, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — Shock wave propagation in diamond crystal along the <110> crystallographic direction was simulated by molecular dynamics (MD) using the Reactive Empirical Bond Order (REBO) potential. In addition to usual regimes of shock wave propagation, such as single elastic wave, two split elastic-plastic waves, and single plastic shock wave, a two-zone *elastic-elastic* single shock wave was observed in the range of piston velocities between 2.0 and 4.1 km/s and longitudinal stresses 126 -278 GPa. The elastic-elastic splitting occurs because the crystal undergoes a stress-induced structural phase transition from a normal, low-pressure, to a high-pressure phase of diamond within the interval of pressures below the Hugoniot elastic limit. The existence of a polymorphic phase transition makes possible a rarefaction shock wave, which was observed in our MD simulations of short piston impact of a diamond sample followed by the formation of a rarefaction shock wave that transforms the high-pressure phase back to the low pressure phase of diamond.

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