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Molecular dynamics simulations of diamond shock compression using different interatomic potentials ROMAIN PERRIOT, XIANG GU, YOU LIN, VASILY V. ZHAKHOVSKY, University of South Florida, Department of Physics, Tampa, Fl 33620, USA, NICOLAS PINEAU, JEAN-BERNARD MAILLET, LAURENT SOULARD, Départment de Physique Théorique et Appliquée, CEA-DAM Ile de France, Bruyères-le-Châtel, 91297 Arpajon Cedex, France, JAN H. LOS, Département Théorie et Simulation Numérique, CINaM, CNRS-UPR 3118, Campus de Luminy, 13288 Marseille, France, CARTER T. WHITE, Naval Research Laboratory, Washington, DC 20375, USA, IVAN I. OLEYNIK, University of South Florida, Department of Physics, Tampa, Fl 33620, USA — Shock wave propagation in diamond crystals were simulated by molecular dynamics (MD) using several interactomic potentials: Reactive Empirical Bond Order (REBO) potential; Screened REBO (S-REBO); and, long-range carbon bond-order potential (LCBOP II). Several shock-wave regimes were observed, including single-wave elastic, plastic, and split two-wave elastic-plastic regimes, as well as a novel steady two-zone elastic-plastic regime. The latter regime is characterized by the leading elastic zone of the metastable material uniaxially compressed above the Hugoniot Elastic Limit, which depends on the specific potential used in the simulations. The results obtained using REBO, S-REBO, and LCBOP II are compared with experiment.

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