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Molecular dynamics simulations of anomalous elastic response of covalent crystals to shock compression KEITH MCLAUGHLIN, IVAN OLEYNIK, University of South Florida, SERGEY ZYBIN, California Institute of Technology, MARK ELERT, U.S. Naval Academy, CARTER WHITE, Naval Research Laboratory — We have performed large-scale molecular-dynamics simulations of shock-wave propagation in single-crystal covalent solids such as diamond and silicon. An anomalous elastic response of these materials has been observed in the intermediate range of shock-wave intensities between the elastic-plastic split shock-wave regime and the shock-induced chemistry regime. The anomalous elastic response is characterized by the absence of plastic deformations in highly uniaxially compressed material. The unusual materials response in shock-compressed diamond is attributed to unique and complex constitutive relationships: both shear and longitudinal stresses are non-monotonic functions of compression. This example clearly demonstrates the necessity of generalization of the notion of the Hugoniot elastic limit (HEL) to include critical shear stresses in a criterion of materials yielding upon shock compression.

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