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Molecular dynamics simulations of anomalous elastic response of covalent crystals to shock compression

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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.

[X] Prefer Oral Session
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