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Shear stresses in shock compressed covalent solids IVAN OLEYNIK, DOUGLAS LOVELADY, University of South Florida, SERGEY ZYBIN, California Institute of Technology, MARK ELERT, U.S. Naval Academy, CARTER WHITE, Naval Research Laboratory — Shear stresses are the driving forces for the creation of both point and extended defects in crystals subjected to high pressures and temperatures. We report DFT results appropriate for shear stresses in shock compressed covalent solids such as diamond and silicon for three low-index crystallographic directions, <100>, <110>, <111>. The non-monotonic behavior of shear stresses predicted by first-principles theory will be discussed in connection to dynamics of plastic deformations and the structure of the shock wave front. In particular, the non-monotonic dependence of shear stresses on uniaxial compression might result in a significant delay or even freezing of the plastic response that was recently observed in MD simulations of strong shock waves in covalent solids.

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