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Structural deformation and instability of strong covalent solids<sup>1</sup> CHANGFENG CHEN, University of Nevada, Las Vegas, HONG SUN, Shanghai Jiaotong University — We employ first principles total-energy calculations to study the structural deformation modes at large strains and the lattice instabilities beyond the elastic limit for several strong covalent solids. We examine the atomistic bonding changes to elucidate the microscopic mechanism for the stress response and the orientational dependence of the peak stresses along different crystallographic directions and the bond breaking modes. Implications for the mechanical properties will be discussed.

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