Abstract Submitted for the SHOCK05 Meeting of The American Physical Society

Strength and Deformation Modes of Strong Covalent Solids¹ CHANGFENG CHEN, University of Nevada, Las Vegas — We present results of first-principles studies on the atomistic deformation modes and the ideal strength of several strong covalent solids, including diamond, cubic boron nitride and recently synthesized cubic B-C-N ternary compounds. We show that the widely used empirical relationship between the elastic moduli and material strength leads to a significant overestimate for the strength of the ternary compounds. The nonelastic stress response at large strains makes it necessary to examine the stress-strain relation up to the breaking point for an accurate determination of the strength and the structural failure mode. Implications for other similar materials will be discussed.

¹This work was supported by DOE under Cooperative Agreement DE-FC52-01NV14049.

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Date submitted: 07 Mar 2005

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