

Abstract Submitted
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Ideal Strength of Hexagonal Diamond and Related B-C-N Compounds¹ CHANGFENG CHEN, YI ZHANG, University of Nevada, Las Vegas, ZICHENG PAN, HONG SUN, Shanghai Jiao Tong University, China — We have performed first principles calculations on the ideal strength of h-diamond, w-BN, and Φ -BC₂N. We have considered structural deformation under pure tensile, pure shear or biaxial stress fields. The calculated results reveal new atomistic fracture mechanism for these materials.

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