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Super-Hard Materials of the B-C binary system

Thursday, 11 July 2019 15:00 (2 hours)

A number of potentially ultra-hard materials were examined using ab-initio methods. Compound phases of varying lattice stoichiometry in the B-C-N-O quaternary system, in the forms, C8-xBx (x = 1, 2, 3, 4), C7-xBNx (x = 1, 2, 3) and C6-xBNOx (x = 1, 2) were proposed as possible super-hard materials with useful applications. Cell structures and elastic properties were studied, systematic trends were established. It was determined that C7B and C6BN were mechanically and dynamically stable compounds with potential super-hard characteristics, C6BN being the harder of the two.
The results showed a graphical minimum in the effective values of the isotropic shear modulus, G and Young modulus, E at x = 3 (C5B3) for the C8-xBx materials, this indicates that a much higher boron concentration, i.e. with x > 4, could possibly increase the hardness of these materials; we present a more detailed and extended study (x = 1-7) of the C8-xBx materials.

Apply to be
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Yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

Phd

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