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Structures and elastic properties of crystalline and amorphous BC_2N solids

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Abstract. Crystalline and amorphous BC_2N supercells with 216 atoms have been constructed by random distributions of B, C, and N atoms in the diamond lattice and amorphous sp^3 carbon structure, respectively. The atomic structures of these two systems were relaxed using density functional theory, and their mechanical properties including the bulk modulus, shear modulus, and Young's modulus were computed. Crystalline BC_2N possess higher elastic moduli than those of cubic BN. Amorphous BC_2N exhibit reasonable elastic moduli and appreciable ductility with a large ratio between the bulk modulus and shear modulus. Both crystalline and amorphous BC_2N are superior candidates as superhard materials.

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Key words: BC_2N, structure, elastic properties, superhard material

1 Introduction

C_2 and BN are isoelectronic with eight valence electrons, which can lead to isoelectronic compound of BC_2N. It is expected that the BC_2N crystals of cubic phase can combine the excellent properties of diamond (high hardness) [1, 2] and cubic-BN (c-BN) (higher chemical inertness) [3] in the field of superhard materials [1, 4]. Therefore, both crystalline [1,4–9] and amorphous BC_2N [10–13] solids have received considerable attentions. However, neither their atomic structures nor physical properties have been well understood [1, 2, 14].

For crystalline BC_2N, previous experiments showed evidences for both diamond-like solid solutions [1, 6, 9] and phase separation into diamond and c-BN [15, 16]. According

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to the absence of (200) peaks in X-ray diffraction (XRD), Knittle *et al*. [9] reported that several cubic B-C-N solid solutions have been synthesized. Solozheko *et al*. [1] employed high-brilliance synchrotron radiation to study in situ the process of phase formation. The presence of 111, 220, and 311 lines and the absence of 200 lines suggested a diamond-like cubic B-C-N phase with BC_2N composition. Under similar high-pressure and high-temperature conditions, however, Sasaki [16] and Nakano [15] observed the simultaneous crystallization of diamond and c-BN. Due to the poor resolution of X-ray detection systems [17], it was unclear whether the synthesized products are B-C-N ternary alloys or just mechanical mixtures of highly dispersed diamond and c-BN [1,17].

Meanwhile, various theoretical models have been proposed to describe the most probable structure of crystalline BC_2N [4,5,7,14]. Typically, in these models, B, C, and N atoms are orderly distributed within the diamond lattice with certain space-group symmetry. However, both XRD data [1, 6, 9, 18] and Raman analysis [19] in previous experiments strongly suggested random distributions of B, C, and N atoms in the diamond lattice. In addition to the unclear crystal structure, there are also some controversies on the physical properties (particularly the mechanical properties) of the BC_2N solids. For example, using shock compression methods, Komatsu *et al*. [8] synthesized the cubic $BC_{2.5}N$ with a bulk modulus of 401 GPa, which is larger than that of c-BN (369 GPa) [20]. However, Solozhenko *et al*. [1] reported a rather small bulk modulus (282 GPa) for cubic BC_2N synthesized under the high pressure and high temperature conditions.

Parallel to the study of crystalline BC_2N, amorphous BC_2N solids have been prepared by chemical vapor deposition (CVD) [13], magnetron sputtering [11, 21, 22] and other techniques [10, 12, 23, 24], and their structures and composition were characterized by means of Fourier Transform-Infrared Spectroscopy (FTIR) and X-ray photoelectron spectroscopic (XPS). Most of these works were focused on structural characterization to verify whether the synthesized films are atomic-level hybridizations [11,13,21] or simple phase separations [10, 23], while the detailed atomic structure of the amorphous BC_2N solid was still unclear. Moreover, the mechanical properties of the BC_2N films were not well understood due to the great influences of the substrates.

To the best of our knowledge, there was no theoretical investigation on the amorphous BC_2N solids yet. In this paper, we carried out a comparative first-principles study on the crystalline and amorphous BC_2N solids within a random solid solution model, in which boron and nitrogen atoms randomly replace the carbon atoms in the diamond lattice and the amorphous sp^3 network structure, respectively. From our theoretical calculations, both crystalline and amorphous BC_2N solids exhibit appreciable mechanical properties with regard to those of c-BN and amorphous carbon, making them good candidates for superhard materials.

2 Structural models and computational details

Our random solid solution models [25] were based on the following considerations: (i) the structural similarities [4] and small lattice mismatch [26] between diamond and c-