Route to high-\(T_c\) superconductivity of \(\text{BC}_7\) via strong bonding of boron–carbon compound at high pressure

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We have analyzed the compositions of boron–carbon system, in which the \(\text{BC}_7\) compound is identified as structural stability at high pressure. The first-principles calculation is used to identify the phase diagram, electronic structure, and superconductivity of \(\text{BC}_7\). Our results have demonstrated that the \(\text{BC}_7\) is thermodynamically stable in the diamond-like \(\text{P4m2}\) structure at a pressure above 244 GPa, and under temperature also. Feature of chemical bonds between B and C atoms is presented using the electron localization function. The strong chemical bonds in diamond-like \(\text{P4m2}\) structure are covalent bonds, and it exhibits the s–p hybridization under the pressure compression. The Fermi surface shape displays the large sheet, indicating that the diamond-like \(\text{P4m2}\) phase can achieve a high superconducting transition temperature (\(T_c\)). The outstanding property of \(\text{BC}_7\) at 250 GPa has manifested very high-\(T_c\) of superconductivity as 164 K, indicating that the carbon-rich system can induce the high-\(T_c\) value as well.

Carbon-rich material at high pressure and high temperature is interesting due to its outstanding properties to be super-hardness and superconductors. With regards to the study of boron carbides, a \(\text{BC}_{1.6}\) phase has been observed using synchrotron-based X-ray diffraction, Raman spectroscopy, and energy-dispersive scanning electron microscopy\textsuperscript{1}. The results have revealed that the \(\gamma\)-\(\text{BC}_{1.6}\) structure transforms to the diamond-like \(\text{BC}_{1.6}\) at a temperature of 2230 K and a pressure of 45 GPa. They demonstrated that \(\text{BC}_x\) can transform to hexagonal-\(\text{BC}_{1.6}\) or orthorhombic-\(\text{BC}_{1.6}\), depending upon the pressure and temperature conditions. However, the heating is not enough to make transformation to the cubic phase. Successfully, a cubic \(\text{BC}_3\) structure has been synthesized at a pressure of 39 GPa and a temperature of 2200 K using a laser-heated diamond anvil cell, which the system is condensed by the \(\text{sp}^3\) hybridization\textsuperscript{2}.

In the progress for finding the word record of the highest superconducting transition temperature (\(T_c\))\textsuperscript{3}, the novel compositions in the interesting compounds have been reported at high pressure conditions. The hydrogen-rich materials of \(\text{H}_3\text{S}_4\) and \(\text{LaH}_{10}\)\textsuperscript{5} were proposed to be superconductor at gigapascal pressures (203 K and 250 K), which the high-\(T_c\) temperature superconductivity depended on the conventional electron–phonon coupling and the shape of density of states around the Fermi level\textsuperscript{6}. The high pressures above 100 GPa on these materials were required for structural stabilities of the rich hydrides. It was introduced that another material to find the better superconductors can be applied by the same concepts and methods\textsuperscript{1}. Therefore, the high-pressure effect is one of the crucial tool for the formation of the atom-rich system, and the discovery of high-\(T_c\) superconductivity. In another way to enhance the high-\(T_c\) superconductivity, alkali-doped \(\text{C}_{60}\) system has been presented as a superconducting material among carbon related compounds. The \(T_c\) in the alkali-doped \(\text{C}_{60}\) was reported as 33 K, which moderated by the coupling of electrons to high-frequency molecular vibrational modes\textsuperscript{7}.

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In the carbon-rich systems, the experimental study has been reported the synthesis of cubic BC$_2$ (c-BC$_2$), which is the diamond-like structure. The c-BC$_2$ was synthesized at a pressure of 24 GPa and a temperature of 2200 K using both laser-heated diamond anvil cell and large-volume multi anvil apparatus. The synthesized c-BC$_2$ showed that it is too high Vickers hardness (H$_v$) up to 71 GPa. Moreover, the BC$_5$ phase is suggested as a candidate structure at high pressure through ab initio random search calculation. The I4/m2 structure was introduced as the most stable structure at high pressure. By the density functional theory (DFT) study, it was reported that the predicted I4m2 structure is metallic, and the estimated $T_c$ of the superconducting phase is as 47 K. In another class of boron carbides, the BC$_7$ was predicted as a candidate structure under high pressure using particle swarm optimization (PSO) methodology. The BC$_7$ compound was the stable composition in the diamond-like I4/m2 structure, and also exhibited to be a super-hard material with the H$_v$ as 75.2 GPa. In addition, the effect of temperature has been presented as an influence for structural phase transformation of boron carbides such as BC$_{1.6}$ and BC$_3$, while the phase diagram boundaries of the boron carbides are still incomplete. Keeping all these carbon-rich in mind, another class of carbides, the BC$_7$ phase predicted as a candidate structure under high pressure using particle swarm optimization (PSO) methodology. Predictions of BC$_7$ revealed that the most stable structure is the diamond-like P4/m2 structure, and also exhibits superhard materials with the Vickers hardness of 75.2 GPa. They suggested that the diamond-like P4/m2 structure can be thermodynamically stable at ambient high pressure (100 GPa). It is known that boron carbides are the most popular materials for experimental and theoretical investigations, in fact, the effect of temperature has an influence for structural phase transformation of boron carbides, such as BC$_{1.6}$ and BC$_3$.

Recently, the phase diagram of B-C system has been investigated from ambient to high pressure and under temperature effect. The report showed that the effect of temperature is an important role for thermodynamically stable structure as well. In this work, the class of BC$_2$ phase is a point of interest for finding phase diagram with quasi-harmonics approximation (QHA), which can calculate thermodynamics properties also. Therefore, the main attention is to investigate the phase diagram of BC$_2$ and the structural searching analysis. The perspective of theoretical inspection displays a thermodynamically stable phase via the QHA calculation. The presence of route to high-Tc superconductivity via decomposition of binary diamond-like BC$_7$ compound is described through the Allen–Dynes equation.

### Computational details

The structure searching of the BC$_7$ was performed by the Universal Structure Predictor: Evolutionary Xtallography (USPEX) code combined with the Vienna ab initio simulation package (VASP) code. In all subsequent generations, the random symmetric algorithm, which consisted of 40% heredity, 20% random symmetric, 20% softmutation, and 20% transmutation operators in the pressure range from 0 to 300 GPa with structures containing up to 4 formula units. All of the DFT calculations in this work used the generalized gradient approximation of the Perdew–Burke–Ernzerhof (GGA–PBE) functional for the exchange-correlation functional. We employed the projector augmented wave (PAW) method, as implemented in the VASP code. The PAW potentials were applied with a plane wave basis set up to a cutoff energy of 700 eV and a $10 \times 10 \times 4$ k-point mesh for the diamond-like P4/m2 structure, which was generated by the Monkhorst–Pack (MP) method. The pseudocore radii of C and B are 1.1 Bohr and 1.1 Bohr, respectively, which are small enough that the overlap of spheres will not occur under applied pressure. All of the structural parameters were fully relaxed by using the Methfessel–Paxton smearing method and the conjugate gradient scheme. All considered structures were relaxed at each pressure until the Hellman–Feynman forces became less than $10^{-3}$ eV/Å. The phonon calculation was calculated using the ab initio lattice dynamics with the linear response method as implemented in the VASP code together with the PHONOPY package, which is an important role for investigation of the phase stability in metallic systems. The cutoff energy and k-point set for the phonon linear response calculation were used as 700 eV and $10 \times 10 \times 4$ for a $3 \times 3 \times 2$ supercell (144 atoms) in the diamond-like P4/m2 structure at 250 GPa. We calculated elastic constants for the diamond-like P4/m2 structure, as implemented in the CAmbridge Serial Total Energy Package (CASTEP) code. In the superconducting phase, we calculated the electron–phonon coupling (EPC) within the density functional perturbation theory via Quantum Espresso (QE) package. The PAW potentials were employed in QE. The plane-wave energy cutoff of 60 Ry was used. The Brillouin zone (BZ) integrations in the electronic and phonon calculations were performed using the MP meshes. The EPC matrix elements were computed in the first BZ on $4 \times 4 \times 2$ q-meshes using individual EPC matrices obtained with a $24 \times 24 \times 16$ k-points mesh. The Allen–Dynes equation was used with the effective Coulomb pseudopotential parameter, $\mu^* = 0.10$ (0.13) as follows;

$$T_c = \frac{\alpha_{\log}}{1.2} \exp \left[ - \frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right],$$

where $\alpha_{\log}$ is the logarithmic average of the spectral function, and $\lambda$ is the total electron–phonon coupling strength. We found that $\lambda$ value are less than 1.5 in most of our work, thus this form of Allen–Dynes equation is quite sufficient.

### Results and discussion

To investigate the structural formation of binary diamond-like BC$_7$ compound, we present the thermodynamically stable structures of B and B-doped diamond in Fig. 1a,b. Structural phase transitions of B under high pressure are analyzed. The $\alpha$-B structure transforms to the $\gamma$-B structure at 26 GPa, and then it transforms to the $\alpha$-Ga-type structure at 98 GPa. The calculation displayed that the $\alpha$-Ga-type structure is the most stable structure (Fig. 1a). It is induced that the direct transformation from graphite to diamond structure at 15 GPa. The diamond structure is the most stable structure and its stable structure can be used for identifying BC$_7$ structure. A
predicted structure can be obtained from USPEX code. It is found that the decomposition of $\alpha$-Ga-type+$\diamond$ transforms to the diamond-like $P\bar{4}m2$. This is shown that the diamond-like $P\bar{4}m2$ structure can be formed above 244 GPa, as seen in Fig. 1b. To investigate a formation of the diamond-like $P\bar{4}m2$ structure in BC7, it is focused on decomposition of B+C above 100 GPa. Convex hull of the B-C system is analyzed at 250 GPa which is the region of stability in the $P\bar{4}m2$ structure and the interesting pressure for $T_c$ calculation (Fig. 2a). The observable compositions of $B_{13}C_2$, $B_4C$, $BC_3$, $BC_5$ and BC7 are compared the formation enthalpy, which can determine the global minimum of structural stabilities in that pressure. The formation enthalpy ($H_f$) can be calculated as follows:

$$H_f = \frac{H_{B_{13}C_2} - (XH_B + YH_C)}{X + Y},$$

where $H_i$ represents the enthalpy of the $i$th compounds in solid form, $X$ and $Y$ are positive numbers. By using the equation (2), the BC7 composition presents the minimum of formation enthalpy in the B-C system at 250 GPa. According to Fig. 2a, we also compute the phonon of the diamond-like $P\bar{4}m2$ structure at 250 GPa, which presents dynamically stable as well (Fig. 2b). All lattice vibration modes are positive. $\Gamma$-point is center of the Brillouin zone (BZ). The boundaries of BZ are given by planes related to points on the reciprocal lattice. The $Z$ point is center of a face of the BZ, while the A point is edge of the BZ. Therefore, the path of $ZA$ mainly represents the transverse acoustic (TA) and longitudinal acoustic (LA) phonons from the lattice vibration. The TA phonons (14–28 THz) are lower frequencies than the LA phonons (30–53 THz). These phonons correspond to shear sound waves for TA, and compressional sound waves for LA. In the diamond-like and zincblende structures\cite{27,28}, it was suggested that the flattening of the TA phonon dispersion near the BZ edge can be explained with introducing long-range interatomic interactions, while the feature of TA and LA phonons in the $ZA$ path exhibits nature of covalent bonds in this crystal. This effect is related to the oscillatory behavior in the phonon dispersion curves.

Figure 1. (a) The enthalpies-pressure relation of boron and (b) the enthalpies-pressure relation of BC7.

Figure 2. (a) Formation enthalpy of BC7 presented in convex hull at 250 GPa and (b) the phonon dispersion and the phonon density of states of the diamond-like $P\bar{4}m2$ at 250 GPa.
in cubic-3C silicon carbide system which gave high energy values of vibrational energies and chemical bonds, when compared with other systems.

In addition, we construct a pressure–temperature (P–T) phase diagram to explore the diamond-like $P\bar{4}m2$ structure in BC$_7$ under temperature effect. The diamond-like $P\bar{4}m2$ is stable within the increasing of pressure and temperature monotonically (Fig. 3a). Figure 3b shows the crystal structure of the diamond-like $P\bar{4}m2$ structure.

The electronic band structure indicated the most significant result in this present study that the diamond-like $P\bar{4}m2$ structure is the metallic structure, in Fig. 4a. The remarkable solution displayed the flat band along the $Z \rightarrow R \rightarrow X \rightarrow \Gamma$-point near Fermi level. Likewise, SH$_3$, YH$_{10}$, and LaH$_{10}$, these flat band exhibited high-$T_c$ superconductivity.$^{29-32}$ One of characteristic features to determine the high-$T_c$ compounds was consulted that it depends on the Van Hove singularities (VHS) around the Fermi level in the density of states.$^6$ The VHS around
They presented that the high-\(T_c\) superconductivity in the \(\text{H}_2\text{Se}\) compound\(^8\), the Fermi level was introduced for characteristic feature of the high-\(T_c\) superconductivity in the \(\text{H}_2\text{S}\) compound\(^8\). The \(\text{H}_2\text{S}\) is much higher than that of \(\text{H}_2\text{Se}\), which the VHS is absent in \(\text{H}_2\text{Se}\) system.

In Fig. 4c, Fermi surface (FS) shows an occupied electron on a surface in reciprocal space, which was derived from the electronic band structure. We found that the FS displayed the large sheet along the \(Z\) direction (Fig. 4c), and corresponds to the band structure and density of state (Fig. 4a,b). From the electronic band structure and the FS viewpoint, it is worth noting that \(\text{BC}_7\) is possible to discover a high-\(T_c\) as well.

We also compute a characteristic of bonding in the diamond-like \(P4m2\) structure using the electronic band structure. We investigated the chemical bonding and the existence of resonance structure of \(\text{BC}_7\) by Voigt–Reuss–Hill (VRH) method\(^{39,40}\), as shown in the Table 1. The calculated elastic constants \((\epsilon)\) of \(\text{BC}_7\) and \(\text{H}_2\text{S}\) compound\(^6\). The calculated elastic constants \((\epsilon)\) of the diamond-like \(P4m2\) structure using the electron localization function (ELF) method\(^{33}\). The ELF displayed the tendency of an accumulated electron, with respect to a uniform electron gas of the same density. The \(P4m2\) plane presents the contour plot of ELF and bonding at 250 GPa, which is a strong bonding due to an electron localization between first NN B–C is 1.449 Å(Fig. 5a).

The coupled frequencies of B and C atoms in diamond-like structure are bonded to their neighbors through the hybridization of electronic states. The \(\text{C}\)-rich in the \(\text{BC}_7\) system has a hole on the B sites, due to having the lower valence electrons of B. The superposition of the orbitals from B and C is expected to induce the electron–phonon coupling constant. The coupling electronic states could induce a resonating valence-bond superconducting state. The coupled frequencies of B and C atoms in \(\text{BC}_7\) obtained from accumulation of electrons between B and C atoms, relating to the systems of strong covalent bonding in \(\text{H}_2\text{Se}\) and \(\text{H}_2\text{O}\)\(^{38}\).

We also calculate bulk modulus (B) and shear modulus (G), which can be obtained from elastic constants \((C_{ij})\) by Voigt–Reuss–Hill (VRH) method\(^{19,40}\), as shown in the Table 1. The calculated \(C_{ij}\) values show all positive, and satisfy with the Born stability criteria\(^{41}\), indicating the mechanical stability in the diamond-like \(P4m2\) structure at 250 GPa. The remarkable result of the \(\text{BC}_7\) conforms the structural stability by phonon dispersion result. By calculated from the VRH method, it is obtained that B is 1157 GPa, and G is 649 GPa. In addition, Tian et al.\(^{42}\) suggested that the positive value of Vickers hardness \((H_v)\) for an interesting material can be evaluated from B and G as follows:

\[
H_v = 0.92 \left( \frac{G}{B} \right)^{1.137} G^{-0.708}, \tag{3}
\]

The spectral function \(\alpha^2F(\omega)\) of the diamond-like \(P4m2\) structure is shown in Fig. 5b, the \(\alpha^2F(\omega)\) referred the electron–phonon coupling (EPC) between an initial state \(k_F\) and all other states on \(k_F\). The calculated \(\alpha^2F(\omega)\) of B and C atoms contributed to the EPC. We investigated \(T_c\) of the diamond-like \(P4m2\) structure using the Allen–Dynes modified McMillan equation\(^{24}\). We found that \(\lambda = 1.27, \omega_{\log} = 1498\ K, \mu = 0.10–0.13,\) and

| \(\text{BC}_7\) | \(P\) (GPa) | \(C_{11}\) | \(C_{12}\) | \(C_{13}\) | \(C_{16}\) | \(C_{33}\) | \(C_{44}\) | \(C_{66}\) | \(B\) | \(G\) | \(H_v\) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| \(P4m2\) | 250 | 2079 | 473 | 871 | 0 | 1839 | 900 | 388 | 1157 | 649 | 46 |
Table 2. The calculated parameters and $T_c$ of $\text{BC}_7$, with solving the Allen–Dynes equations with $\mu^* = 0.10$ (0.13). aReference36. bReference9. cReference43. dReference44. eThis work.

| Metal Carbides | Pressure (GPa) | $\lambda$ | $\omega_{\text{eg}}$ (K) | $T_c$ (K) |
|---------------|---------------|-----------|--------------------------|----------|
| $^{a}\text{XeC}_2$ | 200 | 0.38 | 622 | 38 |
| $^{b}\text{BC}_5$ | 0 | | 810 | 47 |
| $^{c}\text{NaC}_6$ | 0 | 2.92 | | 127 (116) |
| $^{d}\text{AlC}_6$ | 0 | | | $\sim$ 100 |
| $^{e}\text{ClC}_6$ | 0 | | | $\sim$ 40 |
| $^{f}\text{NaC}_5$ | 25–75 | | | $> 100$ |
| $^{g}\text{AlC}_5$ | 25–175 | | | $> 100$ |
| $^{h}\text{BC}_7$ | 250 | 1.27 | 1498 | 164 (154) |

$T_c$ is 164–154 K at 250 GPa. The remarkable solutions manifested that the the diamond-like $P4m2$ structure is the high-$T_c$. Likewise, binary carbon compounds with sodalite structure showed that NaC$_6$ is the high-$T_c$ among of them$^{43}$. Addition, we explored the $T_c$ with the increased C atom, as seen in Table 2. We found that C-rich can enhance $T_c$ at high pressure; however, we suggested that the high-$T_c$ for carbon-rich materials may depend on the characteristic of bonding. Our results showed that carbon-rich materials is one of important effect for making the high-$T_c$, from the strong bonding between B and C-atom (Supplementary Information S1).

Our calculation results showed that the phonon stability of BC$_7$ can be observed $\sim$250GPa. In practical experiment, it is possibly to be found superconductivity of BC$_7$ at the lower pressure in the experiment, which was found in the shift-down of transition pressure in another material. This was discussed in the LaH$_{10}$ system$^{46}$ that the quantum effects are important for the structural stabilities of solids with high electron–phonon coupling constants. The system could be destabilized by the large electron–phonon interaction, thus the reducing of critical pressure may be found in the synthesis.

### Conclusion

In this work, we investigate the decomposition of B–C, and employed the evolutionary algorithm for finding the stable structure at high pressures. The BC$_7$ in the diamond-like $P4m2$ structure exhibits as the minimum of formation enthalpy in the convex hull, and it displays structural stability at pressure above 244 GPa, and under temperature effect. The strong bonding is observed from the electron localization function. The delocalization of states at valence band maximum corresponds to the multicenter bonding of the B–C bonds, which achieves the high temperature superconductivity in BC$_7$. In addition, the electronics properties, such as the band structure, density of states, and the Fermi surface, are discussed as the important key to reach the high-$T_c$ superconductivity for C-rich system at high pressure.

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Competing interests
The authors declare no competing interests.

Additional information

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