

First-principles Study of Structural, Elastic, Anisotropic, and Thermodynamic Properties of R3-B₂C

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The structural, elastic, anisotropy, and thermodynamic properties of R3-B₂C were investigated using first-principles density functional calculations. The calculated equilibrium parameters are in good agreement with the available theoretical results. The elastic constants, elastic modulus, and elastic anisotropies of R3-B₂C were also determined in the pressure range of 0–100 GPa. The calculated elastic modulus indicates that R3-B₂C is a potential superhard material. The calculated elastic anisotropic factors suggest that R3-B₂C is elastically anisotropic. A band structure study shows that R3-B₂C is a direct semiconductor with band gap of 0.170 eV. Moreover, we predict the thermodynamic properties and obtain the relationships among the thermal expansion, temperature, and pressure, as well as the variations of the isothermal bulk modulus, Debye temperature, Grüneisen parameter, and heat capacity.

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I. INTRODUCTION

The search for new superhard materials is an important field of research in materials science and technology owing to their importance in fundamental science and technological applications. Diamond is the hardest material known, and it has found a wide variety of applications [1]. However, the applications of diamond are limited by its poor resistance to oxidation as well as reaction with ferrous metals. The demand for superhard materials in industrial usages has stimulated researches on the synthesis of alternative hard materials. It is known that superhard materials are usually made of light elements such as B, C, N, and O. Zinin *et al.* [2] synthesized a cubic BC₃ phase by direct transformation from graphitic phases at a pressure of 39 GPa and a temperature of 2200 K in a laser-heated diamond anvil cell. A diamond-like BC₅ phase has been synthesized at 24 GPa and a temperature of 2200

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K, which has a similar X-ray diffraction pattern to diamond [3]. Jay *et al.* [4] have found a carbon-rich phase of boron carbide designed from first-principles, thus demonstrating that boron carbide polymorphism can be extended in the carbon-rich domain with the (B11Cp)C-C structure. Its attractiveness comes from the expected improvement of the mechanical properties with respect to B_4C , and its bulk modulus is 231 GPa within GGA calculations. A superhard B_4C_4 [5] phase has been predicted using the particle swarm optimization (PSO) algorithm. The structural stability of B_4C_4 has been confirmed from the calculations of the elastic constants and phonon frequency. The analysis of the electron structure of the predicted B_4C_4 indicates that it is an insulator. The calculated theoretical Vickers hardness of B_4C_4 is 51.54 GPa, indicating that B_4C_4 is a potential superhard material. Lazar *et al.* [6] applied the density functional theory concept to investigate the mechanical properties of the diamond-like compound BC_5 . The calculated bulk modulus of 337 GPa agrees very well with the experimental value, which confirms that the calculated structure is the experimentally claimed one. And its Vickers hardness is estimated to be 83 GPa.

By using a developed particle swarm optimization algorithm on crystal structural prediction, Wang *et al.* [7] explored the possible crystal structures of a B-C system. A new phase of B_2C with structure group R3 was proposed by Wang *et al.* [7]. In the present work, we will investigate the equilibrium crystal structure, elastic properties, elastic anisotropy, and thermodynamic properties of R3- B_2C .

II. THEORETICAL METHOD

In the calculations, the structural optimization and property predictions of the BC polymorphs were performed using DFT [8, 9] with the generalized gradient approximation (GGA) parameterized by Perdew, Burke, and Ernzerhof (PBE) [10] and the local density approximation (LDA) [11, 12] as implemented in the Cambridge Serial Total Energy Package (CASTEP) code [13]. In the structure calculation, a plane-wave basis set with energy cut-off 640 eV was used. The Vanderbilt ultrasoft pseudopotential was used in present work. The k-point samplings with $10 \times 10 \times 10$ in the Brillouin zone were performed using the Monkhorst-Pack scheme [14]. The Broyden-Fletcher-Goldfarb-Shanno (BFGS) [15] minimization scheme was used in geometry optimization. The total energy convergence tests showed that convergence to within 1 meV/atom was achieved with the above calculation parameters. The self-consistent convergence of the total energy was 5×10^{-6} eV/atom; the maximum force on the atom was 0.01 eV/Å, the maximum ionic displacement was 5×10^{-4} Å and the maximum stress was 0.02 GPa.

It is well known that the anisotropy of elasticity has important implications in engineering science and crystal physics. So we go on investigating the anisotropy of R3- B_2C . The directional dependence of anisotropy was calculated using the program Elasticity Anisotropy Measures (ELAM) [16]. The stiffness tensor expresses the stress tensor in terms of the strain tensor: $\sigma_{ij} = C_{ijkl}\epsilon_{kl}$. The components of C_{ijkl} are the elastic stiffness constants. The compliance tensor is the inverse of the stiffness tensor and gives the strain tensor in

terms of the stress tensor: $\varepsilon_{ij} = S_{ijkl}\sigma_{kl}$. The components of S_{ijkl} are the elastic compliance constants. Young's modulus is defined as the ratio of normal stress to linear normal strain (both in the direction of applied load). The shear modulus is defined as the ratio of shear stress to linear shear strain. Poisson's ratio is defined as the ratio of transverse strain (normal to the applied load), to axial strain (in the direction of the applied load).

A fourth order tensor transforms in a new basis set following the rule $S'_{\alpha\beta\gamma\delta} = r_{\alpha i}r_{\alpha j}r_{\alpha k}r_{\alpha l}S_{ijkl}$, where Einstein's summation rule is adopted and where $r_{\alpha i}$ are the components of the rotation matrix (or direction cosines). The transformation can be substantially simplified for the calculation of a specific modulus. The uniaxial stress can be represented as a unit vector, and advantageously described by two angles (θ, ϕ) ; we choose it to be the first unit vector in the new basis set a . The determination of some elastic properties (shear modulus, Poisson's ratio) requires another unit vector, b , perpendicular to the unit vector a and characterized by the angle χ . It is fully characterized by the angles θ $(0, \pi)$, ϕ $(0, 2\pi)$, and χ $(0, 2\pi)$. The coordinates of the two vectors are [16]

$$a = \begin{pmatrix} \sin \theta \cos \varphi \\ \sin \theta \sin \varphi \\ \cos \theta \end{pmatrix}, \quad b = \begin{pmatrix} \cos \theta \cos \varphi \cos \chi - \sin \varphi \sin \chi \\ \cos \theta \sin \varphi \cos \chi + \cos \varphi \sin \chi \\ -\sin \theta \cos \chi \end{pmatrix}. \quad (1)$$

The Young's modulus can be obtained by using a purely normal stress in $\varepsilon_{ij} = S_{ijkl}\sigma_{kl}$ in its vector form, and it is given by $E^{-1}(\theta, \phi) = a_i a_j a_k a_l S_{ijkl}$.

Other properties depending on two directions (if perpendicular this corresponds to 3 angles) which makes them difficult to represent graphically. A convenient possibility is then to consider the minimum and maximum. For each θ and ϕ , the angle χ is scanned and the minimum and maximum values are recorded for this direction. The shear modulus is obtained by applying a pure shear stress in the vector form and results in $G^{-1}(\theta, \phi, \chi) = 4a_i b_j a_k b_l S_{ijkl}$. Poisson's ratio can be expressed as $\nu(\theta, \phi, \chi) = -a_i a_j b_k b_l S_{ijkl} / (a_i a_j a_k a_l S_{ijkl})$.

In order to obtain the thermodynamic properties of B₂C, the quasi-harmonic Debye model was used in this paper; it has been described in detail in Refs. [17–22]. Since this model is very computationally quick and easy, it has been successfully applied to predict the thermodynamic properties of some materials [23–25]. According to standard thermodynamics, if the system is held at a fixed T and suffers a constant and hydrostatic P , the equilibrium state is one that minimizes the availability or non-equilibrium Gibbs energy of the crystal phase [26]:

$$G^*(x; P, T) = E(x) + PV(x) + A_{\text{vib}}(x; T) \quad (2)$$

So the non-equilibrium Gibbs function $G^*(V; P, T)$ takes the form of

$$G^*(V; P, T) = E(V) + PV + A_{\text{vib}}(\Theta(V), T), \quad (3)$$

Here $E(V)$ is the total energy per unit cell for R3-B₂C; $\Theta(V)$ is the Debye temperature. In the next step, the Debye model of the phonon density of states will be used to calculate

the vibrational Helmholtz free energy A_{vib} , which can be expressed as [27–32]:

$$A_{\text{vib}}(\Theta(V) : T) = nKT \left[\frac{9}{8} \frac{\Theta}{T} + 3 \ln \left(1 - e^{-\Theta/T} \right) - D \left(\frac{\Theta}{T} \right) \right], \quad (4)$$

here $D(\Theta/T)$ represents the Debye integral. Assume that y is equal to Θ/T , so

$$D(y) = \frac{3}{y^3} \int_0^y \frac{x^3}{e^x - 1} dx, \quad (5)$$

In Equation (4), n is the number of atoms per formula unit and Θ is the Debye temperature, which is related to an average sound velocity, since in Debye's theory the vibrations of the solid are considered as elastic waves. Assuming an isotropic solid, with Poisson's ratio [33] Θ is expressed as [27]:

$$\Theta = \frac{h}{2\pi k} [6\pi^2 V^{1/2} n]^{1/3} f(\nu) \sqrt{\frac{B_s}{M}}, \quad (6)$$

where M is the molecular mass per formula unit; B_s is the adiabatic bulk modulus, the Poisson ratio ν is taken as 0.14 in our calculation; and $f(\nu)$ is given by [29, 30]:

$$f(\nu) = \left\{ 3 \left[2 \left(\frac{2}{3} \frac{1+\nu}{1-2\nu} \right)^{3/2} + \left(\frac{1}{3} \frac{1+\nu}{1-\nu} \right)^{3/2} \right]^{-1} \right\}^{1/3}, \quad (7)$$

Θ is thus a function of x through its dependence on V , B_S , and σ , and the latter can be considered as a constant for each solid to a good approximation. Therefore, the non-equilibrium Gibbs function $G^*(V; P, T)$ as a function of $(V; P, T)$ can be minimized with respect to volume V as follows:

$$\left(\frac{\partial G^*(V; P, T)}{\partial V} \right)_{P, T} = 0. \quad (8)$$

By solving Eq. (8), the isothermal bulk modulus B_T and other thermal properties, such as the heat capacity at constant volume C_v , the heat capacity at constant pressure C_p , and the thermal expansion α , are taken respectively as [17]:

$$B_T = -x^{-2} B_0 e^{3(B'_0 - 1)(1-x)/2} f(x), \quad (9)$$

$$x = \left(\frac{V}{V_0} \right)^{1/3}, \quad (10)$$

$$f(x) = x - 2 - \frac{3x(B'_0 - 1)(1-x)}{2}, \quad (11)$$

$$C_V = 3nk \left[4D \left(\frac{\Theta}{T} \right) - \frac{3\Theta/T}{e^{\Theta/T} - 1} \right], \quad (12)$$

$$C_P = C_V(1 + \alpha\gamma T), \quad (13)$$

$$\alpha = \frac{\gamma C_V}{B_T V}, \quad (14)$$

where $V_0 = V(0, T)$ is the zero-pressure equilibrium volume, B_0 is the zero-pressure bulk modulus, and B'_0 is the first pressure derivative. In addition, B_0 and B'_0 are the fitting parameters. And in Equations (12) and (13), C_V and C_P are the heat capacities, in equation (14) α is the thermal expansion and γ represents the Grüneisen parameter, it is expressed as $\gamma = -(d \ln \Theta(V) / d \ln V)$.

III. RESULTS AND DISCUSSION

III-1. Structural properties

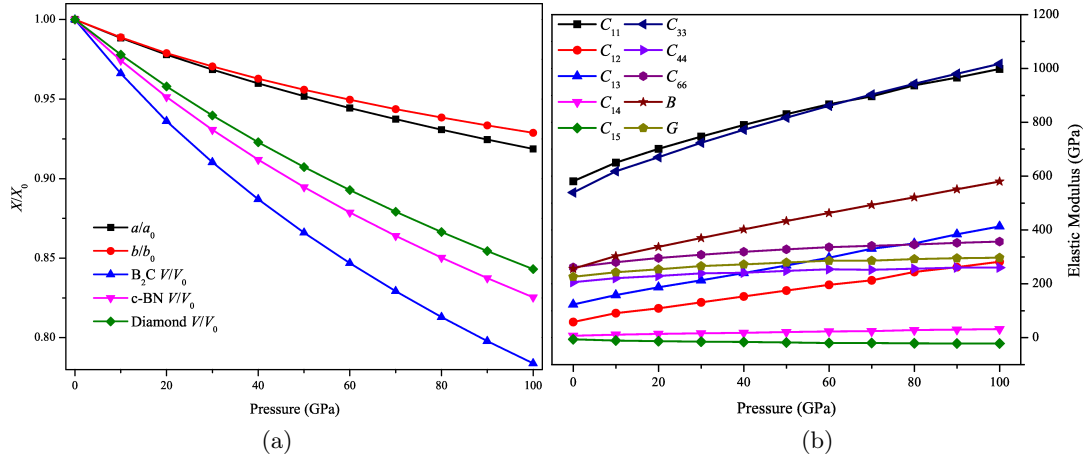
R3-B₂C has a trigonal symmetry that belongs to the R3 space group. The calculated equilibrium lattice parameters with the GGA and LDA methods for R3-B₂C, together with previous results, are listed in Table I. From Table I, it can be seen that our calculated lattice parameters for R3-B₂C are reasonable compared with previous studies [7]. It is clear that the predicted lattice constants and bond lengths with the LDA method are smaller than those with the GGA method, as in the usual cases. For R3-B₂C, there is no available experimental result. However, our predicted lattice parameters using the GGA and LDA methods agree well with the previously reported values of Wang *et al.* [7], which were calculated using the projector augmented wave (PAW) method. The predicted structural constants a and c deviate from the corresponding previous values [7] by 0.27% and 0.04%, respectively. In Fig. 1 (a), the pressure dependence of the equilibrium lattice parameters a/a_0 and c/c_0 are illustrated (where a_0 , and c_0 are the equilibrium conventional lattice constants at ambient pressure). For R3-B₂C, it can be easily seen that the compressibility along the c -axis is more difficult than that along the a -axis (b -axis). To compare the incompressibility of R3-B₂C, c-BN, and diamond under pressure, the volume compressions V/V_0 (where V_0 is the equilibrium primitive cell volume at ambient pressure) as a function of pressure are also plotted in Fig. 1 (a). With the applied pressure increasing from 0 to 100 GPa, the volume V/V_0 of R3-B₂C decreases by 21.6% in the GGA calculations, and the volume V/V_0 of diamond (c-BN) decreases by 15.7% (17.4%) in the GGA calculations, respectively. It is transparent that the incompressibility of R3-B₂C is smaller than that of diamond and c-BN.

III-2. Elastic properties and anisotropic properties

The elastic properties (including elastic constants, elastic modulus, etc.) give important information concerning the nature of the forces operating in solids. Particularly, they

TABLE I: Lattice constants a , c (in Å), and cell volume per formula unit V_0 (in Å³) for R3-B₂C.

Crystal	method	a	c	V
B ₂ C	GGA ^a	4.867	9.115	186.93
	GGA ^b	4.854	9.111	185.94
	LDA ^a	4.866	9.114	177.93

FIG. 1: (a) The lattice parameters a/a_0 and c/c_0 compression as functions of the pressure for R3-B₂C and the primitive cell volume V/V_0 for R3-B₂C, c-BN, and diamond. (b) Elastic constants of R3-B₂C as a function of pressure.

provide information about the stability and stiffness of materials. In this paper, we calculate the elastic constants and elastic modulus of R3-B₂C, together with previous results of BC₇, BC₅, B₄C₄, and B₄C, which are shown in Table II. The criteria for mechanical stability of the trigonal symmetry group are given by:

$$C_{ij} > 0, \quad i, j = 1 \sim 6, \quad (15)$$

$$C_{11} - C_{12} > 0, \quad (16)$$

$$C_{44}(C_{11} - C_{12}) - 2C_{14}^2 > 0, \quad (17)$$

$$C_{11}C_{44} - 2C_{15}^2 - C_{12}C_{44} - 2C_{14}^2 > 0, \quad (18)$$

$$C_{44}(C_{11}C_{33} - C_{13}^2) - C_{33}(C_{14}^2 + C_{15}^2) > 0, \quad (19)$$

$$C_{33}(C_{11} + C_{12}) - 2C_{13}^2 > 0, \quad (20)$$

$$C_{44}(C_{12} - C_{11}) + 2(C_{14}^2 + C_{15}^2) > 0. \quad (21)$$

The calculated results show that the R3-B₂C is mechanically stable under ambient conditions. From Table II, we note that the elastic constants of R3-B₂C are smaller than those of B₄C₄, BC₇, and BC₅, but slightly larger than that of B₄C. The elastic constants versus pressure for R3-B₂C are displayed in Fig. 1 (b). All the elastic constants C_{ij} (except for C_{15}) increase but with different rates under increased pressure. C_{33} of R3-B₂C increases faster than the others, and C_{14} grows the slowest. The B of R3-B₂C is the smallest in these boron-carbide compounds, so is the G . The Young's modulus E and Poisson's ratio ν are taken as: $E = 9BG/(3B + G)$, $\nu = (3B - 2G)/[2(3B + G)]$. From Table II, we note that the elastic modulus of R3-B₂C is smaller than the others in this paper. The Poisson ratio ν of R3-B₂C is 0.16 with the GGA, slightly larger than that of other boron-carbides. The Vickers hardness of R3-B₂C is 51 GPa [7]. That is to say, R3-B₂C is a potential superhard material.

TABLE II: Calculated elastic constant C_{ij} , bulk modulus B (GPa), shear modulus G (GPa), Young's modulus E (GPa), Poisson's ratio ν , and hardness of R3-B₂C, B₄C₄, B₄C, BC₇, and BC₅.

	method	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{33}	C_{44}	C_{66}	B	G	E	ν
B ₂ C	GGA ^a	581	58	123	7	-6	539	206	261	256	226	524	0.16
	LDA ^a	632	75	141	11	-10	597	219	279	286	241	564	0.17
	GGA ^b	603	66	131			564	245	269	270	273	613	0.12
B ₄ C ^c	GGA	491	88	92			534	204	192				
	LDA	512	100	105			561	208	197				
B ₄ C ^d	LDA	562	70	124			536		213				
BC ₇ ^e	GGA	769	196					498			399	891	0.12
	LDA	807	222					537			421	945	0.12
BC ₅ ^e	GGA	865	177	64			1086	382			386	865	0.12
	LDA	931	194	69			1164	401			410	922	0.13
B ₄ C ₄ ^f	GGA	662	185	165			560	307	373	322	309		

^a this work

^b Ref. [7]

^c Ref. [4]

^d Ref. [35]

^e Ref. [36]

^f Ref. [37]

Pugh [34] proposed the ratio of B/G as an indication of ductile or brittle character. The bulk modulus B represents the resistance to fracture, while the shear modulus G represents the resistance to plastic deformation. A higher B/G ratio is associated with ductility, whereas a lower value corresponds to a brittle nature. If $B/G > 1.75$, the material

behaves in a ductile manner, otherwise the material behaves in a brittle manner. In the case of R3-B₂C at 0 K and 0 GPa, our calculated value of B/G is 1.13 with the GGA calculation, which suggests that R3-B₂C is brittle, but B/G is 1.95 at 100 GPa. When the applied pressure changes from 0 GPa to 100 GPa, the ratio B/G value changes from 1.13 to 1.95, which is to say that R3-B₂C becomes ductile with increasing pressure.

Using the above formulas, the calculated Poisson's ratio, shear modulus, and Young's modulus along different directions, as well as the projections in different planes, were shown in Fig. 2 and Fig. 3. We first focus on Poisson's ratio, Fig. 2 (a) displays the 2D representation of Poisson's ratio in the xy , xz , and yz planes for R3-B₂C, respectively. The black represents the maximum value and red represents the minimum value. We found that $0.05 \leq \nu \leq 0.23$, showing that ν remains positive (no negative Poisson's ratio). In order to quantify the anisotropy, we calculated the shear modulus for all possible directions of shear strain, the 2D representation of the shear modulus in the xy , xz , and yz planes for R3-B₂C was shown in Fig. 2 (b). The black represents the maximum and red represents the minimum. We observed that the shear modulus varies between 205 and 262 GPa, and the average value of all directions is 221 GPa, which value is close to the castep value (256 GPa).

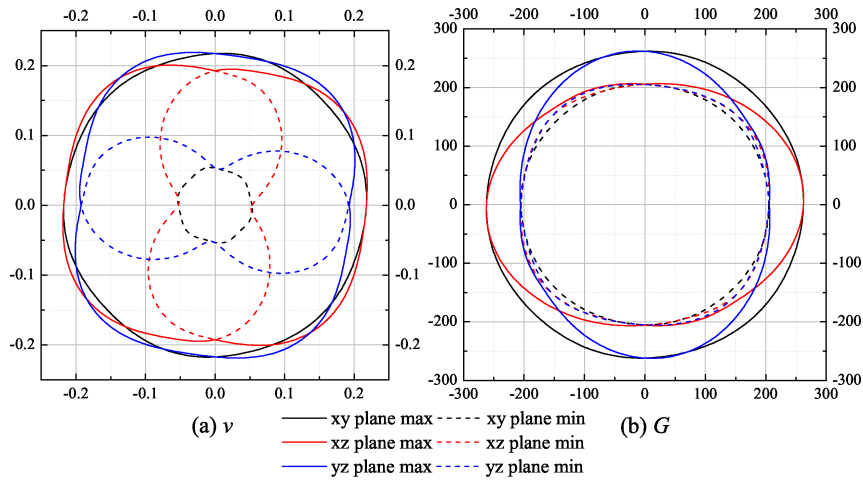


FIG. 2: 2D representation of Poisson's ratio (a) in the xy plane, xz plane, and yz plane for R3-B₂C. 2D representation of the shear modulus (b) in the xy plane, xz plane, and yz plane for R3-B₂C.

Finally, we focus on the Young's modulus, for which is plotted the directional dependence of the Young's modulus at different pressure, the xy , xz , and yz planes for R3-B₂C in Fig. 3 (a), (b), (c), and (d), respectively. It is clear that the Young's modulus for this material is quite anisotropic, with a minimal value of $E_{\min} = 490$ GPa and a maximum of $E_{\max} = 555$ GPa, the average value of all directions is 513 GPa, and the ratio $E_{\max}/E_{\min} = 1.13$. The Young's modulus for R3-B₂C has a minimal value of $E_{\min} = 617$ (660) GPa and a maximum value of $E_{\max} = 753$ (850) GPa, the average value of all directions is 677 (746) GPa, the ratio $E_{\max}/E_{\min} = 1.22$ (1.29) at 50 (100) GPa, respectively.

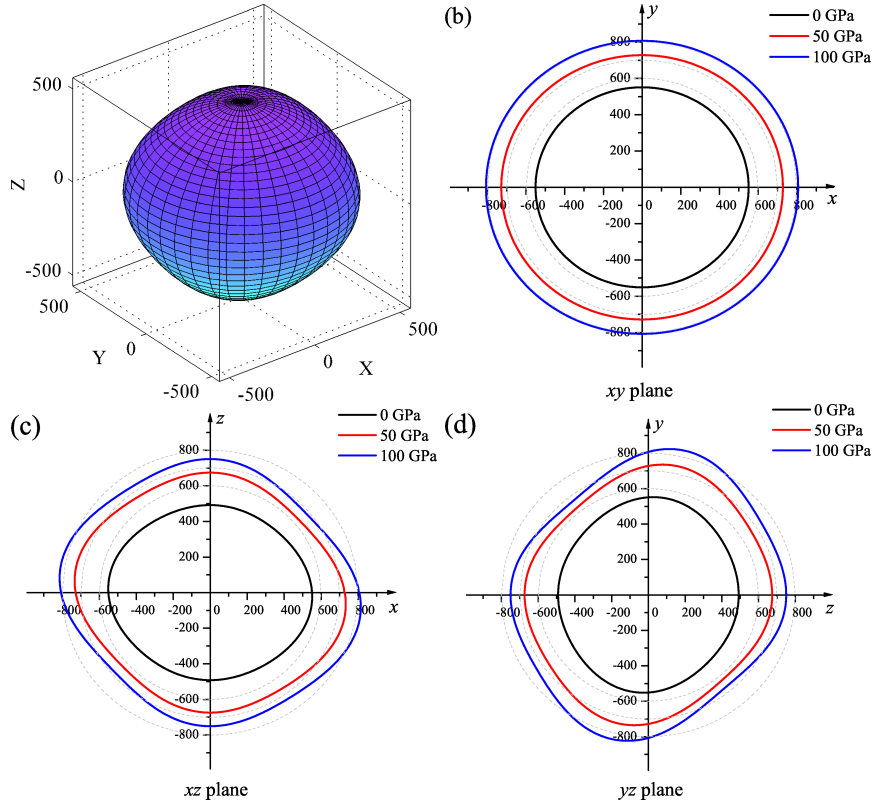


FIG. 3: The directional dependence of the Young's modulus for R3-B₂C (a), 2D representation of Poisson's ratio in the xy plane (b), xz plane (c), and yz plane (d).

So R3-B₂C exhibits a large anisotropy in its Poisson's ratio, shear modulus, and Young's modulus.

III-3. Electronic Properties

The calculated band structures and DOS of R3-B₂C at 0 GPa and 60 GPa are plotted in Fig. 4. The dashed line represents the Fermi level. For R3-B₂C, both the valence band maximum (VBM) and the conduction band minimum (CBM) are at the Γ point, indicating that R3-B₂C is a direct semiconductor with band gap of 0.17 eV. With pressure increasing, R3-B₂C turns into a conductor at 60 GPa. It is known that the calculated band gap with the DFT is usually underestimated by 30–50%, so the true band gap must be larger than the calculated results. The main features of the DOS for R3-B₂C at 0 GPa can be summarized as follows: (i) the peak present in the conduction band DOS (0 to 7.5 eV) of the DOS is mainly due to contributions of the p electrons of B, the contribution of the C atom is very small; (ii) the states from -12.5 eV to the Fermi energy (0 eV) mainly originate from the C- p orbital with less contributions of B- p , the contribution of the C atom s orbital and B atom s orbital are very small. (iii) The peak present in the energy part (-12.5 to -20 eV)

of the DOS is mainly due to contributions of the s electrons of the C atom, the contribution of the C atom p orbital is the smallest. The main features of the DOS for R3-B₂C at 60 GPa are the same as what was analyzed above.

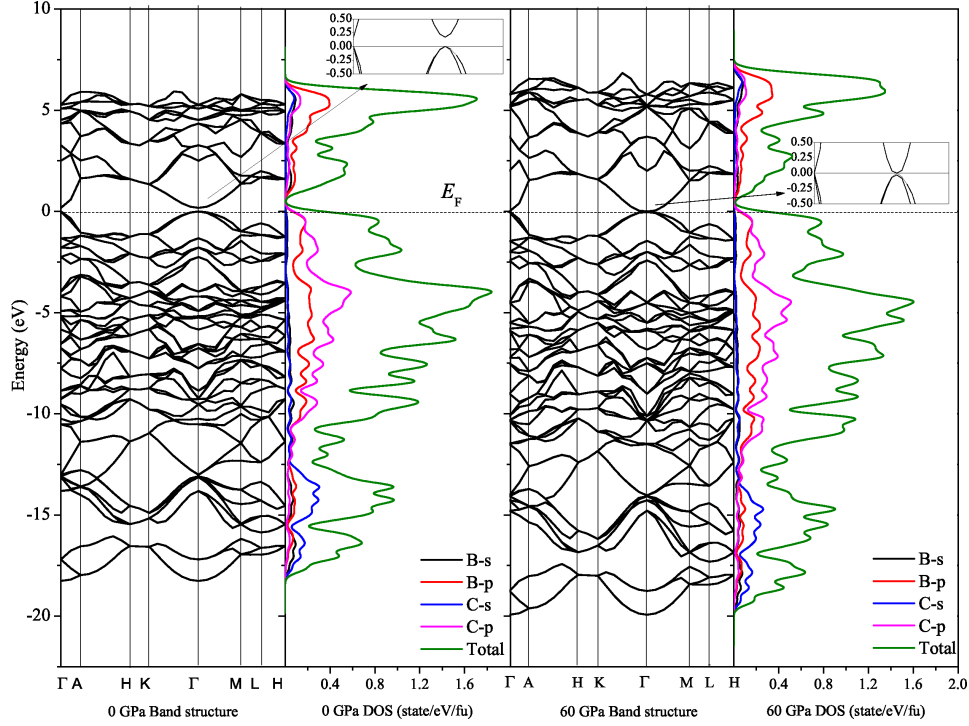


FIG. 4: Electronic band structure, density of state for the R3-B₂C at 0 GPa and 60 GPa.

III-4. Thermodynamic properties

The isothermal bulk modulus B_S of R3-B₂C as a function of pressure and temperature was shown in Fig. 5 (a). Correspondingly, in Fig. 5 (a), when $T < 400$ K the B_S of R3-B₂C has little change; when $T > 400$ K the B_S changes obviously as T increases. From Fig. 5 (a) it is found that the effect of temperature on the B_S is not as significant as that of pressure in our calculated pressure and temperature ranges. The thermal expansion α with pressures and temperatures for R3-B₂C are shown in Fig. 5 (b). From Fig. 5 (b) it can be seen that as the pressure increases the thermal expansion coefficient α decreases. And the higher the temperature is, the faster the thermal expansion coefficient α reduces. It is found that the temperature dependence of α is very small at high temperature and high pressure. As pressure increases, α decreases rapidly at high temperature, and the effects of temperature become less and less pronounced. The effects of pressure on α are small at low temperatures; the effects are increasingly obvious as the temperature increases. This is an indication of the inadequacy of the quasi-harmonic approximation at elevated temperatures and pressures.

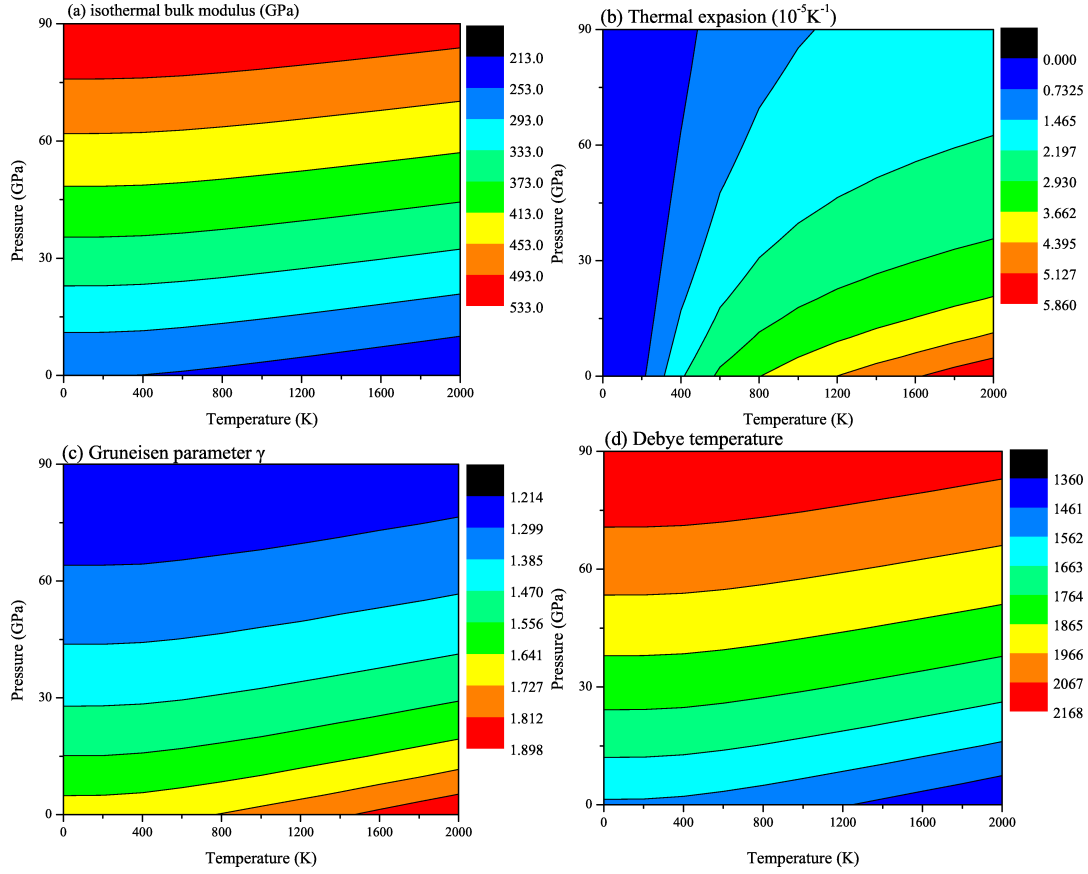


FIG. 5: Two-dimensional contour plots of the isothermal bulk modulus (a), the thermal expansion (b), the Grüneisen parameter(c), and the Debye temperature (d) versus pressure and temperature for R3-B₂C.

The Grüneisen parameter, which describes the alteration in a crystal lattices vibration frequency, can reasonably predict the anharmonic properties of a solid, such as the temperature dependence of phonon frequencies and lattice volume. Usually, the Grüneisen parameter is positive and lies in the range 1.5 ± 1.0 . The calculated relationships of the Grüneisen parameter γ on pressure and temperature are plotted in Fig. 5 (c). It is found that the Grüneisen parameter slightly increases with temperature at a given pressure, but decreases with a pressure change at a given temperature. At low temperature ($T < 800$ K), γ is constant, but it increases slightly linearly with temperature at high temperatures ($T > 800$ K). And from Fig. 5 (c), we can find that the effect of the pressure on the Grüneisen parameter is more significant than that of temperature. The calculated relationships of the Debye temperature Θ_D on the pressure and temperature are plotted in Fig. 5 (d). Θ_D is affected by both the pressure and temperature, and the effect of increased pressure on R3-B₂C is the same as decreased temperature. At a given temperature Θ_D increases quickly with increasing pressure. In a word, we can see that the Debye temperature

decreases with temperature at a certain pressure and increases with pressure at a certain temperature. And it is seen from Fig. 5 (d) that the effect of temperature on the Debye temperature is less significant than that of pressure.

Fig. 6 shows the two-dimensional contour plots of the dependence of the heat capacity on pressure and temperature. The difference between C_P and C_V is very small at low temperatures and low pressures. From Fig. 6, one can also see that the heat capacity (C_P and C_V) increases with the temperature at the same pressure and decreases with the pressure at the same temperature. The effects of the temperature on the heat capacity are much more significant than that of the pressure. It also shows that when $T < 1000$ K the heat capacity is sensitive to both temperature and pressure. At high temperature the calculated heat capacity is expected to converge to a constant $3N_A k_B \approx 74.8 \text{ Jmol}^{-1}\text{K}^{-1}$, according to the law of Dulong and Petit.

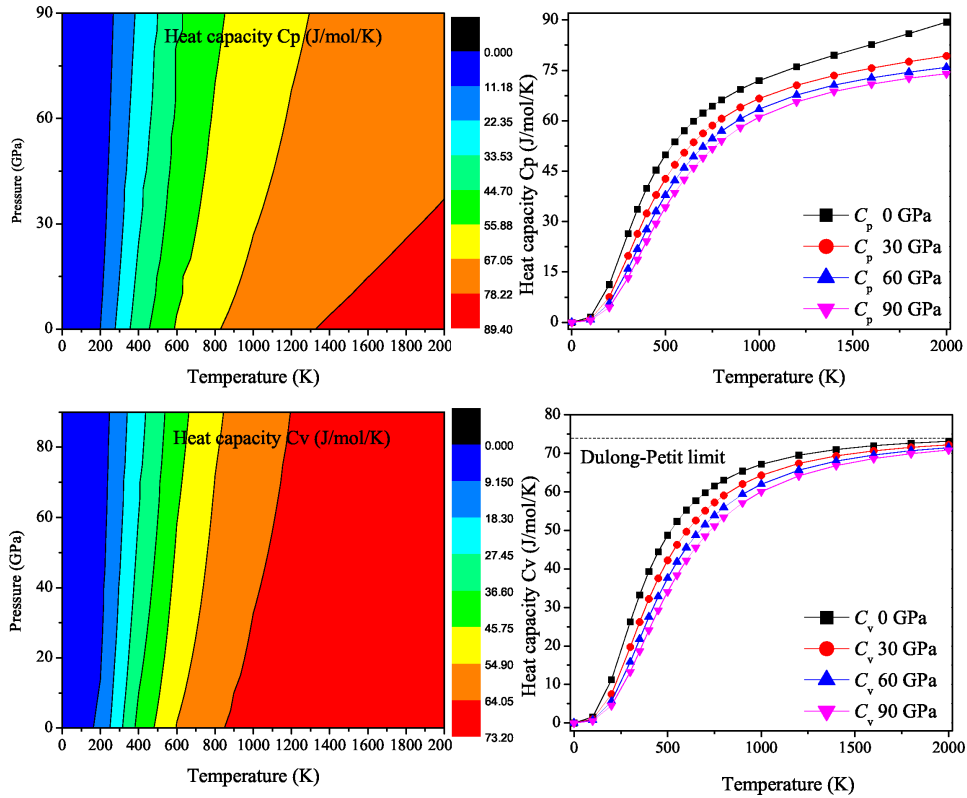


FIG. 6: Calculated specific pressure heat capacity C_P and volume heat capacity C_V as a function of pressure for R3-B₂C at different temperatures: C_P contours (a), C_P - T (b), C_V contours (c), and C_V - T (d).

IV. CONCLUSION

The structural properties, elastic properties, anisotropic properties, electronic properties, and thermodynamic properties of the newly predicted R3-B₂C under high pressure are investigated and analyzed in this paper by the first-principles calculations in combination with the quasi-harmonic Debye model. The obtained results of the ground state structural properties are in good agreement with previous data. The elastic constants under high pressure, elastic modulus under high pressure and high temperature, and the anisotropies of R3-B₂C are also calculated for the first time. With the elastic stability criteria, it is predicted that R3-B₂C is stable. Band structure study shows that R3-B₂C is a direct semiconductor with a band gap of 0.17 eV. Moreover, we predict in the present work the thermodynamic properties and obtain the relationships among the thermal expansion, temperature, and pressure, as well as the variations of the isothermal bulk modulus, Debye temperature, Grüneisen parameter, and heat capacity with pressure.

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