

First-principles study of elastic and thermodynamic properties of orthorhombic OsB₄ under high pressure

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ABSTRACT

The first-principles study on the elastic properties, elastic anisotropy and thermodynamic properties of the orthorhombic OsB₄ is reported using density functional theory method with the ultrasoft pseudo-potential scheme in the frame of the generalized gradient approximation. The calculated equilibrium parameters are in good agreement with the available theoretical data. A complete elastic tensor and crystal anisotropies of the ultra-incompressible OsB₄ are determined in the pressure range of 0–50 GPa. By the elastic stability criteria, it is predicted that the orthorhombic OsB₄ is stable below 50 GPa. By using the quasi-harmonic Debye model, the heat capacity, the coefficient of thermal expansion, and the Grüneisen parameter of OsB₄ are also successfully obtained in the present work.

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1. Introduction

Transition metal borides have attracted considerable attentions from both theoretical and experimental studies due to their chemically inert and extreme hardness as well as high thermal and electrical conductivity [1]. Recently, Kaner et al. have suggested that the introduction of light and covalent-bond-forming elements (B, C, N, and O) into the transition metal (TM) lattices with highly valence-electron density is expected to have profound influences on their chemical, mechanical, and electronic properties [2–4]. Based on this prospect, recent design of new intrinsically potential superhard materials ($H_v \geq 40$ GPa) has concentrated on light element TM compounds with high elastic moduli, in particular the 4d and 5d TM compounds [5–8]. Following the first synthesized ultra-incompressible material OsB₂ [3], extensive experimental and theoretical investigations have been carried out for other TM borides in view of their synthesis is more straightforward. Nowadays, some TM borides such as WB₄, ReB₂, WB₂, RhB_{1.1}, and IrB_{1.35} has been synthesized and were proposed to be superhard with

claimed hardness of >40 GPa [9–12]. Among these superhard TM borides, WB₄ has the largest B contents reported hitherto. WB₄ exhibits a unique three-dimensional boron covalent bonding network which consisted of in-plane honeycomb B sublattice and out-of-plane B₂ dimer. This is responsible for its high hardness [13].

Up to now, the structures of osmium borides with various stoichiometries (OsB, Os₂B₃, and OsB₂) have been synthesized and some related mechanical properties were also investigated. The obtained results indicated that they are all only hard materials. However, a promising material, osmium tetraboride (OsB₄) within WB₄-type structure, was proposed to be superhard with claimed hardness of 46.2 GPa but with a much low shear modulus of 52 GPa through first-principles calculations [13]. Recently, Zhang et al. [14] proposed an orthorhombic *Pmmn* structure for OsB₄, which is energetically much superior to the WB₄-type structure. This *Pmmn* structure consists of irregular OsB₁₀ dodecahedrons connected by edges and is stable against decompression into a mixture of Os and B at ambient pressure. The elastic and electronic properties of this orthorhombic structure are also explored at ambient conditions. However, to our knowledge, the investigations on its elastic and thermodynamic properties of the orthorhombic OsB₄ under pressures are least studied. Especially, the comprehensive analysis of elastic characteristics (elastic constants, bulk and shear modulus, etc.) under pressures can provide a deeper insight into the response of the crystal to external forces, and obviously play an important

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role in determining the strength and hardness of materials. Moreover it is essential for many practical applications, such as load deflection, thermoelastic stress, fracture toughness, anisotropic character of the bonding, and structural stability [15]. The physical properties under pressures and temperatures have important guidable significances to accelerate the synthesis of OsB₄ and other TM borides.

Here, the aim of this paper is to perform a theoretical investigation of structural, elastic and thermodynamic properties of OsB₄ within orthorhombic *Pmmn* structure under pressures up to 50 GPa by first-principles calculations. The elastic properties of orthorhombic OsB₄ under high pressure are investigated for the first time, from which the elastic anisotropy are also determined. In order to further investigate the OsB₄, the thermodynamic properties, such as the heat capacity, thermal expansion, Grüneisen parameters and so on are determined by the Debye model.

2. Computational methodology

2.1. Total energy electronic structure calculations

In the present work, density functional theory calculations are performed with plane-wave ultrasoft pseudopotential [16] using the generalized gradient approximation with the Perdew–Wang functional [17] as implemented in the CASTEP code [18]. The ionic cores are represented by ultrasoft pseudopotentials for B and Os atoms. The B: 2s²p¹ and Os: 4p⁶5d⁶6s² electrons are explicitly treated as valence electrons. The electronic wave functions are expanded in plane-wave basis set with cutoff energy of 540 eV, and the special points sampling integration over the Brillouin zone was employed by using the Monkhorst–Pack method with a grid of 0.03 Å⁻¹. The total energy was well converged within 1 meV/atom and this set of parameters assures the maximum force is 0.01 eV/Å, the maximum stress is 0.02 GPa.

2.2. Elastic properties

The elastic constants are defined by means of a Taylor expansion of the total energy, $E(V, \delta)$, for the system with respect to a small strain δ of the lattice primitive cell volume V . The energy of a strained system is expressed as follows [19]

$$E(V, \delta) = E(V_0, 0) + V_0 \left(\sum_i \tau_i \xi_i \delta_i + \frac{1}{2} C_{ij} \delta_i \xi_i \delta_j \xi_j \right), \quad (1)$$

where $E(V_0, 0)$ is the energy of the unstrained system with equilibrium volume V_0 , τ_i is an element in the stress tensor, and ξ_i is a factor to take care of Voigt index. It is known, there are nine independent components of the elastic tensor for the orthorhombic structure OsB₄, i.e. C_{11} , C_{12} , C_{13} , C_{22} , C_{23} , C_{33} , C_{44} , C_{55} , and C_{66} .

For the specific case of orthorhombic OsB₄ phase, the isotropic Reuss shear modulus G_R and the Voigt shear modulus G_V are [20–22]

$$G_R = \frac{15}{4(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{13} + S_{23}) + 3(S_{44} + S_{55} + S_{66})}, \quad (2)$$

$$G_V = \frac{(C_{11} + C_{22} + C_{33} - C_{12} - C_{13} - C_{23}) + 3(C_{44} + C_{55} + C_{66})}{15}, \quad (3)$$

and the isotropic Reuss bulk modulus B_R and the Voigt bulk modulus B_V are defined as

$$B_R = \frac{1}{(S_{11} + S_{22} + S_{33}) + 2(S_{12} + S_{13} + S_{23})}, \quad (4)$$

$$B_V = \frac{(C_{11} + C_{22} + C_{33}) + 2(C_{12} + C_{13} + C_{23})}{9}, \quad (5)$$

In Eqs. (2) and (4), the S_{ij} are elastic compliance constants. The arithmetic average of the Voigt and the Reuss bounds is called the Voigt–Reuss–Hill (VRH) average and is commonly used to estimate elastic moduli of polycrystals. Hence, The VRH averages for shear modulus (G) and bulk modulus (B) are $G = (G_R + G_V)/2$ and $B = (B_R + B_V)/2$. The Young's modulus, E , and Poisson's ratio, ν , are given by $E = (9BG)/(3B + G)$ and $\nu = (3B - 2G)/(6B + 2G)$.

The Debye temperature can be calculated from the elastic constants using the average sound velocity v_m , by the following equation [23]

$$\Theta_D = \frac{h}{k} \left[\frac{3n}{4\pi} \left(\frac{\rho N_A}{M} \right) \right]^{\frac{1}{3}} v_m, \quad (6)$$

where h is Planck's constant, k is Boltzmann's constant, N_A is Avogadro's number, n is the number of atoms per formula unit, M is the molecular mass per formula unit, and ρ is the density. The average sound velocity v_m is given by

$$v_m = \left[\frac{1}{3} \left(\frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]^{-\frac{1}{3}}, \quad (7)$$

where v_t and v_l are the transverse and longitudinal elastic wave velocity of the polycrystalline materials and are given by Navier's equation [24].

2.3. Thermodynamic properties

The investigations on the thermodynamic properties of the orthorhombic OsB₄ under high temperature and pressure are determined by the quasi-harmonic Debye model [25], in which the phononic effect is considered. However, it should be noted that the Debye model of phonon density of states is essentially a linear extrapolation of the sound speed of acoustic branches but not optical branches in order to get density states. In fact, the thermodynamic properties of the crystal can be obtained by treating the lattice vibrations as quantized (phonons). However, this model is very computationally quick and easy, which has been successfully applied to predict the thermodynamic properties of some materials [26–28]. The model has been described in detail in elsewhere [25], here, we give only a brief description as follows:

In the quasi-harmonic Debye model, the non-equilibrium Gibbs function $G^*(V; P, T)$ is taken in the form of

$$G^*(V; P, T) = E(V) + PV + A_{vib}(\Theta(V); T), \quad (8)$$

where $E(V)$ is the total energy, PV corresponds to the constant hydrostatic pressure condition, $\Theta(V)$ is the Debye temperature, and the vibrational contribution A_{vib} can be written as

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

here $D(\Theta/T)$ represents the Debye integral, n is the number of atoms per formula unit. For an isotropic solid, Θ is expressed as

$$\Theta = \hbar (6\pi^2 V^{1/2} n)^{1/3} f(\sigma) \sqrt{\frac{B_S}{k^2 M}}, \quad (10)$$

here V , M , n , and $f(\sigma)$ is the molar volume, molar mass, the number of atom per formula unit, and a scaling function that depend on Poisson's ratio of the isotropic solid, respectively. The B_S is the

adiabatic bulk modulus, which is equal to the isothermal bulk modulus B_T in the Debye model, leading to the following equation:

$$B_S = B_T = V \left(\frac{d^2 E}{dV^2} \right) \quad (11)$$

where E is the total energy of the crystal at 0 K.

Therefore, the non-equilibrium Gibbs function G^* as a function of $(V; P, T)$ can be minimized with respect to volume V as

$$\left(\frac{\partial G^*(V; P, T)}{\partial V} \right)_{P, T} = 0. \quad (12)$$

By solving Eq. (12), one can get the thermal equation of state (EOS) $V(P, T)$. The heat capacity C_V , C_P and the thermal expansion α are expressed as is given by

$$C_V = 3nk \left[4D(\Theta/T) - \frac{3\Theta/T}{e^{\Theta/T} - 1} \right], \quad (13)$$

$$C_P = C_V(1 + \alpha\gamma T), \quad (14)$$

$$\alpha = \frac{\gamma C_V}{B_T V}, \quad (15)$$

where γ is the Grüneisen parameter defined as

$$\gamma = - \frac{d \ln \Theta(V)}{d \ln V}. \quad (16)$$

3. Results and discussion

3.1. Structural properties

The crystal structure of the OsB_4 with $Pmmn$ space group is shown in Fig. 1. To calculate the equilibrium lattice constants and bulk modulus, the total energy is calculated by varying the volume for the $Pmmn$ - OsB_4 . The calculated E - V data are fitted to the third-order Birch–Murnaghan equation of state (EOS) [29], and the calculated equilibrium structure parameters, bulk modulus, and its pressure derivative are tabulated Table 1 together with other theoretical results for comparison. It is clear that our results agree well with the recent work from the Ref. 14 using PAW + GGA method, and the mismatch of lattice parameter is within 0.3%. Furthermore, the pressure dependence of the normalized parameters a/a_0 , b/b_0 , and c/c_0 as a function of pressure for the $Pmmn$ - OsB_4 is exhibited in Fig. 2, where a_0 , b_0 , and c_0 is its value at $T = 0$ K

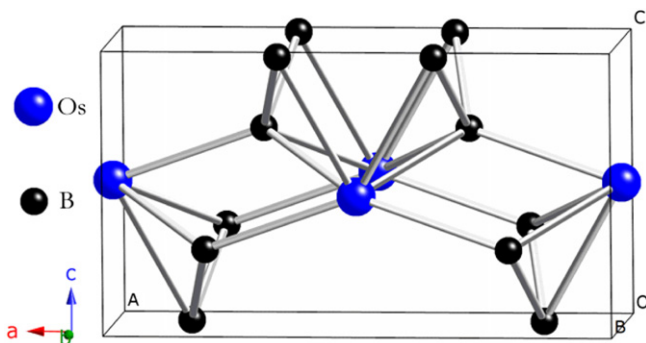


Fig. 1. Crystal structure of the $Pmmn$ - OsB_4 . The large and small spheres represent Os and B atoms, respectively.

Table 1

Calculated equilibrium lattice constants a_0 (Å), b_0 (Å), c_0 (Å), equilibrium volume V_0 (Å³/f.u.), EOS fitted bulk modulus B_0 (GPa), and its pressure derivative B_0' for the $Pmmn$ - OsB_4 at 0 K and 0 GPa.

Source	a_0	b_0	c_0	V_0	B_0	B_0'
This work	7.106	2.888	4.006	82.199	291	4.327
Theoretical ^a	7.119	2.896	4.015	82.776	293	4.119

^a Ref. [14].

and $P = 0$ GPa. By fitting the calculated data with least squares method, we obtained their relationships at the temperature of 0 K as the following relations:

$$\frac{a}{a_0} = 0.99985 - 0.8438 \times 10^{-3}P + 3.65293 \times 10^{-6}P^2 \quad (17)$$

$$\frac{b}{b_0} = 0.99991 - 1.34 \times 10^{-3}P + 5.86437 \times 10^{-6}P^2 \quad (18)$$

$$\frac{c}{c_0} = 0.99979 - 1.05 \times 10^{-3}P + 4.45302 \times 10^{-6}P^2 \quad (19)$$

It can be clear seen that the compression along the b -axis is the largest, and the smallest compression is exhibited along the a -axis. This indicates the clear elastic anisotropy of the $Pmmn$ - OsB_4 . The smallest compression along the a -axis can be attributed to the strong covalent B–B bonding in B layers and B–Os bonding in BOs_{10} dodecahedron along a -axis that has been clarified in our previous work [14].

3.2. Elastic properties

The nine independent elastic constants of the $Pmmn$ - OsB_4 using stress–strain relation derived from the method described above and listed in Table 2. It is shown that our results are in good agreement with data reported in Ref. [14] at 0 K and 0 GPa. Under high pressure, the elastic constants C_{ij} increase monotonically with pressure (Fig. 3). Relatively, the slopes for C_{44} and C_{66} are slower when one carefully checks the augmental interval of these elastic

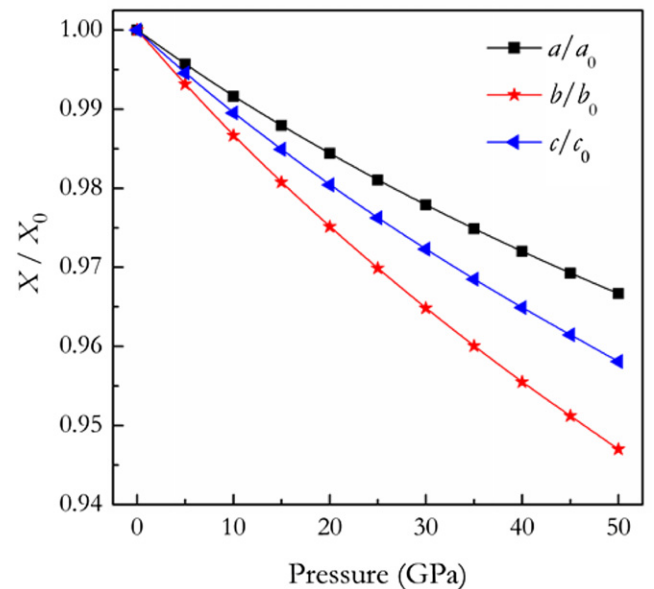


Fig. 2. The normalized parameters a/a_0 , b/b_0 , c/c_0 as a function of the pressure for the $Pmmn$ - OsB_4 .

constants. Moreover, these nine independent elastic constants C_{ij} of the $Pmmn$ -OsB₄ still satisfy the well-known Born stability criteria [30] up to 50 GPa. As shown in Table 2, the calculated elastic moduli also increase monotonically with pressure as expected. The ratio between the bulk and the shear modulus B/G are used to predict the brittle or ductile behavior of materials. According to the Pugh criterion [31], the ductile behavior is predicted when $B/G > 1.75$, otherwise the material behaves in a brittle manner. As shown in Table 2, the ratio of B/G in the $Pmmn$ -OsB₄ increases with pressure and reaches nearly 1.75 at 50 GPa. The results indicate that the $Pmmn$ -OsB₄ is prone to brittleness below 50 GPa, and is strongly prone to ductility above 50 GPa. Such a phenomenon was also found in other transition metal borides [33,34]. Debye temperature correlates with many physical properties of materials, such as specific heat, elastic constants, and melting temperature. The Debye temperatures are predicted deriving from elastic constants under pressures and the result at 0 GPa for the $Pmmn$ -OsB₄ is 781 K, which is close to that of the known intra-incompressible OsB₂ (780 K) [32].

The elastic anisotropy of crystals can exert great effects on the properties of physical mechanism, such as anisotropic plastic deformation, crack behavior, and elastic instability. Hence, it is important to calculate elastic anisotropy in order to improve its mechanical durability [19]. The shear anisotropic factors provide a measure of the degree of anisotropy in the bonding between atoms in different planes. The shear anisotropic factor for the {100} shear planes between the $\langle 011 \rangle$ and $\langle 010 \rangle$ direction is:

$$A_1 = \frac{4C_{44}}{C_{11} + C_{33} - 2C_{13}}. \quad (20)$$

For the {010} shear planes between the $\langle 101 \rangle$ and $\langle 001 \rangle$ directions it is

$$A_2 = \frac{4C_{55}}{C_{22} + C_{33} - 2C_{23}}, \quad (21)$$

and for the {001} shear planes between the $\langle 110 \rangle$ and $\langle 010 \rangle$ directions it is

$$A_3 = \frac{4C_{66}}{C_{11} + C_{22} - 2C_{12}}. \quad (22)$$

For an isotropic crystal the factors A_1 , A_2 , and A_3 must be 1.0, while any value smaller or greater than 1.0 is a measure of the degree of elastic anisotropy. Moreover, for the orthorhombic crystal, the elastic anisotropy which arises from the anisotropy of linear bulk modulus was also considered in addition to the shear anisotropy. The directional bulk modulus along different crystallographic axes can be defined as $B_i = i(dP/di)$ ($i = a, b$, and c) in Ref. [19].

Using the relations mentioned above, the parameters about elastic anisotropy are calculated and shown in Table 3. It is clear

Table 2

Calculated elastic constants C_{ij} , bulk modulus B , shear modulus G , Young's modulus E in unit of GPa of the $Pmmn$ -OsB₄. Also shown are B/G ratio and Debye temperature Θ under pressure.

P	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	B	G	E	B/G	Θ
0 ^a	612	576	630	152	349	178	128	245	51	294	218	524	1.34	
0	605	583	632	149	347	177	127	247	48	293	217	522	1.35	781
10	670	648	702	159	382	188	155	290	69	335	233	567	1.44	807
20	729	710	765	167	413	198	182	329	89	375	248	610	1.51	829
30	785	768	825	174	441	207	210	368	110	414	260	645	1.59	847
40	837	825	880	179	468	219	238	406	130	450	273	681	1.65	865
50	887	878	932	184	493	223	264	444	154	487	282	709	1.73	877

^a Ref. [14].

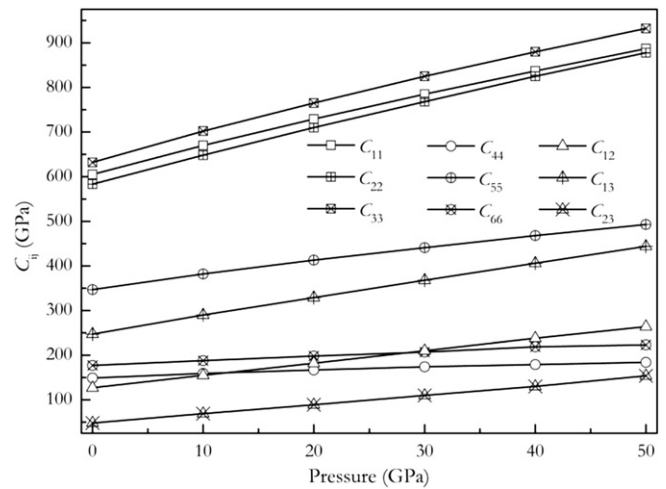


Fig. 3. The calculated pressure dependence of the elastic constants for the $Pmmn$ -OsB₄.

that the $Pmmn$ -OsB₄ is elastic anisotropic. The shear anisotropy results indicate that the elastic anisotropy for {010} shear planes between the $\langle 101 \rangle$ and $\langle 001 \rangle$ directions is close to that of the {001} shear planes between the $\langle 110 \rangle$ and $\langle 010 \rangle$ directions, but larger than that of the {100} shear planes between the $\langle 011 \rangle$ and $\langle 010 \rangle$ directions. The smaller shear anisotropy within {100} shear planes can be explained by the orderly manner of BOs₁₀ dodecahedrons along [001] directions. This result also demonstrates that the {010} and {001} shear planes are easier to be cleavage planes among these principal planes. Moreover, it can be seen that the A_1 remains nearly invariant on the whole, A_2 increases with increasing pressure, and A_3 decrease with increasing pressure. Meanwhile, it is interesting to note that the directional bulk modulus B_a along the a -axis is largest when compared to the B_b and B_c , which is in agreement with the pressure dependence of the normalized lattice parameters (see Fig. 2). However, this result is not consistent with the calculated elastic constants values of C_{11} and C_{33} (see Table 2). This differentia can be explained by the definition of the directional bulk modulus which is proportional to both lattice parameters and the pressure dependence of the lattice parameters. The lattice constant a is almost 1.8 times larger than c for the $Pmmn$ -OsB₄, although the elastic C_{33} is little larger than C_{11} .

An illustrative way of describing the elastic anisotropy is a three-dimensional surface representation showing the variation of elastic modulus with crystallographic direction. This directional dependence of the Young's modulus E for orthorhombic crystal is given by [19]:

$$\frac{1}{E} = l_1^4 S_{11} + l_2^4 S_{22} + l_3^4 S_{33} + 2l_1^2 l_2^2 S_{12} + 2l_1^2 l_3^2 S_{13} + 2l_2^2 l_3^2 S_{23} + l_1^2 l_2^2 S_{66} + l_1^2 l_3^2 S_{55} + l_2^2 l_3^2 S_{44} \quad (23)$$

where S_{ij} are the elastic compliance constants and l_1 , l_2 , and l_3 are the direction cosines. Fig. 4 illustrate the directional dependence of the $Pmmn$ -OsB₄ in the elastic modulus calculated using the

Table 3

Calculated anisotropy factors A_1 , A_2 , and A_3 and the directional bulk modulus B_a , B_b , B_c (in GPa) of the $Pmmn$ -OsB₄ under pressure.

P	B_a	B_b	B_c	A_1	A_2	A_3
0	1118.4	700.3	889.4	0.802	1.240	0.758
10	1284.2	798.3	1020.7	0.803	1.261	0.746
20	1436.6	892.8	1139.6	0.799	1.274	0.737
30	1588.9	984.4	1254.8	0.798	1.286	0.731
40	1742.2	1074.3	1362.3	0.791	1.296	0.739
50	1877.6	1161.2	1478.8	0.790	1.313	0.722

compliance constants computed from the present calculation. The projection of the Young's modulus along ab , ac , and bc planes are also shown in Fig. 4. It can be seen that Fig. 4(a) shows a large deviation from a spherical shape and hence one can conclude that the $Pmmn$ -OsB₄ exhibit a high degree of anisotropy. As expected, the $Pmmn$ -OsB₄ keeps its strong elastic anisotropy along different planes with the increasing pressure as shown in Fig. 4(b) and (c).

3.3. Thermodynamics properties

The thermodynamic properties of the $Pmmn$ -OsB₄ are determined in the temperature range from 0 K to 1800 K where the quasi-harmonic model remains fully valid, meanwhile, the pressure effect is studied in the range 0–50 GPa. The temperature-dependent behavior of the calculated constant pressure heat capacity C_p and constant volume heat capacity C_v at various pressures P are shown in Fig. 5. It clearly shows that the difference between C_p and C_v is very small at low temperatures (<400 K), meanwhile, the C_p and C_v increase rapidly with pressure that this is due to the anharmonic approximations of the Debye model. However, the anharmonic effect on C_v is suppressed at high temperatures, and the C_v approaches a constant value called as Dulong–Petit limit ($C_v(T) \sim 3R$ for mono atomic solids) and the C_p still increases monotonously with increments of the temperature. In addition, one can also see that both the C_p and C_v increase with the temperature at the given pressure and decrease with the pressure at the given temperature, the influences of the

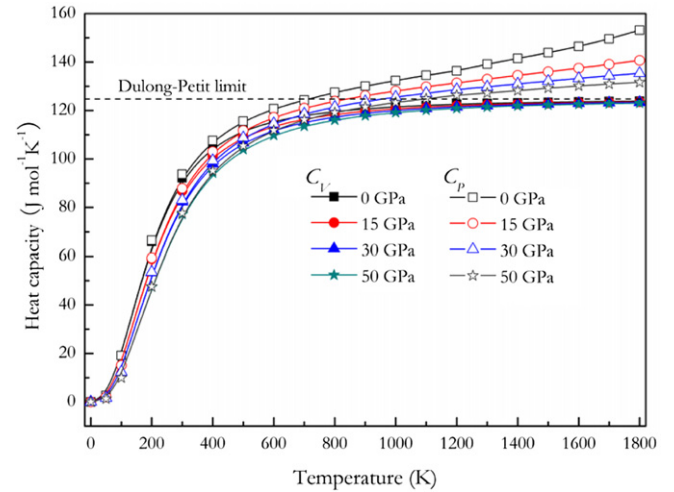


Fig. 5. Temperature dependence of the heat capacity at different pressures for the $Pmmn$ -OsB₄.

temperature on the heat capacity are much more significant than that of the pressure on them.

The pressures and temperatures' dependences of the thermal expansion coefficient α for the $Pmmn$ -OsB₄ are also illustrated in Fig. 6. It is shown that the expansion coefficient α increases sharply at low temperatures especially at 0 GPa and gradually reaches to

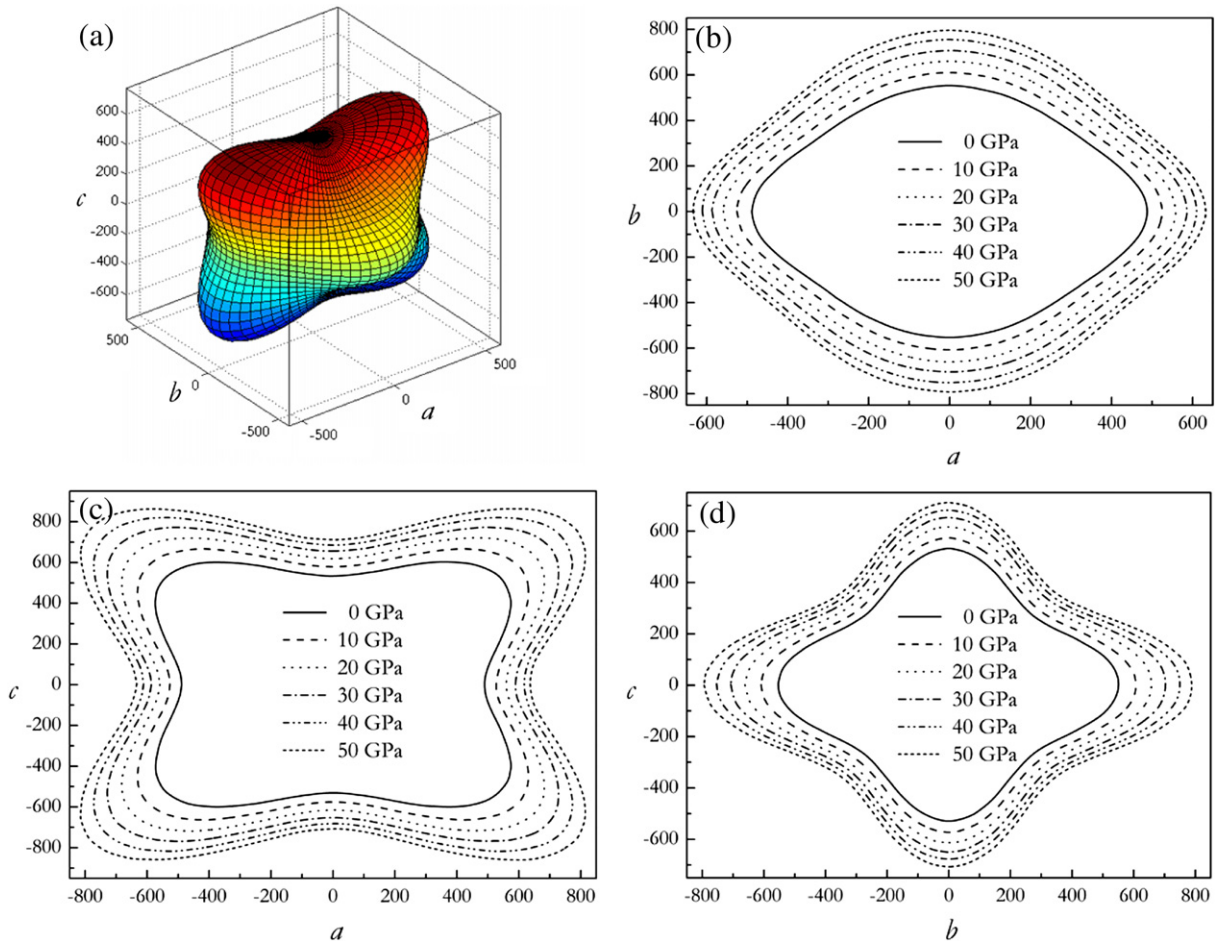


Fig. 4. Illustration of directional dependent Young's modulus of the $Pmmn$ -OsB₄ (a), and the projections of the directional dependent Young's modulus in different planes: ab plane (b), ac plane (c), and bc plane (d).

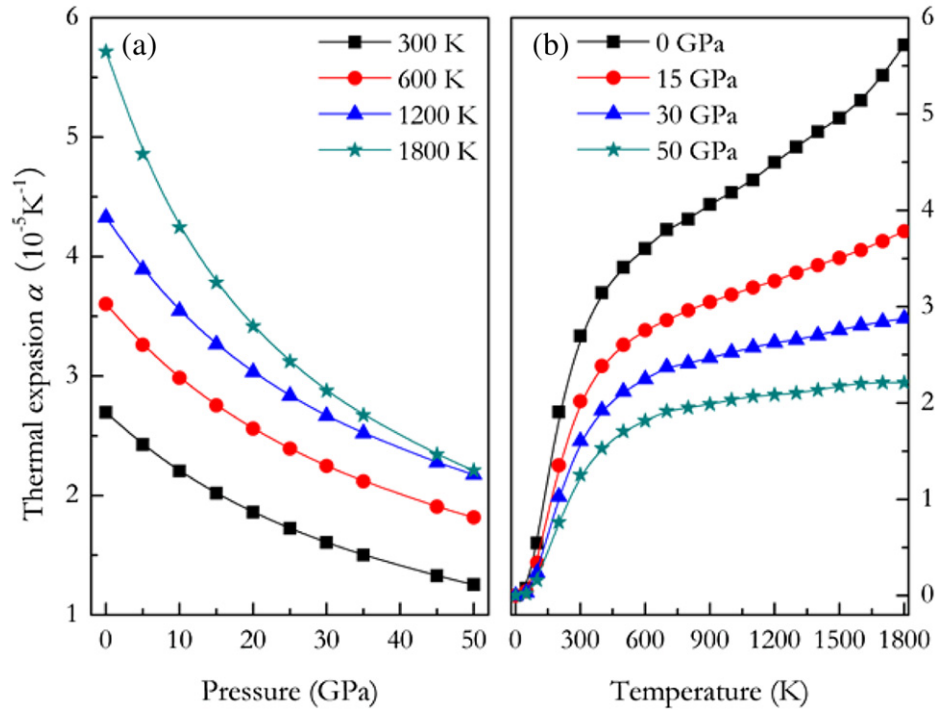


Fig. 6. Pressure (a) and temperature (b) dependence of the thermal expansion coefficient α for the $Pmmn\text{-OsB}_4$.

a linear increase at high temperature in Fig. 6(b). The variations of thermal expansion coefficient with pressures become gently. At a given temperature, the thermal expansion coefficient decreases strongly with pressures and remains very smoothly at high temperatures and high pressures. It can be found that the thermal expansion coefficient α converges to a constant value at high temperatures and pressures. These results are in accordance with the results of the Debye theory which applied to many kinds of materials.

The Grüneisen parameter could describe the alteration in vibration of a crystal lattice based on the increase or decrease in volume as a result of temperature change. Recently, it has been widely used to characterize and extrapolate the thermodynamic properties of materials at high pressures and high temperatures such as the temperature dependence of phonon frequencies and line-widths. Grüneisen parameter [35] is dominated by lower-frequency transverse modes at low temperatures. In Fig. 7, we have plotted the Grüneisen parameter γ of the $Pmmn\text{-OsB}_4$ at

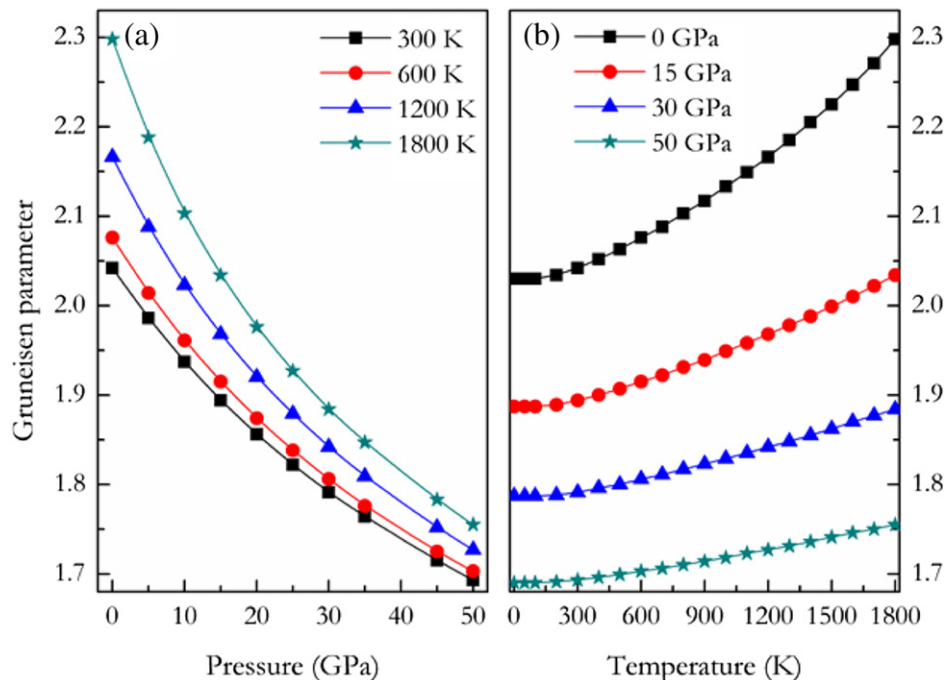


Fig. 7. Pressure (a) and temperature (b) dependence of the Grüneisen parameter γ for the $Pmmn\text{-OsB}_4$.

various temperatures and pressures. It can be observed that the γ decreases dramatically with pressure at given temperature in Fig. 7(a). Meanwhile, at higher temperatures, the γ decreases more rapidly with the increasing pressure. As shown in Fig. 7(b), at fixed pressure ($T > 600$ K), the γ increases monotonously with temperature. These results are due to the fact that the effect of temperature on the Grüneisen parameter γ is not as significant as that of pressure, and there will be a large thermal expansion at a low pressure.

4. Conclusion

In summary, the structural, elastic, and thermodynamic properties of the ultra-incompressible orthorhombic *Pmmn* structure of OsB₄ under pressures have been predicted by first-principles calculations in combination with the quasi-harmonic Debye model. The obtained results of the ground state structural properties and equation of state are in good agreement with previous theoretical calculations. The elastic constants C_{ij} , polycrystalline aggregate elastic moduli, Debye temperature, and the elastic anisotropies of the *Pmmn*-OsB₄ under high pressures are also predicted for the first time. The results indicated that the *Pmmn*-OsB₄ is prone to brittleness below 50 GPa and exhibits larger elastic anisotropy with increasing pressure. In addition, some basic thermodynamical quantities such as the heat capacity (C_V and C_P), thermal expansion coefficient α , and Grüneisen parameter γ are calculated systematically based on the quasi-harmonic Debye model at the pressure of 0–50 GPa and temperature of 0–1800 K, and the results are also interpreted. We hope that our results will stimulate further experimental and theoretical works on this technologically material in the future.

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