Elastic constants and anisotropy of RuB_2 under pressure*

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The structural, elastic constants and anisotropy of RuB_2 under pressure are investigated by first-principles calculations based on the plane wave pseudopotential density functional theory method within the local density approximation (LDA) as well as the generalized gradient approximation (GGA) for exchange and correlation. The results accord well with the available experimental and other theoretical data. The elastic constants, elastic anisotropy, and Debye temperature Θ as a function of pressure are presented. It is concluded that RuB_2 is brittle in nature at low pressure, whereas it becomes ductile at higher pressures. An analysis for the calculated elastic constant has been made to reveal the mechanical stability of RuB_2 up to 100 GPa.

Keywords: elastic properties, density functional theory, RuB_2

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1. Introduction

Since the discovery of superconductivity in MgB_2 at unexpected high temperature $T_c = 39$ K,[1] the physical properties of the transition metal diborides have attracted considerable attention. Many structurally related TB_2 compounds (T=Ti, Zr, Hf, V, Cr, Nb, Ta, Mo) have been investigated in the quest for superconductivity behaviour.[2−7] The metal compound RuB_2 has also been reported to show superconductivity below 1.6 K.[8,9] X-ray diffraction techniques[10,11] showed that RuB_2 had an orthorhombic structure with two formula units per unit cell. Chiodo *et al.*[12] calculated the electronic and structural properties of RuB_2 by using the projector augmented-wave (PAW) method. With the first-principles linear response theory, Wang *et al.*[13] investigated the lattice dynamics and electron–phonon coupling (EPC) of RuB_2. They found that the d electrons of transition metal played the most important role in determining the superconducting behaviour. Recently, Hao *et al.*[14] investigated the elastic anisotropy of RuB_2 at zero temperature and zero pressure. Their results showed that RuB_2 possessed high elastic anisotropic property. Moreover, Chiodo *et al.*[12] and Hao *et al.*[14] reported that RuB_2 was a new kind of superhard material. However, Šimůnek did not believe that RuB_2 was a superhard material.[15]

The comprehensive analysis of elastic constants can provide a deeper insight into mechanical behaviour and hardness of materials. Elastic properties of a solid are important because they are related to various fundamental solid-state properties such as interatomic potentials, equation of state, and phonon spectra. Moreover, elastic properties are also related thermodynamically to the specific heat, thermal expansion, Debye temperature, melting point, Grüneisen parameter and so on.

Recently, the investigations of the elastic properties of RuB_2 at zero pressure and zero temperature have already been conducted.[14] However, the elastic constants and the anisotropy of RuB_2 under pressure have not been studied theoretically yet. It attracts us to investigate the elastic properties of RuB_2 under pressure due to the fact that pressure is a significant variable to tune physical properties. Thus, in the present work, we investigate the elastic properties of RuB_2 under pressure by using the plane-wave pseudopotential density

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functional theory method within the local density approximation (LDA) and the generalized gradient approximation (GGA). The results obtained are well consistent with the available experimental and other theoretical data.

2. Theoretical method

The computations are based on the plane-wave pseudoptential density functional theory within the nonlocal ultrasoft pseudopotential introduced by Vanderbilt,[16] together with both the local density approximation (LDA-CAPZ)[17] as well as the generalized gradient approximation (GGA-PBE).[18] The electronic wave functions are expanded in a plane wave basis set with an energy cut-off of 500 eV. Pseudo-atom calculations are performed for B $2s^2 2p^1$ and Ru $4d^7 5s^1$ separately. For the Brillouin-zone sampling, we use the 6×11×7 Monkhorst–Pack mesh,[19] where the self-consistent convergence of the total energy is 2×10^{-6} eV/atom. This structure has been optimized by using the BFGS algorithm[20] for pressures ranging from 0 GPa to 100 GPa. The tolerance for geometry optimization set as the difference in total energy is within 5×10^{-6} eV/atom, that for the maximum ionic Hellmann–Feynman force is within 0.01 eV/Å (1 Å=0.1 nm), that for the maximum ionic displacement is within 5×10^{-4} Å, and that for the maximum stress is within 0.02 GPa. All these electronic structure calculations are implemented through the CASTEP code.[21]

3. Results and discussion

RuB_2 belongs to the orthorhombic crystallographic system with space group *Pmmn*. Two Ru atoms occupy the 2*a* Wyckoff sites and four B atoms occupy the 4*f* sites with free internal *x* and *z* coordinates. Through the geometries of the structure including cell parameters as well as atomic positions for RuB_2 starting from a six-atom unit cell, we can obtain both lattice geometry and atomic positions to have a fully relaxed structure of RuB_2. After that, a wide range of primitive cell volumes V, i.e from $0.66V_0$ to $1.61V_0$, where V_0 is the equilibrium primitive cell volume at zero pressure, is set to obtain the energy-volume data, which are fitting to the Brich–Murnaghan of state (EOS).[22]

In Table 1, we list the calculated equilibrium lattice parameters, bulk modulus B_0 and its pressure derivative B_0' compared with experimental data[11] and other theoretical results[12,14] at $P = 0$ GPa and $T = 0$ K. Clearly, our results are well consistent with the experimental data and other theoretical data. Compared with the experimental data, our GGA results are a little overestimated and our LDA results are a little underestimated, which implies the validity and the believability of the present calculation. Our GGA results are somewhat in better agreement with the experimental data than other results. When compared with the isomorphous phase OsB_2 (with the bulk modulus 365–395 GPa)[23] and the superhard material diamond (with the bulk modulus 442 GPa),[24] RuB_2 seems to be less stiff (with the bulk modulus 301 GPa (GGA) and 330 GPa (LDA)).

Table 1. Calculated lattice parameters (*a*, *b*, *c*) (Å), primitive cell volume V (Å^3), bulk modulus B_0 (GPa) and its pressure derivative B_0' of RuB_2 at $P = 0$ GPa and $T = 0$ K, together with the experimental and other theoretical data.

	V	a	b	c	B_0	B_0'
LDA (present)	51.80	4.592	2.823	3.994	330	4.1
GGA (present)	53.95	4.650	2.867	4.046	301	4.0
experiment[11]	53.85	4.644	2.867	4.045		
LDA[12]	52.563	4.610	2.837	4.009	334.77	4.1
LDA[14]	51.80	4.596	2.821	3.996	316	
GGA[14]	53.08	4.624	2.847	4.031	290	

The pressure dependence of the normalized lattice parameters a/a_0, b/b_0, c/c_0, and the normalized cell volume V/V_0 (where a_0, b_0, c_0 and V_0 are the zero pressure equilibrium structure parameters) are illustrated in Fig. 1. It is shown that, as pressure increases, the equilibrium ratio b/b_0 decreases more quickly, whereas c/c_0 decreases more slowly indicating that the compression is the largest along the *b*-axis but the smallest along the *c*-axis. Unfortunately, there are no experimental data to be compared with our data.

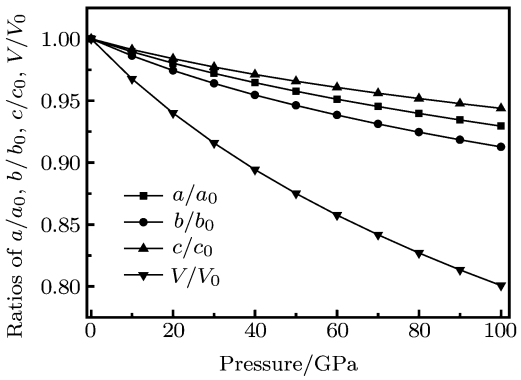


Fig. 1. Normalized parameters a/a_0, b/b_0, c/c_0 and V/V_0 as a function of pressure at $T = 0$.

The elastic stiffness tensor is related to the stress tensor and the strain tensor by Hooke's law. Since the stress tensor and the strain tensor are symmetric, the most general elastic stiffness tensor has only 21 non-zero independent components. For an orthorhombic crystal, they are reduced to 9 components, i.e. c_{11}, c_{22}, c_{33}, c_{44}, c_{55}, c_{66}, c_{12}, c_{13} and c_{23}. These elastic stiffness coefficients (namely the elastic constants) can be determined by computing the stress generated by forcing a small strain to an optimized unit cell.[25] In Table 2, we present the elastic constants of RuB_2 at 0 K and 0 GPa. There is currently no experimental measurements of elastic constants to be compared with our results. However, our results are well consistent with those by Hao *et al.*[14]

Table 2. Elastic constants c_{ij} of RuB_2 at 0 K and 0 GPa, compared with other theoretical data.

	c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}
LDA (present)	562	514	782	126	247	195	199	169	118
GGA (present)	516	459	717	128	225	183	174	160	107
LDA[14]	577	513	784	104	236	191	195	172	133
GGA[14]	540	484	719	116	225	183	174	154	120

The pressure dependence of elastic constants of RuB_2 (up to 100 GPa) with GGA calculations are summarized in Table 3. The elastic constant c_{11} (c_{22} and c_{33}) represents the elasticity in length. The elastic constants c_{12} (c_{13} and c_{23}) and c_{44} (c_{55} and c_{66}) are related to the elasticity in shape. c_{11} can change with longitudinal stain. It is clearly found that c_{11}, c_{22} and c_{33} are sensitive to pressure, while c_{12}, c_{13} and c_{23} vary little under pressure. Furthermore, c_{44}, c_{55}, and c_{66} increase monotonically as the pressure rises. In general, G is the important parameter related to the hardness of a material. Comparing RuB_2 at 0 K and 0 GPa, $G = 184$ GPa with isomorphous phase OsB_2 ($G = 180$ GPa)[14] and the superhard material diamond ($G = 536$ GPa),[24] we predict that the hardness of RuB_2 is almost the same as that of OsB_2, but much smaller than that of diamond. Šimůnek[15] reported on the values of hardness H of RuB_2, OsB_2, and diamond (i.e. $H(RuB_2) = 36.1$, $H(OsB_2) = 35.2$, and H(diamond)=95.4), our prediction agrees with the result of Šimůnek.

Table 3. Values of elastic stiffness constants c_{ij} (GPa), bulk modulus (GPa) along crystallographic axes a, b, c, bulk modulus B (GPa), shear modulus G (GPa), and Debye temperature Θ (K) of RuB_2 under pressure up to 100 GPa at different pressures.

P	c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}	B_a	B_b	B_c	B	G	B/G	Θ
0	516	459	717	128	225	183	174	160	107	879	652	1097	282	184	1.53	783
10	569	526	776	131	250	195	216	172	124	990	779	1163	319	197	1.62	808
20	624	578	867	143	275	208	247	209	150	1113	866	1357	362	214	1.69	837
30	674	633	960	133	296	214	284	246	184	1221	973	1575	407	220	1.85	847
40	726	685	1026	131	318	228	319	274	201	1351	1062	1688	443	230	1.93	864
50	784	737	1089	136	338	238	351	304	221	1491	1148	1804	481	242	1.99	883
60	806	787	1168	135	358	247	376	325	246	1499	1258	1987	513	250	2.05	896
70	862	841	1228	140	377	251	408	356	269	1628	1353	2108	551	260	2.12	911
80	905	888	1292	150	396	261	435	381	285	1722	1433	2228	583	273	2.14	931
90	943	935	1360	142	414	270	462	408	306	1796	1522	2378	617	278	2.22	938
100	987	982	1418	145	431	275	497	438	326	1913	1611	2493	652	286	2.28	949

In Table 3, the elastic constants possess the trend $c_{22} < c_{11} < c_{33}$, which implies the anisotropy of the elasticity. We can depict the mechanical anisotropy of RuB_2 with bulk moduli along the a, b and c axes, i.e. B_a, B_b and B_c, which are defined as[26]

$$B_a = a\frac{dP}{da} = \frac{\Lambda}{1+\alpha+\beta}, \quad (1)$$

$$B_b = b\frac{dP}{db} = \frac{B_a}{\alpha}, \quad (2)$$

$$B_c = c\frac{dP}{dc} = \frac{B_a}{\beta}, \quad (3)$$

where

$$\Lambda = c_{11}+2c_{12}\alpha+c_{22}\alpha^2+2c_{13}\beta+c_{33}\beta^2+2c_{23}\alpha\beta, \quad (4)$$

$$\alpha = \frac{(c_{11}-c_{12})(c_{33}-c_{13})-(c_{23}-c_{13})(c_{11}-c_{13})}{(c_{33}-c_{13})(c_{22}-c_{12})-(c_{13}-c_{23})(c_{12}-c_{23})}, \quad (5)$$

$$\beta = \frac{(c_{22}-c_{12})(c_{11}-c_{13})-(c_{11}-c_{12})(c_{23}-c_{12})}{(c_{22}-c_{12})(c_{33}-c_{13})-(c_{12}-c_{23})(c_{13}-c_{23})}. \quad (6)$$

Our B_a, B_b, and B_c of RuB_2 at 0 K and different pressures are also listed in Table 3. It is noted that the bulk moduli along the c axis is the largest and along the b axis is the smallest, implying that the b axis is the most compressible and the c axis the least compressible at any pressure.

Pugh[27] proposed the ratio of bulk to shear modulus, B/G, as an indication of ductile vs. brittle character. The bulk modulus B represents the resistance to fracture, while the shear modulus G represents the resistance to plastic deformation. A high B/G ratio is associated with ductility, whereas a low value corresponds to 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 RuB_2 at 0 K and 0 GPa, our calculated value of B/G is 1.53 within GGA (1.58 with GGA,[14]) hence describing this material as brittle. For the isomorphous phase OsB_2 at 0 K and 0 GPa, the B/G value is 1.76 with GGA,[14] which suggests that OsB_2 is prone to being ductile. For the superhard material diamond at 0 K and 0 GPa, the experimental B/G value is 0.826.[28] The B/G value of RuB_2 is close to that of OsB_2, and both values are much larger than that of diamond. The ratio B/G reflects the hardness of a material. The smaller the ratio B/G is, the bigger the hardness of the material will be. Thus, the results also show that the hardness of RuB_2 is almost the same as that of OsB_2, but much smaller than that of diamond. When the applied pressure changes from 0 GPa to 100 GPa, the ratio B/G value changes from 1.53 to 2.28, that is to say, RuB_2 becomes more ductile with pressure increasing.

As is known, the Debye temperature is an important fundamental parameter and closely related to many physical properties of solids, such as the specific heat and melting temperature. From the elastic constants, one can obtain the elastic Debye temperature (Θ).[29−31] The obtained Debye temperatures of RuB_2 under pressure are also presented in Table 3. For RuB_2 at 0 K and 0 GPa, we have $\Theta = 783$ K from the elastic constants of GGA calculations, consistent with the theoretical value 780 K by Hao *et al.*[14] Obviously, the Debye temperature increases monotonically with pressure increasing up to 100 GPa.

For an orthorhombic crystal, the mechanical stability leads to restrictions on the elastic constants under isotropic pressure as follows:[32]

$$\begin{aligned}
&(\tilde{c}_{11}+\tilde{c}_{22}-2\tilde{c}_{12})>0, \quad (\tilde{c}_{11}+\tilde{c}_{33}-2\tilde{c}_{13})>0,\\
&(\tilde{c}_{22}+\tilde{c}_{33}-2\tilde{c}_{23})>0,\\
&\tilde{c}_{11}>0, \quad \tilde{c}_{22}>0, \quad \tilde{c}_{33}>0,\\
&\tilde{c}_{44}>0, \quad \tilde{c}_{55}>0, \quad \tilde{c}_{66}>0,\\
&(\tilde{c}_{11}+\tilde{c}_{22}+\tilde{c}_{33}+2\tilde{c}_{12}+2\tilde{c}_{13}+2\tilde{c}_{23})>0, \quad (7)
\end{aligned}$$

where $\tilde{c}_{\alpha\alpha} = c_{\alpha\alpha} - P$ ($\alpha = 1, 2, 3, 4, 5, 6$), $\tilde{c}_{12} = c_{12} + P$, $\tilde{c}_{13} = c_{13} + P$, and $\tilde{c}_{23} = c_{23} + P$. In Table 3, the elastic constants of RuB_2 under pressure satisfy all of these conditions above. Therefore, RuB_2 is mechanically stable at pressure up to 100 GPa.

An appropriate description of an anisotropic behaviour has an important implication in engineering science as well as in crystal physics. The shear anisotropic factors provide a measure of the degree of anisotropy in the bonding between atoms in different planes. The shear anisotropic factors for the {100}, {010}, {001} shear planes are given as follows:[33]

$$A_1 = \frac{4c_{44}}{c_{11}+c_{33}-2c_{13}}, \quad (8)$$

$$A_2 = \frac{4c_{55}}{c_{22}+c_{33}-2c_{23}}, \quad (9)$$

$$A_3 = \frac{4c_{66}}{c_{11}+c_{22}-2c_{12}}. \quad (10)$$

In the case of an isotropic crystal, the factors A_1, A_2, and A_3 must be equal to one, while any value smaller or greater than one is a measure of the degree of elastic anisotropy possessed by the crystal. The anisotropic factors A_1, A_2, and A_3 are plotted as a function of pressure in Fig. 2. There is no experimental data to verify our results. When the applied pressure increases

from 0 to 100 GPa, the anisotropic factors A_1, A_2, and A_3 change 32.4%, 5.4%, 3.4%, respectively, i.e. A_2 and A_3 vary slightly, and A_1 descends sharply with pressure increasing, which is due to the fact that the elastic constants c_{11}, c_{33}, c_{44} and c_{13} are affected by pressure. The anisotropy is dependent only on the symmetry of the crystal. The structure of the crystal changes under applied pressure due to the variations of a, b, and c with pressure. Therefore, the elastic anisotropies are different because of the variations of the elastic constants with pressure. This also corresponds to the stronger covalent bonding in boron layers, ionized ruthenium atoms and weaker interlayer metallic bonding for RuB_2.

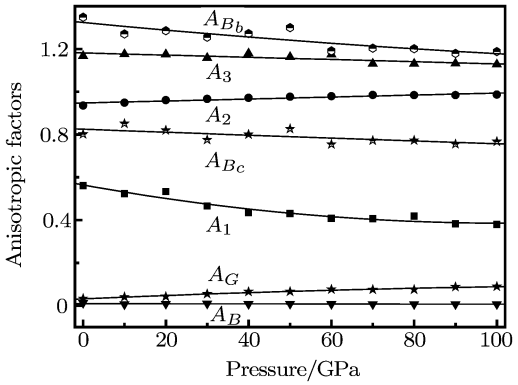


Fig. 2. Anisotropic factors of RuB_2 as a function of pressure.

The anisotropies of the bulk modulus along the a axis with respect to the b and c axes can be written as $A_{B_b} = B_a/B_b$ and $A_{B_c} = B_a/B_c$ respectively. One of them indicates elastic isotropy and the other shows its deviation from the elastic anisotropy indicated by the former. In addition, a more practical measure of the elastic anisotropy is defined as $A_B = (B_V - B_R)/(B_V + B_R)$ and $A_G = (G_V - G_R)/(G_V + G_R)$, where B and G denote the bulk and the shear moduli, and the subscripts V and R represent the Voigt and Reuss approximations respectively. A value of zero ($B_R = B_V$) is associated to isotropic elastic constant, while a value of 100% is associated to the largest possible anisotropy. The pressure dependences of A_B, A_G, A_{B_b} and A_{B_c} are also obtained and presented in Fig. 2. As pressure increases, the anisotropies of the linear bulk moduli A_{B_b} and A_{B_c} reduce 11.9% and 4.2%, respectively. In addition, the percentage bulk modulus anisotropy A_B is smaller than the percentage shear modulus anisotropy A_G as pressure increases, implying that RuB_2 is less anisotropic in compressibility than in shear.

4. Summary

We focus our attention on the elastic properties of RuB_2 under high pressure by means of the *ab initio* plane wave pseudopotential density functional theory within the local density approximation (LDA) and the generalized gradient approximation (GGA). The optimized lattice parameters reproduce perfectly the experimental data. The elastic constants obtained from GGA calculations are found to be in somewhat better agreement with other theoretical values than the LDA calculations. The elastic constants, elastic anisotropy, and Debye temperature Θ as a function of pressure are presented. From our analysis, we also find that RuB_2 is a brittle system at low pressures, whereas it becomes ductile at higher pressures. Moreover, from our elastic constants of RuB_2 under pressure, we have found that RuB_2 becomes more ductile with the pressure increasing, and is mechanically stable at pressures of up to 100 GPa.

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