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Insights into Structure, Electronic and Mechanical Properties of Rubx (X=1, 2, and 3)

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Abstract

The structural, electronic and mechanical properties of RuBx (x=1, 2, 3) are investigated by performing first principles calculations using density functional theory (DFT). The calculated lattice constants agree well with the available results. The chemical bonding is interpreted by calculating the electron localization function (ELF). The covalent Ru-B bond and B-B bond become stronger with the increase of boron's concentrations, which can help improve the hardness of RuBx system. Moreover, RuB has the highest bulk modulus, which means more prominent volume-compression resistance. RuB2 has a certain elastic anisotropy and RuB3 has the best toughness.

Keywords: Superhard materials; Mechanical properties; First-principles calculation; Electron localization function (ELF)

Introduction

Because of the superior property of high hardness, superhard materials have played a vital role in industrial production, including many applications in abrasives, cutting tool materials as well as wear-resistant coatings, etc [1,2]. A recent perspective has reached to the conclusion that diamond remains the hardest known material under normal conditions [3]. In the past decades, many efforts have been devoted into fabricating or designing new type of superhard and ultrahard materials [4-10]. A very important route of synthesizing novel superhard materials is the alloying between low-mass element and transient metal element [11-13]. In a previous research, it was found that RuB2 has high elastic anisotropy [14]. Additionally, the flexibility of RuB2 can be improved with the increase of pressure and temperature can have an obvious impact on the mechanical properties of RuB2 [15]. Modern computational techniques allow the computationally prediction of novel superhard materials with superior properties, which can be promising for practical applications. Computational discovery of hard and superhard materials is a booming field of science, which help predict novel materials with enhanced physical properties [16]. In spite of some experimental advances, a systematic research about physical properties of RuBx (x=1, 2, 3) compounds is still lacking and new computational work is needed strongly. In this paper, the crystal structures, electronic structure as well as mechanical properties of RuBx (x=1, 2, 3) have been reported.

Computational Methods

The density-functional theoretical method (DFT) has witnessed a great success in the computation of the electronic structure of solids. As one of the most accurate methods used for the present work, the structures of RuBx (x=1, 2, 3) are optimized by adopting projector augmented wave (PAW) approach [17]. Exchange and correlation effects are treated by the generalized-gradient approximation (GGA) [18]. The total energy and charge density are integrated in the Brilorine zone by means of Monkhorst-Pack scheme [19]. A suitable plane wave cutting kinetic energy should be selected in order to ensure the accuracy of results. With a test, an energy cutoff of 330 eV is enough for the expansion of plane wave basis set.

Results and Discussion

Structural information

The structural model of Ru-Bx (x=1, 2, 3) system is illustrated in (Figure 1). It can be seen that all these compounds have layered geometry. For RuB (P-6m2), the Ru atomic layer and B atomic layer are in alternating stack arrangement in the form of Ru-B-Ru along the c-axis direction. Each boron atom is located at the center of a triangular columnar formed by six Ru atoms.

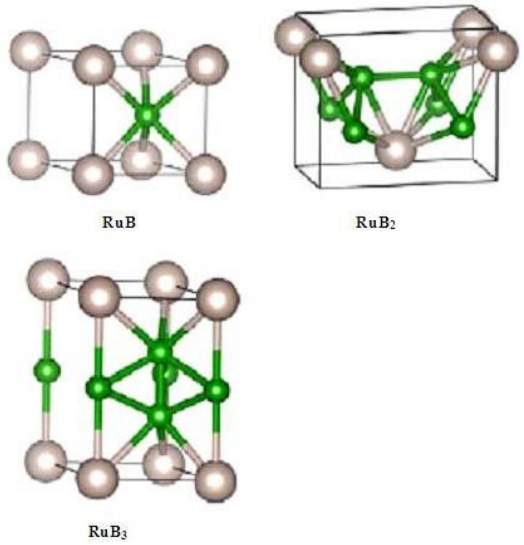

Figure 1: *The Crystal structure of RuBx (x=1,2,3) system, with the bigger ball standing for Ru atom and the B atom are marked in green color.*

Table 1: *lists the optimized lattice constants of RuBx(x=1, 2, 3) in the most stable state, with the reference values denoted in brackets.*

Lattice constants Materials	a(nm)	C(nm)
RuB (P-6m2)	0.288 (0.285[12])	0.287(0.286[12])
RuB_2 (Pmmn)	0.467 (0.465[12,13])	0.406(0.405[12,13])
RuB_3 (P-6m2)	0.290	0.457

Correspondingly, each Ru atom is located at the center of a triangular columnar formed by six boron atoms. RuB2 (Pmmn) is totally a three-dimensional stereo-network structure. The internal structure of RuB3 (P-6m2) is stacked between Ru atomic layer and the triangle double cone layer composed of boron atoms (Table 1). Lists the optimized lattice constants of RuBx (x=1, 2, 3) in the most stable state, with the reference values denoted in brackets. It can be seen that the computed crystal parameters are in fairly good agreement with previous results, with the maximum deviation less that 0.9%.

Electronic Properties

In order to determine the chemical bonding of title materials, the electron localization function (ELF) is calculated and analyzed in the present work [20]. Actually, ELF can help us judge the chemical bonding of a given system. There will be the perfect localization of electron or strong covalent bonding when ELF is adjacent to 1. On the contrary, there will be no electrons in a specific area if ELF=0. ELF of RuBx (x=1, 2, 3) has been presented in (Figure 2). It should be noted that chemical bonding of title materials could be predicted more reasonable after combing ELF with the crystal structure. ELF of RuB shows that Ru layer and B layer are packed in turn along c axis and there is no direct B-B contact or bonding in RuB. As for RuB2, there is strong Ru-B covalent bonding along the direction of c-axis, which means that this type of material possesses good incompressibility along c-axis. Compared with RuB2, there is stronger B-B covalent bonding in RuB3, which means that the hardness of RuB3 has been improved greatly. Additionally, there is strong Ru-B covalent bonding along the direction of c-axis, which has also improved the hardness of RuB3.

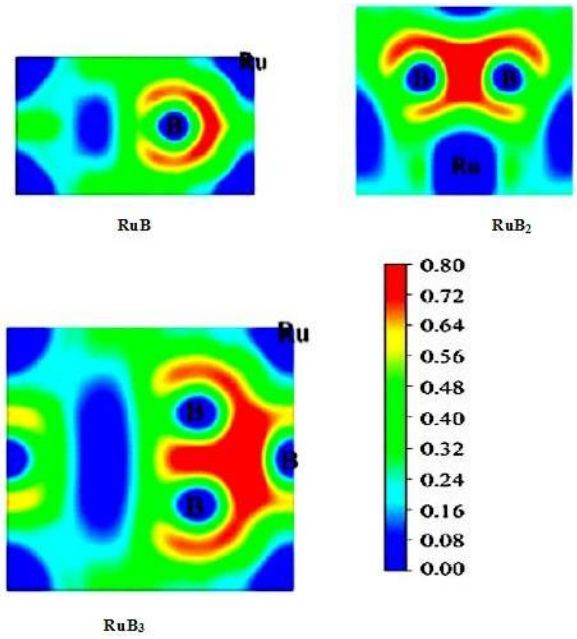

Figure 2: *The electron localization function (ELF) of RuBx (x=1,2,3) system.*

Overall, there is only Ru-B bonding in RuB whereas there exist strong B-B interaction and Ru-B interaction in RuB2 and RuB3. Because of the stronger B-B covalent bonding with the increase of boron's concentrations, the hardness of transition metal boride can be improved further.

Mechanical Properties

Elastic constants (Cij) are often used to describe a given material's rigidity resulting from the external strain. The elastic constants (Cij), bulk modulus (B), shear modulus (G), Young's modulus (E) and Poisson's ratio ( ) of RuBx (x=1,2,3) have been calculated and results are listed in. The bulk modulus and

shear modulus are calculated through the Voigt-Reuss-Hill approximation [21-23]. According to these elastic constants (Cij) and the judgment of mechanical stable conditions, all these compounds (RuB, RuB2 and RuB3) are mechanically stable [24]. It can also be found that C33 value is the largest among all these RuBx compounds, which indicates that there is larger incompressibility for RuBx along c-axis direction.

Table 2: *Calculated elastic constants and the elastic parameters (B, G, E, B/G, □) for RuBx (x=1,2,3) at GGA level.*

Elastic properties Materials	Elastic constants		Elastic parameters	
RuB (P-6m2)	C_{11}=527;	C_{33}=718;	B=312;	G=179;
	C_{44}=157;	C_{12}=190; C_{13}=165	B/G=1.74;	E=449;
			□ =0.26	
RuB_2 (Pmmn)	C_{11}=526;	C_{22}=451;	B=288;	G=181;
	C_{33}=702;	C_{44}=109;	B/G=1.59;	E=448;
	C_{55}=209;	C_{66}=177;	□ =0.24	
	C_{12}=191;	C_{13}=158; C_{23}=129		
RuB_3 (P-6m2)	C_{11}=436;	C_{33}=713;	B=293;	G=161;
	C_{44}=174;	C_{12}=182; C_{13}=186	B/G=1.82;	E=407;
			□ =0.27	

Additionally, it can be predicted that orthogonal RuB2 has a certain elastic anisotropy. It has also been shown in that RuB has the largest bulk modulus, shear modulus and Young's modulus (Table 2). The bulk modulus of RuB is about 332Gpa, which is slightly lower than cubic boron nitride (379Pa) [25]. Therefore, we can predict that RuB has very good volume-compression resistance. According to Pugh model, it is reasonable to adopt B/G or Poisson's ratio (□) to evaluate the toughness or brittleness of a given material [26]. Usually, lower B/G and □ values mean that the material is more brittle and harder. On the contrary, very high B/G and □ values mean that the material is tough and soft. We can see that B/G and □ values of RuB3 are the largest among RuBx (x=1, 2, 3). Therefore, we can confirm that RuB3 is a type of material that has good toughness.

Conclusion

In this systematic study, the crystal structure, electronic structure as well as mechanical properties of RuBx (x=1, 2, 3) compounds have been investigated based on first-principles method. We can draw some conclusions as follows:

- The covalent Ru-B bond and B-B bond become stronger with the increase of boron's concentrations, which can help improve the hardness of RuBx system.
- RuB has the highest bulk modulus, which means more prominent volume-compression resistance. RuB2 has a certain elastic anisotropy and RuB3 has the best toughness.

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