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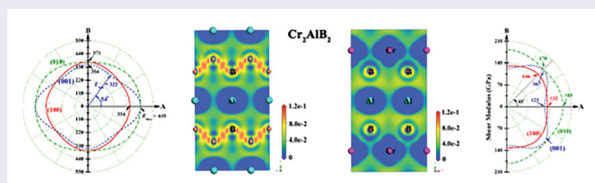
Electrical conductive and damage-tolerant nanolaminated MAB phases Cr_2AlB_2 , Cr_3AlB_4 and Cr_4AlB_6

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ABSTRACT

Theoretical investigations on electronic structure, chemical bonding and mechanical properties reveal that MAB phases $(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$) exhibit anisotropic electrical and elastic properties, low shear deformation resistance and damage tolerance similar to MAX phases. The main contribution to the electrical conductivity is Cr $3d$ states and the anisotropic distribution of Cr atoms results in anisotropic conductivity. The high stiffness originates from the strong covalent B–B bonds, while the low shear deformation resistance is underpinned by metallic B–Cr bonds adjacent to Al layer. The possible slip systems are (100)[010], (010)[100], (010)[001] and (001)[010] for Cr_2AlB_2 , (010)[001] and (001)[010] for Cr_3AlB_4 and Cr_4AlB_6 .



IMPACT STATEMENT

Anisotropic electrical and mechanical properties, damage tolerance of $(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$) are predicted using first-principles calculations and their correlations to the electronic structure and chemical bonding were disclosed.

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KEYWORDS

Transition metal ternary borides; nanolaminated MAB phases; DFT calculations; mechanical properties; deformation mechanism

Ultrahigh temperature ceramics (UHTCs) based on transition metal borides are regarded as the materials of choice for nose tips and sharp leading edges of hypersonic vehicles, hot structure components for scramjet engines [1–3], matrix and/or surface coatings for ultrahigh temperature ceramic matrix composites [4–5]. The intrinsic brittleness, poor thermal shock resistance and difficulty in machining into sharp or complex shapes, however, are main obstacles to impede their applications. Formation of nanolaminated structures like MAX phases, a family of layered ternary carbides and nitrides with a general formulae of $\text{M}_{n+1}\text{AX}_n$ (where M is an early transition metal, X is carbon or nitrogen, A is a III_A – VI_A group element, $n = 1-6$) [6–7], has been proven to be an effective way to overcome the brittleness of transition metal carbides and nitrides. Inspired by the success in development of MAX phases, nanolaminated ternary borides called MAB phases (where M is a transition metal, A is a

III_A or IV_A group element and B is boron) were recently synthesized and characterized by Ade and Hillebrecht [8] and the stacking sequence and defects were observed by Lu et al. [9]. It is expected that MAB phases are damage tolerant, resistant to thermal shock and machinable like MAX phases. However, besides crystal structure and microhardness [8,9], the properties of many MAB phases are not available. Quantum mechanical modeling through first-principles calculations based on density functional theory (DFT) has been proven a powerful tool to predict the intrinsic properties of transition metal borides [10]. It is also helpful in scanning the properties and accelerating the material's design-preparation-application process.

In this work, we report the electronic structure, chemical bonding and mechanical properties of MAB phases in Cr–Al–B system with the general formula $(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$). These materials are selected due

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to the following reasons. Firstly, they contain B, Cr, Al, which can ‘smartly’ form protective B_2O_3 , Cr_2O_3 and Al_2O_3 scales at low, intermediate and high temperatures in oxygen-rich environments. Secondly, similar to nanolaminated ternary carbides, the elastic stiffness is expected to systematically increase with n [11]. Thirdly, the mechanisms that underpin the properties of these MAB phases have not been investigated.

First-principles calculations based on DFT were performed using the Cambridge Serial Total Energy Package code [12], wherein the norm-conserving pseudopotential [13] and generalized gradient approximation based on the revised Perdew–Burke–Ernzerhof (RPBE) scheme [14] for the exchange–correlation functional were used. The plane-wave basis set cutoff was 700 eV and k -points mesh with separation of $0.04 \text{ \AA}^{-1}$ was sampled according to the Monkhorst Pack method in the Brillouin zone [15]. Lattice parameters were modified to minimize the enthalpy and interatomic forces. The Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization scheme [16] was used in geometry optimization with the tolerance of difference on total energy within 5×10^{-6} eV/atom, maximum ionic Hellmann–Feynman force within $0.01 \text{ eV/\AA}$, maximum ionic displacement within $5 \times 10^{-4} \text{ \AA}$ and maximum stress within 0.02 GPa. The elastic stiffness was determined from a linear fit of the calculated stress as a function of strain. Bulk modulus B and shear modulus G were calculated from the second-order elastic constants, c_{ij} , according to Voigt [17] and Reuss [18] approximations, and Young’s modulus E was calculated from Hill’s bulk modulus B_H and shear modulus G_H [19].

The crystal structures of $(CrB_2)_nCrAl$ ($n = 1-3$) are shown in Figure 1. For Cr_2AlB_2 and Cr_4AlB_6 , the space group is $Cmmm$; while for Cr_3AlB_4 , the space group is $Pnmm$. The experimental and fully relaxed structure parameters are given in Table 1. Small deviation on geometry optimized lattice constants and bond lengths demonstrates the reliability of the present calculations. Significant difference in bond lengths and Mulliken populations indicate diversity of chemical bonding, that is, strong covalent B–B bonds, covalent B–Cr bonds, weak covalent–metallic B–Al and Al–Cr bonds, and metallic B–Cr and Cr–Cr bonds.

It is well known that MAX phases are characterized by anisotropic mechanical properties and low shear deformation resistance. For comparison, the elastic properties of the $(CrB_2)_nCrAl$ ($n = 1-3$) and the well-known MAX phases Ti_2AlC , Ti_3AlC_2 and Ti_3SiC_2 are calculated and listed in Tables 2 and 3, respectively. The mechanical properties of MAX phases agree well with the previous published data [20]. The elastic properties of MAB phase obtained in this work are close to those of Li et al. [21]

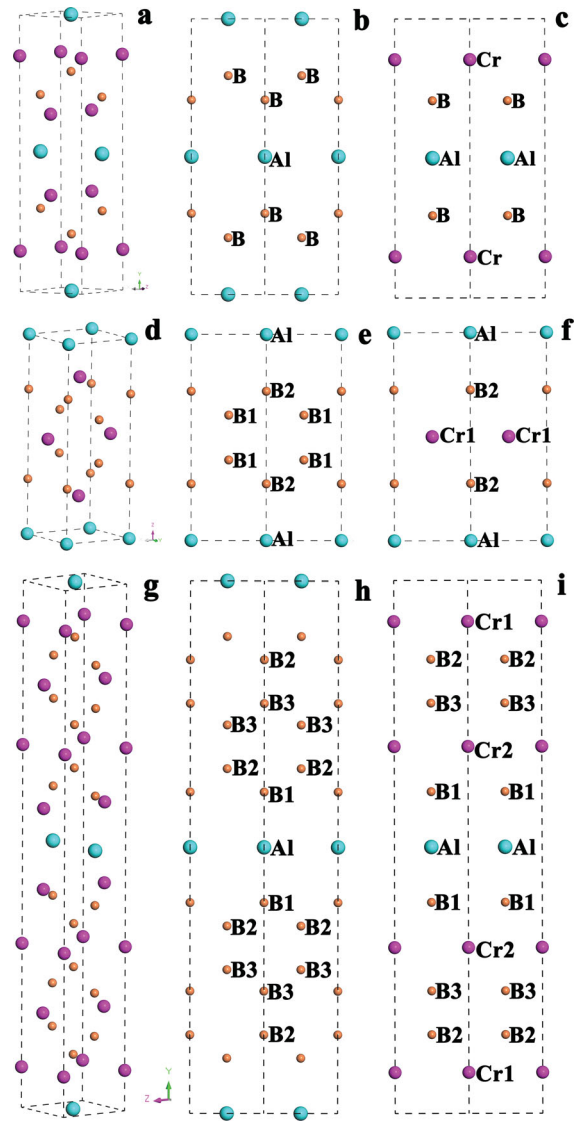


Figure 1. Crystal structures and the distribution of atoms on (002) and (100) plane of Cr_2AlB_2 (a–c), (010) and (100) plane of Cr_3AlB_4 (d–f), and (002) and (100) plane of Cr_4AlB_6 (g–i) (a $2 \times 1 \times 2$ cell is used in (b–c) and (h–i) and a $2 \times 2 \times 1$ cell is used in (e–f)).

but lower than those of Nie et al. [22] due to the fact that ultrasoft pseudopotentials were used by Nie et al. [22], which resulted in underestimation of lattice constants and overestimation of elastic stiffness. Our tests also show that smaller lattice constants and higher elastic moduli are obtained when ultrasoft pseudopotentials were used, so the present calculations are more reliable.

The elastic properties of $(CrB_2)_nCrAl$ ($n = 1-3$) in Table 2 show following features. Firstly, the elastic properties exhibit strong anisotropy. Secondly, the elastic constants that represent stiffness against principle tensile/compression strains are much higher than those against shear deformation strains. Thirdly, the

Table 1. Experimental and geometry optimized lattice parameters of $(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$).

Compound	Cr ₂ AlB ₂	Cr ₃ AlB ₄	Cr ₄ AlB ₆					
Space group	<i>Cmmm</i>	<i>Pmmm</i>	<i>Cmmm</i>					
Z formula units	2	1	2					
Density (g/cm ³)	5.26	5.30	5.26					
Experimental lattice parameters [8]								
Lattice constants (Å)	<i>a</i> = 2.9373 <i>b</i> = 11.0513 <i>c</i> = 2.9675	<i>a</i> = 2.9556 <i>b</i> = 2.9778 <i>c</i> = 8.0539	<i>a</i> = 2.9517 <i>b</i> = 21.2803 <i>c</i> = 3.0130					
Atomic positions	Cr 4i (0, 0.1474, 0) Al 2c (0, 0.5, 0.5) B 4j (0, 0.2941, 0.5)	Cr1 1g (0, 0.5, 0.5) Cr2 2t (0.5, 0.5, 0.188) Al 1a (0, 0, 0) B1 2s (0.5, 0, 0.394) B2 2q (0, 0, 0.288)	Cr1 4i (0, 0.076, 0) Cr2 4i (0, 0.6884, 0) Al 2c (0, 0.5, 0.5) B1 4j (0, 0.6050, 0.5) B2 4j (0, 0.1481, 0.5) B3 4j (0, 0.2298, 0.5)					
Geometry optimized lattice parameters								
Lattice constants (Å)	<i>a</i> = 2.9407 <i>b</i> = 11.0308 <i>c</i> = 2.9642	<i>a</i> = 2.9533 <i>b</i> = 2.9718 <i>c</i> = 8.1043	<i>a</i> = 2.9715 <i>b</i> = 21.3894 <i>c</i> = 2.9610					
Atomic positions	Cr 4i (0, 0.1468, 0) Al 2c (0, 0.5, 0.5) B 4j (0, 0.2940, 0.5)	Cr1 1g (0, 0.5, 0.5) Cr2 2t (0.5, 0.5, 0.2018) Al 1a (0, 0, 0) B1 2s (0.5, 0, 0.3913) B2 2q (0, 0, 0.2752)	Cr1 4i (0, 0.0767, 0) Cr2 4i (0, 0.6886, 0) Al 2c (0, 0.5, 0.5) B1 4j (0, 0.6039, 0.5) B2 4j (0, 0.1478, 0.5) B3 4j (0, 0.2298, 0.5)					
Mulliken population and bond lengths (Å)								
Cr ₂ AlB ₂			Cr ₃ AlB ₄			Cr ₄ AlB ₆		
Bond	Population	Length	Bond	Population	Length	Bond	Population	Length
B–B	1.60	1.7621	B1–B2	1.64	1.7508	B3–B3	1.84	1.7177
B–Cr	0.58	2.1873	B1–B1	0.73	1.7623	B2–B3	0.75	1.7553
B–Cr	−0.39	2.1984	B1–Cr2	−0.14	2.1366	B1–B2	1.64	1.7575
B–Al	0.37	2.2722	B2–Cr2	0.57	2.1776	B2–Cr1	−0.23	2.1215
Al–Cr	0.50	2.6423	B2–Al	0.42	2.2304	B1–Cr1	0.51	2.1764
Cr–Cr	−0.76	2.7098	B1–Cr1	0.20	2.2726	B1–Al	0.43	2.2224
			B2–Cr1	−0.19	2.3509	B2–Cr2	0.07	2.2724
			Al–Cr2	0.25	2.6578	B3–Cr2	0.09	2.2750
			Cr–Cr	−0.83	2.8319	B3–Cr2	0.11	2.2870
						B1–Cr2	−0.20	2.3408
						Al–Cr1	0.31	2.6635
						Cr–Cr	−0.48	2.8173

Table 2. Second-order elastic constants, bulk modulus, shear modulus, anisotropic Young's modulus and Pugh's ratio of $(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$).

Second-order elastic constants c_{ij} (GPa)									
	c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}
Cr_2AlB_2	490	398	419	132	182	123	106	112	117
Cr_3AlB_4	531	486	471	147	185	183	105	137	110
Cr_4AlB_6	561	510	468	148	179	189	135	123	121
Bulk modulus B , shear modulus G , anisotropic Young's modulus (GPa) and Pugh's ratio (G/B)									
	B	G	E	ν	E_x	E_y	E_z	G/B	
Cr_2AlB_2	220	163	392	0.203	445	354	371	0.741	
Cr_3AlB_4	237	182	440	0.203	479	450	421	0.746	
Cr_4AlB_6	254	179	435	0.215	506	459	423	0.705	

Table 3. Second-order elastic constants, bulk modulus, shear modulus, anisotropic Young's modulus and Pugh's ratio of Ti_2AlC , Ti_3AlC_2 and Ti_3SiC_2 .

Second-order elastic constants c_{ij} (GPa)							
Compound	c_{11}	c_{33}	c_{44}	c_{12}	c_{13}	c_{66}	
Ti ₂ AlC	304	274	119	50	57	127	
Ti ₃ AlC ₂	355	292	123	71	68	142	
Ti ₃ SiC ₂	354	344	165	91	103	131	
Bulk modulus B , shear modulus G , anisotropic Young's modulus (GPa) and Pugh's ratio (G/B)							
	B	G	E	ν	E_x	E_z	G/B
Ti ₂ AlC	135	120	278	0.157	287	255	0.889
Ti ₃ AlC ₂	157	130	306	0.176	334	276	0.828
Ti ₃ SiC ₂	183	141	337	0.193	312	296	0.770

elastic stiffness increases with n from 1 to 3. These characteristics are very similar to those of MAX phases.

The anisotropy of elastic properties is reflected from the difference of c_{ij} and E_i ($i = 1-3$). It can also be described by the directional dependence of

Young's modulus. For orthorhombic crystals, the direction dependent Young's modulus is expressed as [23]:

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

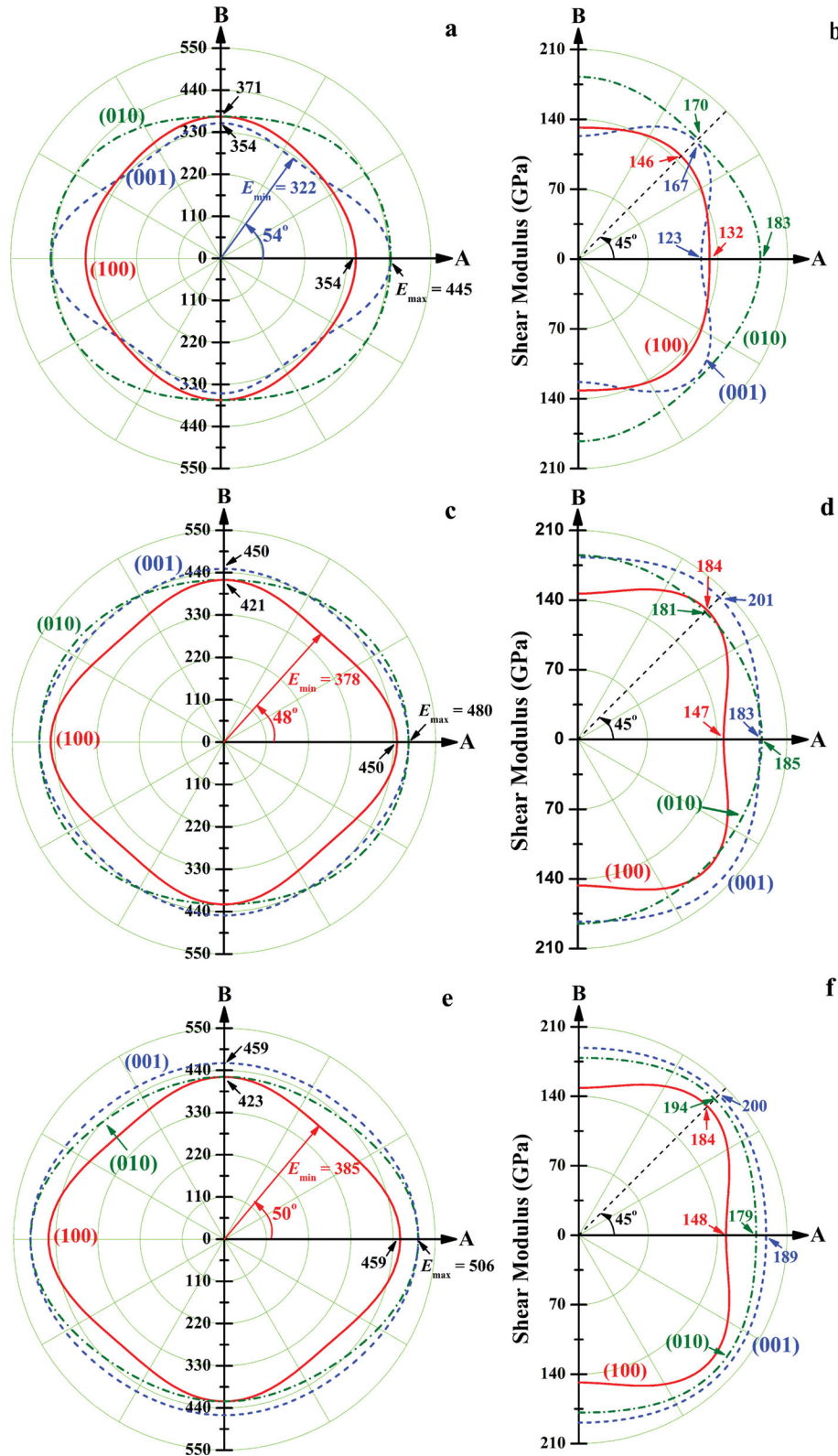


Figure 2. Projection of Young's modulus and shear modulus on (100), (010) and (001) planes of Cr_2AlB_2 (a–b), Cr_3AlB_4 (c–d) and Cr_4AlB_6 (e–f). On (100) plane, A represents [010], B represents [001]; on (010) plane, A represents [100], B represents [001] and on (001) plane, A represents [100], B represents [010].

where s_{ij} is the elastic compliance, l_1 , l_2 and l_3 are the directional cosines of angles with the three principal directions, respectively. Figure 2 shows the directional dependent Young's modulus on (100), (010) and (001) planes of Cr_2AlB_2 , Cr_3AlB_4 and Cr_4AlB_6 . For Cr_2AlB_2 , strongest anisotropy is on (001) plane. The maximum Young's modulus is $E_{\max} = 445$ GPa in [100] direction, and the minimum one is $E_{\min} = 332$ GPa, being 54° inclined to [100] direction (Figure 2(a)). For Cr_3AlB_4 and Cr_4AlB_6 , strongest anisotropy is on (100) plane. For Cr_3AlB_4 , the maximum Young's modulus is $E_{\max} = 480$ GPa in [100] direction and the minimum one is $E_{\min} = 378$ GPa, 48° inclined to the [010] axis (Figure 2(c)); while for Cr_4AlB_6 , the maximum Young's modulus is $E_{\max} = 506$ GPa, and the minimum one is $E_{\min} = 385$ GPa, 50° inclined to the [010] axis (Figure 2(e)).

$(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$) also exhibits low shear deformation resistance (Table 2). For example, Cr_2AlB_2 has both low c_{44} (132 GPa) and c_{66} (123 GPa), but Cr_3AlB_4 and Cr_4AlB_6 exhibit low c_{44} of 147 GPa and 148 GPa, respectively. These values are close to the c_{44} of Ti_2AlC , Ti_3AlC_2 and Ti_3SiC_2 in Table 3, indicating that these two families of materials may share the common low shear deformation resistance and damage-tolerant behavior. The difference in c_{44} , c_{55} and c_{66} also indicates shear anisotropy of $(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$). The shear modulus is related to the compliances as:

$$G'_{ij} = \frac{1}{4s'_{ijij}}, \quad (2)$$

where s'_{ijij} is the compliance under certain coordination system. And the shear modulus on every considered plane can be expressed as:

$$G'_{(100)} = \frac{1}{s_{44} + (s_{22} + s_{33} - 2s_{23} - s_{44}) \sin^2 2\theta}, \quad (3)$$

$$G'_{(001)} = \frac{1}{s_{66} + (s_{11} + s_{22} - 2s_{12} - s_{66}) \sin^2 2\theta}, \quad (4)$$

$$G'_{(010)} = \frac{1}{s_{55} + (s_{11} + s_{33} - 2s_{13} - s_{55}) \sin^2 2\theta}. \quad (5)$$

The projection of shear modulus on (100), (001) and (010) planes are given in Figure 2. For Cr_2AlB_2 , strong anisotropy is on (100) plane (Figure 2(b)). The lowest shear modulus ($G_{\min} = 123$ GPa) is associated with (100)[010] and (010)[100] systems, suggesting that they are the most likely slip systems. In addition, the shear modulus associated to (010)[001] and (001)[010] is as low as 132 GPa, indicating that these systems might also be possible slip systems of Cr_2AlB_2 . For Cr_3AlB_4

and Cr_4AlB_6 , strong anisotropy is also on (100) plane. The lowest shear moduli ($G_{\min} = 147$ GPa for Cr_3AlB_4 (Figure 2(d)) and $G_{\min} = 148$ GPa for Cr_4AlB_6 (Figure 2(f)) are associated with (010)[001] and (001)[010], suggesting that they are the most likely slip systems.

As shown in Table 2, bulk modulus of polycrystalline $(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$) increases from 220 GPa for Cr_2AlB_2 and 237 GPa for Cr_3AlB_4 to 254 GPa for Cr_4AlB_6 , which are close to those of UHTCs like TM_2B_2 (TM = Ti, Zr, Hf, Nb and Ta) [10] and NiB [24], but much higher than those of MAX phases. The shear moduli, however, are in a same level, being 163, 182 and 179 GPa for Cr_2AlB_2 , Cr_3AlB_4 and Cr_4AlB_6 , respectively. Pugh's ratio is often used as a criterion ($G/B < 0.571$) to distinguish ductile materials from brittle ones. The Pugh's ratios of Cr_2AlB_2 , Cr_3AlB_4 and Cr_4AlB_6 are 0.741, 0.746 and 0.705, respectively. These values, although not smaller than 0.571, are lower than those of the typical damage-tolerant MAX phases Ti_2AlC , Ti_3AlC_2 and Ti_3SiC_2 , indicating that these MAB phases are possible damage-tolerant ternary borides.

The above results demonstrate that similar to the well-known MAX phases, MAB phases Cr_2AlB_2 , Cr_3AlB_4 and Cr_4AlB_6 exhibit anisotropic elastic properties, low shear deformation resistance and are possibly damage tolerant. These properties are believed to be underpinned by the electronic structure and bonding properties. To establish the structure-property relationships, we investigated the electronic structure and chemical bonding nature of these MAB phases. The band structure and the total (TDOS) and projected density of states (PDOS) of Cr_2AlB_2 , Cr_3AlB_4 and Cr_4AlB_6 are shown in Figure 3. For all three compounds, valence and conduction bands overlap at the Fermi level and there are finite states at Fermi level in TDOS curves, indicating the presence of metallic bonds in these materials. In addition, similar to MAX phases, there is anisotropy in overlapping along different directions in the band structures, indicating anisotropy in electrical conductivity, that is, high electrical conductivity parallel to (010) of Cr_2AlB_2 and Cr_4AlB_6 , and (001) of Cr_3AlB_4 . The anisotropy in electrical conductivity can be understood from the PDOS curves and the crystal structures. From the PDOS curves, the main contributions to electrical conductivity are from Cr 3d states with smaller contributions from Al 3p and B 2p states. In the crystal structure, Cr atomic planes are parallel to (010) of Cr_2AlB_2 and Cr_4AlB_6 , and (001) of Cr_3AlB_4 , such that the electrical conductivity is higher on these planes. Figure 3 also provides some stability information. For Cr_2AlB_2 , the Fermi level is below the top maximum of the valence band, indicating incomplete filling of the valence bands. For Cr_3AlB_4 and Cr_4AlB_6 , however, the Fermi level is located at the local minimum,

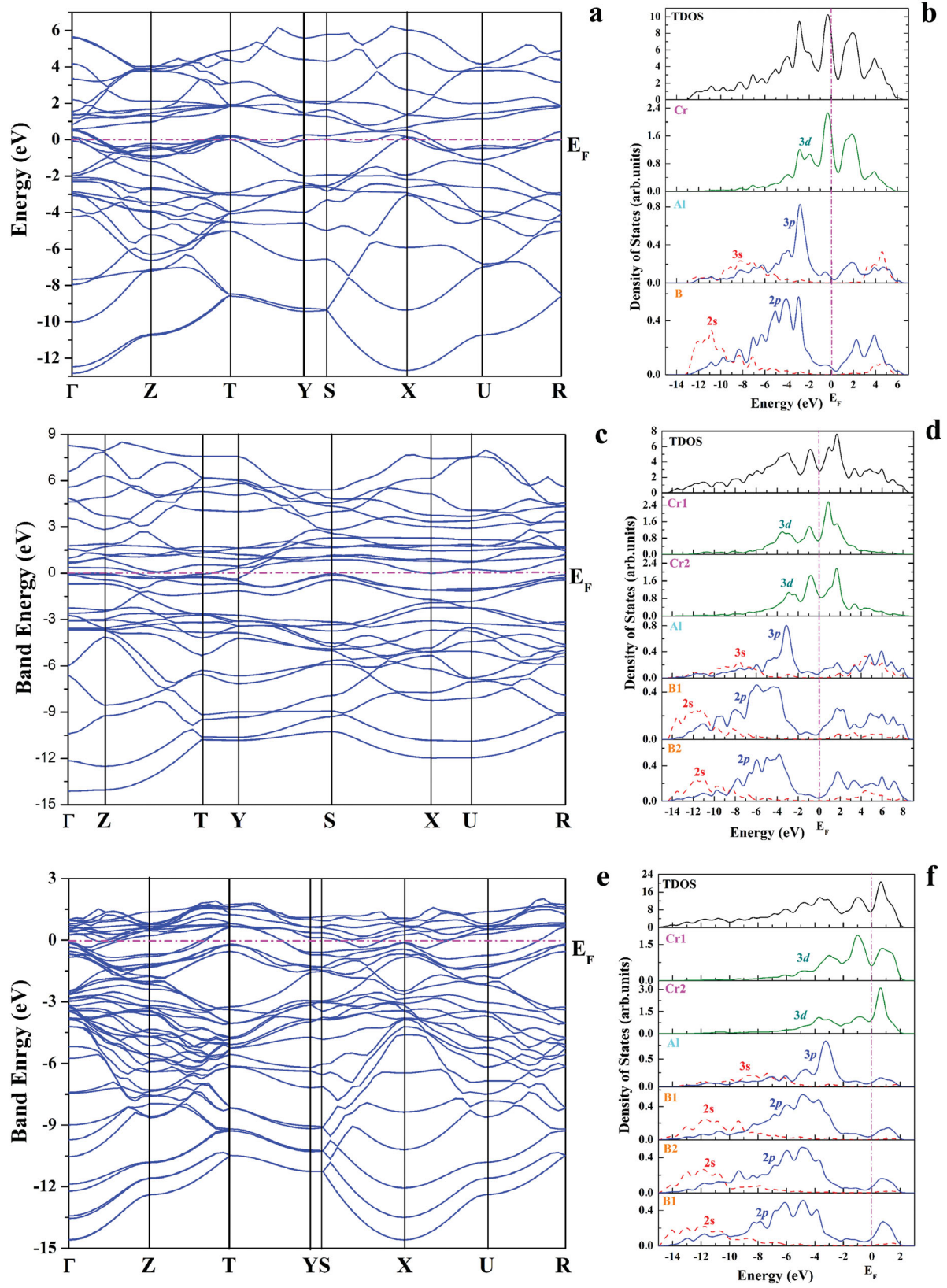


Figure 3. Band structure, TDOS and PDOS of Cr_2AlB_2 (a–b), Cr_3AlB_4 (c–d) and Cr_4AlB_6 (e–f).

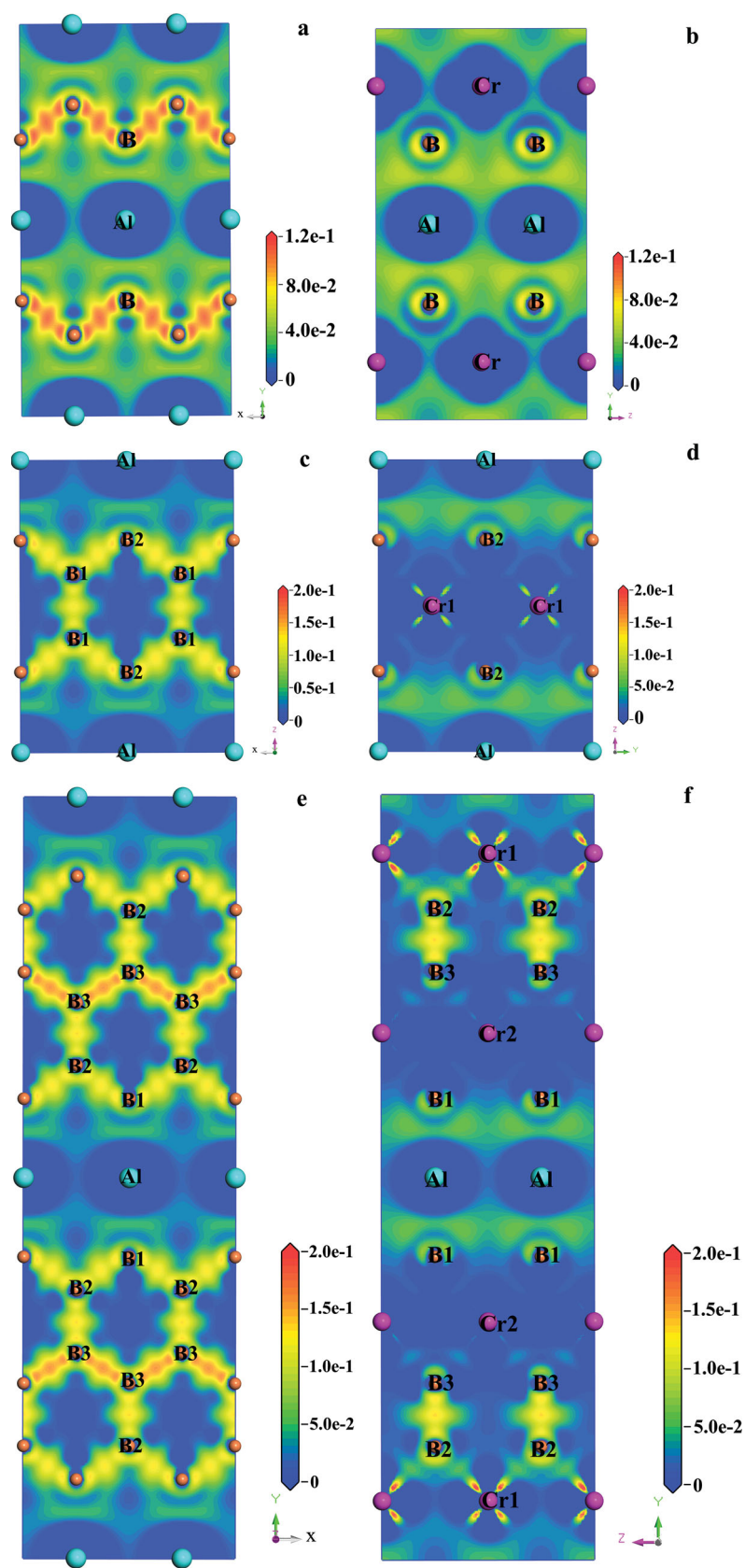


Figure 4. Electron density difference maps on (002) and (100) planes of Cr_2AlB_2 (a–b), (101) and (102) planes of Cr_3AlB_4 (c–d) and (002) and (100) planes of Cr_4AlB_6 (e–f).

indicating complete filling of valence bands and more stability under electronic perturbations.

The mechanisms that drive the high stiffness, low shear deformation resistance and damage tolerance can be understood from the chemical bonding nature in $(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$). Figure 4 shows the electron density difference maps, which illustrate the charge redistribution due to chemical bonding, on (002) and (100) planes of Cr_2AlB_2 , (010) and (100) planes of Cr_3AlB_4 and (002) and (100) planes of Cr_4AlB_6 . Similar to NiB [24], the bonding in the zigzag B–B chains of Cr_2AlB_2 is strong covalent bond formed by overlapping of B sp^2 –B sp^2 orbitals. Since the B–B bond chains are parallel to [100] direction (Figure 4(a)), the stiffness is the highest in [100] (high c_{11} and E_x). The B–Cr bond on (100) plane, however, is metallic because there is no accumulation of electrons between B and Cr (Figure 4(b)) and the Mulliken population is negative. The presence of metallic bond warrants (100)[010], (010)[100], (010)[001] and (001)[010] slips in Cr_2AlB_2 . In Cr_3AlB_4 , four B1 and two B2 atoms form a six-membered ring on (010) plane (Figure 4(c)). Since the B1–B2 bond is stronger than B1–B1 bond, the stiffness is the highest in [100] direction. On (100) plane, the metallic Cr1–B2 bond allows (010)[001] and (001)[010] slips (Figure 4(d)). In Cr_4AlB_6 , B1, B2 and B3 atoms form covalent honeycomb on (002) plane (Figure 4(e)). Since the B3–B3 bond is stronger than B2–B3 and B1–B2 bonds, the stiffness is the highest in [100] direction. On the (100) plane, the metallic B1–Cr2 and B2–Cr1 bonds allow slips along (010)[001] and (001)[010] (Figure 4(e)). The increase of stiffness with n in $(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$) is due to the increase of fractions of strong covalent B–B bonds with n .

In summary, MAB phases $(\text{CrB}_2)_n\text{CrAl}$ ($n = 1-3$) exhibit anisotropic electrical conductivity and elastic properties, low shear deformation resistance and damage-tolerant behavior similar to MAX phases. These properties are underpinned by the electronic structure and anisotropic chemical bonding. The anisotropic electrical conductivity is due to the anisotropic distribution of metallic Cr layers, which mainly contribute to the conductivity through their $3d$ states. High bulk and Young's moduli are originated from the strong covalent B–B bonds, while the low shear deformation resistance and easy slip are due to the presence of metallic Cr–B bonds adjacent to Al layers. The possible slip systems are (100)[010], (010)[100], (010)[001] and (001)[010] for Cr_2AlB_2 , (010)[001] and (001)[010] for Cr_3AlB_4 and Cr_4AlB_6 .

Disclosure statement

No potential conflict of interest was reported by the authors.

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