Electrical conductive and damage-tolerant nanolaminated MAB phases Cr$_2$AlB$_2$, Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$

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ABSTRACT

Theoretical investigations on electronic structure, chemical bonding and mechanical properties reveal that MAB phases (CrB$_2$)$_n$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 3$d$ 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$_2$AlB$_2$, (010)[001] and (001)[010] for Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$.

IMPACT STATEMENT

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

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 M$_{n+1}$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 machineable 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 (CrB$_2$)$_n$CrAl ($n = 1–3$). These materials are selected due
to the following reasons. Firstly, they contain B, Cr, Al, which can ‘smartly’ form protective B2O3, Cr2O3 and Al2O3 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 Å\(^{-1} \) 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 \( 5 \times 10^{-6} \) eV/atom, maximum ionic Hellmann–Feynman force within 0.01 eV/Å, maximum ionic displacement within \( 5 \times 10^{-4} \) Å 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 \((\text{CrB}_2)_n\text{CrAl} (n = 1–3)\) are shown in Figure 1. For \( \text{Cr}_2\text{AlB}_2 \) and \( \text{Cr}_4\text{AlB}_6 \), the space group is \( \text{Cmmm} \); while for \( \text{Cr}_3\text{AlB}_4 \), the space group is \( \text{Pmmm} \). 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 \((\text{CrB}_2)_n\text{CrAl} (n = 1–3)\) and the well-known MAX phases \( \text{Ti}_2\text{AlC} \), \( \text{Ti}_3\text{AlC}_2 \) and \( \text{Ti}_3\text{SiC}_2 \) 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] 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 \((\text{CrB}_2)_n\text{CrAl} (n = 1–3)\) in Table 2 show following features. Firstly, the elastic properties exhibit strong anisotropy. Secondly, the elastic constants that represent stiffness against principal tensile/compression strains are much higher than those against shear deformation strains. Thirdly, the

Figure 1. Crystal structures and the distribution of atoms on (002) and (100) plane of \( \text{Cr}_2\text{AlB}_2 \) (a–c), (010) and (100) plane of \( \text{Cr}_3\text{AlB}_4 \) (d–f), and (002) and (100) plane of \( \text{Cr}_4\text{AlB}_6 \) (g–i) (a 2 × 1 × 2 cell is used in (b–c) and (h–i) and a 2 × 2 × 1 cell is used in (e–f)).
Also be described by the directional dependence of

\[
\text{Cr}_4\text{AlB}_6 \quad 254 \quad 179 \quad 435 \quad 0.215 \quad 506 \quad 459 \quad 423 \quad 0.705
\]

\[
\text{Cr}_3\text{AlB}_4 \quad 237 \quad 182 \quad 440 \quad 0.203 \quad 479 \quad 450 \quad 421 \quad 0.746
\]

\[
\text{Cr}_2\text{AlB}_2 \quad 220 \quad 163 \quad 392 \quad 0.203 \quad 445 \quad 354 \quad 423 \quad 0.741
\]

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

\[
\frac{1}{E} = \frac{s_{11}I_1^4 + 2s_{12}I_1^2I_2^2 + 2s_{22}I_2^4 + 2s_{23}I_2^2I_3^2 + s_{33}I_3^4}{E_i}
\]

\[
+ 2s_{13}I_1^2I_3^2 + s_{44}I_2^4 + s_{55}I_1^2I_3^2 + s_{66}I_1^2I_2^2.
\]

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

| Compound    | \(\text{Cr}_2\text{AlB}_2\) | \(\text{Cr}_3\text{AlB}_4\) | \(\text{Cr}_4\text{AlB}_6\) |
|-------------|----------------|----------------|----------------|
| Space group  | \(\text{Cnmm}\) | \(\text{Pnmm}\) | \(\text{Cnmm}\) |
| Z formula units | 2       | 1            | 2            |
| Density (g/cm³) | 5.26   | 5.30        | 5.26        |

**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).\

| Bond      | Population | Length (Å) | Bond      | Population | Length (Å) | Bond      | Population | Length (Å) |
|-----------|------------|------------|-----------|------------|------------|-----------|------------|------------|
| B–B       | 1.60       | 1.7621     | B–B       | 1.64       | 1.7508     | B–B       | 1.84       | 1.7177     |
| B–Cr      | 0.58       | 2.1873     | B–Cr      | 0.73       | 1.7623     | B–Cr      | 0.75       | 1.7553     |
| B–Al      | –0.39      | 2.1984     | B–Cr      | –0.14      | 2.1366     | B–Cr      | –0.23      | 2.1215     |
| Al–Cr     | 0.50       | 2.2722     | B–Cr      | 0.57       | 2.1776     | B–Cr      | 0.51       | 2.1764     |
| Cr–Cr     | –0.76      | 2.7098     | B–Cr      | 0.20       | 2.2726     | B–Cr      | 0.43       | 2.2224     |

**Table 3.** Second-order elastic constants, bulk modulus, shear modulus, anisotropic Young’s modulus and Pugh’s ratio of \(\text{Ti}_2\text{AlC}, \text{Ti}_3\text{AlC}_2\) and \(\text{Ti}_3\text{SiC}_2\).\

| Compound | \(c_{11}\) | \(c_{12}\) | \(c_{13}\) | \(c_{44}\) | \(c_{55}\) | \(c_{66}\) | \(G/B\) |
|----------|-----------|-----------|-----------|-----------|-----------|-----------|--------|
| \(\text{Ti}_2\text{AlC}\) | 304       | 274       | 119       | 50        | 57        | 127       |
| \(\text{Ti}_3\text{AlC}_2\) | 355       | 292       | 123       | 71        | 68        | 142       |
| \(\text{Ti}_3\text{SiC}_2\) | 354       | 344       | 165       | 91        | 103       | 131       |

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

\[
\frac{1}{E} = s_{11}I_1^4 + 2s_{12}I_1^2I_2^2 + 2s_{22}I_2^4 + 2s_{23}I_2^2I_3^2 + s_{33}I_3^4
\]

\[
+ 2s_{13}I_1^2I_3^2 + s_{44}I_2^4 + s_{55}I_1^2I_3^2 + s_{66}I_1^2I_2^2.
\]
Figure 2. Projection of Young’s modulus and shear modulus on (100), (010) and (001) planes of Cr$_2$AlB$_2$ (a–b), Cr$_3$AlB$_4$ (c–d) and Cr$_4$AlB$_6$ (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$_2$AlB$_2$, Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$. For Cr$_2$AlB$_2$, strongest anisotropy is on (100) plane. The maximum Young’s modulus is $E_{\text{max}} = 445$ GPa in [100] direction, and the minimum one is $E_{\text{min}} = 332$ GPa, being 54° inclined to [100] direction (Figure 2(a)). For Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$, strongest anisotropy is on (001) plane. For Cr$_3$AlB$_4$, the maximum Young’s modulus is $E_{\text{max}} = 480$ GPa in [100] direction and the minimum one is $E_{\text{min}} = 378$ GPa, 48° inclined to the [010] axis (Figure 2(c)); while for Cr$_4$AlB$_6$, the maximum Young’s modulus is $E_{\text{max}} = 506$ GPa, and the minimum one is $E_{\text{min}} = 385$ GPa, 50° inclined to the [010] axis (Figure 2(e)).

(CrB$_2$)$_n$CrAl ($n = 1–3$) also exhibits low shear deformation resistance (Table 2). For example, Cr$_2$AlB$_2$ has both low $c_{44}$ (132 GPa) and $c_{66}$ (123 GPa), but Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$ exhibit low $c_{44}$ of 147 GPa and 148 GPa, respectively. These values are close to the $c_{44}$ of Ti$_2$AlC, Ti$_3$AlC$_2$ and Ti$_3$SiC$_2$ 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 (CrB$_2$)$_n$CrAl ($n = 1–3$). The shear modulus is related to the compliances as:

$$G'_{ij} = \frac{1}{4s'_{ij}},$$

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

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

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

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

The projection of shear modulus on (100), (001) and (010) planes are given in Figure 2. For Cr$_3$AlB$_2$, strong anisotropy is on (100) plane (Figure 2(b)). The lowest shear modulus ($G_{\text{min}} = 123$ GPa) is associated with (100)[010] and (010)[001] 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$_2$AlB$_2$. For Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$, strong anisotropy is also on (100) plane. The lowest shear moduli ($G_{\text{min}} = 147$ GPa for Cr$_3$AlB$_4$ (Figure 2(d)) and $G_{\text{min}} = 148$ GPa for Cr$_4$AlB$_6$ (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 (CrB$_2$)$_n$CrAl ($n = 1–3$) increases from 220 GPa for Cr$_2$AlB$_2$ and 237 GPa for Cr$_3$AlB$_4$ to 254 GPa for Cr$_4$AlB$_6$, which are close to those of UHTCs like TM$_2$B$_2$ (TM = Ti, Zr, Hf, Nb and Ta) [10] and NiB$_2$ [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$_2$AlB$_2$, Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$, 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$_2$AlB$_2$, Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$ 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$_2$AlC, Ti$_3$AlC$_2$ and Ti$_3$SiC$_2$, 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$_2$AlB$_2$, Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$ 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$_2$AlB$_2$, Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$ 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$_2$AlB$_2$ and Cr$_4$AlB$_6$, and (001) of Cr$_3$AlB$_4$. 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$_2$AlB$_2$ and Cr$_4$AlB$_6$, and (001) of Cr$_3$AlB$_4$, such that the electrical conductivity is higher on these planes. Figure 3 also provides some stability information. For Cr$_2$AlB$_2$, the Fermi level is below the top maximum of the valence band, indicating incomplete filling of the valence bands. For Cr$_3$AlB$_4$ and Cr$_4$AlB$_6$, however, the Fermi level is located at the local minimum,
Figure 3. Band structure, TDOS and PDOS of Cr$_2$AlB$_2$ (a–b), Cr$_3$AlB$_4$ (c–d) and Cr$_4$AlB$_6$ (e–f).
**Figure 4.** Electron density difference maps on (002) and (100) planes of Cr$_2$AlB$_2$ (a–b), (010) and (100) planes of Cr$_3$AlB$_4$ (c–d) and (002) and (100) planes of Cr$_4$AlB$_6$ (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 (CrB2)nCrAl (\(n = 1–3\)). Figure 4 shows the electron density difference maps, which illustrate the charge redistribution due to chemical bonding, on (002) and (100) planes of Cr2AlB2, (010) and (100) planes of Cr3AlB4 and (002) and (100) planes of Cr4AlB6. Similar to NiB [24], the bonding in the zigzag B–B chains of Cr2AlB2 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 c11 and E\(_c\)). 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 Cr2AlB2. In Cr3AlB4, 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 Cr4AlB6, 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 (CrB2)nCrAl (\(n = 1–3\)) is due to the increase of fractions of strong covalent B–B bonds with \(n\).

In summary, MAB phases (CrB2)nCrAl (\(n = 1–3\)) 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 3\(d\) 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 Cr2AlB2, (010)[001] and (001)[010] for Cr3AlB4 and Cr4AlB6.

**Disclosure statement**

No potential conflict of interest was reported by the authors.

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