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First-principles study of the ideal cleavage fracture of Cr_2Nb microalloyed by X (Al, Ni, Co, Ti)

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ABSTRACT

The structural properties and elastic constants of the pure Cr_2Nb, the ideal cleavage fracture properties of the Cr_2Nb with the elements X (Al, Ni, Co and Ti) and site preference of the elements X were investigated using the first-principles method. Our calculated lattice parameters and elastic constants of the pure Cr_2Nb are in agreement with the experimental data. Moreover, our calculated results show that the elements X (Al, Ni and Co) occupy the Cr site, and Ti the Nb site in Cr_2Nb. The cleavage energies G_c and critical cleavage stress σ_c with and without the additive elements in the cleavage planes were calculated. The results demonstrate that the elements X (Al, Ni, Co and Ti) could be used to improve the cleavage properties of Cr_2Nb. Finally, the electronic mechanism behind the effects of the additive elements on the ideal cleavage properties of Cr_2Nb was investigated by calculating the electronic structure.

1. Introduction

Laves phases have been attractive for their important applications, such as superconductors, giant magnetostrictive materials and hydrogen storage materials [1,2]. Laves phases are also promising candidates for high-temperature materials due to their high melting point, low density, and good oxidation resistance [3–6]. Cr_2Nb with the C15 cubic structure is a typical Laves phase compound and has many applications due to its attractive properties, such as high melting point (1770 °C), high creep resistance and good oxidation resistance [7,8]. However, the Cr_2Nb compound is very brittle at low and ambient temperatures. Therefore, many studies have been conducted to investigate the mechanical properties of Cr_2Nb in both the experimental and theoretical fields.

From the experimental aspect, Takeyama and Liu [7] examined the mechanical properties of Laves phase alloys based on Cr_2Nb under the high temperature and correlated with microstructures and phase relationships. Kazantzis et al. [8] and Morais Smith et al. [9] investigated the stacking-fault energy, the high temperature mechanical properties and the deformation mechanisms of the Cr_2Nb, respectively. Lee et al. [10] studied the cracking in Cr–Cr_2Nb eutectic alloys due to thermal stresses. The microstructure and mechanical properties of Cr_2Nb with the additive elements X (Re, Al, Ni, Co, V, Mo and Ti) have also been studied [11–13]. The results showed that the elements V and Mo were effective in improving the high temperature deformability, and Re was effective in improving the mechanical properties at room and elevated temperatures. However, alloying with $\geq$ 8% Al, Ni and Co lowers the strength and ductility at elevated temperatures. Ti can slightly increase the toughness of Cr_2Nb. Moreover, Okaniwa et al. [14] investigated the site occupancy of additives V, Mo, W, and Ti in the Cr_2Nb using the atom location by channeling enhanced microanalysis method. From the theoretical aspect, Mayer et al. [15] and Ormeci et al. [16] calculated the elastic constants and electronic structure of Cr_2Nb using the linear muffin-tin orbital method, respectively. At the same time, they also estimated the bulk modulus, Young's modulus, and Poisson's ratio. Hong et al. [17,18] investigated the phase stability, elastic modulus, heat of formation, and the thermoelastic properties of Cr_2Nb using the first-principles calculations. Chan [19] studied the effect of elements Ge and Si on the fracture toughness of Cr_2Nb. The result showed that Ge and Si can improve the fracture toughness of Cr_2Nb. Rosch et al. [20] calculated the elastic constants and reported on the fitting and validation of potentials specifically generated for the fracture of C15 Cr_2Nb. Kellou et al. [21] studied the structural, electronic, and thermal properties of Cr_2Nb using the full-potential linearized

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augmented plane waves method. Yao et al. [22] and Jiang [23] investigated the site occupancy behaviors of ternary additions, such as Ti, V, Zr, Mo, and W in Cr_2Nb, respectively. At the same time, Yao et al. [24] also investigated the defects, elastic properties, and electronic structure of Cr_2Nb. It can be seen that the theoretical study of the mechanical properties of Cr_2Nb is mainly focused on elastic constants, such as shear modulus and Poisson's ratio using the first-principles. There are a few theoretical studies about the effects of the additive elements on the mechanical properties of Cr_2Nb. Although Chan investigated the alloying (Ge and Si) effects on the fracture toughness of Cr_2Nb, he did not provide the electronic mechanism behind the effects of the alloy on the fracture toughness.

Although the fracture is caused by the macroscopic stress field, there is no doubt that at the atomistic level the crack advances by sequential breaking of individual bonds between atoms. This small portion of the total crack energy can still control the whole fracture process [25]. The first-principles method can provide important information at atomic level free from any parameters. Basically, the additive element can alter the electronic structure and bonding nature, which in turn affect the physical and mechanical properties of the materials. The first-principles method has the capability to describe the properties that are determined from the electronic structure. Therefore, it can elucidate the intrinsic effect of the additive element. Moreover, compared with the experimental studies, the theoretical studies are not affected by some uncontrollable factors, such as constitutional defect, impurity content and heat treatment. Of course, the theoretical simulation also neglects many processes at the macroscopic level e.g. the solubility and the interaction of dopants. At present, the first-principles method has been widely used to study material fracture, and provide microscopic insights into the mechanical behavior of solid materials at the atomic level [26–30].

In this paper, the ideal cleavage fracture properties of Cr_2Nb with the elements X (Al, Ni, Co and Ti) were investigated by means of the calculation of the cleavage energies G_c and critical cleavage stress σ_c in the framework of the density functional theory within the generalized gradient approximation. The low cleavage strength is one of the main causes of brittleness in the intermetallic systems. The principal objective of this work is to understand the electronic mechanism behind the effects of the additive elements on the ideal cleavage fracture in Cr_2Nb.

2. Computational method

The calculations were performed using the plane-wave pseudopotential method based on density functional theory (DFT). The generalized gradient approximation (GGA) in the scheme of Perdew–Burke–Ernzerhof [31] was used for the exchange and correlation correction. The structural optimizations were conducted using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization. Charge population was calculated according to the formalism described by Segall et al. [32]. A plane-wave cutoff energy of 400 eV was employed throughout the calculation. For the sampling of the Brillouin zone, the total energy and the electronic structures used an $8 \times 8 \times 1$ k-point grid generated according to the Monkhorst–Pack scheme [33]. The elastic constants were calculated by the 'stress–strain' method.

The ideal cleavage fracture was modeled by a repeated slab construction of atomic layers with three-dimensional translational symmetry. Convergency of the cleavage energy as a function of the slab thickness has been tested. As is shown in Fig. 1, it contains two "slab" and each slab consists of four layers of (1 0 0) planes of Cr_2Nb. The elements X (Al, Ni, Co and Ti) were introduced into the cleavage planes of Cr_2Nb through the substitution of X for the Cr or Nb atoms. It is implicitly supposed that cleavage is initiated in a plane

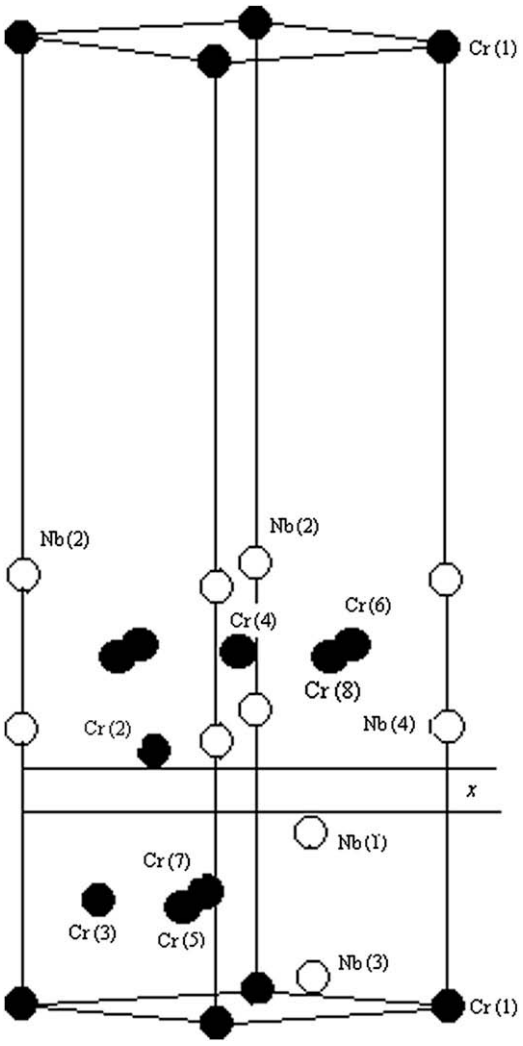

Fig. 1. Model used in the cleavage calculation.

including the additive elements. The ideal cleavage energy G_c is given by $G_c = 2r_s$, where r_s is the surface energy of the two cleaved surface planes. The critical stress σ_c is calculated by $\sigma_c = G_c/el$, where l is critical length. The solving of parameter l depends on the so-called universal binding energy relation (UBER) [34]. The UBER describes the energy-separation law by

$$E_b(x) = -G_c[(1 + x/l)\exp(-x/l) - 1].$$

The change of total energy $E(x)$ with increasing separation x is obtained from DFT total energies.

3. Results and discussion

3.1. Geometry optimization and elastic constants

Cr_2Nb belongs to the space group *Fd*-3*m* (227). There are two Cr_2Nb groups (six atoms) per primitive cell. Niobium and chromium occupy 2a in (0, 0, 0) and 4d in (0.625, 0.625, 0.625) sites, respectively. The crystal structure is optimized by force and energy minimization. The lattice parameters, bulk modulus, and elastic constants were calculated and compared with the experimental and available theoretical results. We also calculated the shear modulus and Poisson's ratio of the pure Cr_2Nb. The results are summarized in Table 1. It can be seen that our calculated lattice parameter and bulk modulus are in good agreement with the

Table 1
The calculated and experimental lattice parameters (Å), bulk modulus B (GPa), shear modulus G, Poisson's ratio υ, and elastic constants (GPa) of Cr_2Nb.

	a (Å)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)	G	υ
DFT–GGA[a]	6.94	308	205	67	239	61	0.39
NFP–LDA[b]	6.85	322	199	69	243		
NFP–GGA[b]	6.92	317	185	83	229	76	0.37
LAPW–LDA[c]	6.82	316	216	71	252	62	0.38
DFT–GGA[d]	6.97	309	198	69	235		
Experimental[e]	6.99				229		

[a] This work.
[b] Ref. [15].
[c] Ref. [17].
[d] Ref. [18].
[e] Ref. [35].

experimental data. Moreover, the calculated elastic constants are also closer to other theoretical results.

3.2. Site preference of the elements X (Al, Ni, Co, Ti)

The energy of formation was calculated because it can directly reflect the site occupancy behaviors of the elements X (Al, Ni, Co and Ti) in Cr_2Nb. The energy of formation is defined as

$$\Delta E = E(Cr_3XNb_2) - 3E(Cr) - E(X) - 2E(Nb) \quad (X \text{ on the Cr site})$$

$$\Delta E = E(Cr_4NbX) - 4E(Cr) - E(X) - E(Nb) \quad (X \text{ on the Nb site})$$

where $E(Cr_3XNb_2)$, $E(Cr_4NbX)$, $E(Cr)$, $E(X)$, and $E(Nb)$ are the total energies of Cr_3XNb_2, Cr_4NbX, the pure Cr, X (Al, Ni, Co and Ti) and Nb bulk metals, respectively. The results are shown in Table 2. It can be seen that X (Ni and Co) preferentially occupy the Cr sites, and Al has a weak site preference for the Cr site, while Ti has a weak site preference for the Nb site in Cr_2Nb. The result is in accordance with the experimental result.

3.3. Ideal cleavage fracture

We calculated the cleavage energy G_c and critical stress σ_c of (1 0 0), (1 1 0), and (1 1 1) planes of Cr_2Nb, respectively. The results are given in Table 3. For pure Cr_2Nb, we obtained the lowest energy $G_c = 5.68\ J/m^2$ and also the lowest critical stress $\sigma_c = 34.79$ GPa which indicate that the (1 1 1) cleavage is preferred. In contrast to the (1 1 1) plane, the (1 1 0) plane is the most stable due to its highest energy $G_c = 6.78\ J/m^2$ and also highest critical stress $\sigma_c = 42.45$ GPa. The result indicates that the cutting Cr–Nb bonds depend strongly on the orientation of the cleavage planes. Furthermore, it can be seen that the elements X (Al, Ni and Co) on Cr sites reduce the ideal cleavage energy and critical stress of the pure Cr_2Nb system, respectively. Therefore, the elements X (Al, Ni and Co) on Cr sites could decline the cleavage strength of the Cr_2Nb system. The result is consistent with the experimental findings that alloying with Al, Ni, and Co can reduce the cleavage strength of Cr_2Nb. Among these elements, the element Ni on Cr site influences the cleavage properties of Cr_2Nb significantly, and Co on Cr site influences the cleavage properties less significantly. It is important to notice, for (1 0 0) plane, that while Ti on Nb site reduces the ideal cleavage energy of the Cr_2Nb system, it increases its critical stress. For (1 1 0) and (1 1 1) planes, Ti on Nb increases the cleavage energy and critical stress of the Cr_2Nb system, respectively. Therefore, we concluded that Ti on Nb site could enhance the cleavage strength of Cr_2Nb.

Table 2
The energy of formation ΔE (eV) and site occupancy behaviors of the additive elements X (Al, Ni, Co and Ti) in Cr_2Nb.

	ΔE	Theoretical site occupancy[a]	Experimental[b]
Al_{Nb}	−54.8	Cr site	
Al_{Cr}	−55.13		
Ni_{Nb}	−56.89	Cr site	
Ni_{Cr}	−58.48		
Co_{Nb}	−57.73	Cr site	
Co_{Cr}	−59.43		
Ti_{Nb}	−57.88	Nb site	Nb site
Ti_{Cr}	−57.61		

[a] This work.
[b] Refs. [14] and [36].

Table 3
The calculated cleavage energy G_c (J/m^2), critical length l (Å), and critical stress σ_c (GPa).

($h\,k\,l$)		G_c	l	σ_c
(1 0 0)	Cr_2Nb	6.14	0.64	35.27
	Ni_{Cr}	5.28	0.65	29.86
	Al_{Cr}	5.49	0.67	29.99
	Al_{Nb}	5.57	0.66	30.89
	Co_{Cr}	5.69	0.69	30.23
	Ti_{Cr}	5.78	0.67	31.58
	Ti_{Nb}	5.63	0.58	35.56
(1 1 0)	Cr_2Nb	6.78	0.59	42.25
	Ni_{Cr}	6.48	0.68	35.03
	Al_{Cr}	6.50	0.68	35.14
	Al_{Nb}	6.15	0.59	38.19
	Co_{Cr}	6.54	0.65	36.93
	Ti_{Cr}	6.49	0.64	37.17
	Ti_{Nb}	6.96	0.60	42.65
(1 1 1)	Cr_2Nb	5.68	0.60	34.79
	Ni_{Cr}	5.17	0.61	31.37
	Al_{Cr}	5.21	0.58	32.91
	Al_{Nb}	4.98	0.58	31.84
	Co_{Cr}	5.45	0.62	32.58
	Ti_{Cr}	5.46	0.62	32.43
	Ti_{Nb}	5.97	0.63	34.83

Al and Ti have a weak site preference for the Cr and Nb sites in Cr_2Nb, respectively. Therefore, we also calculated the cleavage energy and critical stress for Al on Nb site and Ti on Cr site. The results are also shown in Table 3. It can be seen that Al on Nb site can also reduce the ideal cleavage energy and critical stress of Cr_2Nb system. The result indicates that the effect of the element Al on the strength and stability of Cr_2Nb does not depend on its site preference in Cr_2Nb. In contrast to Ti on Nb site, Ti on Cr site reduces the ideal cleavage energy and critical stress of Cr_2Nb system. Therefore, the effect of the element Ti on the strength and stability of Cr_2Nb depends strongly on its site preference in Cr_2Nb.

3.4. Electronic structure

The investigation of electronic structure can provide microscopic insights into the mechanical behavior of solid materials. In order to understand the electronic mechanism behind the effects of the elements X (Al, Ni, Co and Ti) on the ideal cleavage fracture in Cr_2Nb, it is important to study the density of states (DOS) and charge population of the Cr_2Nb with and without the elements X. We used the electronic structure of the (1 0 0) plane of Cr_2Nb as an example to discuss the electronic mechanism behind the effects of the additive elements. In Fig. 2(a)–(c), we show the DOS of the Cr_2Nb with and without the elements X (Al, Ni and Co) on Cr sites, respectively. Fig. 2(d) shows the DOS of the Cr_2Nb with and without the element Ti on Nb sites. The solid lines represent the DOS of the Cr_2Nb with the additive elements. The dotted lines represent the

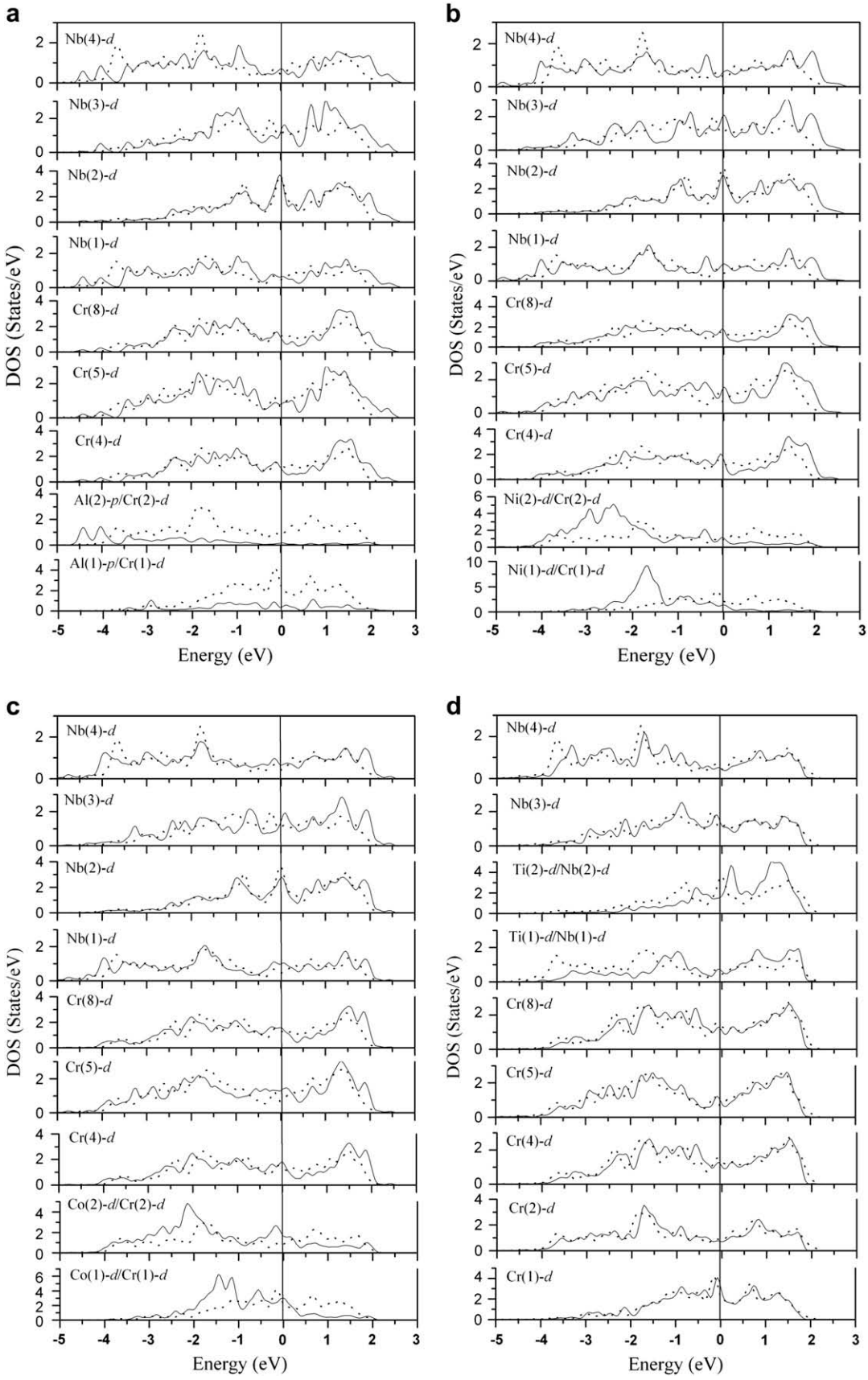

Fig. 2. The calculated DOS of the pure Cr_2Nb (dotted lines) and Cr_2Nb with the additive elements X (Al, Ni, Co and Ti) (solid lines); (a) Cr_3AlNb_2, (b) Cr_3NiNb_2, (c) Cr_3CoNb_2, (d) Cr_4NbTi.

Table 4
The charge population (e) of Cr_2Nb with and without the additive elements X (Al, Ni, Co and Ti).

Cr_2Nb		Cr_3NiNb_2		Cr_3AlNb_2		Cr_3CoNb_2		Cr_4NbTi	
Species	Charge	Species	Charge	Species	Charge	Species	Charge	Species	Charge
Cr (1)	−0.28	Ni (1)	0.1	Al (1)	0.22	Co (1)	0.26	Cr (1)	−0.27
Cr (2)	−0.04	Ni (2)	0.02	Al (2)	0.01	Co (2)	0.11	Cr (2)	−0.11
Cr (3)	−0.16	Cr (3)	−0.25	Cr (3)	−0.3	Cr (3)	−0.25	Cr (3)	−0.2
Cr (4)	−0.36	Cr (4)	−0.32	Cr (4)	−0.35	Cr (4)	−0.33	Cr (4)	−0.48
Cr (5)	−0.16	Cr (5)	−0.25	Cr (5)	−0.30	Cr (5)	−0.25	Cr (5)	−0.2
Cr (6)	−0.36	Cr (6)	−0.32	Cr (6)	−0.34	Cr (6)	−0.33	Cr (6)	−0.48
Cr (7)	−0.16	Cr (7)	−0.25	Cr (7)	−0.3	Cr (7)	−0.25	Cr (7)	−0.2
Cr (8)	−0.36	Cr (8)	−0.33	Cr (8)	−0.35	Cr (8)	−0.33	Cr (8)	−0.48
Nb (1)	0.79	Nb (1)	0.61	Nb (1)	0.63	Nb (1)	0.58	Ti (1)	1
Nb (2)	0.15	Nb (2)	0.25	Nb (2)	0.21	Nb (2)	0.23	Ti (2)	0.57
Nb (3)	0.06	Nb (3)	0.07	Nb (3)	0.15	Nb (3)	−0.05	Nb (3)	0.07
Nb (4)	0.87	Nb (4)	0.67	Nb (4)	0.71	Nb (4)	0.63	Nb (4)	0.78

DOS of the pure Cr_2Nb system. From Fig. 2(a), we found that the overlap between the Al p states and Cr d and Nb d states is significantly reduced, indicating a weaker hybridization between the Al atoms and Cr and Nb atoms. Therefore, the element Al can weaken the metal–metal bond charge network, thereby lowering the strength of Cr_2Nb. From Fig. 2(b) and (c), it can be seen that the elements Ni and Co also weaken the metal–metal bond charge overlap. Both Ni and Co appear some sharp peaks at 2.92 eV, 2.41 eV, 1.68 eV, 2.13 eV, 1.45 eV, and 1.17 eV, respectively, and yet the corresponding peaks of both Cr and Nb are reduced. Thus, the overall hybridization is weakened. This explains why the elements Ni and Co also decline the cleavage strength of Cr_2Nb. On the other hand, as can be seen in Fig. 2(d), the element Ti can increase the overlap between the Ti d states and Cr d and Nb d states, indicating a strong hybridization between the Ti atoms and Cr and Nb atoms. However, we also found that some peaks of the Ti (1) and Ti (2) d states are a little lower than Nb (1) and Nb (2) d states, respectively. This is the reason that the element Ti can enhance the cleavage strength of Cr_2Nb less significantly. Therefore, we look forward to finding a kind of element that can enhance the cleavage strength of Cr_2Nb significantly in the future.

In the following, in order to gain insight at the microscopic level into the effects of the additive elements on the ideal cleavage fracture in Cr_2Nb, we also calculated the charge population of the Cr_2Nb with and without the elements X (Al, Ni and Co) on Cr sites and Ti on Nb site. As it can be seen clearly in Table 4, comparing with the Cr (1) and Cr (2) of the pure Cr_2Nb system, the elements X (Al and Ni) give rise to the depletion of charge, thereby reducing the hybridization between the X (Al and Ni) atoms and Nb and Cr atoms. Although the Co (2) accumulated a little charge, the overlapped charge between the Nb and Cr atoms is depleted. Moreover, the charge depletion between the Nb and Cr atoms is larger than the charge accumulation between the Co (2) and Cr atoms. Therefore, the elements X (Al, Ni and Co) can lower the strength of Cr_2Nb. The Co (1) and Co (2) depleted and accumulated charge, respectively, so that Co influences the cleavage properties significantly less than the elements Al and Ni. In contrast to the elements X (Al, Ni and Co), comparing with the Nb (1) and Nb (2) of the pure Cr_2Nb, the element Ti gives rise to charge accumulation between the Ti and Cr atoms, thereby strengthening the metal–metal bond charge network. Thus, the Ti can enhance the strength of Cr_2Nb. These results are consistent with our calculated DOS.

4. Summary and conclusions

In summary, we have performed first-principles density functional calculation of the structural properties and elastic constants of the pure Cr_2Nb, site preference of the elements X (Al, Ni, Co and Ti), and the ideal cleavage fracture properties of the Cr_2Nb with and without the elements X (Al, Ni, Co and Ti). The results showed that the elements X (Ni and Co) preferentially occupy the Cr site, and Al has a weak site preference for the Cr site, while the element Ti has a weak site preference for the Nb site in Cr_2Nb. The elements X (Al, Ni, Co and Ti) on Cr sites and Al on Nb site can reduce the cleavage strength of Cr_2Nb, while Ti on Nb site can enhance the cleavage strength of Cr_2Nb. These results are in good agreement with the experimental and available theoretical data. The results also indicated that the effect of the element Al on the strength of Cr_2Nb does not depend on its site preference, while Ti depends on its site preference in Cr_2Nb. In order to understand the electronic mechanism behind the effects of the elements X (Al, Ni, Co and Ti) on the ideal cleavage fracture in Cr_2Nb, we also calculated the DOS and charge population of the Cr_2Nb with and without the additive elements X (Al, Ni, Co and Ti). The result indicates that the elements X (Al, Ni and Co) can weaken hybridization between the X (p/d) states and Cr d and Nb d states, while the element Ti gives rise to a strong hybridization between the Ti d states and Cr d and Nb d states. This explains why the elements X (Al, Ni, Co and Ti) can change the cleavage strength of Cr_2Nb.

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