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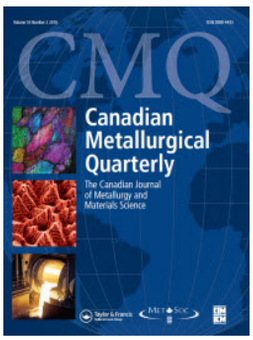

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Effects of ternary elements on the ductility of TiAl

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TiAl alloys have great potential for applications at high temperature due to their excellent material properties. However, the low ductility at the room-temperature restricted its application greatly. It is very important to find approaches of improving the ductility of the material. In this study, effects of ternary elements (Zr, Hf, V, Nb, Ta, Cr, Mo, W, Cu and Zn) on the ductility of TiAl were investigated by first-principle calculations. Results revealed that the addition of the atoms of Zr, Hf, Cu and Zn could improve the ductility of TiAl by changing the lattice parameter, the electronic structure, and the elastic constants of TiAl. The calculation results can be used as a reference for selecting alloying elements for ductility improvement of TiAl alloys.

Alliages TiAl ont des grand applications potentielles dans les zones de température élevée en raison de leurs performances excellentes. Cependant, leur faible ductilité à la température ambiante limitent leurs applications sérieusement.Donc, la méthode de améliorer la ductilité des alliages TiAl se trouve a une grande importance. Ce article calcule les affecters des éléments des alliages (Zr, Hf, V, Nb, Ta, Cr, Mo, W, Cu et Zn) effets sur les alliages TiAl par les premiers principes.Le résultat déclare que Zr, Hf, Cu et Zn peuvent améliorer le ductilité par améliorer les paramètres de maille, structure électronique,et constantes élastiques des alliages TiAl.Le résultat est une référence pour sélectionner le élément pour améliorer les alliages TiAl.

Keywords: Intermetallic compounds, Ab initio calculations, TiAl alloys

Introduction

TiAl (space group P4/mmm, prototype AuCu) has been considered as a candidate material suitable for high-temperature applications due to its high melting point, low density, relatively high hardness, and good oxidation and creep resistance.[1–4] However, applications of TiAl have been severely restricted due to its low ductility at the room-temperature. This weakness can be attributed to the fact that its tetragonal $L1_0$ crystal structure and strong directional chemical bonds lead to difficulties in the activation of slip systems and anisotropy of coefficient of thermal expansion (CTE). Consequently, many methods have been used to improve the ductility of TiAl, including heat treatment, grain refinement, element alloying, as well as the introduction of a second reinforcing phase to fabricate composites, etc.[5–10] Among various methods, element alloying is a simple but quite effective way of improving the ductility of TiAl.[11–14] To economically and effectively design new alloys without using the traditional trial and error method, it is important to study the alloying effect on the properties of TiAl at the atomic and electronic level.

Recently, first-principle calculations have been used to investigate the property of TiAl. However, most studies are focused on the occupation sites of alloying elements in TiAl.[15–17] Calculations on the relationship between the ternary element addition and the ductility of TiAl are limited. Jiang et al. investigated the effect of some transition metal elements on the ductility of TiAl from the aspect of lattice distortion (c/a ratio).[18] Music *et al.* investigated the effect of some transition metal elements (V, Nb, Ta, Cr, Mo, W and Mn) on the ductility of TiAl in terms of elastic properties (bulk-modulus-to-C_{44} ratio). They reported that the largest bulk-modulus-to-C_{44} ratio for TiAl was obtained for the Mn substitution, which possessed the most obvious effect on the ductility

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of TiAl.[19] However, no investigation has been reported regarding to the influence of element additions on the ductility of TiAl from systematical study of the lattice parameter, electronic structure and elastic constants.

In this regard, in order to offer a great insight into the intrinsic ductility of TiAl, the first-principle calculation was employed to systematically study the effect of the addition of different ternary elements (Zr, Hr, V, Nb, Ta, Cr, Mo, W, Cu and Zn) on the ductility of TiAl at the atomic level. This will provide a theoretical basis for the selection of alloying elements.

Calculation setup

The calculation was performed on a 32-atom supercell with the Cambridge Sequential Total Energy Package code (CASTEP),[20,21] in which the plane-wave pseudopotential total energy method was utilised. Ultrasoft pseudopotentials were used to present the interactions of electrons with ion cores.[22] Brillouin zone was set within a $3 \times 3 \times 3$ k point mesh generated by the Monkhorst-Pack scheme.[23] The plane-wave basis cutoff was set as 400 eV for all cases. More precise calculations with a plane-wave cutoff energy of 450 eV have also been performed. The results are very similar to the 400 eV cases. Therefore, the value of 400 eV for plane-wave cutoff energy is precise enough for the investigation.

Results and discussion

Site occupancy

The effects of alloying elements on the lattice parameter, electronic structure and elastic constants of TiAl would be largely influenced by their site occupation in TiAl. Thus, it is necessary to identify the site preference of them first. To identify the crystal site (Ti or Al) of TiAl that the atoms prefer to occupy, the formation enthalpies occupying Ti and Al sites in the $Ti_{16}Al_{16}$ supercell were calculated by the first-principle calculation. The formation enthalpies H_f, an estimation of the structural stability, were calculated according to the definition: $H_f = E_t - n_{Ti}E^{Ti}_{solid} - n_{Al}E^{Al}_{solid} - n_{Me}E^{Me}_{solid}$.[24,25] E_t is the total energy, and the values of E_t for $Ti_{16}Al_{15}Me$ and $Ti_{15}Al_{16}Me$ (Me = Zr, Hr, V, Nb, Ta, Cr, Mo, W, Cu and Zn) were calculated and listed in Table 1. n_{Ti}, n_{Al} and n_{Me} are the total number of Ti, Al and the substitutional atoms in the $Ti_{16}Al_{15}Me$ or $Ti_{15}Al_{16}Me$ supercell, respectively. E^{Ti}_{solid}, E^{Al}_{solid} and E^{Me}_{solid} are the corresponding total energies of the atoms calculated by using their most stable structures, and the calculated values of E^{Ti}_{solid} and E^{Al}_{solid} are –1603.12 eV and –56.48 eV, respectively.

Table 1 Calculated E_t, ΔH_f and the site occupancy of the substitutional atoms in TiAl

Atoms	$E_{Ti_{15}Al_{16}Me}$ (eV)	$E_{Ti_{16}Al_{15}Me}$ (eV)	ΔH_f	Site preference
Zr	–26244.37	–27789.83	–1.18	Ti
Hf	–25372.01	–26917.53	–1.12	Ti
V	–26939.47	–28485.41	–0.7	Ti
Nb	–26514.90	–28060.58	–0.96	Ti
Ta	–25100.49	–26646.18	–0.95	Ti
Cr	–27430.20	–28976.49	–0.35	Ti
Mo	–26899.95	–28446.04	–0.55	Ti
W	–26896.71	–28442.90	–0.45	Ti
Cu	–6309.42	–27856.04	–0.02	Ti
Zn	–26672.57	–28219.30	0.09	Al

Thus, the formation enthalpies of $Ti_{15}Al_{16}Me$ and $Ti_{16}Al_{15}Me$ supercells are defined as follows:

$$H_{Ti_{15}Al_{16}Me} = E_{Ti_{15}Al_{16}Me} - 15E^{Ti}_{solid} - 16E^{Al}_{solid} - E^{Me}_{solid} \quad (1)$$

$$H_{Ti_{16}Al_{15}Me} = E_{Ti_{16}Al_{15}Me} - 16E^{Ti}_{solid} - 15E^{Al}_{solid} - E^{Me}_{solid} \quad (2)$$

The formation enthalpy difference (ΔH_f) between $H_{Ti_{15}Al_{16}Me}$ and $H_{Ti_{16}Al_{15}Me}$ are calculated as follows:

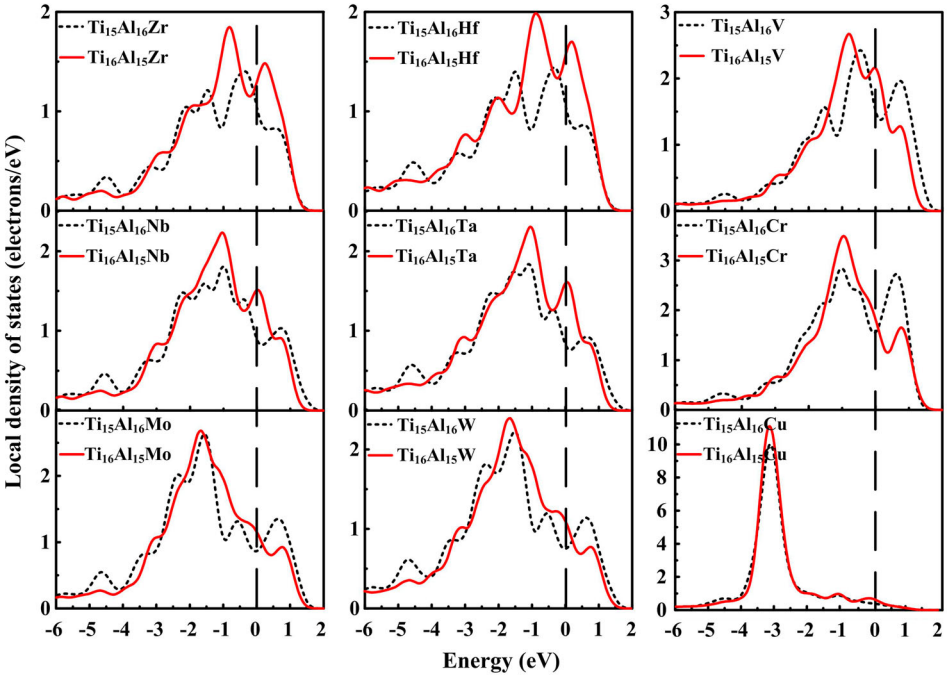
$$\Delta H_f = H_{Ti_{15}Al_{16}Me} - H_{Ti_{16}Al_{15}Me} = E_{Ti_{15}Al_{16}Me} - E_{Ti_{16}Al_{15}Me} + E^{Ti}_{solid} - E^{Al}_{solid} \quad (3)$$

If the formation enthalpy is more negative, it means that the structure is more stable. Thus, when the calculated value of ΔH_f is positive, it represents the substitutional atom prefers to occupy the Al site. Otherwise, it represents the substitutional atom prefers to occupy the Ti site. Table 1 lists the values of the formation enthalpy difference (ΔH_f) between the substitutional atoms occupying Ti and Al sites. It can be seen that the $Ti_{15}Al_{16}Me$ (Me = Zr, Hf, V, Nb, Ta, Cr, Mo, W and Cu) structure possesses the lower formation enthalpies, indicating the more stable structure. Moreover, according to the PDOS of the atoms of Zr, Hf, V, Nb, Ta, Cr, Mo, W and Cu occupying Ti and Al sites in the $Ti_{16}Al_{16}$ supercell as shown in Fig. 1, the numbers of electronic states on the Fermi level of Al^{Me} are lower than those of Ti^{Me}, indicating the more stable structure of $Ti_{15}Al_{16}Me$ (Me = Zr, Hf, V, Nb, Ta, Cr, Mo, W and Cu). It can be confirmed that the atoms of Zr, Hf, V, Nb, Ta, Cr, Mo, W and Cu prefer to occupy the Ti site. While the Zn prefers to occupy the Al site in TiAl, because the formation enthalpy of $Ti_{16}Al_{15}Zn$ is more negative.

The substitution of Al or Ti by the substitutional atoms would cause the changes of the lattice parameter, electronic structure and elastic constants of TiAl. These aspects will be discussed in detail in the following sections.

Lattice parameter

TiAl is an intermetallic compound with an ordered $L1_0$-type crystal structure, with the parameter of c-axes is a little larger than that of a-axes. It has been proposed that the lattice tetragonality of TiAl is one of the basic characteristics that relate to the intrinsic brittleness.[16,26] The lattice parameters of TiAl with and without substitutional atoms were calculated by the first-principle calculation, and shown in Table 2. From the results it can be seen that with the addition of Zr and Hf atoms, the lattice parameters of a-axes



1 Local density of states (LDOS) with different occupying sites by the substitutional atoms in the supercell

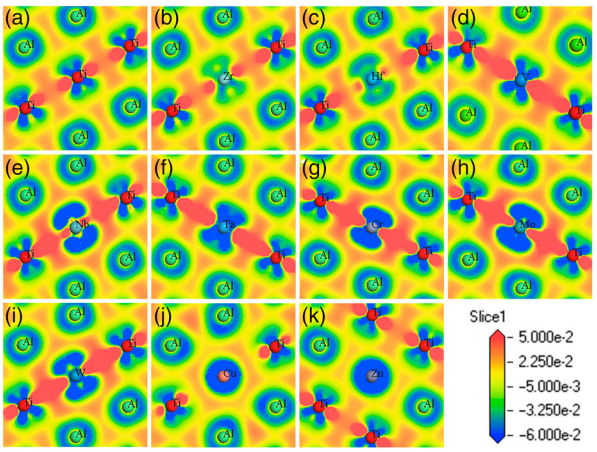
and *c*-axes increased simultaneously, leading to the increase of the crystal volume (V). In the same time, the *c*/*a* ratios of the crystal lattice decreased with the addition of Zr and Hf atoms. With the addition of Cu atoms, the lattice parameters of *a*-axes and *c*-axes decreased simultaneously, leading to the decrease of the V. Meanwhile, the *c*/*a* ratio of the crystal lattice decreased with the addition of Cu atoms. With the addition of V, Nb, Ta, Cr, Mo and W atoms, the lattice parameters of *a*-axes decreased, while the lattice parameters of *c*-axes increased, leading to the increase of the *c*/*a* value. With the addition of Zn atoms, it showed little effect on the *a*-axes of TiAl, while greatly reduced the lattice parameter of *c*-axes. The contraction of the *c*-axes reduced the *c*/*a* ratio of the crystal lattice.

The additions of the substitutional atoms would also cause the changes of the density of TiAl. The atomic weights of the substitutional atoms (Zr, Hr, V, Nb, Ta, Cr, Mo, W, Cu and Zn) are all larger than those of Ti and Al. So the substitution of Al or Ti by the substitutional atoms would increase the weight of the supercell. As shown in Table 2, with the addition of Zr, Hr, V, Nb and Ta atoms, the crystal volume increased. Thus, the addition of Zr, Hr, V, Nb and Ta atoms would have little effect on the density of TiAl. However, with the addition of Cr, Mo, W, Cu and Zn atoms, the crystal volume decreased. Thus, the addition of Cr, Mo, W, Cu and Zn atoms would increase the density of TiAl.

From the discussion above, it can be found that the addition of the atoms of Zr, Hf, Cu and Zn can reduce the value of *c*/*a* ratio of the crystal lattice, and therefore reduce the lattice tetragonality of TiAl. The reduced lattice tetragonality is believed to be beneficial to the ductility improvement because new glide systems could be activated.

Table 2 Lattice parameters of the $Ti_{16}Al_{16}$, $Ti_{15}Al_{16}Me$ and $Ti_{16}Al_{15}Me$ calculated by first-principles calculation

Sample	*a* (Å)	*c* (Å)	*c*/*a*	*V* (Å^3)
$Ti_{16}Al_{16}$	4.006	4.052	1.012	65.027
$Ti_{15}Al_{16}Zr$	4.024	4.065	1.010	65.823
$Ti_{15}Al_{16}Hf$	4.024	4.061	1.009	65.758
$Ti_{15}A1_{16}V$	3.986	4.060	1.019	64.506
$Ti_{15}Al_{16}Nb$	4.001	4.071	1.017	65.169
$Ti_{15}Al_{16}Ta$	4.003	4.070	1.017	65.218
$Ti_{15}Al_{16}Cr$	3.975	4.064	1.022	64.214
$Ti_{15}Al_{16}Mo$	3.985	4.072	1.022	64.664
$Ti_{15}Al_{16}W$	3.985	4.073	1.022	64.680
$Ti_{15}Al_{16}Cu$	3.998	4.037	1.010	64.527
$Ti_{16}Al_{15}Zn$	4.006	4.042	1.009	64.866



2 Charge density difference with different occupying sites by the substitutional atoms in the supercell

Table 3 Elastic constants of the $Ti_{16}Al_{16}$, $Ti_{16}Al_{15}Me$ and $Ti_{16}Al_{15}Me$ calculated by first-principles calculation

Sample	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B	G	E	B/G
$Ti_{16}Al_{16}$	182.0	69.0	82.3	167.2	112.6	75.5	111.0	74.7	135.7	1.49
$Ti_{15}Al_{16}Zr$	180.9	73.3	83.8	165.0	110.5	73.2	112.0	72.5	131.6	1.54
$Ti_{15}Al_{16}Hf$	186.5	72.5	82.2	168.6	110.9	74.9	112.8	74.8	139.2	1.51
$Ti_{15}A1_{16}V$	184.7	77.4	85.6	170.2	113.5	84.8	115.2	76.0	133.4	1.52
$Ti_{15}Al_{16}Nb$	175.9	76.8	83.5	169.3	113.2	84.2	112.1	74.5	125.3	1.50
$Ti_{15}Al_{16}Ta$	184.9	78.4	85.3	170.4	112.9	85.6	115.3	76.1	133.3	1.52
$Ti_{15}Al_{16}Cr$	182.9	82.9	83.7	176.3	113.6	90.2	115.8	77.3	130.2	1.50
$Ti_{15}Al_{16}Mo$	181.7	87.3	83.9	177.4	113.9	90.9	116.7	76.8	126.1	1.52
$Ti_{15}Al_{16}W$	185.8	88.0	83.5	181.6	114.4	94.1	118.1	78.8	130.7	1.50
$Ti_{15}Al_{16}Cu$	176.2	72.4	84.6	157.8	105.8	77.5	110.4	70.1	125.3	1.57
$Ti_{16}Al_{15}Zn$	164.1	78.7	87.2	158.0	110.9	65.1	110.3	65.7	108.0	1.68

Electronic structure

Figure 2*a–k* shows the charge density difference of $Ti_{16}Al_{16}$, $Ti_{15}Al_{16}Me$ and $Ti_{16}Al_{15}Me$, which reflect the charge distribution directly. In Fig. 2*a*, it shows an obvious anisotropic electron density in $Ti_{16}Al_{16}$, which is due to the strong directional d–d bonding between the Ti atoms. Hence, there are strong covalent bondings between Ti–Ti atoms. The anisotropy of charge density distribution will decrease the ductility of TiAl. However, when the atoms of Zr, Hf and Cu substitute the Ti site, the directionality of the Ti–Ti bondings is weakened as shown in Fig. 2*b*, *c* and *j*. On the other hand, when the atoms of V, Nb, Ta, Cr, Mo and W substitute the Ti site, covalent bondings with stronger directionality between Me (Me = V, Nb, Ta, Cr, Mo and W) and Ti will be formed. Therefore, the atoms of V, Nb, Ta, Cr, Mo and W would enhance the anisotropy of charge density distribution in TiAl, thus decrease the ductility of TiAl. As shown in Fig. 2*k*, the Zn addition has little effect on the charge distribution, and is not able to improve the ductility of TiAl by affecting the electronic structure.

From the discussion above, it can be found that the additions of the Zr, Hf and Cu atoms have beneficial effect on the ductility of TiAl through improving the electronic structure.

Elastic constants

TiAl, as a tetragonal crystal, has six different elastic constants (C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, C_{66}). The second order elastic constants (C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, C_{66}), bulk-modulus (B), shear modulus (G) and Young's modulus (E) were calculated and listed in Table 3.

The calculated second order elastic constants satisfied the generalised elastic stability criteria for tetragonal crystals under hydrostatic pressures (Formula (4)–(6)), making the tetragonal cell mechanically stable.

$$C_{11} - C_{12} > 0; (C_{11} + C_{33} - 2C_{13}) > 0 \quad (4)$$

$$2C_{11} + 2C_{12} + C_{33} + 4C_{13} > 0 \quad (5)$$

$$C_{11} > 0; C_{33} > 0; C_{44} > 0; C_{66} > 0 \quad (6)$$

The Young's modulus E is an important property of materials. According to the calculated values listed in Table 3, the addition atoms decrease the Young's modulus of TiAl, except for the atoms of Hf. Therefore, it is concluded that the atoms of Hf are beneficial to increase the Young's modulus of TiAl.

Moreover, according to Pugh's study,[27] the quotient of B/G reflects the extend of ductility for metals and intermetallic compounds; that is, a high value of B/G means better ductility, while a low value indicates a tendency for brittleness. For TiAl, as shown in Table 3, the calculated value of the B/G is 1.49, showing the brittleness of the material in nature. This would hinder it from being used to important practical applications. It is noted that these atom additions have little effect on the value of the B/G, except for the addition of Zn atoms. The addition of Zn atoms could obviously improve the value of B/G, from 1.49 for $Ti_{16}Al_{16}$ to 1.68 for $Ti_{16}Al_{15}Zn$. Thus, it is expected that the atoms of Zn could improve the ductility of TiAl through changing the elastic constants.

Conclusions

The addition of Zr, Hf, Cu and Zn atoms reduced the lattice tetragonality of TiAl. The addition of Zr, Hf and Cu atoms weakened the directionality of the Ti–Ti bondings. The addition of Zn atoms obviously improved the value of B/G. All of the above aspects are believed to be beneficial to the ductility improvement of TiAl. Thus, it can be concluded that the atoms of Zr, Hf, Cu and Zn could improve the ductility of TiAl alloys.

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