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Electronic structure and physical properties of hcp Ti_3Al type alloys

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Abstract: According to the basic information of sequences of Ti and Al characteristic atoms in hcp Ti-Al system, the compositional variations of the electronic structure, atomic potential energies, atomic volumes, lattice constants and cohesive energies of the ordered hcp Ti_3Al type alloys were calculated by the framework of systematic science of alloys(SSA). The electronic structure of the hcp Ti_3Al compound consisted of ψ_{4h}^{Ti} and ψ_{0h}^{Al} atoms is 0.75[Ar] $(3d_n)^{0.573}(3d_c)^{2.1685}(4s_c)^{0.972}(4s_f)^{0.3093}$+0.25[Ne]$(3s_c)^{1.32}\cdot(3p_c)^{1.19}(3s_f)^{0.49}$. The factors of controlling lattice stability are electronic structure, atomic energies and atomic concentration. The ψ_{4h}^{Ti} atoms play a determinative role in forming $D0_{19}$ structure with a=0.287 2 nm, c=0.456 4 nm, atomic cohesive energy ε=4.810 8 eV/atom and heat of formation ΔH=−0.332 8 eV/atom. These calculated values are in good agreement with experimental values (a=0.287 5 nm, c=0.46 0 nm, ΔH=−0.27, −0.29 eV/atom). The calculated cohesive energy of the hcp Ti_3Al compound is slightly bigger than that of the fcc Ti_3Al.This is a good sign that makes it feasible to stabilized $L1_2$ structure of the hcp Ti_3Al compound by ternary element. The new element should have more d_c-electrons than Ti-metal and occupy at the Ti-lattice points.

Key words: Ti_3Al alloy; electronic structure; physical property

1 Introduction

The intermetallic compound hcp Ti_3Al with $D0_{19}$ structure has been the subject of considerable attention by experimentalists[1−3]. It is considered as a desirable candidate for application in aircraft turbine engines because its static strength and stiffness do not degrade rapidly as temperature increase. The calculations of the Ti-Al phase diagram using a variety of models have been performed[4−8]. But these Gibbs energy functions do not be associated with electronic structure, atomic energies, atomic volumes and lattice constants. The knowledge of the Ti-Al system obtained from Gibbs energy functions is not complete.

According to the framework of systematic science of alloys(SSA)[9], the Ti-Al system has fcc, hcp and bcc lattice systems, besides a liquid system. It has been found that the compositional variations of the electronic structure, atomic potential energies, atomic volumes, lattice constants, cohesive energies and Gibbs energies of these four phases can be calculated from the basic information of the same sequences of the characteristic atoms in the fcc Ti-Al lattice system[10−13].

In this study, the basic information of the sequences of Ti and Al characteristic atoms in the hcp Ti-Al lattice system was determined. The properties of hcp Ti_3Al alloys as a function of composition were obtained and the controlling factors for crystalline stability of hcp Ti_3Al compound were analyzed.

2 Basic information of Ti and Al characteristic atoms

According to the basic clusters overlapping(BCO) model in SSA framework, there are two basic cluster sequences that include 13 kinds of Ti and Al basic clusters in hcp Ti-Al system. The disordered and ordered alloys with hcp Ti_3Al type can be formed by arrangements of these 26 kinds of characteristic atoms, or by mixing the following 26 kinds of characteristic crystals. According to information about experimental lattice constants of some hcp $Ti_xAl_{(1-x)}$ alloys and on the basis of experimental value and theoretical analysis, we have determined the basic information about the electronic structures, volumes, lattice constants, potential

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energies and cohesive energies of the characteristic atoms and corresponding characteristic crystals in the hcp Ti-Al system (Tables 1 and 2).

In Tables 1 and 2, s_c, p_c and d_c are respectively the covalent electrons in *s*, *p* and *d* orbitals, s_f and p_f are the near-free electrons in *s* and *p* orbitals, and d_n is the nonbonded electrons in *d* orbital.

As shown in Fig.1, for hcp Ti-Al system, the relationships of the ε_i^{Ti}, ε_i^{Al}, v_i^{Ti} and v_i^{Al} with the number *i* can be described by following equation, where *Q* can respectively denote ε and *v*.

$$\begin{cases} Q_i^{Ti} = Q_O^{Ti} + (i/I)^2 (Q_I^{Ti} - Q_O^{Ti}) \\ Q_i^{Al} = Q_I^{Al} + [(I-i)^2/I^2](Q_O^{Al} - Q_I^{Al}) \end{cases} \quad (1)$$

3 Basic information of ordered hcp Ti_3Al type alloys

Since the complex interactions between atoms in the alloys are reflected by the electronic structure, potential energies, atomic volumes, lattice constants, cohesive

Table 1 Structural parameters and properties of Ti-characteristic atoms and Ti-characteristic crystals in hcp Ti-Al system

i	s_f	s_c	d_c	d_n	v/(10^{-3}nm^3·atom^{-1})	c/nm	a/nm	ε/(eV·atom^{-1})	E_c/(kJ·mol^{-1})
0	0.314 5	0.932 0	2.124 5	0.629 0	17.653	0.468 00	0.295 00	−4.841 1	467.09
1	0.312 5	0.936 0	2.126 5	0.625 0	17.629	0.4679 30	0.294 96	−4.852 5	468.19
2	0.307 5	0.942 0	2.135 5	0.615 0	17.557	0.467 30	0.294 56	−4.885 9	471.41
3	0.298 5	0.956 0	2.148 5	0.597 0	17.437	0.4662 30	0.293 89	−4.941 4	476.77
4	0.286 5	0.972 0	2.168 5	0.573 0	17.268	0.464 72	0.292 94	−5.022 0	484.54
5	0.271 5	0.989 0	2.196 5	0.543 0	17.052	0.462 18	0.291 71	−5.119 2	493.92
6	0.253 5	1.090 0	2.230 5	0.507 0	16.787	0.460 37	0.290 19	−5.241 0	505.68
7	0.233 5	1.025 0	2.274 5	0.467 0	16.474	0.451 03	0.288 38	−5.385 0	519.57
8	0.210 5	1.042 0	2.326 5	0.421 0	16.113	0.454 12	0.286 26	−5.551 9	535.67
9	0.186 5	1.045 0	2.395 5	0.373 0	15.705	0.450 25	0.283 82	−5.741 0	553.92
10	0.162 0	1.017 0	2.497 0	0.324 0	15.248	0.445 84	0.281 04	−5.952 0	574.28
11	0.135 5	0.981 0	2.612 5	0.271 0	14.742	0.440 85	0.277 90	−6.185 2	586.78
12	0.108 5	0.932 0	2.742 5	0.217 0	14.189	0.435 27	0.274 38	−6.440 6	621.42

c/a=1.586 4

Table 2 Structural parameters and properties of Al-characteristic atoms and Al-characteristic crystals in hcp Ti-Al system

i	s_f+p_f	s_c	p_c	v/(10^{-3}nm^3·atom^{-1})	c/nm	a/nm	ε/(eV·atom^{-1})	E_c/(kJ·mol^{-1})
0	0.490 0	1.300 0	1.190 0	15.800	0.459 95	0.281 66	−4.177 2	403.04
1	0.560 0	1.300 0	1.140 0	15.944	0.461 35	0.282 51	−4.042 1	390.00
2	0.620 0	1.311 0	1.069 0	16.073	0.462 59	0.283 27	−3.918 6	378.08
3	0.678 0	1.310 0	1.012 0	16.200	0.463 80	0.284 02	−3.806 7	367.29
4	0.725 0	1.332 0	0.943 0	16.307	0.464 82	0.284 64	−3.707 2	357.69
5	0.766 0	1.355 0	0.879 0	16.402	0.465 72	0.285 19	−3.619 2	349.20
6	0.800 0	1.382 0	0.818 0	16.483	0.466 49	0.285 66	−3.542 3	341.78
7	0.830 0	1.400 0	0.770 0	16.555	0.467 17	0.286 08	−3.477 9	335.56
8	0.854 0	1.416 0	0.730 0	16.614	0.467 72	0.286 42	−3.425 3	330.49
9	0.870 0	1.436 0	0.694 0	16.654	0.468 09	0.286 65	−3.384 2	326.52
10	0.885 0	1.441 0	0.674 0	16.690	0.468 43	0.286 85	−3.354 7	323.67
11	0.891 0	1.451 0	0.658 0	16.706	0.468 58	0.286 94	−3.338 3	322.10
12	0.893 0	1.454 0	0.653 0	16.711	0.468 63	0.286 97	−3.331 3	321.42

c/a=1.633

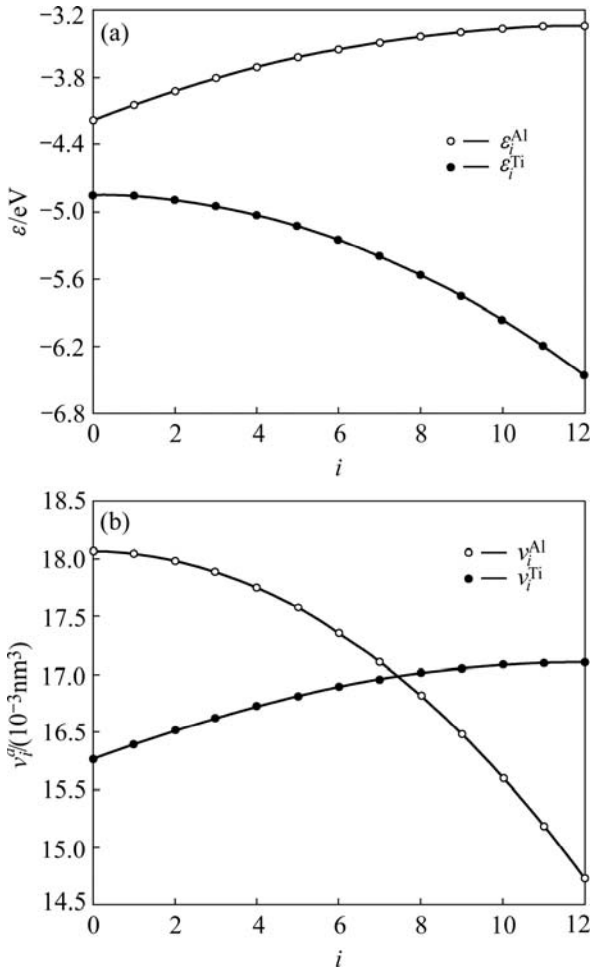

Fig.1 Relationships of ε_i^{Ti} and ε_i^{Al} (a), v_i^{Ti} and v_i^{Al} (b) of ψ_i^{Ti} and ψ_i^{Al} atoms with number i of nearest neighbor Al atoms in hcp Ti-Al system

energies and Gibbs energies of the characteristic crystals, the basic information of the alloys can be obtained by the additive law of characteristic crystals (Eqn.(2)):

$$\begin{pmatrix}\psi(x,T)\\ \varepsilon(x,T)\\ v(x,T)\\ E_c(x,T)\\ G'(x,T)\end{pmatrix}=\sum_{i=0}^{I}\left\{x_i^{Ti}\begin{pmatrix}\psi(T)\\ \varepsilon(T)\\ v(T)\\ E_c(T)\\ G'(T)\end{pmatrix}^{Ti}+x_i^{Al}\begin{pmatrix}\psi(T)\\ \varepsilon(T)\\ v(T)\\ E_c(T)\\ G'(T)\end{pmatrix}^{Al}\right\} \quad (2)$$

where x_i^{Ti} and x_i^{Al} are concentrations of the Ti and Al characteristic atoms in the alloys.

For the ordered hcp Ti_3Al type alloys with maximal ordering degree, the concentrations x_i^{Ti} and x_i^{Al} as a function of composition are shown in Fig.2. The basic information about the compositional variations of electronic structure, atomic potential energies, atomic volumes, lattice constants and cohesive energies of the hcpTi_3Al alloys and their components Ti and Al are listed

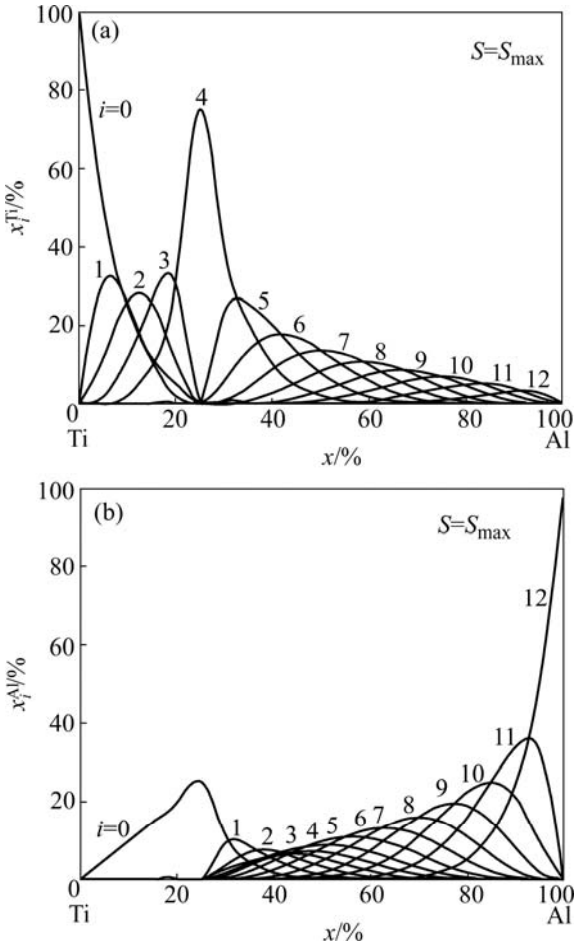

Fig.2 Concentrations x_i^{Ti} and x_i^{Al} of ordered $Ti_xAl_{(1-x)}$ alloys with hcp Ti_3Al-type and maximal ordering degree as functions of composition x_{Al}

in Table 3. It can be known that the hcp Ti_3Al compound is formed by ψ_{4h}^{Ti} and ψ_{0h}^{Al} atoms.

4 Crystalline structures of Ti_3Al type alloys

4.1 Relationship of lattice stability with electronic structure for Ti_3Al compound

The factors of controlling lattice stability are electronic structure, atomic energy and atomic concentration. The perfectly ordered $Ti_{0.75}Al_{0.25}$ alloy may be hcp Ti_3Al compound with $D0_{19}$ structure, or fcc Ti_3Al compound with $L1_2$ structure.

In order to understand the effect of electronic structure factor on lattice stability, the average electronic structures of hcp Ti_3Al and fcc Ti_3Al[12] compounds are shown as follows:

$$\begin{aligned}\psi(\text{hcp } Ti_3Al)&=0.75\psi_{4h}^{Ti}+0.25\psi_{0h}^{Al}\\&=0.75[Ar](3d_n)^{0.573}(3d_c)^{2.1685}(4s_c)^{0.972}(4s_f)^{0.2865}+\\&\quad 0.25[Ne](3s_c)^{1.32}(3p_c)^{1.19}(3s_f)^{0.49}\end{aligned} \quad (3)$$

Table 3 Electronic structure and properties of ordered Ti_xAl_{1-x} alloys with hcp Ti_3Al-type having maximal ordering degree and their components of Ti and Al

x_{Al}	Alloy									
	s_f	s_c	p_c	d_c	d_n	v/(10^{-3}nm^3·atom^{-1})	ε/(eV·atom^{-1})	c/nm	a/nm	E_c/(kJ·mol^{-1})
0	0.314 5	0.932 0	0	2.124 5	0.629 0	17.653 0	−4.847 0	0.468 00	0.295 00	467.09
0.10	0.323 0	0.995 8	0.105 5	1.919 0	0.556 7	17.401 0	−4.813 0	0.468 32	0.292 94	463.82
0.25	0.337 4	1.054 0	0.297 5	1.626 4	0.429 8	16.924 0	−4.817 0	0.456 35	0.287 16	464.17
0.30	0.355 1	1.135 5	0.295 6	1.529 0	0.389 4	16.800 0	−4.762 0	0.453 28	0.292 57	458.94
0.40	0.415 5	1.206 3	0.348 3	1.332 8	0.311 3	16.614 0	−4.639 0	0.466 29	0.286 86	447.02
0.50	0.480 5	1.267 1	0.391 1	1.134 0	0.238 3	16.462 0	−4.494 0	0.465 91	0.285 66	433.03
0.60	0.549 4	1.323 8	0.428 4	0.930 8	0.172 2	16.357 0	−4.324 0	0.465 64	0.284 83	416.68
0.75	0.658 6	1.409 2	0.482 0	0.611 8	0.088 7	16.313 0	−4.017 0	0.465 69	0.284 43	387.07
0.80	0.696 2	1.437 7	0.501 0	0.499 4	0.065 7	16.332 0	−3.899 0	0.465 69	0.284 44	375.69
0.90	0.772 8	1.495 4	0.543 3	0.261 1	0.027 4	16.427 0	−3.637 0	0.466 53	0.285 16	350.45
1.00	0.893 0	1.454 0	0.653 0	0	0	16.71 1	−3.335 0	0.468 63	0.286 97	321.42

x_{Al}	Ti component								
	s_f	s_c	d_c	d_n	v/(10^{-3}nm^3·atom^{-1})	ε/(eV·atom^{-1})	c/nm	a/nm	E_c/(kJ.mol^{-1})
0	0.314 5	0.932 0	2.124 5	0.629 0	17.653 0	−3.335 0	0.468 00	0.295 00	467.09
0.10	0.309 3	0.940 0	2.132 3	0.618 5	17.588 0	−4.883 0	0.467 58	0.294 74	470.54
0.25	0.286 5	0.972 0	2.168 5	0.573 0	17.298 0	−5.028 0	0.464 99	0.293 11	484.54
0.30	0.278 1	0.988 0	2.184 2	0.556 3	17.186 0	−5.084 0	0.463 98	0.292 48	489.96
0.40	0.259 4	1.024 1	2.221 4	0.518 9	16.930 0	−5.213 0	0.461 67	0.291 02	502.40
0.50	0.238 3	1.039 1	2.268 0	0.476 7	16.629 0	−5.364 0	0.458 92	0.289 28	516.95
0.60	0.215 2	1.038 7	2.327 1	0.430 4	16.283 0	−5.538 0	0.455 71	0.287 26	533.65
0.75	0.177 5	1.021 7	2.447 3	0.355 0	15.683 0	−5.839 0	0.450 04	0.283 69	562.69
0.80	0.164 2	1.010 6	2.497 1	0.328 5	15.461 0	−5.951 0	0.447 91	0.282 34	573.44
0.90	0.136 9	0.978 0	2.611 3	0.273 8	14.983 0	−6.190 0	0.443 25	0.279 40	596.53
1.00	0.108 5	0.932 0	2.742 5	0.217 0	14.189 0	−6.441 0	0.435 27	0.274 28	621.42

x_{Al}	Al component							
	s_f	s_c	p_c	v/(10^{-3}nm^3·atom^{-1})	ε/(eV·atom^{-1})	c/nm	a/nm	E_c/(kJ.mol^{-1})
0	0.490 0	1.320 0	1.190 0	15.800 0	−4.182 0	0.459 95	0.281 66	403.04
0.10	0.490 0	1.320 0	1.190 0	15.800 0	−4.182 0	0.459 95	0.281 66	403.04
0.25	0.490 0	1.320 0	1.190 0	15.800 0	−4.182 0	0.459 95	0.281 66	403.04
0.30	0.534 7	1.479 8	0.985 5	15.897 0	−4.011 0	0.460 89	0.282 44	386.56
0.40	0.649 7	1.479 6	0.870 7	16.140 0	−3.777 0	0.463 23	0.283 67	363.95
0.50	0.722 6	1.495 2	0.782 2	16.296 0	−3.623 0	0.464 72	0.284 58	349.10
0.60	0.772 1	1.513 9	0.713 9	16.407 0	−3.515 0	0.465 77	0.285 22	338.70
0.75	0.818 9	1.538 4	0.642 7	16.523 0	−3.409 0	0.466 86	0.285 99	328.52
0.80	0.829 2	1.544 5	0.626 3	16.550 0	−3.386 0	0.467 12	0.286 05	326.25
0.90	0.843 4	1.552 9	0.603 7	16.587 0	3.353 0	0.467 47	0.286 26	323.10
1.00	0.893 0	1.454 0	0.653 0	16.711 0	−4.847 0	0.468 63	0.286 97	321.420

$$\psi(\text{fcc Ti}_3\text{Al}) = 0.75\psi_{4f}^{Ti} + 0.25\psi_{0f}^{Al}$$
$$= 0.75[\text{Ar}](3d_n)^{0.229}(3d_c)^{2.5169}(4s_c)^{0.5448}(4s_f)^{0.6593} + 0.25[\text{Ne}](3s_c)^{1.772}(3p_c)^{1.008}(3s_f)^{0.22} \quad (4)$$

It should be pointed out that the ψ_{4h}^{Ti} and ψ_{0h}^{Al} atoms belong in the sequences of Ti- and Al-characteristic atoms in the hcp lattice system, and the ψ_{4f}^{Ti} and ψ_{0f}^{Al} atoms belong in the sequences of Ti- and Al-characteristic atoms in the fcc lattice system.

The ψ_{4f}^{Ti} atoms have a tendency to form hcp and bcc structures, because their d_c electrons would rather be in the e_g state with lower potential energy than in the t_{2g} state with higher potential energy. Only when the Al atoms or other elements have stronger tendency to form fcc structure than the tendency to form hcp and bcc structure of the Ti atoms, can the d_c electrons be in the t_{2g} state due to strong effect of Al atoms, and can the Ti_3Al compounds have fcc lattice structure.

The ψ_{0f}^{Al} atoms have a tendency to form fcc structure. The ψ_{0f}^{Al} atoms in the fcc Ti_3Al compound have less concentration (x_{0h}^{Al}=25%, mole fraction), less s_c spherical covalent electrons and more p_c directional electrons (1.008 eV/atom) than other atoms. Thereby, the ψ_{0f}^{Al} atoms have weaker role in forming fcc lattice than other atoms in the fcc $TiAl_3$ compounds.

The ψ_{4h}^{Ti} atoms have the most concentration (x_{4h}^{Ti}=75%, mole fraction) and the strongest tendency to form hcp and bcc structures, because their d_c electrons (2.156 eV/atom) are less than that of ψ_{4f}^{Ti} atoms, and would rather be in the e_g state. The ψ_{0h}^{Al} atoms have the least concentration (x_{0h}^{Al}=25%) and the weakest tendency to form fcc structure, because their s_c electrons (1.32 electrons/atom) are less than that of ψ_{0f}^{Al} atoms. Therefore the ψ_{4h}^{Ti} atoms play the leading role in forming hcp lattice for $D0_{19}$- Ti_3Al compound.

4.2 Relationship of lattice stability with atomic energies and concentration for Ti_3Al type alloys

The atomic cohesive energies and heat of formation of the hcp and fcc Ti_3Al compounds are as follows:

$$\varepsilon(\text{hcp Ti}_3\text{Al}) = -(0.75\,\varepsilon_{4h}^{Ti} + 0.25\,\varepsilon_{0h}^{Al}) = 4.810\ 8 \text{ eV/atom} \quad (5)$$

$$\varepsilon(\text{fcc Ti}_3\text{Al}) = -(0.75\,\varepsilon_{4f}^{Ti} + 0.25\,\varepsilon_{0f}^{Al}) = 4.795\ 2 \text{ eV/atom} \quad (6)$$

$$\Delta\varepsilon = \varepsilon(\text{hcp Ti}_3\text{Al}) - \varepsilon(\text{fcc Ti}_3\text{Al}) = 0.015\ 2 \text{ eV/atom} \quad (7)$$

$$\Delta H(\text{hcp Ti}_3\text{Al}) = \varepsilon(\text{hcp Ti}_3\text{Al}) - (0.75\varepsilon_0^{Ti}(\text{hcp})) + 0.25\varepsilon_{12}^{Al}(\text{fcc}) = -0.332\ 8 \text{ eV/atom} \quad (8)$$

$$\Delta H(\text{fcc Ti}_3\text{Al}) = \varepsilon(\text{fcc Ti}_3\text{Al}) - (0.75\varepsilon_0^{Ti}(\text{hcp})) + 0.25\varepsilon_{12}^{Al}(\text{fcc}) = -0.317\ 2 \text{ eV/atom} \quad (9)$$

The ε(hcp Ti_3Al) is slightly larger than ε(fcc Ti_3Al), so the hcp Ti_3Al compound is more stable than the fcc Ti_3Al compound. The calculated heat of formation of the ΔH(hcp Ti_3Al) is smaller than its experimental values (−0.27 and −0.29 eV/atom)[14].

From the compositional variation of cohesive energies of the hcp Ti_3Al, fcc Ti_3Al, fcc TiAl and fcc $TiAl_3$ type ordered $Ti_xAl_{(1-x)}$ alloys (see Fig.3), it can be known that the hcp Ti_3Al type ordered $Ti_xAl_{(1-x)}$ alloys are more stable than other ordered alloys in the range of 0-40% Al (mole fraction).

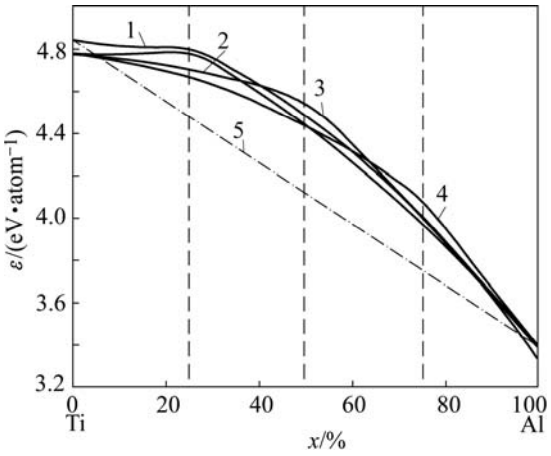

Fig.3 Atomic cohesive energies of hcp Ti_3Al(1), fcc Ti_3Al(2), fcc TiAl(3) and fcc $TiAl_3$(4) type ordered $Ti_xAl_{(1-x)}$ alloys and mixed solution [hcp Ti+fcc Al](5)

The calculated energy difference between hcp and fcc Ti_3Al compounds is very small, which makes it feasible to stabilize the $L1_2$ phase by ternary alloy additions. Considering electronic structure and that the ψ_{4h}^{Ti} atoms play the leading role in forming hcp lattice for $D0_{19}$ Ti_3Al compound, these ternary element additions should occupy the Ti-lattice points, and have much more d_c-electrons than Ti-atoms.

4.3 Relationship of lattice constants and concentration of hcp Ti_3Al type alloys

The average atomic volumes of several ordered $Ti_xAl_{(1-x)}$ alloys with hcpTi_3Al type are listed in Table 3. Because we still can not establish the function between the ratio c/a and concentration in theory for the ordered $Ti_xAl_{(1-x)}$ alloys with hcp Ti_3Al type, we have drawn the polynomial equation of the c/a—x_{Al} curve from the experimental data of ratio c/a:

$$c/a = 1.586\ 4 + 0.131\ 7x_{Al} - 0.085\ 07\,x_{Al}^2 \quad (10)$$

The lattice constants of several hcp Ti_3Al type $Ti_xAl_{(1-x)}$ alloys are listed in Table 3. The lattice constants of the hcp Ti_3Al compound are a=0.287 2 nm and

c=0.456 4 nm, c/a=1.614, which are in good agreement with experimental values (a=0.287 5 nm, c=0.460 nm)[15].

5 Conclusions

1) It has been proved that the compositional variations of the electronic structure, atomic potential energies, atomic volumes, lattice constants and cohesive energies of the ordered hcp Ti_3Al type alloys can be obtained from the basic information of sequences of Ti and Al characteristic atoms and corresponding characteristic crystals in the Ti-Al hcp lattice system.

2) The hcp Ti_3Al compound is formed by ψ_{4h}^{Ti} and ψ_{0h}^{Al} atoms. The electronic structure is $0.75[Ar](3d_n)^{0.573}\cdot(3d_c)^{2.168\,5}(4s_c)^{0.972}(4s_f)^{0.309\,3}+0.25[Ne](3s_c)^{1.32}(3p_c)^{1.19}\ (3s_f)^{0.49}$. The calculated lattice constants and heat of formation of the hcp Ti_3Al compound are in good agreement with experimental values.

3) The factors of controlling crystalline structure are electronic structure, atomic potential energies and atomic concentration. Comparing ψ_{4h}^{Ti} and ψ_{0h}^{Al} atoms in the hcp Ti_3Al compound with the ψ_{4f}^{Ti} and ψ_{0f}^{Al} atoms in the fcc Ti_3Al compound, it has been found that the ψ_{4h}^{Ti} atom has the least d_c-electrons and the strongest tendency to form hcp and bcc structures, and the ψ_{0h}^{Al} atom has the least s_c-electrons and the weakest tendency to form fcc structure. Therefore, the ψ_{4h}^{Ti} atoms play the leading role in forming hcp Ti_3Al compound.

4) The calculated cohesive energy of the hcp Ti_3Al compound is slightly bigger than that of the fcc Ti_3Al.This is a good sign that makes it feasible to stabilized $L1_2$ structure of the hcp Ti_3Al compound by ternary element. The new element should have more d_c-electrons than Ti-metal and occupy at the Ti-lattice points.

References

[1] THOMAS M, VASSEL A, VEYSSIERE P. Dissociation of superdislocations in the intermetallic compound Ti_3Al [J]. Scr Metall, 1987, 21: 501−506.

[2] FLEISCHER R L, DIMIDUK D M, LIPSITT H A. Electronic structure, cohesive properties, and phase stability of Ti_3Al and Ni_3Al [J]. Annu Rev Mater Sci, 1999, 19: 231−239.

[3] YAMAGUCHI M, UMAKASHI Y. In-situ TEM study of fracture mechanisms of poly synthetically twinned(PST) crystals of TiAl alloys [J]. Prog Mater Sci, 1997, 34: 1−9.

[4] CHUBB S R, PAPACONSTANTOPOULOS D A, KLEIN B M. First-principles study of $L1_0$ Ti-Al and V-Al alloys [J]. Phys Rev B, 1998, B38: 12120−12124.

[5] HONG T, WATSON-YANG T J, FREEMAN A J, OGUCHI T, XU J H. Crystal structure, phase stability, and electronic structure of Ti-Al intermetallics: $TiAl_3$ [J]. Phys Rev B, 1990, B41: 12462−12467.

[6] HONG T, WATSON-YANG T J, FREEMAN A J. Crystal structure, phase stability and electronic structure of Ti-Al Intermetallic: Ti_3Al [J]. Phys Rev B, 1991, B43: 1940−1947.

[7] ZHANG F, HUANG W, CHANG Y A. Equivalence of the generalized bond-energy model, the wagner-schottky-type model and the compound-energy model for ordered phases [J]. Calphad, 1997, 21: 337−348.

[8] ASTA M, DE FONTAINE D. First-principles study of phase stability of Ti-Al intermetallic compounds [J]. J Mater Res, 1993, 8: 2554−2569.

[9] XIE You-qing. The framework of metallic materials systematic science [J]. Mater Rev, 2001, 15(4): 12−15.

[10] XIE Y Q, PENG K, LIU X B. Influences of x_{Ti}/x_{Al} on atomic states, lattice constants and potential energy planes of ordered FCC TiAl type alloys [J]. Physica B, 2004, 344: 5−20.

[11] XIE Y Q, LIU X B, PENG K. Atomic states, potential energies, volumes, brittleness and phase stability of ordered FCC $TiAl_3$ type alloys [J]. Physica B, 2004, 353: 15−33.

[12] XIE Y Q, PENG H J, LIU X B. Atomic states, potential energies, volumes, brittleness and phase stability of ordered FCC Ti_3Al type alloys [J]. Physica B, 2005, 362: 1−17.

[13] XIE Y Q, TAO H J, PENG H J. Atomic states, potential energies, volumes, brittleness and phase stability of ordered FCC $TiAl_2$ type alloys [J]. Physica B, 2005, 366: 17−37.

[14] BRANDES E A. Smithells metals reference book [M]. London: Butterworths Press, 1983: 275.

[15] PEARSON W B. A handbook of lattice spacings and structures of metals and alloys [M]. New York: Pergamon, 1958: 103.

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