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Influence of chemical composition and alloying elements on microdefects and electron density in Ni-Al alloys①

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[Abstract] Positron lifetime spectra have been measured in binary Ni-Al alloys with different chemical composition and NiAl alloys doped with Cr, Zr, Fe and Mg. The results indicate that in B2-NiAl and $L1_2$-Ni_3Al alloys, some of the valance electrons of Ni and Al atoms are localized, which leads to a lower free electron density of the alloy. The mean free electron density of the binary Ni-Al alloy decreases with increasing Al content. The open volume of defects on grain boundary of the Ni_3Al is larger than that of monovacancy or dislocation. Structural vacancies and microvoids are found in B2-NiAl alloys with Al content above 45% (mole fraction), and the concentration of the vacancies and open volume of microvoids will increase with higher Al content. The addition of Cr, Zr and Fe into a NiAl alloy can increase its mean free electron density and reduce the open volume of defects on its grain boundary, while with addition of Mg into the NiAl alloy, its mean free electron density decreases and open volume of boundary defects increases.

[Key words] Ni-Al alloy; chemical composition; alloying element; microdefect; electron density
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1 INTRODUCTION

$L1_2$-Ni_3Al and B2-NiAl are important intermetallic compounds in NiAl alloys. A Ni_3Al alloy has relatively high strength and presents remarkable positive effects of temperature and strength in certain temperature region as well as it has good creep resistance, fatigue durability and oxidation resistance[1]. A NiAl alloy, with low density, high melting temperature, high thermal conductivity and good anti-oxidation ability, can be applied as a coating material for high temperature turbine blades and aero-engines[2]. All these advantages of Ni_3Al and NiAl will help them to be developing structural materials of high temperature. However, they have different mechanical properties, for example, at room temperature, a Ni_3Al alloy of single crystal has preferable plasticity[3] while polycrystal one is quite brittle[1]. As for NiAl, its application has been hindered as it's an intermetallic compound of intrinsic brittleness and is brittle in single or polycrystals[2].

Brittleness of multiple-crystal Ni_3Al is regarded as the result of grain-boundary weakness[4] and plastication research on it has made a progress. Aoki and Izumi firstly[5] found that with small amount of B, the plasticity of alloy can be largely improved and alloying elements Fe, Mn, Ag and Pd are useful for its plasticity as well[6~8]. However, it's not so successful on plasticity of NiAl. Many experiments and theoretical researches have been done to find out both brittleness mechanism of NiAl alloys at room temperature and methods on improving NiAl tenacity. Results show that additions of B, C or Be in NiAl alloys can't largely improve the plasticity of alloy and cause no change of fracture model[2,9], while Cr, Co, Fe Mn, etc can reduce the ordering energy of alloy and improve their plasticity, among which tensile elongation of Ni50Al20Fe30 at room temperature is 8%[10]. Vacancy concentration in NiAl alloy is related to its chemical composition[11]. Some researchers studied on microdefects and electron structure of $L1_2$-Ni_3Al and B2-NiAl and discussed influence of material microstructure on its mechanical properties[11~13], but experiment results seldom involve deeply into electron structure.

Positron is quite sensitive to microdefects in metals and alloys[14,15]. Positron annihilation technique is useful for studies on microdefects and electron structure of materials, which can provide information about size and concentration of microdefects, local electron density and so on[16,17]. In this paper, positron lifetime spectra of binary Ni-Al alloys with different chemical composition and NiAl alloys with different alloying elements are measured and ana-

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lyzed. Microdefects and electron density of binary Ni-Al are studied. Behaviors of alloying elements in NiAl alloys, their influences on microdefects and electron density in alloys and relationship between microstructure and mechanical properties of alloy are discussed as well.

2 SAMPLE PREPARATION

Chemical composition of tested alloys are listed in Table 1, according to which alloys were prepared by pure Ni (99.95%), Al (99.98%), Zr (99.9%), Cr (99.92%), Fe (99.96%), Mg (99.93%). To unify composition, every alloy was melted in non-consumable electrode arc furnace for more than 3 times and represented by nominal chemical composition since mass losses in melting process were less than 0.01%. Uniform heat treatment was taken on obtained ingots for 12 h in vacuum furnace at 1 000 ℃. Thin plates (1 mm × 10 mm × 10 mm) were cut from ingots by spark-erosion and selected to be samples of positron lifetime spectra after planishing and polishing their surface.

Table 1 Chemical compositions of alloys tested (mole fraction, %)

Alloy No.	Ni	Cr	Fe	Zr	Mg	Al
1	77.0	–	–	–	–	23.0
2	55.0	–	–	–	–	45.0
3	50.0	–	–	–	–	50.0
4	48.0	7.0	–	–	–	45.0
5	48.0	–	7.0	–	–	45.0
6	50.0	–	30.0	–	–	20.0
7	50.0	–	–	2.0	–	48.0
8	50.0	–	–	–	2.0	48.0

3 EXPERIMENT METHODS

Fast-fast coincidence lifetime spectrometer of ORTEC company is taken to measure all these alloys' positron lifetime spectra. In our experiment, the resolution of the apparatus (FWHM) was determined to be 240 of ^{22}Na source with backing Kapton film is 3.7×10^5Bq. The source is splinted between two identical samples as a sandwich structure of "sample-source-sample" and laid in the middle of the start and stop detector. Positron annihilation experiments are taken at room temperature (25 ℃) and 10^6 counts are accumlated for each spectrum.

POSITRONFIT EXTENDED program[18] is used to fit the spectra. Three lifetime components (τ_1, τ_2, τ_3) and corresponding intensity (I'_1, I'_2, I'_3) are obtained by subtracting source composition and background. τ_3($\approx$1 200) in each spectrum with an extremely small intensity I'_3(< 1%) is considered as the results of positron annihilation on the surface of samples and source. This was disregarded in our discussion. Renormalizing I'_1, I'_2 and marking them as I_1, I_2, it's found that the shorter the positron lifetime (τ), the bigger the positron annihilation rate (λ) and $\lambda = \tau^{-1}$. Correspondingly, $\lambda_1 = \tau_1^{-1}$, $\lambda_2 = \tau_2^{-1}$ and the mean positron annihilation rate $\lambda_m = I_1\lambda_1 + I_2\lambda_2 = I_1\tau_1^{-1} + I_2\tau_2^{-1}$. Suppose that positron exist in two states: free or trapped by defects then according to two-state trapped model[19], its annihilation rate (λ_b) in the bulk of alloy equals its mean value (λ_m), i.e. $\lambda_b = \lambda_m$. Electron density n at different annihilation sites can be calculated by formulation of Brandt and Reinheimer[20]: $n = (\lambda - 2)/134$, where, unit of λ is ns^{-1}, unit of n is atom unit, i.e. a.u. (to electron density, 1a.u. = 6.755×10^{30} m^{-3}). In lattice of metals or alloys, positron are mainly annihilated with free electrons.

4 RESULTS AND DISCUSSION

Parameters of positron lifetime specctra and electra density of tested alloys are listed in Table 2. Bulk positron lifetime[21,22], position annihilation rate, electron density and electronic configurations of pure Ni, Al, Zr, Cr, Fe and Mg metals are also listed in Table 3 for discussion.

4.1 Electron density of binary Ni-Al alloys

The positron first component lifetime of Ni77Al23 (τ_1(Ni77Al23)) is 106.0 ±2, lower than that of pure Ni and Al metal (τ_b(Ni) = 110, τ_b(Al) = 166), while its corresponding intensity (I_1 = 71.0%) is relatively high. Compared with other tested alloys, the second positron lifetime component of Ni77Al23 is the shortest (τ_2(Ni77Al23) = 201 ±6, see Table 2 and Table 3), which is caused by the phenomena that most positron annihilates in the bulk of the alloy (free-state annihilation) and others are trapped by defects. Therefore, positron two-state trapped model[19] can be applied in Ni77Al23 alloys, by which positron annihilation rate in the bulk of Ni77Al23 metal (λ_b) equals its mean positron annihilation rate (λ_m) i.e. $\lambda_b = \lambda_m = I_1\tau_1^{-1} + I_2\tau_2^{-1} = 8.14\ n \cdot s^{-1}$, and correspondingly its free electron density equals each other as $n_b = n_m$(Ni77Al23) = 0.045 8a.u. (see Table 2).

As for binary alloys composed by metals A and B, positron annihilation rate in the bulk of the alloy λ_{eb}(alloy) based on them can be calculated by theory of Lock and West[23] as well as Stott and Kubica[24] et al if positrons are homogenously distributed in lattice and atoms are combined by pure metallic bonds. With some mathematics treatments, λ_{eb}(alloy) can be expressed as[25]:

$$\lambda_{eb}(\text{alloy}) = \varphi_{(a)}\,\lambda_a(A) + \varphi_{(b)}\,\lambda_b(B) \qquad (1)$$

Table 2 Parameters of positron lifetime spectra and electron densities of alloys tested

Alloy	τ_1	τ_2	I_1/%	I_2/%	λ_m/ns^{-1}	λ_2/ns^{-1}	n_m/a.u.	n_2/a.u.	n_{cb}/a.u.
Ni77Al23	106.0±2	201±6	71.0±2	29.0±2	8.14	4.98	0.0458	0.0222	0.0476
Ni55Al45	167.4±1	295±11	86.4±2	13.6±2	5.62	3.39	0.0270	0.0104	0.0426
NiAl	177.9±2	317±18	87.0±2	13.0±2	5.30	3.15	0.0246	0.0086	0.0415
Ni48Al45Cr7	170.4±2	294±13	81.3±3	18.7±3	5.41	3.40	0.0254	0.0105	–
Ni48Al45Fe7	174.8±2	305±12	83.4±2	16.6±2	5.32	3.28	0.0248	0.0096	–
Ni50Al20Fe30	117.9±1	267±4	73.4±1	26.6±1	7.22	3.75	0.0390	0.0131	–
Ni50Al48Zr2	168.3±1	313±12	85.6±1	14.4±1	5.55	3.19	0.0265	0.0089	–
Ni50Al48Mg2	179.3±1	331±16	88.4±1	11.6±1	5.28	3.02	0.0245	0.0076	–

Table 3 Bulk positron lifetimes, positron annihilation rates, electron densities and electronic configurations of Ni, Al, Zr, Cr, Fe and Mg elements

Element	τ_b	λ_b/ns^{-1}	n_b/a.u.	Electronic configuration
Ni	110	9.09	0.0529	(Ar) $3d^8 4s^2$
Al	166	6.02	0.0300	(Ne) $3s^2 3p^1$
Zr	165	6.06	0.0303	(Kr) $4d^2 5s^2$
Cr	120	8.33	0.0472	(Ar) $3d^5 4s^1$
Fe	106	9.43	0.0554	(Ar) $3d^6 4s^2$
Mg	225	4.44	0.0182	(Ne) $3s^2$

where λ_a(A) and λ_b(B) are positron mean annihilation rate, respectively in pure metal A and B base, $\varphi_{(A)}$ and $\varphi_{(B)}$ are respectively the mole fractions of A and B in the alloys.

In Ni77Al23 alloy, if Ni and Al are combined by pure metallic bonds, positron annihilation rate of the bulk of Ni77Al23 alloy, λ_{cb}(Ni77Al23) can be obtained as λ_{cb}(Ni77Al23) = 8.38ns^{-1}, by Eqn. (1), where positron annihilation rates in pure metal Ni and Al are λ_b(Ni) = 9.09ns^{-1} and λ_b(Al) = 6.02ns^{-1} (Table 3) and the mole fractions of A, B in the alloy are respectively $\varphi_{(Ni)}$ = 0.77 and $\varphi_{(Al)}$ = 0.23. Then free electron density in the bulk of the alloy can be calculated as n_{cb}(Ni77Al23) = 0.0476a.u. by n = (λ − 2)/134. Our measured value of free electron density in the bulk of Ni77Al23 is n_b = n_m(Ni77Al23) = 0.0458a.u. (see Table 2), which is lower than n_{cb}(Ni77Al23). Therefore, it's concluded that when Ni and Al are aggregated to form Ni77Al23 alloys, some valance electrons of Ni and Al are localized, which leads to the decrease of free electron density in the alloy.

Electronic configurations of Ni and Al are shown in Table 3. Some 3d electrons in Ni atom have localized properties. Due to hybridism of Ni d+Al p of nearest neighbor Ni-Al atoms in lattice, 3p electrons of Al and 3d electrons of Ni are localized to form covalent bonds[12, 13] in their formation of Ni77Al23 alloys, which reduces the amount of free electrons in metallic bonding.

Free electron density in the bulk of Ni55Al45 and NiAl can be calculated by Eqn. (1) as well and the result is listed in Table 2. It is shown that

$$n_m(\text{Ni77Al23}) = 0.0458\text{a.u.} < n_{cb}(\text{Ni77Al23}) = 0.0476\text{a.u.}$$
$$n_m(\text{Ni55Al45}) = 0.0270\text{a.u.} < n_{cb}(\text{Ni45Al45}) = 0.0426\text{a.u.}$$
$$n_m(\text{NiAl}) = 0.0246\text{a.u.} < n_{cb}(\text{NiAl}) = 0.0415\text{a.u.}$$

It's found that measured mean free electron density n_m is less than corresponding n_{cd} and their difference increases with higher concentration of Al in the alloy, which means that with increasing Al content, localized valance electrons increase and free electrons in metallic bonding become less. When Al content in binary Ni-Al alloys increases from 23% (mole fraction) to 50% (mole fraction), their mean free electron density (n_m) decreases from 0.0458a.u. to 0.02466a.u. (Table 2).

4.2 Microdefects in binary Ni-Al alloys

Positron lifetime in defects can be a function of the size of open volume defect, i.e. longer positron lifetime implies larger open volume defects[14].

τ_2(Ni77Al23) = 201±6 is larger than positron lifetime in monovacancies of Ni_3Al (τ_v(Ni_3Al) = 180±5) or dislocation (τ_v(Ni_3Al) = 187±5)[26], so it's deduced that of the open volume defects in Ni77Al23 are bigger than that of monovacancy or dislocation.

τ_1(NiAl) = 177.9±2 is higher than bulk positron lifetime of pure Ni and Al (τ_b(Ni) = 110, τ_b(Al) = 166) (see Table 2 and Table 3) but close to what Wurschum et al[29] obtained in NiAl vacancy (τ_v(NiAl) ≈ 180), which indicates τ_1(NiAl) is positron lifetime in NiAl vacancies. As is shown in Table 2 that I_1(NiAl) = (87.0±2)% is relatively high, this means that many structural vacancies exist in NiAl with their concentration relating to alloys' chemical composition[11], and most positron electrons are trapped by these vacancies and annihilated with electrons in vacancies.

τ_2(NiAl) = 317±18 is larger than positron lifetime in metal Ni and Al monovacancies (τ_v(Ni) = 160, τ_v(Al) = 240)[21], which leads to the conclusion that some microvoids besides vacancies can also be found in NiAl alloys.

Results in Table 2 can be presented as follows:

with Al content in binary NiAl alloys increasing from 23% (mole fraction) to 50% (mole fraction), τ_1 increases from 106.0 ±2 to 177.9 ±2, τ_2 increases from 201 ±6 to 317 ±18 and I_1 increases from 71% to 87%, i.e. the concentration of vacancies and open volume of microvoids will increase with higher Al content in Ni-Al alloys.

Such defect structure characteristics of B2-NiAl and Ll_2-Ni_3Al alloys relate to their bonding properties. Due to coexistence of metallic and covalent bonds in these alloys, their crystal structure presents relatively simple ordering structure and high ordering energy since covalent bonding has distinguished space directivity. As for multiple-crystal alloys of high ordering energy, inner atom arrangements of neighboring grains are highly ordering, i.e. a boundary atom can only belong to a grain to keep highly ordering arrangements of the grain's inner atoms. Relaxation is difficult to happen for boundary atoms, which causes the appearance of column pores with comparably large open volume on boundaries. With increasing Al content, localized valence electrons become more in alloys while free electrons that take part in metallic bonding decrease, and bonding force is more non-homogenous, which enhances open volume of microvoids in alloys. When Al content increases from 23% (mole fraction) to 50% (mole fraction), n_2 decreases from 0.0222 a.u. to 0.0086 a.u.

Mechanical properties are closely related to bond structure and microdefects in alloys[28]. Therefore, the higher density the free electrons that engage in formation of metal bonding, the stronger the metallic bonding force; and vice versa. As metallic and covalent bonding coexists in Ni-Al and bonding force of covalence is often higher than that of metallic bonding, i.e. relatively strong covalent bonding and weak metallic bonding caused by low free electron density can both exist in alloys, which leads to inhomogeneous of bonding force: it's stronger along the directions of forming covalent bonding than any other directions. Materials can easily be destroyed along the direction of weak bonding force by the means of external stress.

Free electron density in the bulk of polycrystal Ni77Al23 is visibly high (n_b = n_m(Ni77Al23) = 0.0458 a.u.) while it's relatively low in boundary defects (n_2(Ni77Al23) = 0.0222 a.u.) (see Table 2), which means that metallic bonding force is strong in inner atoms of Ni77Al23 alloys while boundary is a weak bonding force region. Therefore, the phenomena that single-crystal Ni_3Al has good plasticity but polycrystal Ni_3Al is quite brittle[1,3] at room temperature can be explained by what mentioned above. As for NiAl alloys, their mean free electron density and boundary electron density are relatively low (n_m(NiAl) = 0.0246 a.u. and n_2(NiAl) = 0.0086 a.u.). Boundary cohesion of NiAl is very weak and metallic force of inner atoms is not strong as well, so, NiAl is an intrinsic brittle intermetallic compounds and it's quite brittle at room temperature no matter it's single or polycrystals[2].

4.3 Influence of alloying elements on electron density and microdefects in NiAl alloys

Bulk electron density of metal Cr is higher than that of metal Al, but lower than that of metal Ni (see Table 3) so that in alloying, Cr atoms will possibly supply more valance electrons than Al atoms while less than Ni atoms to form metallic bonding. Add Cr element into a NiAl alloy, mean free electron density of the alloy will rise if Cr atoms take place of Al; but, if Cr atoms take place of Ni atoms in the alloy, its mean free electron density will decrease. Our experiments show that n_m(Ni48Al45Cr7) = 0.0254 a.u. which is larger than that of n_m(NiAl) = 0.0246 a.u. (Table 2), it means the addition of Cr gets increase to mean free electron density of the alloy. As for τ_2 (Ni48Al40Cr7) = 294 ±13 (smaller than τ_2(NiAl) = 317 ±18 (Table 2)), it's a result of that addition Cr increase mean free electron density of the alloy to make electric charge more evenly distributed and decrease alloys' ordering energy. Alloy boundary is easily relaxed and its open volume defect is reduced. Moreover, appearance of Cr on the boundary can enhance boundary's electron density, i.e. n_2(Ni48Al45Cr7) > n_2(NiAl) (Table 2). Similarly, bulk electron density of metal Zr is higher than metal Al but lower than metal Ni (Table 3). Thus, analogy results can be obtained in Ni50Al48Zr2 and Ni48Al45Cr7. Respectively adding Cr and Zr element to NiAl alloys can increase metallic bonding force in them and improve boundary structure.

Bulk electron density of metal Fe is higher than metal Al and Ni (Table 3). Adding Fe element into a NiAl alloy, no matter Fe atoms substitute Al or Ni atoms, the alloy's mean free electron density will increase and n_m(Ni48Al45Fe7) is larger than n_m(NiAl) (Table 2). As it's shown in Table 2, n_m(Ni50Al20Fe30) is bigger than both n_m(NiAl) and n_m(Ni48Al45Fe7), this means that the more Fe element be added in the alloy, the larger increase of alloy's free electron density. τ_2(Ni50Al20Fe30) is less than τ_2(Ni48Al45Fe7) and τ_2(NiAl) as well (Table 2), which can be explained as follows: with increasing Fe added, free electron density increases in the alloy, ordering energy reduces and boundary relaxes. Fe atoms exist near boundary regions and electron density of boundary increases as n_2(Ni50Al20Fe30) > n_2(Ni48Al45Fe7) > n_2(NiAl). Therefore, adding high content of Fe element can effectively changed alloys' brittleness at room temperature. Tensile elongation of 8% at room temperature in a Ni50Al20Fe30

alloy has been obtained[10].

Bulk electron density of metal Mg is lower than metal Al and Ni (Table 3). Adding Mg element into a NiAl alloy, no matter Mg atoms substitute Al or Ni atoms, the alloy's mean free electron density will decrease and n_m(Ni50Al48Mg2) is smaller than n_m(NiAl) (Table 2). τ_2(Ni50Al48Mg2) = 331 ±16 is larger than τ_2(NiAl) = 317 ±18, which indicates that adding Mg element to a NiAl alloy can enhance open volume of boundary defects. When Mg atoms appear on boundary, electron density on it will decrease, i.e. n_2(Ni50Al48Mg2) < n_2(NiAl) (Table 2). Therefore, adding 2% (mole fraction) Mg element to a NiAl alloy will not improve the alloy's tenacity.

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