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ARTICLE

Microscopic Phase-field Simulation for the Influence of Aging Process on the Precipitation Process of $Ni_{75}Al_{15}Ti_{10}$ Alloy

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Abstract: The precipitation process of $Ni_{75}Al_{15}Ti_{10}$ alloy was simulated by a microscopic phase-field kinetics model. The microscopic morphology evolution was studied, which indicates that the precipitation process can be divided into two stages: the first is the transformation from $L1_0$ phase to $L1_2$ phase, and the second is the formation of the stoichiometric $L1_2$ phase. The effect of single aging temperature on the microstructure, atomic occupation probability and atomic diffusion was investigated. The result shows that the shape of γ' precipitates transforms from irregular shape to regular cuboid and the degree of orientation growth increases with increasing aging temperature. But the higher the aging temperature, the lower the occupation probability and the order degree. Meanwhile, the path of diffusion of Al atom is from the interface of the γ' phase to the internal, and the diffusion of Ti atom is the opposite. Furthermore, we studied the dual aging to improve occupation probability of γ' precipitates and to discuss their influence on the γ' phase. Dual aging can not only obtain a stable γ' phase with regular shape, but also increase the occupation probability of Al and Ti and inhibit the formation of anti-site defects.

Key words: aging temperature; dual aging; microscopic phase-field; microstructure; occupation probability

Ni-Al-based alloys with the excellent high temperature properties, such as fatigue resistance, corrosion resistance, and mechanical property, have been widely used for turbine blades in most advanced aero-engines[1-3]. This material is mainly composed of coherent γ' precipitates of Ni_3Al ($L1_2$-structure cubes), which are dispersed in a γ matrix formed by solid solution of Ni with other elements, and primarily determined the thermo-mechanical properties of Ni-Al-based alloys[4-6]. However, the main obstacle of Ni-Al-based alloys is low creep resistance which severely restricts their application as engineering materials[7,8]. Thus, understanding the formation mechanism and microstructure of γ' phase with different process parameters (such as aging temperature) is useful for improving the thermo-mechanical properties of alloys. Recently, the researches about microstructure, coarsening orientation and stability of γ' phase have attracted much attention, and many researches on the γ' phase in Ni-Al-based superalloys have been reported.

The phase separation process determines the microstructure and mechanical properties of nickel-aluminum-based superalloys[9-12]. Nunomura et al[9] studied the phase relation and microstructure in Ni-Al-Ti system, and finally obtained the phase diagram of pseudo-binary Ni_3Al-Ni_3Ti alloy. Doi et al[10] investigated the effect of precipitate morphology on the phase separation behavior of γ' precipitates in Ni-Al-Ti alloy. The results indicated that γ' precipitates exhibit a phase separation phenomenon, in which γ particles newly appear in the γ' precipitates due to the influence of chemical free energy and elastic energy. Furthermore, Vogel et al.[6,11,12] successfully mapped the evolution of hierarchical microstructures. They clarified the origin of γ particles occurring in ordered γ' precipitates ($L1_2$ phase) in $Ni_{86.1}Al_{8.5}Ti_{5.4}$ alloy by atom probe tomography, and analyzed the governing driving forces of the phase separation of γ' precipitates in different stages. In

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addition, the coarsening of the γ' precipitates, as a critical phenomenon in precipitation process, has attracted much attention as well[13,14]. Mushongera et al[13] studied the effect of Re on directional γ'-coarsening in commercial single crystal Ni-base superalloys. The results indicated that Re, as a solid-solution strengthener, significantly plays a major role in reducing the rafting rate because Re can reduce the interface mobility by accumulating along the growth path. Masoumi et al[14] applied Semi-analytical models for dissolution and coarsening kinetics. The results suggested that γ' coarsening occurs during the dissolution process which is attributed to the agglomeration and Ostwald ripening. Furthermore, γ' volume fraction, its average size and size distribution play a critical role in the microstructure evolution in the dissolution and coarsening processes.

In recent years, Ni-Al-Ti alloy has become one of the most important Ni-Al-based superalloys due to the solid solution strengthening effect of Ti atom in Ni_3Al, which can greatly improve its mechanical property[15,16]. Meanwhile, aging process is a critical method to optimize the microstructure and phase orientation of γ' precipitates in Ni-Al-based alloys[17,18]. However, previous researches about Ni-Al-Ti alloy are focused on the experimental methods rather than computational simulation analysis, which is very poor for clarifying the pre-precipitation of Ni-Al-Ti alloy. Moreover, few studies have been done about the effect of aging process on the precipitation process of $Ni_{75}Al_{15}Ti_{10}$ alloy.

In this work, we studied the precipitation process of $Ni_{75}Al_{15}Ti_{10}$ alloy by microscopic phase-field simulation. Effects of single aging temperature and dual aging process (re-aging process) on the precipitation process of $Ni_{75}Al_{15}Ti_{10}$ alloy including the formation and transformation of γ', the path of atomic diffusion, atomic occupation probability and volume fraction of γ' phase were systematically investigated.

1 Microscopic Phase-field Model

The phase-field dynamics model has recently appeared as a powerful computational approach to predict the microstructure evolution in materials[19]. The microscopic phase-field kinetics model based on Ginzburg-Landau theory was first proposed by Khachaturyan[20] and developed by Chen[21], which can successfully predict grain growth, coarsening, phase transformation processes by the occupation probability of atoms P(r, t) at different crystal lattice site.

For ternary systems like Ni-Al-Ti alloy, the evolution of morphologies can be described by $P_A(r,t)$, $P_B(r,t)$, and $P_C(r,t)$, which indicate probabilities of occupying A, B and C atoms at a given lattice site r and a certain time t, respectively. Each lattice site is represented by two independent equations due to $P_A(r,t)+P_B(r,t)+P_C(r,t)=1$. Thus, microscopic diffusion kinetics equation is written as follow

$$\begin{cases}\dfrac{\mathrm{d}P_A(r,t)}{\mathrm{d}t}=\dfrac{1}{K_BT}\sum_{r'}\left[L_{AA}(r-r')\dfrac{\partial F}{\partial P_A(r',t)}+L_{AB}(r-r')\dfrac{\partial F}{\partial P_B(r',t)}\right]+\xi(r,t)\\ \dfrac{\mathrm{d}P_B(r,t)}{\mathrm{d}t}=\dfrac{1}{K_BT}\sum_{r'}\left[L_{BA}(r-r')\dfrac{\partial F}{\partial P_A(r',t)}+L_{BB}(r-r')\dfrac{\partial F}{\partial P_B(r',t)}\right]+\xi(r,t)\end{cases} \quad (1)$$

where K_B is Boltzmann constant ($\approx 1.3807\times10^{-23}$), T is the temperature, t is time step, $L_{\alpha\beta}(r-r')$ is a constant that is related to the exchange probability of α and β at lattice site r and r' in unit time, $\xi(r, t)$ is random thermal fluctuation term which is added in Eq.(1) to describe nucleation process, and F is the total free energy of the system.

In the mean-field theory, F is expressed by the following equation:

$$\begin{aligned}F=&-\frac{1}{2}\sum_r\sum_{r'}\begin{bmatrix}V_{AB}(r-r')P_A(r)P_B(r')+V_{BC}(r-r')P_B(r)P_C(r')+\\ V_{AC}(r-r')P_A(r)P_C(r')\end{bmatrix}\\ &+k_BT\sum_r\left[P_A(r)\ln(P_A(r))+P_B(r)\ln(P_B(r))+P_C(r)\ln(P_C(r))\right]\end{aligned} \quad (2)$$

where $V_{\alpha\beta}$ is the interaction energy of a pair of atoms. In order to accurately describe free energy of the system, the fourth nearest-neighbor interatomic potential is adopted. $V^1_{\alpha\beta}$, $V^2_{\alpha\beta}$, $V^3_{\alpha\beta}$, $V^4_{\alpha\beta}$ represent the first, second, third and fourth nearest-neighbor interaction energy parameter between α and β, respectively. According to the reciprocal space of the fcc lattice, we can finally obtain the interaction energy $V_{\alpha\beta}(k)$:

$$\begin{aligned}V_{\alpha\beta}(k)=&4V^1_{\alpha\beta}(\cos\pi h\cdot\cos\pi k+\cos\pi h\cdot\cos\pi l+\cos\pi k\cdot\cos\pi l)+\\ &2V^2_{\alpha\beta}(\cos2\pi h+\cos2\pi k+\cos2\pi l)+\\ &8V^3_{\alpha\beta}(\cos2\pi h\cdot\cos\pi k\cdot\cos\pi l+\cos\pi h\cdot\cos2\pi k\cdot\cos\pi l+\\ &\cos\pi h\cdot\cos\pi k\cdot\cos2\pi l)+\\ &4V^4_{\alpha\beta}(\cos2\pi h\cdot\cos2\pi k+\cos2\pi h\cdot\cos2\pi l+\cos2\pi k\cdot\cos2\pi l)\end{aligned} \quad (3)$$

where h, k, l are the constant related to reciprocal lattice sites, and reciprocal vector $\boldsymbol{k}$ can be acquired by the following Eq.(4):

$$\boldsymbol{k}=(\boldsymbol{k}_x,\boldsymbol{k}_y,\boldsymbol{k}_z)=2\pi(h\boldsymbol{a}_1^*+k\boldsymbol{a}_2^*+l\boldsymbol{a}_3^*) \quad (4)$$

In Eq. (4), $\boldsymbol{a_1}^*$, $\boldsymbol{a_2}^*$, $\boldsymbol{a_3}^*$ are reciprocal vectors along [100], [010], [001] crystal orientation in unit reciprocal cell of fcc lattice, respectively.

Substituting Eq.(2) into Eq.(1), and applying Fourier-transform to Eq.(1). Hence, we can obtain the microscopic Langevin equation in the Fourier space. The occupation probabilities of the atoms at different time steps are acquired by solving Eq.(1) with Eiler method. Through occupation probabilities of atoms, we can observe atomic migration and clustering, phase transformation and decomposition, and coarsening in pre-precipitation of alloys.

2 Results and Discussion

2.1 Effect of single aging temperature on the phase structure, occupation probability and atomic diffusion

Fig.1 shows the 3D structure of the ordered phase and its 2D structure along [010] projection of $L1_2$ phase, I-type of $L1_0$ phase and II-type of $L1_0$ phase. In addition, $L1_2$ structure is classified into α site and β site, corresponding to the center site

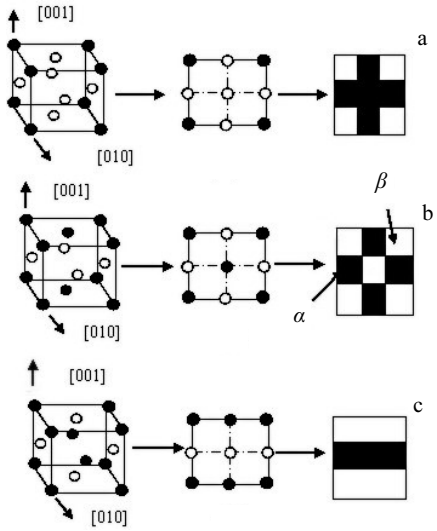

Fig.1 Ordered γ' phase structure and the [010] direction of 2D projection: (a) $L1_2$ phase, (b) $L1_0$ (I) phase, and (c) $L1_0$ (II) phase

of the side face and the corner site in fcc structure, respectively.

In this simulation, 128×128 lattice points are used as computational matrix, and periodic boundary conditions in all directions are applied. In order to precisely predict the process of nucleation and phase transformation, the value of random thermal fluctuation and elastic strain energy are set to 30 and 550, respectively. Occupation probabilities of atoms are represented by different colors in which the dark blue is Ni atom, the red is Al and the green indicates Ti atom when the value of occupation probability is 1.0. Through the evolution of atomic images and alloy morphology, we can directly observe the details of atomic configuration at the same position for different time steps.

Fig.2 shows the atomic figures of microstructure evolution of $Ni_{75}Al_{15}Ti_{10}$ at different temperatures. It can be seen that there are random concentration fluctuations in the disordered matrix at the initial stage of precipitation when the time step is approximately 5000 steps, and some pre-precipitated phase with low ordered degree forms. When the time step is up to 10 000, a large amount of ordered phase appear in the matrix but ordered regions are unclear and its lattice site is similar to Fig.1c, which indicates that the pre-precipitated phase is mainly composed of $L1_0$ (II) phase. Furthermore, a little $L1_2$ phase with lower order degree appears in the matrix (partially enlarged regions are located at the left and right corner in Fig.2a_2).

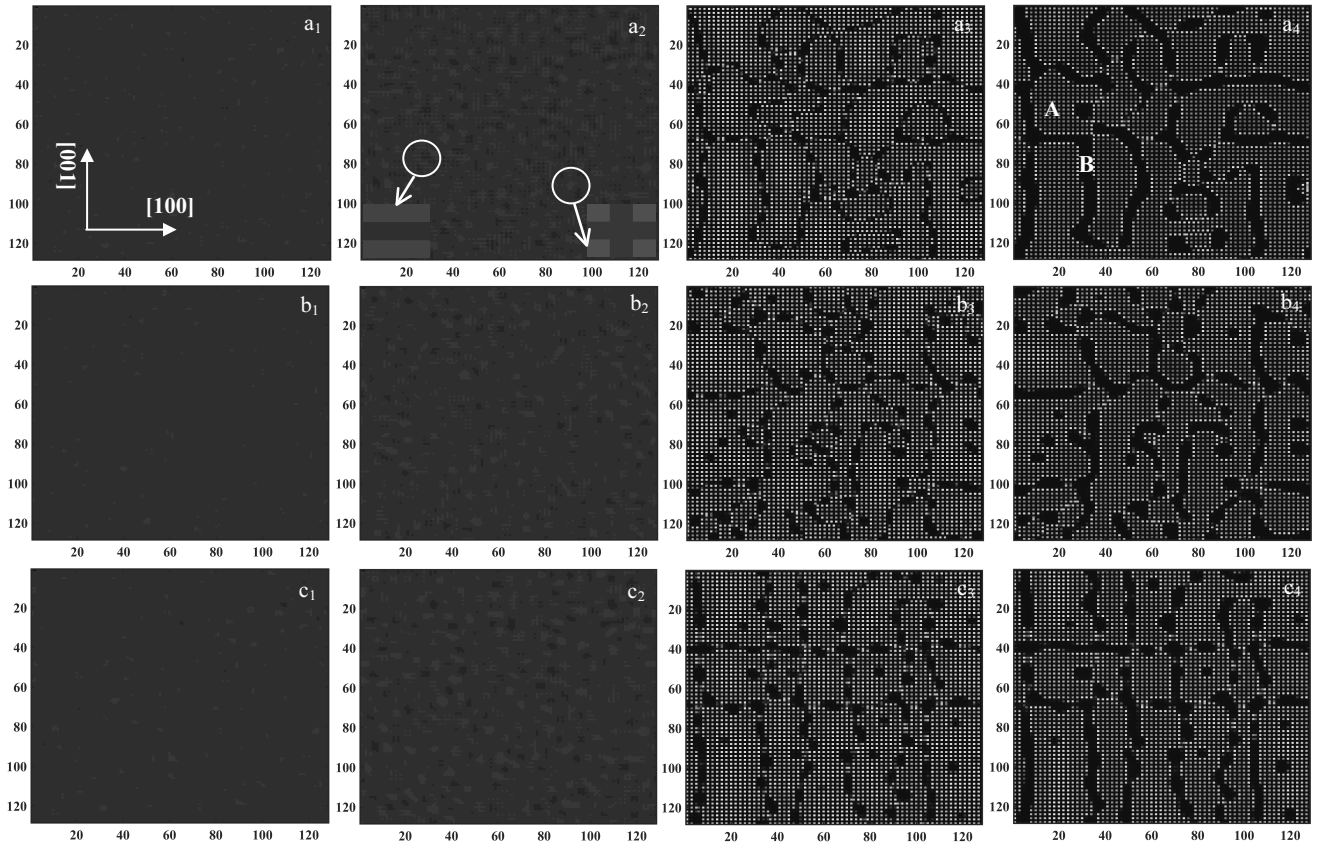

Fig.2 Microstructure evolution of $Ni_{75}A1_{15}Ti_{10}$ alloy at different temperatures: (a_1) T=1173 K, t=5000; (a_2) T=1173 K, t=10 000; (a_3) T=1173 K, t=50 000; (a_4) T=1173 K, t=140 000; (b_1) T=1273 K, t=6000; (b_2) T=1273 K, t=12 000; (b_3) T=1273 K, t=70 000; (b_4) T=1273 K, t=140 000; (c_1) T=1373 K, t=10 000; (c_2) T=1373 K, t=18 000; (c_3) T=1373 K, t=90 000; (c_4) T=1373 K, t=140 000

Subsequently, $L1_0$ phase gradually transforms into $L1_2$ phase with a lower order degree, and the small precipitated γ' particles are close to each other and integrate into larger particles, which indicates that the precipitation process enters into the coarsening stage. With time going, the $L1_0$ phase completely converts to $L1_2$ phase, and eventually that precipitated phase is composed of two-phase, which is γ' phase (A region) and Ni matrix phase (B region). Meanwhile, anti-phase domain boundary forms between γ' phase and γ phase, and the interfaces become clear and narrow (Fig.2a_4). In addition, the occupation probability of lattice site inside the $L1_2$ ordered phase gradually increases, the colors of blue and red lattice point of Ni and Al deepen from Fig.2a_3~2c_3 to Fig.2a_4~2c_4, which indicates that $L1_2$ is in the process of the transformation from the non-stoichiometric to stoichiometric state.

Through the comparison of microstructure evolution of $Ni_{75}Al_{15}Ti_{10}$ at different temperatures, we can draw the following conclusions. With the increase of single aging temperature, the structure of precipitated phase becomes more uniform, that is, γ' phase changes its shape from the irregular to a cuboid. Meanwhile, γ' precipitates are aligned along the elastic "soft directions" of [100] and [001] directions, which is the result of preferred orientation. Furthermore, the interfaces of γ'/γ become clear and the grain size of γ' phase slightly increases with the increase of the aging temperature due to the growth of disordered Ni matrix phase inside the γ' precipitated phase and the spilt of γ' at low temperature. Moreover, we also find that the depth of the lattice of $L1_2$ ordered phase gradually decreases by the rise of aging temperature, and it deepens from the inside to theinterface in γ' phase. On the one hand, it is indicated that the diffusion way of Al and Ti atoms is from the γ'/γ interface to the internal γ' phase, and the concrete analysis will be illustrated hereinafter; on the other hand, it shows that higher temperature can hinder this trend of diffusion. Meanwhile, through the depth of lattice site in γ' phase, especially at the β site, we find that the color of β site is not pure red, which indicates that the β site is occupied by df ferent atoms, and quantitative analyses will be listed in the following part.

The occupation probabilities of atoms at different lattice points are considered to further understand the occupation process of Ni, Al, Ti atoms in γ' phase, and finally clarify the structural transformation. The variation of occupation probabilities of Ni, Al, Ti atoms at α site and β site with different aging temperatures is shown in Fig.3 and specific values are listed in Table 1. It is obvious that there are three stages in the atomic occupation process of α site and β site. Firstly, occupation probabilities of Ni, Al, Ti atoms remain unchanged because the alloy system is in a disordered state and their values maintain the initial level. This stage is called as nucleation incubation period. We can also find that the nucleation incubation period is prolonged with increasing aging temperature, as higher temperature can weaken nucleation driving force, leading to the difficulty of precipitation. Secondly, the occupation probability of Ni in β site decreases rapidly and finally reaches its equilibrium value.

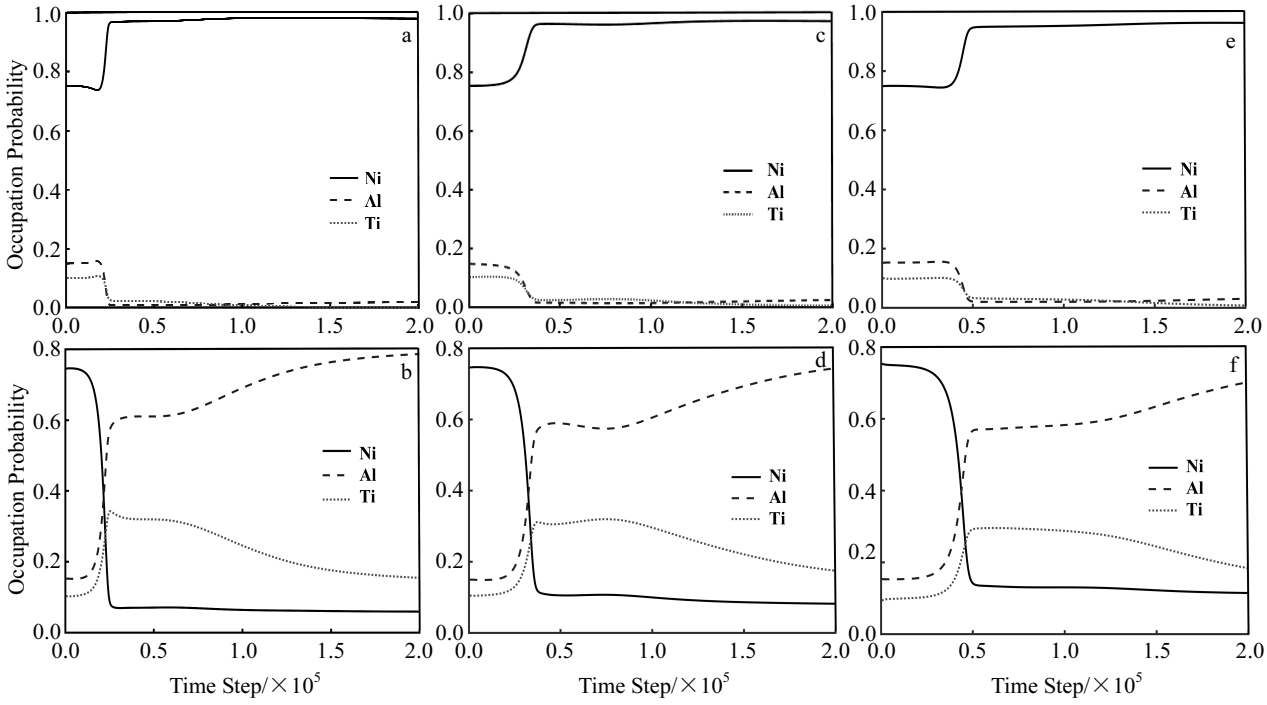

Fig.3 Variation of occupation probabilities of Ni, Al, Ti atoms at α site (a, c, e) and β site (b, d, f) with different aging temperatures: (a, b) T=1173 K, (c, d) T=1273 K, and (e, f) T=1373 K

Table 1 Occupation probabilities of Ni, Al, Ti atoms at α site and β site with different aging temperatures

Temperature/K	Occupation probability					
	Ni atom		Al atom		Ti atom	
	α site	β site	α site	β site	α site	β site
1173	0.9801	0.0591	0.0181	0.7864	0.0018	0.1544
1273	0.9728	0.0818	0.0232	0.7438	0.0040	0.1745
1373	0.9625	0.1143	0.0301	0.7022	0.0074	0.1835

While the values of Al and Ti atoms in β site rise quickly, which indicates that there are clustering of atoms in the alloy system, and this stage corresponds to nucleation, which includes the appearance of $L1_0$ phase and the conversion from $L1_0$ to $L1_2$. At α site, the occupation probability of Ni rises quickly until to the maximum, while the values of Al and Ti atoms are opposite. Hence, α site is the anti-position of Al and Ti atoms and β site is the anti-position of Ni. Furthermore, the lasting time of this stage also increases as the aging temperature rises. It indicates that higher temperature can restrain the process of structural transformation and reduce the degree of order. Thirdly, the occupation probability of Ni remains basically unchanged whether in α site or β site. Although occupation probabilities of Al and Ti atoms in α site remain unchanged, that value in β site changes significantly. First, the occupation probabilities of Al goes up, and that value of Ti gradually drops to the value of 0.15~0.2, which can also validate that the final precipitated phase is the complex compound $Ni_3(AlTi)$. And then, the curves of Al and Ti atoms remain stable, and the equilibrium value of Ti is related to the solid solubility of Ti atom. This stage is corresponding to the process of the transformation from a non-stoichiometric to a stoichiometric state. Through the comparison of occupation probabilities of all atoms at different aging temperatures in Table 1, we can get the point that the occupation probabilities of anti-site atoms increase as the temperature rises, which illustrates that higher temperature can promote the formation of anti-site defects.

To clarify the law of atomic diffusion, we choose a single particle as an object to research the occupation probabilities of Al and Ti from interface to the core with aging time going. Since the aging temperature only influences the atomic motion velocity from the analysis of atomic occupation, we take 1173 K as an instance to discuss the law of atomic diffusion. Fig.4 shows the occupation probabilities of Al and Ti atoms in lattice plane, in which lattice point 1 and 9 represent the interface of γ' phase. At the early stage of precipitation, the occupying value of all atoms remains stable, which is corresponding to the disordered stage of precipitation process. Then, the occupation probabilities of both Al and Ti atoms greatly increase. However, the curve of Al is higher at the edge while lower at the middle, and the curve gradually levels off as the aging time goes on, which indicates that the path of diffusion of Al in the formation of stoichiometric $L1_2$ phase is from the interface to the core of γ' phase. Through a similar analysis of the occupation probability of Ti atom, we can draw the conclusion that the path of diffusion of Ti is from the core to the interface of γ' phase.

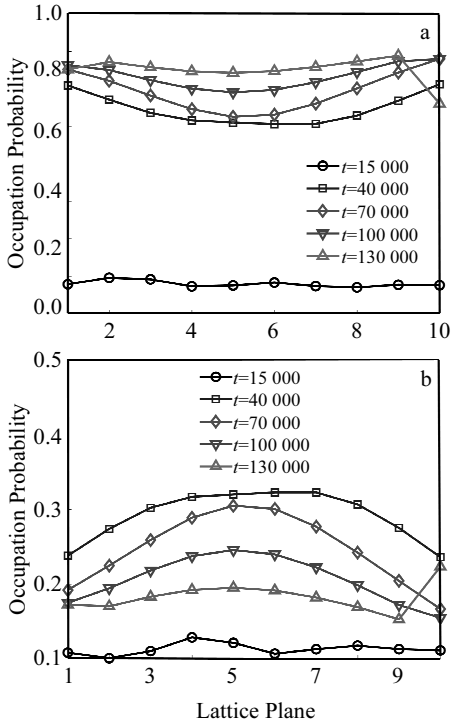

Fig.4 Variation of occupation probabilities of γ' phase in $Ni_{75}A1_{15}Ti_{10}$ aged at 1173 K on lattice plane: (a) Al and (b) Ti

2.2 Effect of dual aging process on the phase structure, occupation probability, volume fraction

Through the study of the precipitation process of $Ni_{75}Al_{15}Ti_{10}$ with one-step aging, we can learn that higher temperature may inhibit the diffusion of Al and Ti atoms to the corresponding lattice site, but it also influences the growth orientation, leading to a result that precipitated phase aligns along [100] and [001] crystal orientation, eventually forming a regular cuboid. In addition, the precipitated phase with high occupation probability, ordering degree and regular shape is expected to exhibit better mechanical property. Hence, the dual aging process can be considered to improve the structure of γ' phase. According to above conclusions, the sample prepared by the two-step aging process (high temperature (1373 K) for a short time and then lower temperature (1173 K) for a long time) is chosen as the candidate to investigate the

effect of dual aging process on phase structure, volume fraction and occupation probability by comparison with the single aging process.

Fig.5 shows the atomic figures of microstructure evolution of $Ni_{75}Al_{15}Ti_{10}$ alloy aged with the two-step aging process of 1373 K (60 000 steps)+1173 K (140 000 steps). In the first 60000 steps, the conversion from $L1_0$ phase to $L1_2$ phase has been basically completed, and the precipitation process is at the stage of coarsening and formation of stoichiometric $L1_2$ phase. Meanwhile, we can also observe that γ' precipitates are oriented in an array along the [100] and [001] crystal orientation (Fig.5a). When precipitation process enters the second step, in which the aging temperature is 1173 K, we can find that the depth of the lattice of $L1_2$ ordered phase is rapidly deepened from Fig.5b, which indicates that the rates of diffusion of all atoms increase suddenly, and the Al, Ni, Ti atoms quickly occupy their corresponding lattice sites. With aging time going, γ' precipitates gradually grow and coarsen, and finally the microstructure of precipitated phase is shown in Fig.5d.

From the final precipitated phase structure graph, it is obvious that the two-step aging process can not only induce γ' precipitates along [100] and [001] crystal orientation but also improve the atomic occupancy compared with the one-step aging at 1173 and 1373 K.

In order to further understand the phase structure and find out the component of γ' phase, we calculate the specific value of occupation probability of Ni, Al and Ti atoms of γ' phase at β site with different aging methods, as shown in Fig.6. We can observe that the value of occupation probability of Ti is up to 0.15~0.2, which is the same as the sample with one-step aging process. Furthermore, the occupation probability of Al with 1373 K+1173 K aging process is higher than that of sample simulated at 1373 K, but the occupation probability of Ni is adverse, and the occupation probability of Ni and Al is similar to that of the sample prepared at 1173 K. It illustrates that the re-aging process can maintain the good performance of Al and Ni atoms of $Ni_{75}A1_{15}Ti_{10}$ aged at 1173 K and has no effect on the solid solution strengthening of Ti atoms.

In addition, the volume of γ' phase in the alloy is an important index to characterizing alloy properties. It is characterized by a volume fraction (VF) which is obtained by the ratio of the volume of ordered phase to the total volume of the system. To further compare the size of γ' phase of different shapes, its equivalent radius are considered, and defined as $R=(A/\pi)^{0.5}$, where $A=a\times b$ is the area of a γ' precipitates determined by measuring the perpendicular sides a and b[11]. And the lattice constant of Ni_3Al is 0.357 94 nm[22]. Compared with that of the alloy aged with one-step aging process of 1173 K, the average particle size (APS) of the alloy with the two-step process increases from 3.42 nm to 4.84 nm, which is attributed to the rapid growth of order precipitates at the first temperature of 1373 K, indicating that the two-step aging process can greatly inherit the microstructure of the precipitated phase at the former temperature, which can be noted as the organization genetic effect of the precipitated phase. Through the comparison of volume fractions, we find that the value of volume fraction of $Ni_{75}A1_{15}Ti_{10}$ aged at 1373 K+1173

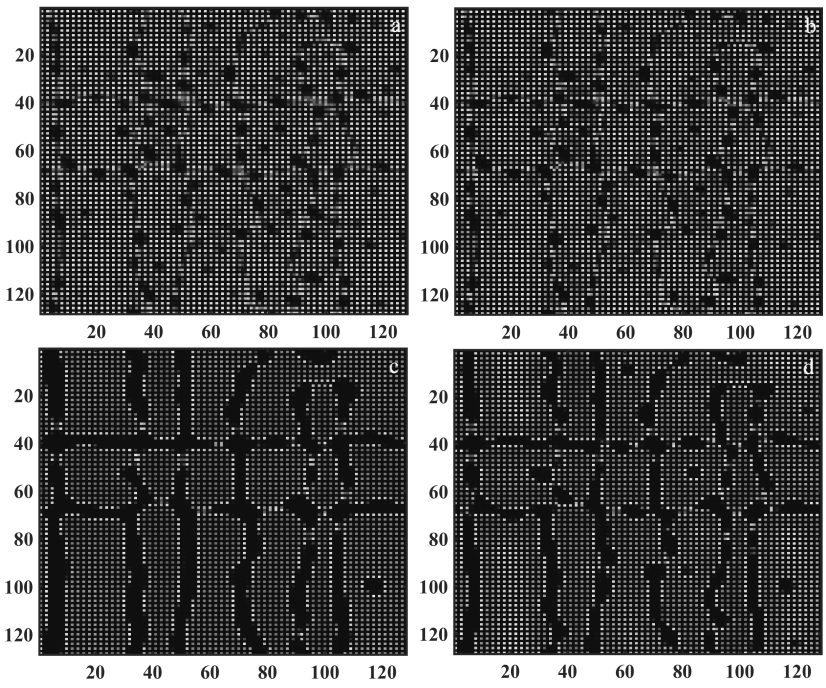

Fig.5 Microstructure evolution of $Ni_{75}A1_{15}Ti_{10}$ aged at 1373 K+1173 K: (a) t=60 000, (b) t=63 000, (c) t=120 000, and (d) t=200 000

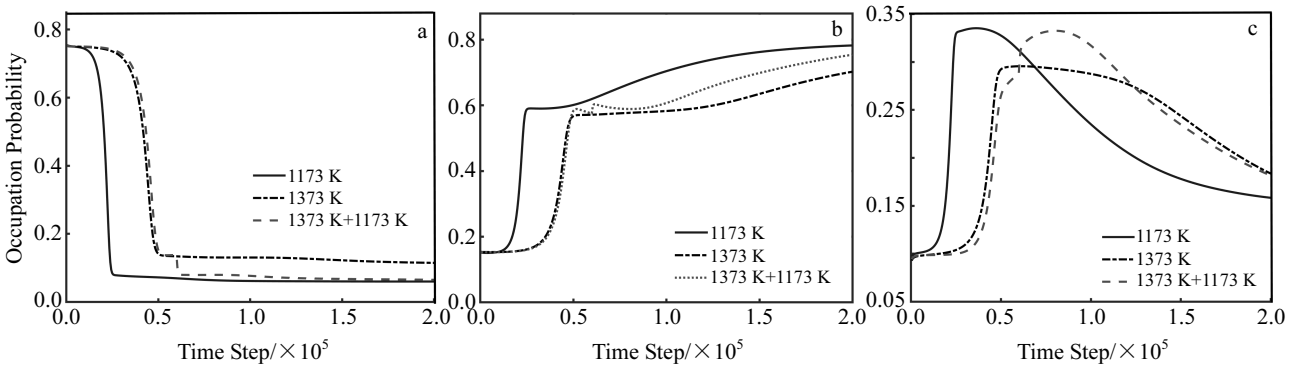

Fig.6 Variation of the occupation of different atoms at β site in the $Ni_{75}Al_{15}Ti_{10}$ alloy aged with different aging processes at different time: (a) Ni, (b) Al, and (c) Ti

K (VF=0.758) is higher than that of the sample aged with one-step process at 1173 K (VF=0.711). It indicates that the two-step aging process is mainly in favor of the formation of γ' phase.

Since the pre-precipitation process is transient, it is difficult to observe by experimental methods. Thus, in order to validate the accuracy of simulation results, we compare them with similar experiment results, which are shown in Fig.7. We studied the microstructure of γ' phase and γ phase in $Ni_{75}Al_{15}Ti_{10}$ aged at 1373 K+1173 K for t =200 000, as shown in Fig.7a. Fig.7b is the DF-TEM image of γ' phase and γ phase of a $Ni_{86.1}Al_{8.5}Ti_{5.4}$ model aged at 1548 K (4 h)+1213 K (0.75 h). From the comparison, we can find that all arrays of γ' phase

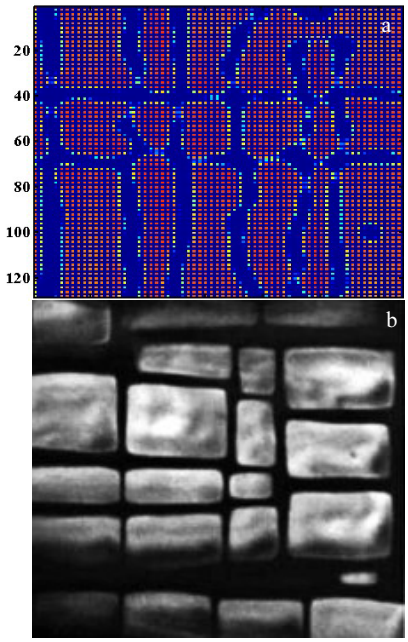

Fig.7 γ' phase morphology obtained from simulated results (a) and experiment observation (b)

along [001] matrix directionshave a regular cuboid shape, and the precipitate microstructure is basically similar.

3 Conclusions

1) In the evolution of phase transformation, the ordering mechanism has two stages: the first is the occurrence of $L1_0$ and its transformation from $L1_0$ to $L1_2$, and the second is the conversion of $L1_2$ phase from non-stoichiometric to stoichiometric state.

2) The higher temperature can drive γ' precipitates aligning along the elastic “soft directions” of [100] and [001] matrix directions, but will lead to lower occupation probability and order degree. Through occupation probabilities of Al and Ti atoms, it can be concluded that the path of diffusion of Al is from the interface to the core of γ' phase, while that of Ti is from the core to the interface of γ' phase.

3) The dual aging process can obtain high occupation probability, order degree and regular shape of γ' phase, which is attributed to the organization genetic effect of the precipitated phase. Meanwhile the VF and APS of $Ni_{75}A1_{15}Ti_{10}$ aged at 1373 K+1173 K go up to 0.758 and 4.84 nm from 0.711 and 3.42 nm, respectively.

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时效工艺对 $Ni_{75}Al_{15}Ti_{10}$ 合金沉淀过程影响的微观相场模拟

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摘　要：通过微观相场动力学模型模拟了 $Ni_{75}Al_{15}Ti_{10}$ 合金的沉淀过程。首先通过原子演化图发现，沉淀过程分为两步，第一步为 $L1_0$ 相向 $L1_2$ 相的转变，第二步为化学计量比的 $L1_2$ 相的形成。其次研究了单级时效温度对微结构，原子占位以及原子扩散的影响。结果表明：随着温度升高，无规则形状的 γ'相变为规则立方体状并且择优取向显著，同时 Al 原子从 γ'相界面向内部扩散，Ti 原子正好相反。但是温度越高，原子占位以及有序化程度越低。为了提高 γ'相的原子占位，进一步比较了双级时效对 γ'相的影响。发现双级时效不仅能获得规则排列稳定的 γ'相，同时还可以提高 Al 与 Ti 原子在其正位处的原子占位并抑制反位缺陷的产生。

关键词：时效温度；双级时效；微观相场；微结构；原子占位

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