Microscopic Phase-Field Simulation for the Influence of Interatomic Potential on the Precipitation Process of $\text{Ni}_{75}\text{Al}_{14}\text{Mo}_{11}$ Alloy

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Abstract The process of γ' phase precipitating from $\text{Ni}_{75}\text{Al}_{14}\text{Mo}_{11}$ is studied by a computational simulation technique based on microscopic phase-field kinetics model. We studied the phase transformation with the purpose of clarifying the influence of the nearest interatomic potential $V_{\text{Ni-Al}}$ (the nearest interatomic potential) on the precipitation process of γ' phase. The result demonstrates that there are two kinds of ordered phases, respective L1_0 and L1_2 in the early stage, and L1_0 phase transforms into L1_2 phase subsequently. For L1_2 phase, Ni atoms mainly occupy α site (face center positions), while Al and Mo atoms occupy β sites (the vertex positions). When $V_{\text{Ni-Al}}$ is increased by 10 MeV, the occupation probability of Ni atoms on α sites and Al atoms on β sites are enhanced. Enhanced $V_{\text{Ni-Al}}$ facilitates clustering and ordering of Al atom, which promotes the formation of the γ' phase. At last, the simulation result was discussed by employing the thermodynamic stability.

KEY WORDS: Interatomic potential; Phase transformation; Microscopic phase-field; Occupation probability

1 Introduction

Interatomic potential and molecular dynamics are of great significance to the development of materials science and technology. The atomic simulation of the materials is based on the interatomic potential, and by this method we can study the properties of the materials at the atomic level and the change process when external conditions changed.

Interatomic potential decides interatomic ordering energy. While the interatomic ordering energy is related to the parameters such as electron density, temperature,

electric field intensity and its variation trend along with plus potential field is more complicated. Changes of interatomic potential can be used to study the impact of external fields (electric field, magnetic field, etc.) on the precipitation of the alloy indirectly. Ustinovshikov [1] studied the microstructure evolution of the $\text{Ni}_{75}\text{Mo}_{20}\text{Al}_{15}$ alloy at the temperatures ranging from 600 to 1600 °C using transmission electron microscopy. By the phase-field method, Miao et al. [2] investigated the relationship between occupation probability changes of Al and Cr atoms on (100) and (200) planes, respectively, and the structure evolution of $\text{Ni}_3(\text{AlCr})$ and found that there are twice in situ transformation during the very early stage. Lu et al. [3] investigated the pre-precipitation process of Ni–Al–Cr alloy using the microscopic phase-field kinetics model and found that temperature plays a significant effect on the pre-precipitated phase with L1_0 ($M = 1$) structure. With increasing temperature, the incubation period and existent time of L1_0 ($M = 1$) pre-precipitated phase are prolonged. It is also found that elastic strain energy has a little effect on the precipitation sequence of Ni–6.8 at.%

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Al–18.2 at.% Cr alloy [4]. With elastic strain energy increasing, the occupation probabilities of Cr atoms at β sublattices and α sublattices in DO₂₂ phase both increase, the occupation probabilities of Cr atoms at β sublattices in L1₂ phase decrease and that of α sublattices in L1₂ phase increase. By graphical demonstration of the anti-site defect-diffusion mechanism, Zhang et al. [5] explained the contribution and the potential harm of anti-site defect to the intermetallic structure materials. Dong et al. [6, 7] studied the formation and transformation of the pre-precipitated phase in the early stage of Ni_{0.75}Al_{0.05}Fe_{0.2} alloy by using the interatomic potential during early-stage precipitation. Zhao et al. [8] studied Cr substitution behavior in Ni₇₅-Al₁₅Cr₁₀ alloy aged at 1073 K using the microscopic phase-field model and found that different interatomic potential can change the Cr occupation probability in α and β sites of γ' phase.

Pasianot et al. [9] developed an interatomic potential method to investigate the microstructure evolution and point defects of the Fe-Cu system based on the embedded atom method (EAM). Oramus et al. [10] simulated the precipitation mechanism of Ni₃Al alloy using MD method on the basis of embedded atom interaction potential.

Although previous studies reported the influence of interatomic potential on the precipitation process in different alloys, few studies have been done about Ni₇₅Al₁₄Mo₁₁ alloy, and almost no reasonable explanation is there on how interatomic potential influence phase precipitation.

In this paper, considering the effect of external field on the atomic ordering behavior, we investigated how Ni–Al interatomic potential influences the precipitation process of the γ' phase in Ni₇₅Al₁₄Mo₁₁ alloy aged at 1073 K, including ordering and clustering of Al and Mo as well as the incubation period of γ' phase and occupation probability of different atoms in α and β sites. By studying the influence of interatomic potential, we hope to design the microstructure of the alloy by control external field.

2 Phase-Field Model

The microscopic phase-field kinetics model based on Ginzburg–Landau theory was found by Khachaturyan [11] and developed by Chen [12–15]. It is a deterministic phase-field method which can describe all diffusion processes, including atomic clustering, ordering, boundary migration, growing and coarsening by using occupation probability $P(r, t)$, indicating occupation probability on lattice r at time t , and it is a discrete lattice form of Cahn–Hilliard diffusion equation [16]. In addition, this model can produce microstructures, composition and order degree changes of system in early precipitation stage thoroughly. The kinetic equation of ternary system is written as

$$\begin{cases} \frac{dP_A(r, t)}{dt} = \frac{1}{k_B T} \sum_{r'} \left[L_{AA}(r - r') \frac{\partial F}{\partial P_A(r', t)} + L_{AB}(r - r') \frac{\partial F}{\partial P_B(r', t)} \right] \\ \frac{dP_B(r, t)}{dt} = \frac{1}{k_B T} \sum_{r'} \left[L_{BA}(r - r') \frac{\partial F}{\partial P_A(r', t)} + L_{BB}(r - r') \frac{\partial F}{\partial P_B(r', t)} \right] \end{cases} \quad (1)$$

Equation (1) is a microscopic Langevin equation, where $L_{\alpha\beta}(r - r')$ is the atom transition probability constant of α and β , which changes from lattice r to r' ; and $\alpha, \beta = A, B$ or C ; k_B is Boltzmann constant; t is time step; T is the temperature; $P_A(r, t)$, $P_B(r, t)$ and $P_C(r, t)$ stand for occupation probabilities of A , B and C at a certain time step, and $P_C(r, t) = 1 - P_A(r, t) - P_B(r, t)$; F is the total free energy of system, it comes from the mean field theory

$$\begin{aligned} F = & -\frac{1}{2} \sum_r \sum_{r'} [V_{AB}(r - r') P_A(r) P_B(r') \\ & + V_{BC}(r - r') P_B(r) P_C(r') + V_{AC}(r - r') P_A(r) P_C(r')] \\ & + k_B T \sum_r [P_A(r) \ln(P_A(r)) + P_B(r) \ln(P_B(r)) \\ & + P_C(r) \ln(P_C(r))], \end{aligned} \quad (2)$$

$$\begin{aligned} V_{AB}(r - r') &= W_{AA}(r - r') + W_{BB}(r - r') - 2W_{AB}(r - r') \\ V_{BC}(r - r') &= W_{BB}(r - r') + W_{CC}(r - r') - 2W_{BC}(r - r') \\ V_{AC}(r - r') &= W_{AA}(r - r') + W_{CC}(r - r') - 2W_{AC}(r - r'), \end{aligned} \quad (3)$$

where $V_{\alpha\beta}$ is a useful interaction energy among atoms and in the Fourier space is $V(k)$; $W_{\alpha\beta}(r - r')$ is the elastic interaction energy and in Fourier space is $B(e)$. In this model, the fourth nearest-neighbor interatomic potential is adopted. $V_{\alpha\beta}^1$, $V_{\alpha\beta}^2$, $V_{\alpha\beta}^3$, and $V_{\alpha\beta}^4$ are the first-, second-, third- and fourth-nearest interatomic potentials between α and β , respectively. Then, substituting them into the FCC, the reciprocal space is as follows:

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

where h, k , and l are reciprocal lattice sites obtained from the following:

$$\vec{k} = (k_x, k_y, k_z) = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^* \quad (5)$$

where $\vec{a}_2^*$, $\vec{a}_2^*$, and $\vec{a}_3^*$ are the unit reciprocal lattice vectors of the FCC lattice structure along three directions.

A Fourier transform was applied to Eqs. (1) and (2), and the free energy was added to the microscopic Langevin equation in the Fourier space. We solved the equation using the Euler method and obtained the occupation probabilities of the atoms at different time steps, and the evolution morphology of the precipitates is obtained according to the variation of occupation probability.

Theoretically, it has a great advantage in studying the pre-precipitation phase and the phase precipitation process [17]. We chose a computational matrix consisting of 128×128 lattice points and use dark blue for the Ni atoms, light green for the Al atoms and red for the Mo atoms. The lattice site is dark blue if the occupation

probability of Ni is 1.0, light green if the occupation probability of Al is 1.0 and red if the occupation probability of Mo is 1.0. The color defines the atoms occupation probability at the lattice site. The figures for the precipitation process are obtained to investigate and analyze the microstructure and how the interatomic potential influences the precipitation process.

3 Results and Analysis

3.1 Microstructure Evolution

Figure 1 shows the structures of ordered phase and their projections along [010]. Figure 1a is the crystal structure of $L1_0$ ($M = 1$) and its projection, while Fig. 1b is that for

Fig. 1 Schematic diagrams of the crystal structure and projections along direction [010]: **a** structure of $L1_0$ ordered phase; **b** structure of $L1_2$ (γ' phase) ordered phase

L1₂. In Fig. 1, the black dots indicate X atoms and white dots indicate Ni atoms.

Figure 2 shows the atomic figures of microstructure evolution of Ni₇₅Al₁₄Mo₁₁ alloy under 1073 K. The color assigned to each lattice site is a mixture of red, green, and blue. From Fig. 2a, we can see that there are concentration fluctuations and atom clustering in the disordered matrix at 10,000 steps. It is difficult to distinguish the structures because of low ordered degree of pre-precipitated phase. Ordered structure appears in the matrix since 22,000 steps, which randomly distributes in the matrix with diffuse interfaces among them. We enlarge the ordered phase shown as the box on the lower corner. But at this moment, these ordered particles are unclear and belong to non-stoichiometric ordered phase. In addition, compare Fig. 1a with b, the pre-precipitated phases are respective L1₀ and L1₂ with lower ordered degree. As time goes on, L1₀ ordered transition phase gradually reduces and L1₂ phase gradually increases. The L1₀ structure transforms into L1₂ phase in situ as the occupation portability changes (Fig. 2c, d). At the same time, non-stoichiometric L1₂ phase gradually transforms into stoichiometric L1₂ phase. Over time, collision and fusion of these ordered phases occur, and some small particles are blended in larger particles nearby which is called coarsening process—small domains disappear, large domains grow up and the interfaces form between the ordered phases. As the time goes continuously, the L1₀ structure turns into L1₂ structure completely, and only γ' (L1₂)—ordered phase exists eventually. Therefore, anti-phase domain boundary forms among the ordered phases, and the interfaces are clear and narrower. With increasing Ni occupation probability, Ni atoms cluster in the anti-phase domain boundaries, forming the blue area. At the same time, as the occupation probability of Mo atoms increases gradually, the color of red lattice point gradually deepens as shown in Fig. 2e and f. At $t = 500,000$ step, the ordered phases become more uniform and the interface widen.

From the atomic microstructure evolution of Ni₇₅Al₁₄Mo₁₁ alloy at 1073 K, we can see two kinds of ordered phases during the aging process and L1₀ phase transforms into L1₂ phase gradually.

3.2 Analysis of Occupation Probability

Through analysis of the occupation probability of atom at different lattice points, we can qualitatively observe the occupation process of the atoms in the precipitation phase and further clarify the structure transformation. The partial enlarged figures of L1₀ phase transforming into L1₂ phase are shown in Fig. 3.

At 22,000 step, there are two kinds of ordered structures including L1₀ and L1₂ as shown in Fig. 3a, b. As time prolonged, the L1₀ transforms into L1₂ (Fig. 3c) at $t = 70,000$. We can find clearly the color of different lattices changes gradually as time going on (Fig. 3b, c, d). In order to further clarify the structural transformation of γ' phase, we need to compute the occupation probability of Ni, Al and Mo atoms at α , β_1 and β_2 lattice points.

Figure 4 shows the variation of occupation probability of Ni, Al and Mo atoms with time at different sites in Ni₇₅Al₁₄Mo₁₁ alloy aged at 1073 K. Figure 4 shows that before about 10,000 steps, since the alloy system is in disorder, three occupation probability curves are linear. The occupation probabilities of Ni, Al, and Mo atoms at any lattice are the same, which are the initial values.

After 10,000 step, the occupation probability of Ni atom at α site goes up to about 0.9836 rapidly and then it remains unchanged. While the occupation probabilities of Al and Mo atoms reduce rapidly until to the minimum values about 0.0153 and 0.0011, respectively. Therefore, Ni atoms gradually occupy α site, and the occupation probabilities of Al and Mo atoms at α site are very small. So α site is occupied by Ni atom, which is Al and Mo atoms' anti-site. Figure 4b shows that after 8000 step, the occupation probability of Ni atom at β_1 rises again to a maximum 0.9829 and remains unchanged after reducing to a certain value, and those of Al and Mo atoms reduce to small values 0.0154 and 0.0027, respectively, after going up to a certain value. So β_1 site is occupied by Ni atom, which is Al and Mo atoms' anti-site. Comparing Fig. 4a with b, the occupation probabilities at α and β_1 sites during the atomic initial disordered state and the eventual equilibrium state are the same, but the intermediate process is different. At about $t = 22,000$ step shown in Fig. 4b, both Al and Mo atom occupation probabilities at β_1 rise to over 0.2, and at β_2 site rise to over 0.4. So L1₀ pre-precipitated phase is formed at this stage, which corresponds to Fig. 3a, b. In the same way, as shown in Fig. 4c, we can see that after 8000 step, the occupation probability of Ni atom gradually reduces to a small equilibrium value and remains the same; the occupation probability of Al atom slowly rises to a equilibrium value of 0.8422 and that of Mo atoms reduces to the value of 0.1139, meaning that the L1₀ pre-precipitated phase begins to transform toward L1₂ phase. Finally, the occupation probabilities at different sites reach the equilibrium values, meaning that the L1₀ pre-precipitated phase is completely transformed into L1₂ phase. So β_2 sites are occupied by Al and Mo atoms and the occupation probability of Al atom is always bigger than Mo atom. Ni atoms occupy the surface center positions (α site) and Al, Mo atoms occupy the vertex positions (β site).

Fig. 2 Atomic figures of microstructure evolution of $\text{Ni}_{75}\text{Al}_{14}\text{Mo}_{11}$ alloy at 1073 K: **a** $t = 10,000$; **b** $t = 22,000$; **c** $t = 27,000$; **d** $t = 33,000$; **e** $t = 70,000$; **f** $t = 100,000$; **g** $t = 250,000$; **h** $t = 500,000$

Fig. 3 Partial enlarged figures from L1₀ phase to L1₂ phase of Ni₇₅Al₁₄Mo₁₁ alloy aged at 1073 K: **a** $t = 22,000$; **b** $t = 27,000$; **c** $t = 70,000$; **d** $t = 500,000$

Fig. 4 Variation of the occupation probabilities of Ni, Al and Mo atoms with time at different sites in Ni₇₅Al₁₄Mo₁₁ alloy aged at 1073 K: **a** α site; **b** β_1 site; **c** β_2 site

3.3 Influences of the Nearest Interatomic Interaction Energy on the γ' Phase Precipitation Process

Phase precipitation is a process of atomic diffusion. In other words, the change of phase structure is a variation process of the

occupation probability at the lattice. In order to investigate the effect of the interatomic potential on the precipitation process of γ' phase, we changed the nearest interatomic potential $V_{\text{Ni-Al}}$ ($V_{\text{Ni-Al}} = 122.30$ MeV) [18] and then computed the occupation probability of L1₂ phase (Figs. 5, 6), order parameters (Fig. 7) and the volume fraction of γ' phase (Fig. 8).

Fig. 5 Variation of the occupation probabilities of different atoms at α site of γ' phase in $\text{Ni}_{75}\text{Al}_{14}\text{Mo}_{11}$ alloy aged at 1073 K: **a** Ni; **b** Al; **c** Mo

Fig. 6 Variation of the occupation probability of different atoms at β site of γ' phase in $\text{Ni}_{75}\text{Al}_{14}\text{Mo}_{11}$ alloy aged at 1073 K at different time: **a** Ni; **b** Al; **c** Mo

Figure 5 shows the variation of the occupation probabilities of different atoms at α site of L_{12} phase under the condition that $V_{\text{Ni-Al}}$ is changed ± 10 MeV. From Fig. 5, we can find that when the $V_{\text{Ni-Al}}$ increases 10 MeV, the occupation probability of Ni atom at α site increases gradually after about 7000 steps and then goes up rapidly to about 0.9880 and finally remains unchanged, which is bigger than value acquired when the $V_{\text{Ni-Al}}$ is unchanged (Fig. 5a). While the occupation probabilities of Al and Mo atoms decrease after about 7000 steps and then go down rapidly to about 0.0112 and about 0.008, respectively (Fig. 5b, c). It is not hard to find that the curves shift to the left, and the time point that the occupation probability begins to go up earlier.

The changing process of the occupation probability of the atoms at β site of L_{12} phase is given in Fig. 6 when $V_{\text{Ni-Al}}$ is changed ± 10 MeV. In the same way, from Fig. 6 we can find that when the $V_{\text{Ni-Al}}$ increases 10 MeV, the occupation probability of Ni atom at β site decreases gradually after about 7000 steps and then goes up rapidly to about 0.0370 and finally remains unchanged for a long time, which is smaller than the value acquired when the $V_{\text{Ni-Al}}$ is unchanged (Fig. 6a). While the occupation probability of Al atom increases gradually after about 7000

steps and then goes up rapidly to a certain value and then keeps going up slowly to about 0.8524 at last (Fig. 5b, c), which is bigger than the value acquired when the $V_{\text{Ni-Al}}$ is unchanged (Fig. 6b). The occupation probability of Mo atom increases gradually after about 7000 steps and then goes up rapidly to a certain value at first and then goes down slowly to about 0.1116 eventually. With $V_{\text{Ni-Al}}$ increased 10 MeV, the occupation probability of Mo atom becomes smaller. From the occupation probability curves in Fig. 5, it can be seen that all the curves shift to the left, too.

From the above observation and analysis, it can be concluded that during the γ' phase precipitation process in $\text{Ni}_{75}\text{Al}_{14}\text{Mo}_{11}$ alloy aged at 1073 K, the increase in nearest interatomic interaction energy $V_{\text{Ni-Al}}$ can promote the occupation probability of Ni atom at α site and the occupation probability of Al atom at β site, meaning the precipitated phase is not changed. Moreover, the increase in $V_{\text{Ni-Al}}$ makes the transformation time point go ahead meaning the incubation period of γ' phase becomes shorter. So the increase in nearest interatomic interaction energy $V_{\text{Ni-Al}}$ has a promoting effect on the formation of γ' phase.

The changes of Al and Mo average long-range-order parameter (ALROP) and average composition order

Fig. 7 Changes of the average long-range-order parameter (a, c) and average composition parameter (b, d) of Al and Mo with time

Fig. 8 Effect of the nearest interatomic interaction energy on the volume fractions of γ' phase

parameter (ACOP) with time in $\text{Ni}_{75}\text{Al}_{14}\text{Mo}_{11}$ alloy aged at 1073 K are shown in Fig. 7. It shows that clustering process and the ordering process of the atom exist in the phase

precipitation process. The average long range order parameter and average composition order parameter present the atomic ordering–disordering transformation process and clustering process of the atom, respectively. So we can use the ordering of Al and Mo atoms to present the ordering of γ' phase. From Fig. 7a and b, we know the formation process of γ' phase has incubation period. In addition, with $V_{\text{Ni-Al}}$ increased by 10 MeV, both the average long-range-order parameter and average composition order parameter of Al atom increase with time and the curves shift to the left. Figure 7c and d shows the variation of average long range order parameter and average composition parameter of Mo with time in $\text{Ni}_{75}\text{Al}_{14}\text{Mo}_{11}$ alloy aged at 1073 K. It comes to the same conclusion in the same way.

The average long order parameter can reflect the order degree of the precipitated phase and the average composition parameter can reflect the clustering. By these two parameters, the phase precipitation process including the incubation period can be observed clearly. From Fig. 7 and

above analysis, it can be seen clearly that the increase in the nearest interatomic potential $V_{\text{Ni-Al}}$ is helpful for the clustering and the ordering of Al and Mo. The incubation period is shortened. So it has a promoting effect on the formation of γ' phase.

In addition, we also studied how the $V_{\text{Ni-Al}}$ affects the volume fractions of γ' phase. Figure 8 shows the effect of the nearest interatomic potential on the volume fraction of γ' phase. When $V_{\text{Ni-Al}}$ is increased by 10 MeV, the volume fraction curve shifts to the left and the volume fraction of γ' phase goes up to about 91.81%, which increases 33.31% compared to the original volume fraction (68.87%). Therefore, we come to the conclusion that the increase in the nearest interatomic potential $V_{\text{Ni-Al}}$ can promote the formation of γ' phase.

4 Discussion

Chen *et al.* [19] thought that the main factor that influences the second phase precipitation is the driving force leading to the change of local long-range-ordering fluctuations. $\delta\eta(r)$, the second free energy parameter introduced, is related to the corresponding long-range-order parameters:

$$\Delta f \rightarrow \int \left(\frac{\partial^2 f}{\partial \eta^2} \right)_{\eta=0} (\delta\eta)^2 d^3r \rightarrow C(T - T_-) \int (\delta\eta)^2 d^3r, \quad (6)$$

where C is a constant and T_- is the ordering instability temperature below which $(\partial^2 f / \partial \eta^2)_{\eta=0}$ can be negative. Therefore, it is the driving force for local long-range-order fluctuation which is relevant to the rate of ordering. Equation (6) also shows that the driving force for local fluctuation is proportional to the undercooling below the ordering instability line, $(T - T_-)$.

Khachaturyan [20] pointed out the relationship of T_- and $V_{\alpha\beta}(k_0)$.

$$T_- = \frac{\varphi(c)}{k_B} \cdot V_{\alpha\beta}(k_0), \quad (7)$$

where $\varphi(c)$ is a function, which is associated with atomic concentration c . $V_{\alpha\beta}(k_0)$ is the interatomic potential. $V_{\text{Ni-Al}}$ is the interatomic potential of L_{12} phase. From Eq. (7), we can find that the change of $V_{\text{Ni-Al}}$ can only change the ordering instability temperature T_- . And it is easy to find that the undercooling $(T - T_-)$ of L_{12} will increase along with increasing $V_{\text{Ni-Al}}$. And then the driving force increases.

According to this theory above, when the $V_{\text{Ni-Al}}$ increases, the undercooling $(T - T_-)$ of L_{12} will increase following, and then, the driving force of L_{12} phase will become stronger. So the increase in $V_{\text{Ni-Al}}$ can speed up

the precipitation of ordered phase. Thus, in the γ' phase precipitation process of $\text{Ni}_{75}\text{Al}_{14}\text{Mo}_{11}$ alloy aged at 1073 K, it shows that the incubation period of γ' phase becomes shorter and the volume fraction of γ' phase goes up greatly. Here, we just combine these two theories to speculate some phenomena presented in this simulation. Further studies are needed to explain these changes.

5 Conclusions

Two kinds of ordered phases L_{10} and L_{12} precipitate from the systems. Both of them are occupied by Ni, Al and Mo atoms. In addition, the L_{10} transforms into L_{12} as the occupation portability changing.

In the γ' phase (L_{12} phase), α site is occupied by Ni atom and Al and anti-site defect Mo, while Al and Mo atoms occupy β sites together with anti-site defect Ni. The occupation probability of Al atom is always bigger than the occupation probability of Mo atom.

The increase in the nearest interatomic potential $V_{\text{Ni-Al}}$ is helpful for clustering and ordering of Al and Mo atoms, and clustering and ordering of atom appear earlier. The volume fraction of γ' phase increases as $V_{\text{Ni-Al}}$ increases, too. So the increase in $V_{\text{Ni-Al}}$ can shorten the incubation period of γ' phase and promote phase formation.

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References

- [1] Y. Ustinovshikov, J. Alloys Compd. **582**, 119 (2014)
- [2] S.F. Miao, Z. Chen, Y.X. Wang, C. Xu, R. Ma, M.Y. Zhang, Acta Metall. Sin. **45**, 630 (2009) (in Chinese)
- [3] Y.L. Lu, Z. Chen, X. Li, Comput. Mater. Sci. **99**, 247 (2015)
- [4] Y.L. Lu, D.W. Jia, T.T. Hu, Z. Chen, L.C. Zhang, Superlattices Microstruct. **66**, 105 (2014)
- [5] J. Zhang, Z. Chen, Y.X. Wang, L.J. Tong, China Sci. Technol. Pap **16**, 1894 (2015)
- [6] W.P. Dong, Y.X. Wang, K. Yang, Chin. Sci. Bull. **56**, 2055 (2011)
- [7] W.P. Dong, Y.X. Wang, Z. Chen, K. Yang, Trans. Nonferrous Met. Soc. China **21**, 1105 (2011)
- [8] Y. Zhao, Z. Chen, Y.X. Wang, M. Zhang, Acta Metall. Sin. **45**, 635 (2009) (in Chinese)
- [9] R.C. Pasianot, L. Malerba, J. Nucl. Mater. **360**, 118 (2007)
- [10] P. Oramus, C. Massobrio, M. Kozłowski, Comput. Mater. Sci. **47**, 186 (2003)
- [11] A.G. Khachaturyan, *Theory of Structural Transformation in Solids* (Wiley, New York, 1983), p. 129

- [12] L.Q. Chen, A.G. Khachaturyan, *Scr. Metall. Mater.* **25**, 61 (1991)
- [13] R. Poduri, L.Q. Chen, *Acta Mater.* **46**, 1719 (1998)
- [14] L.Q. Chen, W. Yang, *Phys. Rev. B* **50**, 15752 (1994)
- [15] L.Q. Chen, *Annu. Rev. Mater. Res.* **32**, 113 (2002)
- [16] Y. Wang, A.G. Khachaturyan, *Acta Metall. Mater.* **43**, 1837 (1995)
- [17] J.W. Cahn, J.E. Hillard, *Chem. Phys.* **28**, 258 (1958)
- [18] N.T. Wilson, M.S. Bailey, R.L. Johnston, *J. Inorg. Chim. Acta* **359**, 3649 (2006)
- [19] R. Poduri, L.Q. Chen, *Acta Mater.* **46**, 1719 (1998)
- [20] A.G. Khachaturyan, *Theory of Structural Transformations in Solids* (Wiley, New York, 1983), p. 133