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Phase-field study the effects of elastic strain energy on the occupation probability of Cr atom in Ni–Al–Cr alloy

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ABSTRACT

The occupation probability (OP) of Cr atom at α sublattices and β sublattices of DO_{22}–Ni_3Cr and $L1_2$–Ni_3Al in Ni–Al–Cr alloy was studied by using phase-field microelasticity model. The elastic strain energy (ESE) arised by a coherent misfit has little effect on the precipitation sequence of alloy while it changes the behavior of the temporal evolution OP of Cr atom in DO_{22} and $L1_2$ phases. With the ESE increasing, the OP of Cr atom at both α sublattices and β sublattices in DO_{22} phase increases, the OP of Cr atom at β sublattices in $L1_2$ phase decreases, and the OP of Cr atom at α sublattices in $L1_2$ phase increases. Eventually, the ESE leads to directional coarsening of coherent microstructure.

1. Introduction

Ni_3X intermetallic compound generated from the precipitation process of Nickel base alloy plays a significant role on the mechanical properties of high temperature structure materials [1–4], wherein, the yield strength of Ni_3Al phase with $L1_2$ structure increases with temperature, thus most nickel-based alloys possess excellent property of high strength at high temperature. In solid solution, Cr atom may replace Al or Ni atom, or both alternatives [5]. Compared with Cr atom substituting Ni atom, Cr atom substituting Al atom can better improve the yield strength, so the occupation probability (OP) of Cr atom is closely related to the high temperature yield strength of alloy. The elastic strain energy (ESE) arised by lattice mismatch between the ordered precipitates and the disordered matrix affects

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occupation behavior of Cr atom. Therefore investigating the occupancy behavior of Cr atom in the elastic constrained system is important to predict and improve alloy mechanical properties.

The phase-field dynamic model [6–9] has recently emerged as a powerful computational approach for modeling and predicting microstructure evolution in materials. In this model, the composition of alloy is related to a long-range order parameter by a nonequilibrium free energy function of atom single-site occupation probabilities, the nonhomogeneous system is described at atomic scale, and the precipitation process caused by atoms jumping at crystal sites can be simulated. In this work, we investigate the effect of ESE on OP of Cr atom and morphologies evolution of DO_{22} and $L1_2$ phase in Ni–6.8at.%Al–18.2at.%Cr alloy.

2. Model and numerical methods

2.1. Microscopic phase-field dynamic model

The precipitation process can be described by the microscopic phase-field model, which was found by Khachaturyan [10] and developed by Chen [11,12]. In this model, the atomic configuration and morphologies are described by single-sublattices occupation probability function. $P_A(\boldsymbol{r}, t)$, $P_B(\boldsymbol{r}, t)$, and $P_C(\boldsymbol{r}, t)$, respectively represents the probabilities of finding A, B, or C atom at a given sublattices and time. In the ternary system, the occupation functions $P_A(\boldsymbol{r}, t) + P_B(\boldsymbol{r}, t) + P_C(\boldsymbol{r}, t) = 1$, so there are only two equations independent at each lattice sublattice. The microscopic phase-field kinetic model of ternary system is described as follows:

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

where $\boldsymbol{L}_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}')$ is a constant related to the lattice sublattices $\boldsymbol{r}$ and $\boldsymbol{r}'$ per unit time, α, β = A, B, or C. k_B is the Boltzmann constant; $\xi(\boldsymbol{r}, t)$ is the thermal noise term, which is assumed to be Gaussian-distributed with an average value of zero, be uncorrelated with space and time, and obey the so-called fluctuation dissipation theory; F is the total free energy of system and can be given by the following equation:

$$\begin{aligned} F = -\frac{1}{2}\sum_{\boldsymbol{r}}\sum_{\boldsymbol{r}'}\left[\begin{array}{l} V_{AB}(\boldsymbol{r}-\boldsymbol{r}')P_A(\boldsymbol{r})P_B(\boldsymbol{r}') + V_{BC}(\boldsymbol{r}-\boldsymbol{r}')P_B(\boldsymbol{r})P_C(\boldsymbol{r}') \\ +V_{AC}(\boldsymbol{r}-\boldsymbol{r}')P_A(\boldsymbol{r})P_C(\boldsymbol{r}') \end{array}\right] \\ + k_B T\sum_{\boldsymbol{r}}[P_A(\boldsymbol{r})\ln(P_A(\boldsymbol{r})) + P_B(\boldsymbol{r})\ln(P_B(\boldsymbol{r})) + P_C(\boldsymbol{r})\ln(P_C(\boldsymbol{r}))] \end{aligned} \tag{2}$$

where $V_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}') = V_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}')_{ch} + \boldsymbol{B}(e)_{el}$ is the interaction energies between α and β at lattice sublattices γ and γ', $V_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}')_{ch}$ is short-range chemical interaction and $\boldsymbol{B}(e)_{el}$ is long-range strain-induced elastic interaction.

2.2. Microelasticity field

In the microelasticity theory, the ESE of solid solution is given as a sum of two physically distinct terms [13]: (1) the configuration-independent term describing the self-energy and image force-induced energy, (2) the configuration dependent term associated with concentration inhomogeneity. The first term is not affected by the spatial redistribution of solute atoms and therefore it can be ignored. The second term gives a substantially nonlocal elastic strain energy change associated with spatial distribution of solute atoms, so it affects the morphology of the precipitation phase.

In a real space, the configuration-dependent elastic strain energy associated with an arbitrary atomic distribution $P(\boldsymbol{r})$ is [14]