Materials Chemistry and Physics 217 (2018) 23–30

Contents lists available at ScienceDirect

Materials Chemistry and Physics

journal homepage: www.elsevier.com/locate/matchemphys

Morphology and kinetics evolution of γ′ phase with increased volume fraction in Ni–Al alloys

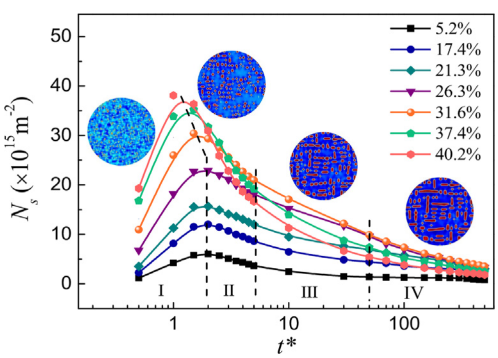
Chengwei Liu[a,b], Yongsheng Li[a,b,*], Lihui Zhu[a,b], Shujing Shi[a,b], Shi Chen[a,b], Shengshun Jin[a,b]

[a] School of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing, 210094, China
[b] MIIT Key Laboratory of Advanced Metallic and Intermetallic Materials Technology, Nanjing, 210094, China

HIGHLIGHTS

- Precipitation kinetics of γ′ phase at different volume fractions are studied.
- Average aspect ratio of precipitates increases with increased volume fraction.
- Coarsening rate decreases first and then increases with increased volume fraction.
- Particles size distribution deviates from LSW's predication for large volume fraction.

GRAPHICAL ABSTRACT



ARTICLE INFO

Keywords:
Ni–Al alloys
Volume fraction
Precipitation kinetics
Phase-field

ABSTRACT

The morphological evolution and precipitation kinetics of γ′ phase in Ni–Al alloys with the variation of volume fraction are studied by using phase-field simulation. The variation of morphology, particles number density and coarsening rate constants are quantitatively clarified with increased volume fraction. The shape of γ′ phase changes from square to rectangular and then to connected strip structure, so the average aspect ratio of γ′ phase increases. The change rate of particles number density has an uniformly increase at the nucleation and growth stage, while it increases firstly and then decreases for volume fraction greater than 30% at the coarsening stage. The coarsening rate constants decrease for the volume fraction less than 20%, while increase when the volume fraction is greater than 30%. In addition, the width of the particles size distribution (PSD) broadens and the peak value decreases, the peak position shifts from 1.0 to 0.5, the PSDs deviate from the theoretical value by the Lifshitz-Slyozov-Wagner for the large volume fraction.

1. Introduction

Ni-based superalloys have been served as the high temperature structure materials in the aerospace fields, such as working blades of aero-engine, combustion chamber and turbine disk, for the excellent toughness, high temperature creep strength, oxidation resistance, corrosion resistance and anti-fatigue properties of the superalloys [1–5]. The high-temperature mechanical properties of Ni-based superalloys are obtained mainly from the precipitation strengthen of ordered $L1_2$-γ′ precipitates, which is embedded into the γ–matrix through aging treatment, and hinders the movement of dislocations, thereby enhancing the mechanical properties of the alloys. Therefore, the properties

* Corresponding author. School of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing, 210094, China.
E-mail addresses: cwliu16@163.com (C. Liu), ysli@njust.edu.cn (Y. Li), zlhqjulie@163.com (L. Zhu), ssj3677@163.com (S. Shi), chenshi6211@163.com (S. Chen), jinshengshun@163.com (S. Jin).

https://doi.org/10.1016/j.matchemphys.2018.06.038
Received 3 April 2018; Received in revised form 10 June 2018; Accepted 18 June 2018
Available online 19 June 2018

of Ni-based superalloys are closely related to the volume fraction of the precipitates, which has a great influence on the particles size and spatial distribution of precipitates [6,7]. It is necessary to study the influence of volume fraction of the precipitates on the precipitation kinetics of the γ′ phase, including the particles size and particles size distribution [8,9].

The introduction of coherent precipitates by the heat treatment is a vital method of alloys strengthening, and the volume fraction of precipitates affects the morphology and coarsening kinetics of the γ′ phase. Ardell et al. [10,11] have pointed out that the coarsening rate decreases with increased volume fraction in the small volume fraction of Ni-based superalloys, which is contrary to the coarsening theory and the coarsening kinetics under unstressed systems, this phenomenon is called "abnormal" coarsening. Kim and Ardell [12] showed that the coarsening rate of Ni_3Ge decreases and the width of the PSD is broadened with increased volume fraction, simultaneously, the peak value of PSD is less than that of Lifshitz-Slyozov-Wagner (LSW), because the LSW theory assumes a small volume fraction and ignores the effect of the elastic interaction [13,14]. The elastic interaction is infinitely long range, which can lead to the strong spatial correlation between the precipitates, resulting in their coarsening along a certain crystal direction. In the presence of coherency stress, the precipitates display different coarsening behaviors compared to that without stress. Vaithyanathan et al. [15] also verified this inference by phase-field simulation. The simulated results showed that the morphology of the precipitates changes from square to rectangular, and then to the plate-shaped with increased volume fraction. When the volume fraction of γ′ phase is less than 20%, the coarsening rate constants decrease with increased volume fraction, and the coarsening rate remains constant when the volume fraction of γ′ phase is in the range of 20–50%, but when the volume fraction is more than 50%, the coarsening rate increases instead, The reason is that the large volume fraction promotes the particles coalescence, resulting in an increase in the coarsening rate constants. The particles size distribution (PSD) shows that when the volume fraction is less than 50%, the peak position and width of the distribution have no obvious change, and when the volume fraction is greater than 50%, the peak position moves to the left and the distribution is widened.

Cho et al. [16] studied the coarsening kinetics of Ni_3Si at a volume fraction of 3–30%. Their research indicates that when the volume fraction is less than 10%, the coarsening rate constants decrease with increased volume fraction, when the volume fraction is greater than 10%, the coarsening rate constants are not affected by the volume fraction, the experimental results are similar to Vaithyanathan's results. However, Jayanth et al. [17] showed that the coarsening rate constants increase with increased volume fraction. Vaithyanathan argued that this phenomenon is due to the prolonged aging, which produces non-equiaxed and non-cubic precipitates [15], therefore, Jayanth's results can not be compared with the coarsening in the shape of equiaxed precipitates.

In addition, the volume fraction of the precipitates has substantial effects on the mechanical properties. Trevisiol et al. [18] found that the hardness increases with increased martensite volume fraction in low alloy steels. Chen et al. [19] conducted a creep test on Inconel 718 alloy aged at 625 °C with 795 MPa loading, and found that when the volume fraction of the δ phase is below 45%, the rupture time and total creep strain decrease as the volume fraction increases, however, when the value is greater than 45%, the rupture time and the total creep strain increase. Therefore, it is generally accepted that a suitable volume fraction improves the creep resistance of Inconel 718 alloy, and that is an advantage on enhancing ductility and toughness [20].

Nowadays, the experiment and simulation calculation can be performed to study the high temperature alloys, the simulation has advantages on the longtime calculation and discovers the phenomenon that is difficult to be observed by experiments. Such as the phase-field [21,22] simulation for the early stage and continuum phase transformation, and the ab initio molecular dynamics on revealing the structure change of molecular cluster to a high enough temperatures [23,24].

Therefore, the effects of the volume fraction of γ′ phase in the Ni–Al alloys aged at 1103 K were studied by using phase-field simulation. The morphology of γ′ phase, coarsening rate constants and the PSD were quantitatively simulated with the Al compositions from 16.7 at. % to 17.7 at. % Al, and the volume fractions of γ′ phase change from $Vf = 5.2\%$ to 40.2%. The classical theory predicts that the coarsening rate constants increase with the volume fraction when the volume fraction satisfies a certain range, and the PSD shows a distinct difference with the change of the volume fraction. The selected range of the volume fraction will help to clarify the kinetics evolution of γ′ phase and will compare with the previous results. Several new points will be showed in the present work, which supplies the full understanding of the precipitation kinetics dependent on volume fraction.

2. Model and methods

2.1. Chemical free energy

The total free energy F of the Ni–Al alloy consists of chemical free energy, gradient energy and elastic strain energy, and is expressed by:

$$F = \int_V \left[f(c,\eta) + \frac{\alpha}{2}(\nabla c)^2 + \frac{3\beta}{2}(\nabla\eta)^2 + E_{\mathrm{el}} \right] \mathrm{d}V \tag{1}$$

where V is the volume of the system, $f(c, \eta)$ is the bulk chemical free energy density, $f(c, \eta) = G(c, \eta)/V_m$ [25], V_m is the mole volume, $G(c, \eta)$ is the chemical free energy. α and β are the gradient energy coefficients, which control the diffuse-interface thickness, they need to be determined from the experimentally measured interfacial energy and anti-phase boundary energy, we used the value $\alpha = 2.5 \times 10^{-9}$ J/m, $\beta = 6.0 \times 10^{-12}$ J/m [25], E_{el} is the elastic strain energy density.

By using the CALPHAD method and the thermodynamic database, the chemical free energy of the Ni–Al superalloys, can be expressed by Refs. [26–28]:

$$\begin{aligned} G(c,\eta) = {} & cG_0^{\mathrm{Al}} + (1-c)G_0^{\mathrm{Ni}} + c(1 - c[L_0 + L_1(2c-1) + L_2(2c-1)^2 + L_3(2c-1)^3] \\ & + 12U_1c^2\eta^2 + 36U_4(1-2c)c^2\eta^2 - 48U_4c^3\eta^3 \\ & + (RT/4) \times \begin{Bmatrix} [c(1+3\eta)]\ln[c(1+3\eta] + [1-c(1+3\eta)]\ln[1-c(1+3\eta)] \\ +3[c(1-\eta)]\ln[c(1-\eta)] + 3[1-c(1-\eta)]\ln[1-c(1-\eta)] \end{Bmatrix} \end{aligned} \tag{2}$$

where G_0^{Al} and G_0^{Ni} are the Gibbs free energy of Al and Ni, respectively, c is the composition of Al, η is the order parameters, L_0, L_1, L_2 and L_3 are the interaction parameters of excess free energy, U_1, U_4 are the bonding energy parameters, these parameters are functions of temperature [29,30], R is the gas constant, and T is the absolute temperature. The parameters were chosen such that the chemical free energy curve provides a qualitative description of the thermodynamics of the Ni–Al alloy system at 1103 K. Fig. 1 (a) shows the chemical free energy of the γ phase and γ′ phase of the Ni–Al alloy as a function of Al composition