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Phase-field modeling of the γ'-coarsening behavior in Ni-based superalloys

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Abstract

Microstructural changes during heat treatment of the Ni-based CMSX-4 and CMSX-6 superalloys have been investigated experimentally and simulated using a phase-field multi-component model incorporating elastic driving forces in the presence of a lattice misfit. Furthermore, a theoretical model of the coarsening of anisotropic particles is proposed for the prediction of the main kinetic parameters of the coarsening process. A comparison of the main characteristics of the microstructural evolution during non-directional γ'-coarsening, provided from both experiments and phase-field simulations, gives a good agreement of the coarsening kinetics of the CMSX-4 superalloy. However, for the CMSX-6 superalloy, phase-field simulation results and theoretical predictions are not entirely consistent with experimental results, and show that additional effects, for example, those caused by plastic deformation, might be a reason for the slow coarsening rate.

Keywords: Phase transformation; Diffusion; Coarsening; Elastic behavior; Phase-field modeling

1. Introduction

Nickel-based superalloys are used as the material for turbine blades due to their excellent mechanical properties. These excellent properties are a result of the microstructure, which consists of the hard intermetallic γ' phase that is coherently embedded in the Ni-based γ phase. The mechanical properties of these superalloys largely depend on the size, morphology and distribution of the γ' particles. Both the γ and γ' phases have fcc crystallographic lattices, although a small misfit between the two is present. This mismatch results in internal stresses, which strongly influence the microstructural evolution during operation at high temperatures. Typically, the optimum microstructure is a monodispersion of γ' particles but, due to the misfit and other driving forces, the larger particles grow at the expense of the smaller ones. In the end, the microstructure is made up a few large precipitates, which is detrimental to the properties of the superalloy. This happens during the late stages of the precipitation process or during operation. Therefore, knowledge of the coarsening process is an important aspect for the design and optimization of superalloys.

The main goal of this work is to investigate numerically the influence of components with slow diffusivity on the stability of the γ'/γ microstructure at high temperatures. Such knowledge will help in the development of a stable material with an appropriate alloy composition.

Previous studies in this context deal with the coarsening process in the presence of external stresses (see the overview by Wang and Li [1] and the references in Ref. [2]). In this case, the driving force of the coarsening is the difference in the strain in directions normal and parallel to the applied force. The direction of growth of the platelets depends on the sign of the lattice misfit and the applied

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stress. This kind of coarsening, so-called directional coarsening or rafting, has largely been studied by experimental and numerical methods.

In this paper, we simulate the coarsening process in Ni-based superalloys in the absence of external forces. The driving force of the coarsening is the combination of the curvature effect and the elastic strain energy due to the lattice misfit, and it has a similar physical meaning as Ostwald ripening. This type of coarsening has not been sufficiently investigated numerically, particular in the context of the selection of the optimum alloy composition needed to achieve minimal coarsening effects. The development of the γ/γ' microstructure during annealing has been investigated experimentally by Pyczak et al. [3], where the contents of alloying elements, in particular rhenium, ruthenium and iridium, vary. Experimental data has shown that the development of the γ' precipitates is controlled by diffusion. Therefore, in order to understand the effects of alloying elements on the evolution of the γ' precipitates, the modifications to the diffusion rate caused by the alloying elements have to be taken into account.

Several studies [2,4–8] have been carried out to investigate the directional coarsening of misfitting precipitates in the presence of an applied force by means of the the Cahn–Hilliard equation for the evolution of the concentration field and the Allen–Cahn or Ginzburg–Landau equation for the evolution of the order parameter. The thermodynamic model was extended by the elastic energy contribution. The elastic strain energy as a function of the concentration field or a function of the phase-field variable was added to the total energy functional. Recent numerical studies [6] used the model of Kim et al. for binary alloys [9], which is based on thermodynamic databases, to achieve quantitative simulation results. However, the simulations of the directional coarsening was limited to binary alloys.

On the other hand, many studies have focused on the influence of the elastic field from the misfit on the growth and coarsening kinetics of the particles. Phase-field simulations of the Ostwald ripening of spherical γ' precipitates with a small γ'–γ lattice misfit were carried out by Grafe et al. [10] in a ternary Ni–Al–Cr alloy using the extended multi-component Kim–Kim–Suzuki model [11]. They showed good agreement with the experimental data and the classical LSW theory [12]. Phase-field simulations of the γ'-coarsening in a binary Ni–Al alloy carried out for a larger misfit [13] also showed agreement between the coarsening kinetics and experiments and the classical LSW theory at coarsening times of up to 10 h.

In the present work, we apply the quantitative multi-component phase-field model developed in the previous work [14], which continues the theoretical investigations of Kim et al. [9], Tiaden et al. [11] and Eiken et al. [15]. To model the coarsening process and to investigate the influence of the different components, the model was extended by including elastic driving forces from the misfit stress. The thermodynamic properties were modeled in Thermo-Calc using the database TTNi8 and DICTRA software. To make a quantitative kinetic analysis, an analytical expression was evaluated for the definition of the main quantitative characteristics of the coarsening, such as the mean distance between the particles. This analytical model is based on previous works in this field [12,16] and considers the cross-dependencies between the components in multi-component diffusion. Phase-field simulation is used to investigate the kinetics of the coarsening in two commercially available Ni-based superalloys, CMSX-4 and CMSX-6. The results of the phase-field simulation are compared with experimental data and a theoretical expression derived specially for the case of the coarsening of anisotropic particles. We show that, for one investigated alloy, CMSX-4, the coarsening occurs in a purely elastic regime; therefore, preliminary plastic deformation or other effects do not need to be considered. For the CMSX-6 superalloy, a deviation of the experimental data from the theoretical and simulation results can be observed.

In the following section, we introduce the phase-field model that we used to predict the microstructural evolution. The calculation of the elastic energy and its inclusion in the phase-field model is then presented in Section 3. In this section, the various ways to include the elastic effects are compared and analyzed. A coarsening law, which represents the influence of the multi-component diffusion is described in Section 4. The results of the phase-field simulations and their comparison to the analytical expressions and experimental results are presented and discussed in Section 5.

2. The multi-component model with elastic effects

For the simulation of the aging heat treatment process of Ni-based alloys we used the phase-field model developed in our previous work for multi-component alloys [14] and the model successfully used for the simulation of the transformation with elastic effects [1].

The investigated system contains two phases, γ and γ'. In the following, we denote the γ' phase by index p and the γ phase by index q. The phase-field variables are defined on the interval [0,1] as ϕ_p for the γ' phase and $\phi_q = 1 - \phi_p$ for the γ phase.

A non-linear partial differential equation describes the evolution of the interface between the phases

$$\tau \frac{\partial \phi_p}{\partial t} = -\frac{1}{H} \frac{\delta F}{\delta \phi_p} \tag{1}$$

where F is the total free energy in the system, H is a constant with dimensions of energy per unit volume and τ is a relaxation time.

The phase-field kinetic equation following from Eq. (1) has the form

$$\tau \frac{\partial \phi_p}{\partial t} = W^2 \nabla^2 \phi_p - f_{\phi_p} + \frac{\sqrt{2} W}{3\sigma} g_{\phi_p} (\Delta G_{\mathrm{ch}} - \Delta G_{\mathrm{el}}) \tag{2}$$

where ΔG_{ch} is the chemical driving force of the transformation, ΔG_{el} is the elastic driving force, which will be