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Microstructure simulation on recrystallization of an as-cast nickel based single crystal superalloy

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ABSTRACT

Recrystallization (RX) in an as-cast single crystal (SX) nickel-based superalloy was investigated using simulation and experiments. One cellular automaton (CA) method was proposed to predict RX microstructure of SX superalloys. The stored energy was obtained using one macroscopic phenomenon-based elastic–plastic model in this research, and the orthotropic mechanical properties were taken into account. Kinetics parameters were used on the basis of physical fundamentals, and different values were employed in the dendritic arms and interdendritic regions. In order to validate the simulation model, heat treatments under inert atmosphere were conducted on compressed cylinder samples to induce RX. The RX microstructures on the middle section perpendicular to the cylinder axis were observed using EBSD technique. Both simulation and experiments show that the kinetics of recrystallization were significantly different in dendritic arms and interdendritic regions, and simulated microstructure agrees well with experimental. The proposed model in this research can predict the kinetics, microstructural evolution during recrystallization of as-cast SX superalloys.

1. Introduction

Nowadays, nickel-based single crystal (SX) superalloys have been widely used for turbine blades. However, great care should be taken to prevent defects such as stray grains [1,2], freckles [3–5], recrystallization [6–8], etc. Recrystallization (RX) can introduce high-angle grain boundaries and degrade the creep [8,9] and fatigue [10] properties significantly.

RX, which is intolerant in single crystal components, may arise during heat treatment and service term, and can be ascribed to the plastic deformation during manufacturing process. RX behaviors in wrought [11,12], powder metallurgy [13] and oxide dispersion strengthened [14] superalloys have been studied by many researchers. Most of previous work on RX of SX superalloys focuses on the influence of annealing conditions [15,16] and orientational dependence [17,18], microstructural features [19,20] and mechanical properties [8,21,22]. In addition, modeling and simulation have been employed to predict plastic strains and sites where RX can occur [6,7,23,24]. However, microstructural simulations of recrystallization in SX nickel-based superalloys were rarely reported.

Till now, simulation on RX behavior has been conducted in many materials [25–30], most on aluminium [31–35], magnesium [36,37], and steel [38,39]. Nevertheless, little work has been done on the simulation of RX in SX nickel-based superalloys. Many methods, such as monte carlo [40,41], phase field [28,42] and cellular automaton [34,43,44], have been employed to predict the microstructural evolution during RX process. Among these models, CA has gained the highest popularity for its simplicity and higher calculation efficiency. Difficulty of predicting RX microstructure of SX superalloys may result from two facts. First, this alloy consist at least two phases, and secondly little was known about the kinetics. The first problem can be solved by treating the gamma and gamma prime phases as only one phase, taking account into the highly similar lattice parameters. The other one can hardly be solved in previous work, because the growth kinetics of RX in SX superalloys has been little researched and it is difficult to obtain the kinetic parameters from experiments. One microstructural simulation on RX of SX superalloys was reported by Zambaldi et al. [18], and the activation energy for RX grain boundary motion was set as high as 1290 kJ/mol with no physical basis given. This value violated the real condition obviously, though simulation and experimental results can agree with each other in his research. Furthermore, his model seems a little simple and many critical details were not given.

In the present paper, one modified CA model was proposed to conduct the simulation of RX in as-cast SX superalloys. Driving force for RX was obtained using one macroscopic

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phenomenon-based deformation model, considering the anisotropy of SX superalloys. Key simulation parameters were employed based on physical fundamentals in this research. To make the model more accurate, the influence of as-cast dendritic microstructure on RX kinetics was also taken into account. Different grow kinetics parameters were used in the dendritic arms and the interdendritic regions. In this research, experimental and simulated RX microstructures were compared, and this model can give us a better understanding of the influence of as-cast inhomogeneity on RX in SX superalloys.

2. Mathmatical models

2.1. Driving force

Deformed metal or alloys will experience three main stages during heating: recovery, recrystallization and grain growth, as shown in Fig. 1. The effect of recovery is strong for metals and alloys (such as Al) with high stacking fault energy (Al [45], 166 mJ/m^2). The stacking fault energy of pure Ni [46] is about 125 mJ/m^2, while most research indicates that the value for most single crystal nickel-based superalloys is below 20 mJ/m^2, as a result of alloying elements Re, Mo, Nb, W, etc. [46–49]. Thus, the recovery of SX superalloy is very weak, which is also demonstrated by some experiments [16]. Therefore, recovery will be omitted in this research.

Generally, deformed stored energy provides the driving force for recrystallization of deformed metals and alloys during heat treatment. In most previous work, the deformation stored energy was expressed in terms of dislocation density using dislocation-based constitutive models [50,51]. However, these models can hardly describe the deformation behaviors of SX superalloys due to the large amount of the coherent precipitates. Another method is crystal plasticity finite element [18,25,52] (CPFEM), which has gained a great popularity in describing the heterogeneous characteristics of deformation on mesoscale during last two decades. Nevertheless, it can hardly describe the stored-energy distribution on the entire component scale as a result of its limitation of computing amount.

Hence, one macroscopic phenomenon-based deformation model is adopted in the present modeling to obtain the driving force for RX. This model can describe the mechanical behavior of SX nickel-based superalloys, and gain popularity for its concise equations as well as calculation speed. In this model, nickel-based single crystal superalloys can be treated as orthotropic materials, though inhomogeneity exists in single crystal components [6,7]. An elastic–plastic model was employed to describe the mechanical behavior, together with the elastic orthotropy and the Hill yield criterion. Fig. 2 shows Young's modulus in all orientations at 980 °C and 1070 °C. High anisotropy of SX superalloy DD6 can be derived, and elastic modulus decreases with increasing temperatures.

Most of the work expended in deforming a metal is given out and only a very small amount (~1%) remains as energy stored in the material [45]. Hence, the driving force (P) for recrystallization can be calculated using the following form:

$$P = 0.01U^{pl} \tag{1}$$

where U^{pl} denotes plastic dissipated energy, and is obtained as follows:

$$dU^{pl} = \int_0^{\varepsilon_{pl}} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}_{pl} \tag{2}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}_{pl}$ are the stress and plastic strain vector. Hill's flow function is introduced in the following form:

$$f(\boldsymbol{\sigma}) = \frac{1}{\sqrt{2}}\sqrt{(\sigma_{22}-\sigma_{33})^2+(\sigma_{33}-\sigma_{11})^2+(\sigma_{11}-\sigma_{22})^2+2K(\sigma_{23}^2+\sigma_{31}^2+\sigma_{12}^2)} \tag{3}$$

Here, K denotes anisotropic plastic parameter, and can be obtained by tensile or compression tests of the material in different orientations. Isotropic hardening criterion was employed in this paper. One commercial available FEM software (Abaqus) was used for the deformation calculation. More details and model parameters can be found in Ref. [6].

2.2. Nucleation model

Nucleation tends to occur in sites with high deformation stored energy. In this research, nucleation model takes account into real physical influences, e.g., annealing temperature and as-cast concentration inhomogeneity. A continuous nucleation law is implemented. The nucleation rate $\dot{N}$ is controlled by the following equation:

$$N = C_0(P - P^c)\exp\left(-\frac{Q_a}{RT}\right) \tag{4}$$

with R the universal gas constant, T the absolute temperature, and Q_a the activation energy, and P the driving force, which can be determined using above deformation model. C_0 is a scaling parameter ($1.0\times10^9\ s^{-1}\ J^{-1}$ in this research). P^c is the critical stored energy below which recrystallization will not occur. Q_a has different values in dendritic arms (DAs) and interdendritic regions (IDRs).

The value of P^c was computed with the following relation [53]:

$$P^c = \frac{10^7\varepsilon^c}{2.2\varepsilon^c + 1.1}\gamma_{lagb} \tag{5}$$

where ε^c is the critical plastic strain (here set to 2%) and γ_{lagb} is the low angle grain boundary energy, which is assumed as 0.6 J/m^2 in the present work.

2.3. Recrystallization and grain growth model

The movement of the recrystallization front is treated as a strain-introduced boundary migration process. The contribution of driving pressure arising from boundary curvature is neglected for its relative small amount in this stage. Thus, the main driving force in this stage is also the deformation stored energy. The velocity of the RX front, V, moving into the deformed matrix can be expressed as follows:

$$V = MP \tag{6}$$

where M is the grain boundary mobility for the primary static recrystallization and P is driving pressure for the grain boundary movement. The mobility can be estimated by

$$M = M_0\exp\left(-\frac{Q_b}{RT}\right) = \frac{D_0b^2}{kT}\exp\left(-\frac{Q_b}{RT}\right) \tag{7}$$

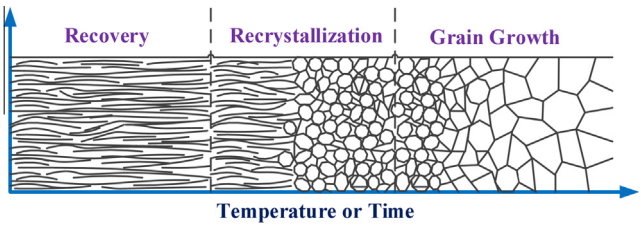

Fig. 1. General change of deformed metal during heat treatment.