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Deformation and recrystallization of single crystal nickel-based superalloys during investment casting

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ABSTRACT

A semi-quantitative, macroscopic, phenomenon-based, thermo-elastic–plastic model was developed to predict the final plastic strains of single crystal nickel-based superalloys by considering their orthotropic mechanical properties. Various cases were considered and simulated to investigate the basic factors that influence the final plasticity. Thermo-mechanical numerical analysis was conducted to predict the recrystallization sites of simplified cored rods, with the results in good agreement with the experimental results. These hollowed rods with thin walls showed an increased propensity for recrystallization. The geometric features, especially stress concentration sites, are more significant to the induced plasticity than the material's orientation or shell/core materials. This paper also attempts to provide useful suggestions, such as introducing filets, to avoid causing plastic strains during the casting process that induce recrystallization.

1. Introduction

Turbine blades for gas turbine applications are fabricated by investment casting, often in single crystal form, which can allow higher inlet gas temperatures to be used and increase efficiency. However, the external and internal geometries of single crystal blades are becoming increasingly complicated, making them more difficult to cast as greater care is required to prevent defects, such as stray grains and freckles, being introduced during the manufacturing process. Recrystallization (RX) is one of the major difficulties and can be ascribed to plastic deformation, as demonstrated by Burgel et al. (2000). During the manufacture of new parts, plastic deformation can be caused by several possible sources: thermal contraction during solidification and subsequent cooling, removing the ceramic mold and core material mechanically, stamping identification marks, grinding the airfoil, etc. In practice, plastic deformation will induce RX during subsequent heat treatments or long-term service. For example, RX can introduce high-angle grain boundaries, which are obviously undesirable. As demonstrated by Meng et al. (2010) and Moverare et al. (2009), RX is potentially detrimental to creep and fatigue properties, respectively.

Work has been done to study the phenomenon of RX in single crystal nickel-based superalloys. Some research has focused on the influence of microstructural features on RX, such as γ′-precipitates, carbides, and γ/γ′ eutectics. For example, Dahlen and Winberg (1980) have discussed the influence of γ′-precipitation on the RX of nickel-based superalloys. Wang et al. (2013) and Xiong et al. (2010) have investigated the effect of carbon content on the RX of single crystal (SX) nickel-based superalloys. In addition, Wang et al. (2009) studied the influence of eutectics on plastic deformation and the subsequent RX of the SX nickel-based superalloy CMSX-4. Meanwhile, some research has concentrated on the effect of different annealing conditions and crystallographic orientations on RX behavior. Wu et al. (2012) conducted surface RX of a Ni_3Al-based SX superalloy at different annealing temperatures and blasting pressures. Xie et al. (2012) studied the crystallographic orientation dependence of RX in a Ni-based SX superalloy. However, little attention has been paid to the effect of geometric features, ceramic shell and core material, and processing details. Certain critical questions need to be answered, such as at what temperature will RX occur? What is the critical plastic deformation required to induce RX?, and what is the influence of the geometric features, including holes and platforms? Answers to these questions will allow more efficient foundry processes, even process-friendly blade designs, to be developed. Modeling has been used to analyze the directional

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solidification of SX superalloys from thermal and microstructural perspectives. Pan et al. (2010) conducted multiscale modeling and simulations of the directional solidification process of turbine blade casting, which resulted in good predictions of temperature profiles and grain number. Dai et al. (2011) investigated grain selection in spiral selectors during investment casting of SX turbine blades through both experimental and numerical modeling techniques. One advantage simulation provides over experiments is that it can predict the plastic strains that cause RX.

The overarching goal of this study was to build a physics-based tool for predicting casting-induced plasticity and subsequent RX during the heat treatment of SX superalloys by considering the material's anisotropic mechanical properties. Panwisawas et al. (2013a,b) developed a mathematical model to predict plasticity and RX in investment-cast SX superalloys. However, this model considered SX superalloys as isotropic materials, which does not conform to the reality. Many mechanical models have been proposed to describe the mechanical properties of anisotropic materials. Ding et al. (2004) proposed a macroscopic phenomenon-based model built on a modified Hill plasticity model. Zambaldi et al. (2007) employed a microscopic crystal plasticity model, which was built on the physical deformation mechanisms of materials, to predict the distribution of crystallographic slip in SX nickel-based superalloys. The former gained great popularity for its concise equations, as well as its convenience and speed of calculations, though the latter model can give more accurate predictions of slips and grain size.

This paper proposed a mathematical thermo-mechanical model using the Hill's plasticity model as a basis, which considers the orthotropic mechanical properties of SX superalloys, and took into account both the scale effect and convenience. Numerical analysis using this model was performed to identify the major factors that cause the plasticity during investment casting and RX during the subsequent heat treatment. A series of simplified thermo-mechanical numerical analyses with the DD6 superalloy were conducted and compared with experimental results to test the validity of the model. This model could be employed to optimize processing conditions to reduce the likelihood of RX.

2. Mathematical model of SX superalloys

Plastic deformation during investment casting mainly occurs because of the different thermal expansion coefficients of the metals, and the ceramic shell and core. Assuming the plasticity is rate-independent, the thermal strain (ε_{th}), elastic strain (ε_{el}), and plastic strain (ε_{pl}) follow the relation below:

$$\varepsilon_{th} + \varepsilon_{el} + \varepsilon_{pl} = 0 \tag{1}$$

The thermal strain can be calculated as

$$\varepsilon_{th} = \alpha \Delta T = \alpha (T - T_{ref}) \tag{2}$$

Here, T_{ref} is the reference temperature, which is usually room temperature. The variable α denotes the thermal expansion coefficient, which is usually considered isotropic for SX materials (Green, 1998).

2.1. Orthotropic elastic properties

The elastic strain part of the model for SX superalloys considers the orthotropic characteristics. For materials with cubic structures (BCC or FCC), where the three principal orientations (denoted 1, 2, and 3) are identical, the elastic constitutive equation is determined with the generalized Hooke law, which can be expressed as follows:

$$\begin{aligned} &\{\varepsilon\} = [S]\{\sigma\} \\ &\{\sigma\} = [S]^{-1}\{\varepsilon\} = [C]\{\varepsilon\} \end{aligned} \tag{3}$$

$$\begin{aligned} &\{\varepsilon\} = [\varepsilon_{11}\varepsilon_{22}\varepsilon_{33}\gamma_{12}\gamma_{23}\gamma_{31}]^T \\ &\{\sigma\} = [\sigma_{11}\sigma_{22}\sigma_{33}\tau_{12}\tau_{23}\tau_{31}]^T \\ &[S] = [C]^{-1} \end{aligned} \tag{4}$$

$$[S] = \begin{pmatrix} 1/E & -\mu/E & -\mu/E & 0 & 0 & 0 \\ -\mu/E & 1/E & -\mu/E & 0 & 0 & 0 \\ -\mu/E & -\mu/E & 1/E & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G \end{pmatrix} \tag{5}$$

where $\{\sigma\}$ and $\{\varepsilon\}$ are the stress and strain vectors, respectively. S_{ij} and C_{ij} denote the elastic compliance and stiffness constants, respectively, which measure the strain (or stress) necessary to maintain a given stress (or strain). E, μ, and G are the Young's modulus, Poisson's ratio, and shear modulus, respectively, in the three principal orientations: ⟨0 0 1⟩, ⟨0 1 0⟩, and ⟨1 0 0⟩. The stiffness and compliance constants have the following relations:

$$S_{11} = \frac{C_{11} + C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \tag{6}$$

$$S_{12} = \frac{C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \tag{7}$$

$$S_{44} = \frac{1}{C_{44}} \tag{8}$$

The matrix phase, γ, and precipitate phase, γ′, both exhibit FCC structures and have coherent interfaces. Therefore, the nickel-based SX superalloys can be considered approximately orthotropic materials with three identical principal orientations. There are only 3 independent constants in [S].

By applying spatial geometry transformations, the Young's modulus, E', and shear modulus, G', in a given crystallographic orientation can be obtained as follows:

$$\frac{1}{E'} = S'_{11} = S_{11} - 2JS\left(\frac{S_{11} - S_{12} - S_{44}}{2}\right) \tag{9}$$

with the orientation parameters J and S given by:

$$J = l^2m^2 + l^2n^2 + m^2n^2 \tag{10}$$

$$S = 2S_{11} - 2S_{12} - S_{44} \tag{11}$$

where l, m, and n represent the directional cosines relative to the axes 1, 2, and 3, respectively. Thus, the degree of anisotropy depends on the orientation parameter, which has a minimum value of zero along ⟨0 0 1⟩, a maximum value of 1/3 along ⟨1 1 1⟩, and a value of 1/4 along ⟨0 1 1⟩. For a pure nickel SX at room temperature, typical values for the compliance constants are $S_{11} = 0.799 \times 10^{-5}\,\mathrm{MPa}^{-1}$, $S_{12} = -0.312 \times 10^{-5}\,\mathrm{MPa}^{-1}$, and $S_{44} = 0.844 \times 10^{-5}\,\mathrm{MPa}^{-1}$. It can be seen that the ⟨1 0 0⟩ direction is the least stiff, while the ⟨1 1 1⟩ direction is the stiffest, with ⟨1 1 0⟩ between these two limits. The values of Young's modulus along these crystallographic orientations are $E_{\langle 0\,0\,1\rangle} = 125$ GPa, $E_{\langle 0\,1\,1\rangle} = 220$ GPa, and $E_{\langle 1\,1\,1\rangle} = 294$ GPa. SX superalloys display a similar degree of anisotropy. To determine the degree of elastic anisotropy in SX cubic materials, the anisotropic factor, A, is defined as:

$$A = \frac{2C_{44}}{C_{11} - C_{12}} = \frac{2(S_{11} - S_{12})}{S_{44}} \tag{12}$$

where $A = 1$ for isotropic materials. For example, the following cubic metals have A values of 2.44 (Ni), 3.19 (Cu), 2.97 (Ag), 2.90 (Au), 1.65 (Ge), and 1.22 (Al). Thus, Ni displays a fair degree of anisotropy, but it is not the most anisotropic cubic metal.

The Young's and shear moduli over a wide range of temperature can be obtained using many methods, with tensile testing and