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Numerical study of the flow responses and the geometric constraint effects in Ni-base two-phase single crystals using strain gradient plasticity

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Abstract

The [0 0 1] tensile flow of a single-crystal superalloy (CMSX-4) having a high volume fraction of regularly-arrayed cuboidal γ' precipitates was simulated using a gradient-dependent plasticity model for the constitutive description of the γ-matrix. The simulated flow curves showed flow softening in the early stage of straining. Flow softening was accompanied by the organized catastrophic plastic flow of the γ-matrix, which resulted from the breakdown of the geometric (or kinematic) constraints imposed by the γ/γ' microstructure. The flow-softening behavior was influenced by the thickness of γ-matrix channels (a volume fraction of the γ' precipitates), the flow property of the γ-matrix and the geometry of the γ'-precipitate edge. In particular, changing the radius of the γ'-precipitate edge resulted in a dramatic variations in the flow curves. The present unit-cell simulations exhibited good predictions for the γ'-precipitate size dependence of the flow stress at moderate strains.

Keywords: Single crystal superalloy; Unit cell; Strain gradient plasticity; Geometric constraint; [0 0 1] Tension

1. Introduction

Single-crystal superalloys having a high volume fraction of Ni_3Al (γ') precipitates distributed within a matrix of solution-strengthened Ni (γ phase) exhibit outstanding high-temperature mechanical performance, making them the designer's choice for turbine blades. The high-temperature strengthening of these single-crystal superalloys has been the subject of numerous experimental and theoretical studies. The unique geometry and spatial arrangement of the γ and γ' phases is known as one of the major factors influencing the strengthening of single-crystal superalloys. For instance, the γ/γ' microstructure of the CMSX-4 or SRR99 alloys can be described as a roughly-periodic array of large (0.5–1 μm) cuboidal γ' precipitates surrounded by narrow channels (<0.1 μm) of the γ-matrix; the details vary depending upon heat-treatment conditions and alloying elements. Recent work has tried to model the mechanical behavior of superalloys for ideal microstructures using the finite element method (FEM) [8,9,11,12]. Numerical modeling of idealized alloy microstructures using FEM can be used to critically examine the effects of grain- or precipitate-level morphology on the flow response of the overall body. In addition, these simulations can also be used to further develop and evaluate constitutive descriptions for each of the microstructural phases; for example, constitutive descriptions that have an associated microstructural length scale. These constitutive descriptions could be potentially used in higher-level simulations, such as those used in actual component design.

Numerical analysis of single-crystal superalloys using FEM can be categorized into two basic approaches. The first approach is to use a periodic "unit cell" representation of the microstructure, where the two phases are represented by a parallelepiped having assigned attributes of the γ' precipitate, which is embedded inside another having assigned attributes of the γ-matrix. Within this unit cell the cuboidal γ' precipitate is separated by channels of the γ-matrix, so that the cubic unit cell contains 1/8 of a γ' precipitate surrounded

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by channels of the γ-matrix. In this approach one can apply separate constitutive descriptions for the γ-matrix and the γ' precipitate, and investigate the local flow distributions and the macroscopic flow responses under the various γ/γ' geometries [1–12]. The second approach uses a homogenized constitutive description for the γ and γ' phases without a distinct delineation of the γ and γ' phases in the finite element mesh [13–20]. Each element can be described as a representative volume element (RVE), which is assumed to represent the microstructural details of the γ and γ' phases under a homogenized constitutive description. The second approach is conceptually more global in representing microstructure as a volume element, and hence is more simplified in comparison with an element in a unit cell approach. In the present work, we focus on the first approach, i.e., the unit cell approach.

The early numerical studies of single-crystal superalloys using a unit-cell approach mainly focused on characterization of the distribution of the local stresses, the thermal misfit stresses caused by differences in thermal expansion between the γ and γ' phases [1–4], and the variation of stress distribution upon change of the γ' morphology [1,2,4–6]. The analysis was initially performed using 2D plane-strain or plane-stress elements [1–3], and treated the γ and γ' phases as elastic [1], or elastic γ' and elasto-viscoplastic γ using a conventional power-law creep formulation [3,5,6]. The FE simulations were extended to 3-D elements [4–9], and somewhat more elaborate viscoplastic constitutive descriptions were employed for the γ-matrix [7–9]. For example, Kuttner and Wahi explored the unit-cell approach using deformation-mechanism-based constitutive descriptions for single-crystal superalloys [9]. They developed a constitutive model (modified Norton's law) that incorporated the deformation mechanisms of single-crystal superalloys such as Orowan bypassing and interfacial climb of the dislocation loops in the γ channels, and a creation of anti-phase boundaries (APB) in the γ' precipitates by the cutting dislocation pairs [9]. Another rather different deformation-mechanism-based constitutive description for single-crystal superalloys can be found in the numerical work done by Fedelich [21,22]. He incorporated the detailed deformation mechanisms of the γ and γ' phases into the internal state variables, and homogenized these variables using a Fourier series under the assumption of the periodic γ/γ' microstructure in order to derive the macroscopic flow formulations [21,22]. The limitation of constitutive models done by Kuttner and Wahi [9] and Fedelich [21,22] was that length-scale dependence was explicitly introduced as part of the constitutive law and was spatially uniform everywhere in the unit cell. One can find more analytical approaches, other than a unit-cell approach, in references [23–28].

The most recent numerical analysis of single-crystal superalloys using a unit-cell approach can be found in the work done by Busso and co-workers [10–12]. Their simulations targeted prediction of the experimentally-measured flow behavior for [0 0 1] oriented single-crystal superalloy (CMSX-4) in tension at elevated temperatures (850 and 950 °C). In their early work [10] they simulated the deformation of a unit cell for a γ' volume fraction of 65–70% using the constitutive descriptions of an elastic γ' precipitate embedded in an elasto-viscoplastic γ-matrix without any strain hardening, and found that they could predict a flow softening at the early stage of straining. They noted that "*softening is a geometric effect – as the deformation proceeds the material in the γ channel rotates and activates additional slip systems*." [11]. They also suggested that this softening behavior decreased with increasing channel width of the γ-matrix (hence a decrease in a volume fraction of the γ' precipitate). In their later simulations, they adopted a form of non-local gradient-dependent plasticity for the constitutive description of the γ-matrix, and simulated a γ' size dependence of the flow stress [11]. The simulations were also performed to capture the effect of the morphological change of the γ' precipitate [12]. These studies mark the first efforts that predicted the effect of precipitate size and volume fraction on the stress–strain curve of a single-crystal superalloy using FEM.

Through a study of selected aspects of the microstructure on the flow behavior of single-crystal superalloys, the present study extends the work of Busso et al., although through use of an alternate non-local gradient-dependent plasticity formulation. The work examines how the local geometries of the γ and γ' phases influence the local and global flow responses of a unit cell representation of a [0 0 1]-oriented single-crystal superalloy (CMSX-4) by performing a numerical analysis using FEM. It is generally believed that upon loading at high temperatures the continuous γ-matrix will deform first due to the metallurgical requirement of the presence, multiplication and propagation of dislocations for plasticity. The γ' precipitates, being harder and of small sizes, have to wait for dislocations to be generated in the matrix before they can be sheared. However, the γ' precipitate also induces geometrical constraints that result in locally complex stress states that affect the deformation of the γ-matrix and hence the flow properties of the crystal. The results show that the flow behavior is sensitive to changes in the γ/γ' morphologies, the constitutive responses assigned to the γ and γ' phases, and the boundary conditions applied during simulation. These and selected other simulation results, such as flow softening and the effect of the edge and corner geometry of the γ' precipitate, are discussed in order to clarify their causes and how such effects are linked to the plastic responses of the γ-matrix. The present study also discusses the applicability and limitations of a strain-gradient-based continuum plasticity model in simulating the flow behavior of single crystal superalloys.

2. Simulation outline

2.1. Numerical details

The constitutive descriptions used for the γ matrix followed the framework of the non-local gradient-dependent