Evaluation of Creep Deformation and Mechanical Properties of Nickel-based Superalloys through FE Analysis Based on Crystal Plasticity Models

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Abstract

The shape and the size of the γ' phase s are the controlling factors for the mechanical and creep properties of nickel-based super-alloys. In order to take into account of the effect of these underlying microstructures on the deformation behavior of these alloys, a multi-scale approach is essential. In this work, a homogenized dislocation density based crystal plasticity model has been developed from a detailed model containing γ−γ' phase s exclusively at the lower length scale. The mechanisms like anti-phase boundary shearing and micro-twinning etc. have been incorporated. The model has been used to simulate the creep deformation behavior of single crystal experiments. The results of simulation were compared to those of experiment and were found to be satisfactory.

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Selection and peer-review under responsibility of the Indira Gandhi Centre for Atomic Research.

Keywords: Nickel-based super-alloy, crystal plasticity, finite element simulation, creep deformation, homogenization

1. Introduction

Nickel-based super-alloys have been widely used in nuclear industry as steam generator tubes, through-wall nozzles and weld material etc. due to their superior strength and corrosion resistance properties. The superior strength and creep resistance properties of these nickel-based super-alloys are dependent on the mechanisms which inhibit the motion or slow down the speed of dislocations within the crystal structure. In these alloys, the γ' phase [Ni3(Al, Ti)] acts as a coherent barrier to dislocation motion and is a precipitate strengthener in the primary γ matrix [1]. The shape and size of γ' phase can be precisely controlled by careful precipitation-hardening heat-treatments. It is very important to take into account of the underlying micro-structure in order to develop a reliable constitutive model for predicting the strength and creep deformation behavior of these alloys. The aim of this work is to develop a physically motivated multi-scale approach for simulation of response of
these types of alloys. At the lower scale, a dislocation-density based crystal plasticity model is developed which simulates the response of various types of micro-structures within a single crystal. The micro-structures are designed with various shapes and volume fractions of $\gamma'$ precipitates.

A new model for simulation of the mechanism of anti-phase boundary (APB) shearing of the precipitates (with matrix dislocations) is also developed in this work. This mechanism is activated when the stress along with the interface dislocation density are sufficient to form super-dislocations in order to enter the ordered $\gamma'$ phase, thereby inducing softening in the material. The dislocations in the [111] plane form super-dislocations at the interface and enter the $\gamma'$ phase when the resolved shear stress and the dislocation reaches critical values [2]. The results of the lower scale model are homogenized as a function of various micro-structural parameters and the homogenized model is used at the next level (i.e., grain level) of multi-scale framework. In addition, a new criterion for initiation of micro-twin and a constitutive model for twin strain accumulation are also used. Micro-twin is a deformation mechanism in these alloys when the dislocations at the interface of the precipitates separate into partials and the leading partials move on adjacent planes to create a re-ordering assisted micro-twinned region. This new formulation along with the homogenized crystal plasticity model has been used to simulate the stress-strain response as well as the tension-compression asymmetry as observed in single crystal experiments of these nickel based super-alloys.

2. Dislocation density based crystal plasticity model at the lower scale

The constitutive formulation of the dislocation density based crystal plasticity model is based on the simulation of shear strain rate $\dot{\gamma}^\alpha$ on slip system $\alpha$ and it can be written as (Orowan’s Equation)

$$\dot{\gamma}^\alpha = \rho_m^\alpha b v^\alpha$$

(1)

where $\rho_m^\alpha$ is the density of mobile dislocations on slip system $\alpha$, $b$ is the Burger’s vector and $v^\alpha$ is the velocity of dislocations on slip system $\alpha$. This velocity of dislocations is a function of applied shear stress $\tau^\alpha$, effective stress $\tau_{\text{eff}}^\alpha$ in the slip system and other slip system resistances and can be written mathematically as [3]

$$v^\alpha = \lambda \nu e^{(-Q_{\text{act}}/k_B \theta)} \sinh \left( \frac{\tau_{\text{eff}}^\alpha V_{\text{act}}^\alpha}{k_B \theta} \right) \text{sgn}(\tau^\alpha)$$

(2)

where $\lambda$ is the distance moved by the dislocation in each step (as it is a discontinuous process which depends upon the probability of overcoming the barriers and the presence of other mechanisms) and it is sometimes called dislocation jump, $\nu$ is the frequency of oscillation of the dislocations, $Q_{\text{act}}$ is the activation energy barrier to be overcome by the dislocations (which depends upon the mechanism of interaction of dislocations with matrix and other barriers, e.g., precipitates or other phases), $k_B$ is Boltzmann’s constant, $\theta$ is the applied absolute temperature in Kelvin, $V_{\text{act}}^\alpha$ is the activation volume which again depends upon the mechanism of deformation being active at the applied stress and temperature and many other parameters.

During the process of dislocation motion and their interaction with other dislocations and obstacles, the process of generation and annihilation of dislocations continues which gives rise to the net dislocation density. Two types dislocations [4], viz. statistically stored dislocations (SSD) and geometrically necessary dislocations (GND) are considered in this model. Their evolution with slip strain rate gives rise to hardening and softening in the slip system response.

For simulation of APB shearing in the $\gamma'$ phase and the subsequent plastic deformation, the following constitutive equations are proposed in this work. The shear strain rate $\dot{\gamma}^\alpha$ and the velocity of dislocations $v^\alpha$ in the slip plane $\alpha$ of the $\gamma'$ phase can be written as the following.
\[
\dot{\gamma}^\alpha = H(\rho_m^\alpha - \rho_c^\alpha)\rho_m^\alpha b v^\alpha
\]

\[
v^\alpha = \lambda ve^{-Q_{act}/k_B\theta} \sinh\left(\frac{\tau^\alpha - \tau_{pass}}{k_B\theta} H(\tau^\alpha - \tau_c)V_{act}\right) sgn(\tau^\alpha)
\]

where \(H(\ )\) is the heavy-side function. The dislocation-density based crystal-plasticity framework as discussed above has been implemented in an in-house finite element based code. The calculation of all the constitutive state variables is done at a material point except the geometrically necessary dislocation density \(\rho_{GND}^\alpha\) which is a nonlocal parameter.

2. Results and discussion

The dislocation-density based crystal plasticity model as described in the previous section has been used to simulate the deformation behavior of single crystal experiments of nickel based super-alloy CMSX-4. The experimental results have been taken from Ref. [5]. This alloy contains around 70 % of \(\gamma^\prime\) precipitates and the precipitate are of primarily cubical shape. The experiment has been conducted at 800 deg. C and the loading is along the [001] direction of the crystal. The FE mesh of the precipitate along with the matrix is shown in Fig. 1. The representative volume element (RVE) is loaded in the vertical direction with symmetric boundary conditions in x, y and z-directions. The other faces use periodic boundary conditions except the loading face. The FE mesh consists of 8-noded 3D brick elements. The results of the simulation with and without activation of APB shearing of the precipitates are shown in Fig. 2. The experiment is carried out at a strain rate of 1e-4 per second. The experimental data is also plotted in Fig. 2. As the precipitates have zero initial dislocation density and the volume fraction of the precipitates in the matrix is very high (i.e., of the order of 70\%), the response is very stiff if the mechanism of APB shearing is not activated in the constitutive model.

Fig. 1. FE mesh of the matrix along with the cubic precipitates loaded along the vertical <001> direction.

The response of the \(\gamma\) phase only (i.e., without the precipitates) is also plotted in Fig. 2. It can be noted that the yield stress as well the hardening are very low for the RVE containing no \(\gamma^\prime\) phases. The super-alloy gets
its high yield stress and the hardening behavior from the presence of $\gamma'$ phases in the matrix. However, with accumulation of dislocation density at the interfaces of matrix and the precipitates at high stresses, the condition is satisfied so that the dislocations can form super-dislocations and enter the $\gamma'$ phase. Hence, with incorporation of the criteria for APB shearing, the stress-strain response can be simulated satisfactorily as shown in Fig. 2. The material constants are also calibrated from this single crystal experimental data. Once the parameters are calibrated, these are used to simulate other micro-structures with various shapes and volume fraction of the $\gamma'$ precipitates.

![Stress-strain response of a single crystal nickel based super-alloy CMSX-4 for loading along <001> direction at 800 deg. C.](image)

The precipitate shape is described by the parameter ‘$n$’ in the following equation for a generalized 3D ellipsoid.

$$\left(\frac{x}{a}\right)^n + \left(\frac{y}{b}\right)^n + \left(\frac{z}{c}\right)^n = 1$$  \hspace{1cm} (5)

where $a$, $b$, and $c$ are the dimensions of the precipitate in three principal directions and ‘$n$’ is the shape exponent. The shape exponent ‘$n$’ is equal to 2 for a sphere and tends to infinity for a cube. In order to parameterize the shape exponent in the homogenized model, the shape exponent has been converted to the shape factor $n_1$ through

$$n_1 = \tan^{-1}(n)$$  \hspace{1cm} (6)

The analysis has been carried out for various volume fractions of cubical precipitates ($n=\infty$) with volume fractions ranging from 12.5% to 75.1%. Similarly, the shape exponent has been varied and analysis has been carried out for six different shape exponents with values ranging from 1.5 to 9.55 and the cubical shape. The nature of stress-strain response of various types of micro-structures with different volume fraction and shape of precipitates has been studied through these simulations. It was observed that the yield stress increases with increasing volume fraction of precipitates. The increase in yield stress is initially small. However, it becomes significant at larger volume fractions of the $\gamma'$ phase. The hardening response also changes with volume fraction of precipitates. Both the precipitate shape and the volume fractions affect the onset of yielding and plastic hardening response, though these effects are more sensitive to the change in volume fraction compared to the change in shapes of the precipitates.
In order to use this model in the higher length scale, the results of the simulation with various microstructural features have been homogenized. The parameter \( n_1 \) along with the precipitates volume fraction \( (v_p) \) serve as the micro-structural parameters with which the homogenized variables has been expressed in suitable functional forms in the homogenized crystal plasticity framework. The volume-averaged slip strain rate in each slip system has been evaluated and its evolution (maximum of all the slip systems) with volume-averaged resolved shear stress is presented in Fig. 3 for various values of precipitate volume fractions \( (v_p) \) for a micro-structural system with cubical precipitates. Similar analyses have been carried out for micro-structural systems with different shapes of precipitates. The onset of plastic deformation is related to the value of the homogenized activation energy \( Q_{\text{hom}} \) which is a function of the micro-structural variables \( v_p \) and \( n_1 \). The ratio of \( Q_{\text{hom}} \) to \( Q_{\text{ref}} \) (reference value of activation energy for the \( \gamma \) phase only) has been determined from the analysis of individual micro-structures and a functional fit has been obtained, i.e.,

\[
\frac{Q_{\text{hom}}}{Q_{\text{ref}}} = f_0 \left( v_p, n_1 \right) \tag{7}
\]

Similar exercise has been carried out for the homogenized passing stress \( \tau_{\text{hom}}^p \) and homogenized activation volume \( V_{\text{act}}^{\text{hom}} \) respectively. The dependence of homogenized passing stress on \( v_p \) and \( n_1 \) has been determined from the values of homogenized resolved shear stress after the APB shearing process of the precipitates as shown in Fig. 3. Similarly, the homogenized resolved shear stress changes with continued plastic deformation and hence, the homogenized activation volume not only depends upon the parameters \( v_p \) and \( n_1 \), but also the the volume averaged plastic work \( W_p \). The volume averaged plastic work density can be evaluated from the FE results as

\[
W_p = \int \int \tau \cdot \dot{\gamma} \, dt \, dV \left/ \int \right. \, dV \tag{8}
\]

Hence, we can represent the homogenized passing stress and activation volumes in the following functional forms, i.e.,

\[
\frac{\tau_{\text{hom}}^p}{\tau_{\text{ref}}^p} = f_p \left( v_p, n_1 \right) \tag{9}
\]

\[
\frac{V_{\text{act}}^{\text{hom}}}{V_{\text{act}}^{\text{ref}}} = f_V \left( v_p, n_1 \right) f_{W_p} \left( W_p \right)
\]

where the subscripts ‘\( \text{hom} \)’ refers to the homogenized quantity and ‘\( \text{ref} \)’ corresponds to that of \( \gamma \) phase only. The homogenized parameters of the dislocation density based crystal plasticity model can now be used in the next level of simulations where we don’t need to consider the explicit FE discretization of the \( \gamma - \gamma' \) phases.

The homogenized dislocation density based crystal plasticity model has been used along with the micro-twin nucleation and propagation laws to simulate the creep response of single crystal nickel-based super-alloy with stress applied along different orientations of the crystal. The criterion for micro-twin formation and its propagation can be found in Ref. [2]. The nickel based alloy is CMSX-4 and it contains 57.8% volume fraction of precipitates. The experimental data has been taken from Ref. [6]. Significant tension-compression asymmetry is observed as can be seen from the experimental data presented in Fig. 4 when the single crystal specimen is loaded along <001> direction. For the loading in <001> tension, micro-twin formation is not observed as confirmed from transmission electron microscopy (TEM) observation in Ref. [6]. However, when loaded in <001> compression, significant micro-twin development is observed in the alloy and the deformation is dominant by the strain accumulation due to micro-twin. The experimental conditions have been simulated in the model and the predictions of the model are compared with those of experiment in Fig. 4.

It can be observed that the tension-compression asymmetry has been successfully modeled with the new formulation and the creep response with time as predicted by the model is very close to those of experiment both in <001> tension and <001> compression mode [Fig. 4]. It can be observed that the new model developed
in this work has been very successful in satisfactorily predicting the single crystal experimental data. The micro-twin induced tension-compression asymmetry has also been satisfactorily predicted by the new model.

3. Conclusions

The stress-strain behavior and creep response of nickel-based super-alloys depend upon the morphology and distribution of the $\gamma'$ precipitates in the primary $\gamma$ matrix. When simulating the response through the advanced crystal-plasticity based formulations, it is not possible to incorporate the $\gamma' - \gamma$ morphology in the FE model explicitly though it is possible to obtain the detailed information regarding the distribution of size, shape, spacing and volume fraction of these $\gamma'$ phases from the analysis of the microstructure. Through a multi-scale framework, it is now possible to consider the effects of the underlying micro-structure in the homogenized crystal-plasticity based constitutive relations, which has been the focus of this work.

At the lower length scale of the multi-scale framework, a dislocation density based crystal plasticity model has been used along with the consideration of the mechanism of APB shearing in the $\gamma'$ phases. The constitutive responses in the slip system level have been homogenized in order to develop a parametric form of the model in the higher length scale. The homogenized model as a function of the micro-structural parameters have been used along with the model for micro-twin nucleation and propagation to simulate the observed tension-compression symmetry behavior in the creep responses of single crystal specimens. The results of the new model have been compared with those of experiment and it was observed that the simulated results compare well with those of experiment. The model also predicts tension-compression asymmetry (due to presence of micro-twin) very satisfactorily.

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