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Incorporating strain gradient effects in a multi-scale constitutive framework for nickel-base superalloys

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An efficient multi-scale constitutive framework for nickel-base superalloys is proposed that enables the incorporation of strain gradient effects. Special interface regions in the unit cell contain the plastic strain gradients that govern the development of internal stresses. The model is shown to accurately simulate the experimentally observed size effects in the commercial alloy CMSX-4. The limited complexity of the proposed unit cell and the micromechanical simplifications make the framework particularly efficient in a multi-scale approach. This is demonstrated by applying the model in a gas turbine blade finite element analysis.

Keywords: Superalloys; Crystal plasticity; Dislocations; Strain gradients; Size effects.

1 Introduction

Strain gradient effects are only quite recently recognized as an important factor in mechanical modelling at small length scales. At these length scales, the material strength is observed [1] to be size dependent, with an increase of strength at decreasing dimensions, i.e. smaller is stronger. The existence of a strain gradient dependent back stress and its relevance for crystal plasticity of small components undergoing inhomogeneous plastic flow has been reported in several papers. The work of Gurtin and co-workers [2-5] is here emphasized in particular.

Strain gradient effects are also relevant for single crystal nickel-base superalloys, which are widely used as gas turbine blade materials because of their high resistance against high temperature inelastic deformation. The superior high temperature behaviour is attributed to the two-phase composite microstructure consisting of a γ -matrix containing a large volume fraction of γ '-particles (see Figure 1). Cubic Ni₃Al (γ ') precipitates are more or less regularly distributed in a Ni-matrix (γ -phase). The typical precipitate size is 0.5 µm and the matrix channel width is typically 60 nm. Since these very narrow matrix channels bear the majority of the plastic deformation, considerable plastic strain gradients develop in the material.

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Therefore, strain gradient effects should be included in superalloy constitutive models, as was done by Busso and co-workers [6,7] and Choi et al. [8]. They used a detailed unit cell FE model of an elastic γ' precipitate embedded in an elasto-viscoplastic γ -matrix. Busso and co-workers [6,7] adopted a non-local gradient dependent crystal plasticity theory to describe the behaviour of the γ -matrix. The flow resistance and hardening of the matrix were based on the densities of statistically stored and geometrically necessary dislocations. This enabled the prediction of a precipitate size dependence of the flow stress and allowed to capture the effect of morphological changes of the precipitate. Choi et al. [8] extended this work using a more phenomenological crystal plasticity formulation with no direct relation to dislocation densities. However, a strain gradient dependence was incorporated in the model, which also resulted in the prediction of precipitate size effects and an influence of the microstructure morphology.

[Insert Fig. 1 about here]

The ability to perform a reliable life time assessment is crucial for both gas turbine component design and maintenance. Therefore, a vast amount of work has been done on modelling the mechanical behaviour of superalloys. Initially the material was treated as a homogeneous single phase material [10-20]. In all these approaches conventional crystal plasticity theory was used to model the material response, which means that constitutive laws were defined on the slip system level. Since these solution methods address the macroscopic level, they can easily be used as a constitutive description in a finite element (FE) analysis, which is nowadays the common method used for component stress analysis and life time assessment.

However, to be able to quantify strain gradients in the material and to assess their effect on the macroscopic response, the two-phase nature of superalloys has to be modelled explicitly. In the resulting microstructural models the shape, dimensions and properties of both phases are considered as model parameters. However, the length scale of the microstructure, which is in the order of micrometers, is much smaller than the engineering length scale. Modelling a macroscopic component completely, i.e. taking into account all microstructural details, is therefore not feasible in the engineering practice.

One way to bridge this gap in length scales is to use a multi-scale approach in which an appropriate homogenization method is applied to connect the microscopic to the macroscopic level. A large number of multi-scale frameworks has been developed in the past decades and applied to different materials. Examples are Eshelby-type homogenization methods [21] for materials with (elastic) inclusions, variational bounding methods

 [22,23] and asymptotic homogenization methods [24,25]. Some more recent examples applicable to the class of unit cell methods are the first order [26,27] and second order [28] computational homogenization methods and the crystal plasticity work by Evers [29] that considered the effect of multiple differently oriented grains in an FCC metal. Finally, Fedelich [30,31] used a Fourier series homogenization method to model the mechanical behaviour of Ni-base superalloys.

Another way to overcome the length scale problem is to use microstructural models that predict the material response in a closed-form set of equations on the level of the material point [6-8,32-35]. The microstructural results are then used to develop constitutive descriptions that fit in traditional methods at the macroscopic level. Clearly, the analyses on the microscopic and the macroscopic level are completely separated in this case. Svoboda and Lukas [33,35] developed an analytical unit cell model consisting of a γ '-precipitate and three γ -channels. The deformation in the distinct regions was assumed to be uniform and power law creep behaviour was used for the matrix material. The required compatibility at the γ/γ' -interfaces resulted in a relatively high overall stiffness. Kuttner and Wahi [34] used a FE method to model a unit cell representing the γ/γ' -microstructure. A modified Norton's creep law was assumed for both phases and threshold stresses for different deformation mechanisms were included. The latter models [33-35] as well as the model by Fedelich [30,31] adopted the Orowan stress as a threshold stress for plastic deformation. Since the Orowan stress is related to the spacing of the γ' -precipitates, a length scale dependence was explicitly introduced into the constitutive description. However, apart from the models by Busso and co-workers [6,7] and Choi et al. [8], that were discussed before, none of these models includes strain gradient effects, whereas the FE based unit cell models are detailed but usually too complex to be used efficiently in a multi-scale analysis of structural components. Therefore, in this paper a new framework is proposed that is particularly developed to incorporate strain gradient effects, and to be computational efficient, thus enabling application in a multi-scale approach (FE analyses on real components).

A new unit cell approach is forwarded, in which the role of the γ/γ' -interfaces is included. More specifically, each phase in the material is represented by a combination of a bulk material unit cell region and several interface regions. In the interface regions internal stresses will develop as a result of the lattice misfit between the two phases and the plastic strain gradients, represented by non-uniform distributions of geometrically necessary dislocations (GNDs). Conditions requiring stress continuity and strain compatibility across the γ/γ' -interfaces are specified in these regions. Continuous dislocation densities and slip gradients, as typically used in a continuum formulation, are approximated here by piece-wise constant fields. The comprehensible complexity of the adopted unit cell and the micromechanical simplifications, which render a composition of 10 piece-wise uniformly deforming regions, make the framework particularly efficient in a multi-scale approach. The unit cell response is determined numerically on a material point level (integration point level) within a macroscopic FE code, which is computationally much more efficient than a fully detailed FE-based unit cell. The material response is predicted accurately by using an extended version of an existing non-local strain gradient crystal plasticity model [36,37] for the matrix material. The precipitate is treated as an elastic anisotropic solid.

Finally, to reduce the model complexity, the mechanisms of precipitate shearing and rafting are omitted, which limits the application range of the present model somewhat. In the majority of industrial gas turbines single crystal Ni-base superalloy blades operate at temperatures well below 950 °C and are not allowed to deform by more than 1 to 2%. Since the matrix phase of the material is known to accommodate the majority of the deformation, it is justified, at these operating conditions, to assume that the γ '-precipitates remain elastic during deformation. This means that the mechanism of precipitate shearing by dislocations is not considered. Experimental work [19,35,38-46] has shown that precipitate shearing becomes important at temperatures above 950 °C and at larger strains (later stages of steady-state creep). At lower temperatures considerable stresses in the range of 500 to 600 MPa are required to initiate particle shearing. Moreover, the morphology of the microstructure is assumed to remain the same during deformation, which also neglects the mechanism of rafting. Again experimental work [47] has shown that precipitate coarsening is completed rapidly at temperatures above 950 °C and after proportionally longer times at lower temperatures. Consequently, the assumption of an elastic precipitate and a fixed morphology limits the application region of the present model to temperatures below 950 °C and strains smaller than about 5% and also to relatively short loading times. However, this limited application range is sufficient to demonstrate the importance of strain gradient effects in nickel-base superalloys. Moreover, future extension of the model with precipitate deformation mechanisms and rafting kinetics can remove the present limitations.

To summarize, the original aspect of the present model is the incorporation of strain gradient effects, which are not included in the majority of the existing models, in an efficient multi-scale framework. Due to the micromechanical simplifications, the present model is computationally much more efficient than the strain gradient FE unit cell models.

In the next section the multi-scale framework is outlined, providing definitions of the unit cell and the interaction laws. Then the strain gradient effects are implemented, both in the hardening law and through internal

stresses: section 3 describes the constitutive models that are used, focusing mainly on the strain gradient crystal plasticity concepts, while section 4 considers the internal stresses, describing the formulation of misfit and strain gradient induced back stresses. In section 5, the model is applied to the Ni-base superalloy CMSX-4. Simulated stress-strain curves and size effects are compared to experimental results, showing that the present framework is able to describe the material response and size effects to a level of detail similar to complex FE unit cell models, while being computationally much more efficient. The computational efficiency is demonstrated by applying the model to a gas turbine blade finite element analysis. Finally, section 6 forwards some concluding remarks.

2 Multi-scale model description

The strain gradient effects are incorporated in a newly developed multi-scale model for the prediction of the superalloy mechanical behaviour. This model covers several length scales, which is shown schematically in Figure 2a. The *macroscopic* length scale characterises the engineering level on which a finite element (FE) model is commonly used to solve the governing equilibrium problem. The *mesoscopic* length scale represents the level of the microstructure within a macroscopic material point. At this length scale the material is considered as a compound of two different phases: γ' -precipitates embedded in a γ -matrix. Finally, the *microscopic* length scale reflects the crystallographic response of the individual material phases. The constitutive behaviour is defined on this level using a strain gradient crystal plasticity framework.

[Insert Fig. 2 about here]

Considering the overall deformation level, a small strain approximation will be used in the model. The intended application of the model is the analysis of gas turbine components in which deformations are small. Consequently, the initial and deformed state are geometrically nearly identical. Instead of a large deformation strain tensor, the linear strain tensor (ε) will be used with the Cauchy stress tensor (σ) as the appropriate stress measure.

In this section the different aspects of the material point model are described. Firstly the mesoscopic unit cell is defined, after which the scale transitions and interaction laws are described.

2.1 Unit cell definition

On the material point level the Ni-base superalloy microstructure, consisting of γ' -precipitates in a γ -matrix, is represented by a unit cell containing 16 regions (see Figure 2b):

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- 1 γ'-precipitate region
- 3 γ -matrix channel regions (γ_j , j = 1... 3) with different orientations (normal to the [001], [010] and [100] direction)
- 12 interface regions (I_k^m and I_k^p , k = 1...6) containing the γ/γ' -interfaces. A matrix and a precipitate region together form a bi-crystal, which is located on each face of the γ' -precipitate.

The interface between the two different phases plays an important role in the mechanical behaviour of the material, especially due to the large strain gradients that develop here. Therefore, special interface regions were included in the model to take into account the processes that take place at the γ/γ' -interfaces. Consequently, each phase in the two-phase material, either a precipitate or a matrix channel, is represented by two types of regions in the unit cell. The first type represents the bulk material behaviour and in the second type all short-range interface effects, including dislocation induced back stress and interaction with other phases, are incorporated. Inside each individual region quantities, like stresses and strains, are assumed to be uniform, which leads to a particularly efficient framework. The only relevant quantity that is not uniformly distributed inside a region is the GND density, as will be shown in section 4.2,

Thus, in the present framework the behaviour of a specific phase in the real material, e.g. a matrix channel, is given by the (weighted) average behaviour of the bulk unit cell region and the appropriate sides of the interface regions. This also means that the individual unit cell regions will not necessarily describe the real deformation behaviour on their own. Finally note that, throughout this paper, the word *phase* refers to a specific component in the real material, either matrix or precipitate, and the word *region* refers to a specific part of the model unit cell.

The constitutive behaviour of the matrix and precipitate fractions of the interface is identical to the behaviour of the bulk matrix and precipitate phases, respectively. However, additional interface conditions (section 2.2) are specified and short-range internal stresses (back stress, see section 4) are included in these regions, which distinguishes them from the matrix and precipitate regions. Another internal stress, the lattice misfit stress, is a long-range stress field, which is consequently included in both bulk and interface regions.

[Insert Fig. 3 about here]

The morphology of the microstructure is defined by the values of the geometrical parameters *L*, *w* and *h*, as shown in Figure 3. The precipitate (γ') size, including the γ' -interface region, is given by the value of *L* in

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three directions (L_1 , L_2 and L_3). These values also determine two of the three dimensions of the three matrix channel regions (γ_i) and the six interface regions (I_k). The total channel width, including one channel and two γ interface regions, is given by the parameter h_i for γ -channel *i*. Finally, the width of the interface regions is related to the values of *L* and *h*. The width of the matrix phase layer in the interface (I_i^m) is defined as 30% of the matrix channel width ($w_i^m = 0.30 h_i$) and the width of the precipitate layer in the interface (I_i^p) as 5% of the precipitate size ($w_i^p = 0.05 L_i$). The selection of these values will be motivated in section 5. The CMSX-4 microstructure (Figure 1) is rather regular, so for the present model the precipitates are assumed to be cubic with $L_1 = L_2 = L_3 =$ 500 nm. The matrix channel width is taken as $h_1 = h_2 = h_3 = 60$ nm. These values yield a γ' volume fraction of 72%.

As will be shown later, the interface regions at opposite sides of the precipitate (e.g. I_1^m and I_4^m) are assumed to behave identically in terms of deformation, internal stress development, etc. Therefore, to the benefit of computational efficiency, only half of the interface regions need to be included in the equations in the next subsections, thereby effectively reducing the number of regions from 16 to 10. The opposite regions are then incorporated in the volume averaging by doubling the respective volume fractions.

2.2 Scale transitions and interaction law

The relations between the different length scales of the model are shown schematically in Figure 4. Conventionally, a finite element method is used on the macroscopic level to solve the engineering problem with its boundary conditions. In the present multi-scale approach the usual standard procedure to obtain the stress response for a given deformation (i.e. a local closed-form constitutive equation) is replaced by a mesoscopic calculation at the unit cell level as indicated in Figure 4.

[Insert Fig. 4 about here]

The deformation (total strain) for a certain macroscopic material point during a time increment is provided by the macro scale and the stress response is returned after the computations at the mesoscopic level. The quantities used for this macro-meso scale transition are denoted as the mesoscopic average strain (ε_{tot}) and the mesoscopic average stress (σ_{tot}). The stress tensor σ_{tot} is determined from the strain tensor ε_{tot} based on the specified mesoscopic configuration and the local constitutive equations of the different phases at the micro level.

The mesoscopic strain is obtained by averaging the microstructural quantities in each of the regions,

defined as

$$\sum_{i} f^{i} \boldsymbol{\varepsilon}_{tot}^{i} = \boldsymbol{\varepsilon}_{tot} \qquad i = \gamma', \gamma_{1}, \gamma_{2}, \gamma_{3}, \mathbf{I}_{1}^{p}, \mathbf{I}_{1}^{m}, \mathbf{I}_{2}^{p}, \mathbf{I}_{3}^{m}, \mathbf{I}_{3}^{m}$$
(1)

where f^i are the volume fractions and ε_{tot}^i the total strain tensors in the 10 different regions of the model.

The relation between the mesoscopic and microscopic level is provided by the constitutive models, which relate the stress tensors to the individual strain tensors for all 10 regions

$$\boldsymbol{\varepsilon}^{i} \rightarrow \text{constitutive box} \rightarrow \boldsymbol{\sigma}^{i} \qquad i = \gamma', \gamma_{1}, \gamma_{2}, \gamma_{3}, \mathbf{I}_{1}^{p}, \mathbf{I}_{1}^{m}, \mathbf{I}_{2}^{p}, \mathbf{I}_{3}^{m}, \mathbf{I}_{3}^{p}, \mathbf{I}_{3}^{m}$$
 (2)

The constitutive model at the micro level, for the matrix phase, is based on a strain gradient enhanced crystal plasticity theory and will be described in section 3. The precipitate phase is treated as an elastic medium. Also, only at this point the internal stresses (misfit and back stress, see section 4) play a role in the stress analysis. They are combined with the externally applied stress, as obtained from the equilibrium calculation, to form an effective stress that is used in the constitutive box. They are thus not part of the equilibrium calculation itself, as is also indicated in Figure 4. This separation of external and internal stress calculation is particularly possible in the context of the adopted Sachs approach (to be outlined in the following), as will be discussed in section 4.1.

Inside each of the different regions, both stress and deformation are assumed to be uniform. To specify the coupling between the regions an interaction law has to be defined. Two frequently adopted limit cases can be distinguished:

- Taylor interaction: deformation is uniform across the regions, stresses may vary;
- Sachs interaction: stresses are uniform across the regions, deformation may vary.

These two approaches form an upper and a lower bound for the stiffness, so the real mechanical behaviour intermediates between these cases. A Taylor-type interaction usually yields a response that is too stiff, thereby overestimating the resulting stresses for a given deformation, whereas a Sachs type interaction yields an overly weak response. A Taylor interaction model is inappropriate for the present application, since the deformation is highly localized in the γ -matrix phase. A Sachs-type approach is actually a much better approximation, but it lacks the ability to incorporate kinematical compatibility conditions at the interface. Also, it would not correctly represent the stress redistribution between the two phases that occurs when the matrix starts to deform plastically. Therefore, a hybrid interaction law [48] or a modified Taylor / Sachs approach [29] is best suited here.

 For the present model a modified Sachs approach is used, in which the requirement of a uniform stress state is relaxed for the interface regions. In the γ - and γ '-regions the stresses are required to be equal to the mesoscopic stress. In each pair of interface regions however, only the *average* stress is enforced to be equal to the mesoscopic stress. This results in the following equations:

- Sachs interaction between γ '- and γ -regions:

$$\boldsymbol{\sigma}^{\gamma} = \boldsymbol{\sigma}^{\gamma_1} = \boldsymbol{\sigma}^{\gamma_2} = \boldsymbol{\sigma}^{\gamma_3} = \boldsymbol{\sigma}_{tot}$$
(3)

- Modified Sachs interaction for the bi-crystal interfaces:

$$f^{I_{k}^{p}}\boldsymbol{\sigma}^{I_{k}^{p}} + f^{I_{k}^{m}}\boldsymbol{\sigma}^{I_{k}^{m}} = \left(f^{I_{k}^{p}} + f^{I_{k}^{m}}\right)\boldsymbol{\sigma}_{tot} \qquad k = 1, 2, 3$$
(4)

where σ^i are the stress tensors in the different regions, σ_{tot} is the mesoscopic stress tensor and f^i are the volume fractions of the respective regions.

The fact that each partition of the interface region may respond differently to a mechanical load enables the possibility (and necessity) to define additional conditions at the interfaces. Both stress continuity (across the interface) and kinematical compatibility (in the plane of the interface) are therefore added as additional requirements. This leads to the following supplementary equations, where \vec{n}^k is the unit normal vector on the k^{th} interface.

(5)

- Compatibility between the matrix (I_k^m) and the precipitate side (I_k^p) of the k^{th} interface:

$$\boldsymbol{\varepsilon}^{\mathrm{I}_{k}^{\mathrm{p}}} \cdot \left(\mathbf{I} - \vec{n}^{k} \vec{n}^{k}\right) = \boldsymbol{\varepsilon}^{\mathrm{I}_{k}^{\mathrm{m}}} \cdot \left(\mathbf{I} - \vec{n}^{k} \vec{n}^{k}\right) \qquad k = 1, 2, 3$$

- Stress continuity at the same interface:

$$\boldsymbol{\sigma}^{\mathrm{I}_{k}^{\mathrm{p}}} \cdot \vec{n}^{k} = \boldsymbol{\sigma}^{\mathrm{I}_{k}^{\mathrm{m}}} \cdot \vec{n}^{k} \qquad k = 1, 2, 3 \tag{6}$$

where σ and ϵ are the stress and strain tensors in the different regions.

For the material point model the mesoscopic deformation (total strain) is provided by the macro scale analysis and the mesoscopic stress must be calculated. Since the model consists of 10 distinct regions in which the deformation and stress are homogeneous, and the symmetric stress and strain tensors contain 6 independent components, a total of 120 unknowns results. The systems (1) and (3)-(6) represent a total number of 60 equations, while the constitutive model (2) adds another 60 equations, which completes the description.

In summary, the stresses in the bulk material regions and the *average* stresses of the interface regions are coupled, whereas for the interface regions additional interface conditions in terms of stress and strain are specified. The assumption of uniform stress and strain inside the unit cell regions in combination with the

conditions proposed above completely determine the problem. Additional conditions are not required nor allowed, which means that, for example, the absence of traction continuity between bulk material and interface is accepted for the sake of efficiency.

Constitutive behaviour

A strain gradient enhanced crystal plasticity approach is used to model the constitutive behaviour of the matrix phase, whereas the precipitate is treated as an elastic anisotropic material. After a general introduction concerning the underlying crystal plasticity formulation, the matrix and precipitate constitutive models will be described. Note that the matrix phase constitutive model is applied to both bulk matrix unit cell regions and the matrix sides of the interface regions. The precipitate regions and the precipitate sides of the interface regions remain elastic.

3.1 Strain gradient crystal plasticity

In a conventional crystal plasticity framework, the plastic deformation of metals is a natural consequence of the process of crystallographic slip. For each type of crystal lattice a set of slip systems exists along which the slip process will take place. A slip system is commonly characterised by its slip plane and its slip direction. For the considered superalloy, with a face-centred cubic (FCC) lattice, 3 slip directions on each of the 4 octahedral slip planes can be identified, resulting in 12 slip systems. In addition to the plastic slip, elastic deformation is accommodated by distortion of the crystallographic lattice. In many superalloy crystal plasticity models [6,11,31] an additional set of cubic slip systems is incorporated to account for the cross slip mechanisms that occur when the material is loaded in a direction other than <001>. The present model here is only applied to the technologically important <001> loading direction, corresponding to the direction of centrifugal loading in turbine blades. However, a set of cubic slip systems can easily be incorporated when dealing with other orientations is required.

Clearly, crystallographic slip is carried by the movement of dislocations. Yet, also the hardening behaviour of metals is attributed to dislocations. Plastic deformation causes multiplication of dislocations and their mutual interaction impedes the motion of gliding dislocations, which causes strengthening. The total dislocation population can be considered to consist of two parts:

- statistically stored dislocations (SSDs)
- geometrically necessary dislocations (GNDs) [49]

The SSDs are randomly oriented and therefore do not have any directional effect and no net Burgers vector. They accumulate through a statistical process. On the other hand, when a gradient in the plastic deformation occurs in the material, a change of the GND density is required to maintain lattice compatibility. Individual dislocations cannot be distinguished as SSDs or GNDs. The GNDs are therefore the fraction of the total dislocation population with a non-zero net Burgers vector. Moreover, as will be shown later, a gradient in the GND density causes an internal stress which affects the plastic deformation. These strain gradient dependent influences give the model a non-local character. They enable the prediction of size effects which cannot be captured by conventional crystal plasticity theories.

In the present model it is assumed that all SSD densities are of the edge type, whereas for the GNDs both edge and screw dislocations are considered. This implies that for an FCC metal 12 edge SSD densities are taken into account, next to 12 edge and 6 screw GND densities [50]. A complete overview of the dislocation densities, including their type and slip system is given in Table 1. Each screw dislocation can move on either of the two slip planes in which it can reside. This is indicated in Table 1 by the two corresponding slip system numbers, where a negative number means that the defined slip direction should be reversed.

The elastic material behaviour is modelled using a standard formulation for orthotropic materials with cubic symmetry. The three independent components of the elastic tensor ${}^{4}C$ of both phases in CMSX-4 at 850 ${}^{\circ}C$ are given in Table 2 [6].

[Insert Table 1 about here]

[Insert Table 2 about here]

The next subsection shows how the strain gradient based crystal plasticity framework is used to elaborate the matrix phase constitutive model.

3.2 Matrix constitutive model

The basic ingredient of the crystal plasticity framework is the relation between the slip rates $\dot{\gamma}^{\alpha}$ and the resolved shear stresses τ^{α} for all the slip systems α . The following formulation is proposed here:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left\{ \frac{\left| \tau_{eff}^{\alpha} \right|}{s^{\alpha}} \right\}^m \left\{ 1 - \exp\left(-\frac{\left| \tau_{eff}^{\alpha} \right|}{\tau^{or}} \right) \right\}^n \operatorname{sign} \left(\tau_{eff}^{\alpha} \right)$$
(7)

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where τ^{or} denotes the Orowan stress, s^{α} the actual slip resistance and τ^{α}_{eff} the effective shear stress on slip system α , obtained from the effective stress tensor σ_{eff} by

$$\tau_{eff}^{a} = \mathbf{\sigma}_{eff} : \mathbf{P}^{a} \tag{8}$$

where \mathbf{P}^{α} is the symmetric Schmid tensor defined as

$$\mathbf{P}^{\alpha} = \frac{1}{2} \left(\vec{s}^{\alpha} \vec{n}^{\alpha} + \vec{n}^{\alpha} \vec{s}^{\alpha} \right) \tag{9}$$

The unit length vectors \vec{n}^{α} and \vec{s}^{α} are the slip plane normal and slip direction, respectively. The effective stress tensor is defined as the combination of the externally applied stress, the back stress and the misfit stress (see section 4) according to

$$\boldsymbol{\sigma}_{eff} = \boldsymbol{\sigma} + \boldsymbol{\sigma}_{misfit} - \boldsymbol{\sigma}_{b} \tag{10}$$

The formulation in equation (7) is an extended version of the slip law used in the work of Evers et al. [36,37] for a single phase FCC material. For the present two-phase material an additional threshold term is added to account for the Orowan stress, which is the stress required to bow a dislocation line into the channel between two precipitates. This stress is given by [51] as

$$\tau^{or} = \frac{\mu b}{2\pi d} \ln\left(\frac{d}{r_0}\right) = \alpha \frac{\mu b}{d} \tag{11}$$

where μ is the shear modulus, *b* the length of the Burgers vector, *d* the spacing between two precipitates (equal to the channel width) and r_0 the dislocation core radius (in the order of *b*). There is no generally accepted value for the constant *a*. The used values range from 0.238 to 2.15 for different materials and conditions [6,30-34,41,51], where in some cases the constant *a* was used as an adjustable parameter. A value of $\alpha = 0.85$ is taken here, as was done by Busso et al. [6]. If the effective stress exceeds this Orowan stress threshold, dislocation lines enter the matrix channel and the typical slip threshold (governed by s^{α}) determines whether or not they can move any further. This is the case if the effective stress exceeds the slip resistance. The slip resistance is in a certain sense also an Orowan type stress related to the average spacing of obstacles inside the matrix phase, such as other dislocation segments. While both thresholds are a result of microscopic phenomena, the Orowan threshold is related to a mesoscopic length scale. Moreover, the slip resistance threshold term determines the actual slip rate value, whereas the Orowan threshold τ^{or} is exceeded by the effective stress or when the growth of the dislocation density triggers an increase of the slip resistance s^{α} to a value that exceeds the Orowan threshold, the slip resistance contribution becomes the active threshold that determines the slip rate.

Slip resistance

Generally speaking, slip resistance or dislocation drag is caused by several obstacles such as solute atoms, precipitates (e.g. carbides, intermetallics) and other dislocations, each having a contribution to the overall slip resistance. The physical mechanism associated with an increasing slip rate at increasing temperature is the decrease of dislocation drag (related to the slip resistance). The temperature dependence of all these contributions is assumed to be identical, resulting in a classical expression for the temperature dependent slip resistance

$$s^{\alpha} = s_0^{\alpha} \exp\left[\frac{Q}{kT}\right]$$
(12)

where s_0^{α} is the athermal slip resistance, Q is an activation energy for overcoming the barriers, $k = 1.38 \times 10^{23} \text{ J}$ K⁻¹ is the Boltzmann constant and T the absolute temperature.

The amount and spacing of solute atoms and precipitates (other than γ') in the matrix phase is assumed to be constant, which means that the isothermal lattice slip resistance due to these obstacles is constant as well. The second contribution to the total slip resistance depends on the dislocation densities in the material. This contribution is related to the resistance of sessile / forest dislocations and therefore depends on the total dislocation density, composed of the SSDs and the GNDs. The relation between the slip resistance and the dislocation density is defined according to

$$s_{disl}^{\alpha} = c \mu b \sqrt{\left| \rho_{SSD}^{\alpha} \right| + \left| \rho_{GND}^{\alpha} \right|}$$
(13)

Evers et al. [36] used an interaction matrix containing experimentally determined entries to define the interactions between dislocations on different slip systems. These values are not available for Ni-base superalloys, so only interactions with dislocations on the same slip system (self hardening) will be taken into account, as was done by Busso et al. [6]. Interactions with dislocations on other slip systems (cross hardening) are neglected. Also the contribution to the slip resistance of the screw-type GND densities ($\xi = 13...18$) whose slip plane is ambiguous (see Table 1) is neglected.

The exploitation of equation (13) requires the knowledge of all dislocation densities (12 edge dislocation densities for the SSDs and 12 edge and 6 screw dislocation densities for the GNDs). The GND densities can be obtained from the plastic deformation gradients in the material as will be explained in section 4.2 dealing with the back stresses. The SSD densities are calculated on the basis of an appropriate evolution equation [36], starting from their initial value $\rho_{SSD,0}$:

$$\dot{\rho}_{SSD}^{\alpha} = \frac{1}{b} \left(\frac{1}{L^{\alpha}} - 2y_c \rho_{SSD}^{\alpha} \right) \dot{\gamma}^{\alpha} \, , \quad \rho_{SSD}^{\alpha} (t=0) = \rho_{SSD,0} \tag{14}$$

which is the net effect of dislocation accumulation (left term) and annihilation (right term). The parameter y_c represents the critical annihilation length, i.e. the average distance below which two dislocations of opposite sign annihilate spontaneously. The accumulation rate is linked to the average dislocation segment length of mobile dislocations on system α , which is determined by the current dislocation state through

$$L^{\alpha} = \frac{K}{\sqrt{\left|\rho_{SSD}^{\alpha}\right| + \left|\rho_{GND}^{\alpha}\right|}} \tag{15}$$

where *K* is a material constant.

Further, the experimental tensile curves in section 5 of this paper show that after some amount of yielding strain softening occurs in the material. This phenomenon is typical for superalloys and has been the subject of several studies. Busso and co-workers [6,16,52] and Choi et al. [8] performed unit cell finite element analyses and concluded that the softening might be attributed to lattice rotations around the corners of the precipitates. These rotations induce activation of additional slip systems and result in a fast increase of plastic slip. In these analyses, the precipitate was assumed to behave elastically. On the other hand, Fedelich [31] states that the softening is related to the onset of precipitate shearing, a phenomenon which was not accounted for in the FE unit cell analyses mentioned above.

The present model is specifically developed to be efficient in a multi-scale approach. The consequential choice for small strain kinematics and uniform stress and strain in the unit cell regions mean that local lattice rotations cannot be predicted. Also the mechanism of precipitate shearing is not included. Therefore, in the present framework the softening effect is incorporated in a phenomenological way by adding a softening term

$$s_{soft}^{\alpha} = C_{soft} \left(1 - \sqrt{\frac{\rho_{SSD}^{\alpha}}{\tilde{\rho}_{SSD}^{\alpha}}} \right)^{p}$$
(16)

to the slip resistance, where C_{soft} and p are constants and $\tilde{\rho}_{SSD}^{\alpha}$ is the equilibrium value of the SSD density. This equilibrium value follows from equation (14) by requiring that the creation and annihilation terms are equal. Rather than a real slip resistance, the contribution s_{soft}^{α} should be considered as a reflection of the lack of dislocation mobility. It represents, in a phenomenological way, the increase of dislocation mobility, and consequential decrease of s^{α} , associated with either local lattice rotations or precipitate shearing. In forthcoming work, a precipitate constitutive model will be proposed to properly capture precipitate shearing. The need for a phenomenological term that accounts for softening will then be re-assessed.

Finally, it is assumed that the athermal *lattice* slip resistance is caused by an initial SSD density $\rho_{SSD,0}$, which means that its effect on the total slip resistance is incorporated in the *dislocation* slip resistance as given by equation (13). Therefore, combination of equations (13) and (16) yields the total athermal slip resistance to be used in equation (12):

$$s_0^{\alpha} = s_{disl}^{\alpha} + s_{soft}^{\alpha} \tag{17}$$

3.3 Precipitate constitutive model

In the present approach, the precipitate in the superalloy is assumed to be elastic, which implies that both the unit cell precipitate region and the precipitate sides of the interface regions are treated as anisotropic elastic media. As was mentioned in the introduction, this assumption is only acceptable under certain conditions. The precipitate may deform inelastically when it is sheared by a dislocation or bypassed by dislocation climb. However, these processes have considerable thresholds in terms of stress and temperature. Therefore, at temperatures below 950 °C and moderate stress levels the simplification of an elastically deforming precipitate is justified. These conditions are, nevertheless, sufficient to demonstrate the importance of strain gradient effects, which is the aim of the present paper. The development of an enhanced constitutive model that includes crystal plasticity in the precipitate for more extreme conditions, is the subject of future work.

4 Internal stresses

The interface between the two different phases plays an important role in the mechanical behaviour of the multiphase material, because of the development of significant internal stresses that interact with the externally applied stress, see equation (10). In the present model the following internal stresses are incorporated:

- misfit stress: stress that originates from the lattice misfit between the γ and γ' -phases at the level of the coherent interface that is formed. This is a *long-range* stress field that spans the complete unit cell.
- back stress: stress that originates from deformation-induced plastic strain gradients inducing a gradient in the GND density at the interfaces. This is a *short-range* stress field that only acts in the interface regions.
 Apart from these two explicitly defined internal stress fields, an internal redistribution of stresses occurs due to differences in plastic deformation between both phases.

4.1 Lattice misfit

The γ and γ '-phases both have an FCC lattice structure with a slightly different lattice (dimension) parameter. They form a coherent interface, which means that the crystal lattice planes are continuous across the interface, but a misfit strain exists to accommodate the difference in lattice parameter. For most superalloys the misfit is called negative, which means that the lattice parameter of the precipitate is smaller than the matrix lattice parameter. To bridge the misfit, both the precipitate and matrix are strained, causing compressive misfit stresses in the matrix (parallel to the interface) and tensile stresses in the precipitate.

The amount of straining of the matrix and precipitate is dependent on the magnitude of the misfit, the elastic moduli of both materials and their relative sizes [53]. The unconstrained misfit is defined as

$$\delta = \frac{a_{\gamma} - a_{\gamma}}{a_{\gamma}} \tag{18}$$

with $a_{\gamma'}$ and a_{γ} the lattice parameters of the γ' and γ -phases respectively. If the coefficient of thermal expansion is not equal for both phases, the misfit is temperature dependent, since the difference in lattice parameter changes with temperature. The misfit is assumed to be accommodated equally by both phases, leading to a misfit strain

$$\varepsilon_{misfit} = \frac{\frac{1}{2} (a_{\gamma} - a_{\gamma})}{a_{\gamma}}$$
(19)

in the matrix (in the two directions in the plane of the interface) and the same strain with opposite sign in the precipitate. Using the normal vector of the interface \vec{n}^i , the components of the misfit strain tensor are defined as

$$\varepsilon_{misfit}^{i} = \varepsilon_{misfit} \left(\mathbf{I} - \vec{n}^{i} \vec{n}^{i} \right) + \varepsilon_{n}^{i} \vec{n}^{i} \vec{n}^{i}$$
(20)

with ε_{misfit} given by (19) for the matrix regions and with ε_n^i the misfit strain in normal direction resulting from the requirement that the associated stress component vanishes. This misfit strain tensor represents an initial elastic strain (also called eigenstrain), triggering an initial stress in each of the regions. Since the misfit is accommodated *elastically* in both phases, the misfit stress and strain tensor are directly related to each other by a modified (plane stress) elastic stiffness tensor ${}^4\mathbf{B}_{misfit}^i$, which ensures that only the stress components parallel to the interface are non-zero

$$\mathbf{\sigma}_{misfit}^{l} = {}^{4}\mathbf{B}_{misfit}^{l} : \mathbf{\varepsilon}_{misfit}^{l}$$

Usually, the misfit strain is used as an initial strain in the equilibrium calculation of the local stresses. However, in an approach that is based on the Sachs interaction law this is not straightforward, since the different regions are coupled by their stresses, which affects the stress redistribution due to the misfit strains. At the same time, the use of the Sachs interaction law makes it possible to superpose a separately calculated internal stress (e.g. misfit stress, equation (21)) to the calculated local stress to constitute an effective stress tensor. The effective stress tensor is then used in the constitutive law, equation (2), to calculate the plastic strains.

(21)

The misfit between the two phases can be partially relaxed by plastic deformation of one or both phases. Plastic deformation generates misfit dislocations at the interface resulting in a loss of coherency between the phases and a corresponding relaxation of the misfit. When the total misfit strain would be completely accommodated by plastic slip, the effective stresses in both phases would be similar and the misfit would effectively vanish. For the interface regions this is automatically ensured by the compatibility requirements, according to equation (5). Plastic deformation in one region causes a local stress redistribution across the two phases and a corresponding decrease of the misfit. For the bulk regions (1 precipitate and 3 matrix regions), which are not subject to compatibility requirements, the absolute values of the misfit strain components (equation (20)) are reduced by the absolute value of the plastic strain difference ($\Delta \varepsilon_{pl}^{i}$) between the two phases, until the misfit completely vanishes:

$$\left| \boldsymbol{\varepsilon}_{misfit,ij}^{i} \right| \rightarrow \left| \boldsymbol{\varepsilon}_{misfit,ij}^{i} \right| - \left| \Delta \boldsymbol{\varepsilon}_{pl,ij}^{i} \right|$$

$$(22)$$

This simulates the loss of coherency due to plastic deformation in one or both phases. When a tensile stress is applied to the material, the effective stress in the matrix channels parallel to the loading direction will be lowered by the compressive misfit stress. This is not the case for the channels perpendicular to the loading axis, and it was observed that the deformation is initially localized in these matrix channels.

4.2 Strain gradient induced back stress

The back stress on a slip system originates from the spatial distribution of dislocations and is therefore only related to the GND density. For SSDs, which usually have a random orientation, the back stress contribution will be negligible. The value of the back stress tensor is calculated by summation of the internal stress fields caused by the individual edge and screw dislocation densities.

(23)

$$\mathbf{\sigma}_{\mathbf{b}} = -\left(\mathbf{\sigma}_{e}^{\mathrm{int}} + \mathbf{\sigma}_{s}^{\mathrm{int}}\right)$$

For a field of edge dislocations the stress field in a point is approximated by summation of the contributions of all dislocation systems ξ in a region with radius R around that point [54], resulting in

$$\boldsymbol{\sigma}_{e}^{\text{int}} = \frac{\mu b R^2}{8(1-\nu)} \sum_{\xi=1}^{12} \vec{\nabla} \rho_{GND}^{\xi} \cdot \left(3\vec{n}\,^{\xi}\vec{s}\,^{\xi}\vec{s}\,^{\xi}-\vec{s}\,^{\xi}\vec{s}\,^{\xi}\vec{n}\,^{\xi}-\vec{s}\,^{\xi}\vec{n}\,^{\xi}\vec{s}\,^{\xi}+\vec{n}\,^{\xi}\vec{n}\,^{\xi}\vec{n}\,^{\xi}+4\nu\vec{n}\,^{\xi}\vec{p}\,^{\xi}\vec{p}\,^{\xi}\vec{p}\,^{\xi}\right) \tag{24}$$

where the vectors \vec{s} and \vec{n} are in the direction of the Burgers vector and slip plane normal respectively and \vec{p} is defined as $\vec{p} = \vec{s} \times \vec{n}$, i.e. the dislocation line vector for an edge dislocation.

For the field of screw dislocations the stress field is given by

$$\boldsymbol{\sigma}_{s}^{\text{int}} = \frac{\mu b R^{2}}{4} \sum_{\xi=13}^{18} \vec{\nabla} \rho_{GND}^{\xi} \cdot \left(-\vec{n}^{\xi} \vec{s}^{\xi} \vec{p}^{\xi} - \vec{n}^{\xi} \vec{p}^{\xi} \vec{s}^{\xi} + \vec{p}^{\xi} \vec{s}^{\xi} \vec{n}^{\xi} + \vec{p}^{\xi} \vec{n}^{\xi} \vec{s}^{\xi} \right)$$
(25)

where $\vec{p} = \vec{s} \times \vec{n}$ is now perpendicular to the dislocation line direction (since the Burgers vector is parallel to the dislocation line). Note that only a non-zero gradient of the GND densities causes a non-vanishing contribution.

To calculate the back stress, it is necessary to know the distribution of the dislocation densities for all individual slip systems. These densities can be obtained from the slip gradients in the material. Since the two phases form a coherent interface this can be done on the slip system level [37,54]. Slip gradients in the direction of the slip will be accommodated by edge dislocations while slip gradients perpendicular to the slip direction will be accommodated by screw dislocations. For the edge dislocations ($\xi = 1...12$) the GND densities are obtained from the slip gradients by

$$\rho_{GND}^{\xi} = \rho_{GND,0}^{\xi} - \frac{1}{b} \vec{\nabla} \gamma^{\xi} \cdot \vec{s}^{\xi}$$
(26)

and for the screw dislocations ($\xi = 13...18$) by

$$\rho_{GND}^{\xi} = \rho_{GND,0}^{\xi} + \frac{1}{b} \left(\vec{\nabla} \gamma^{\alpha_1} \cdot \vec{p}^{\alpha_1} + \vec{\nabla} \gamma^{\alpha_2} \cdot \vec{p}^{\alpha_2} \right)$$
(27)

The screw dislocation densities are the result of the combined effect of the slip gradients on the two available slip planes α_1 and α_2 , as given in Table 1. The initial values of the GND densities, $\rho_{GND,0}^{\xi}$, can be used to account for pre-deformation effects, if necessary.

Since the real deformation distribution in the unit cell is simplified by assuming uniform deformation inside each region, gradients in slip are captured through discrete steps in between regions only. This is illustrated in Figure 5, where the solid curve represents the expected distribution of plastic slip and the set of horizontal solid lines the piecewise uniform approximation. The GND density distribution corresponding to the real deformation is approximated by the dashed line. The gradients in the dislocation density and slip, as used in the equations (24) to (27), are replaced by their piece-wise discrete analogons. For example, when defined relative to a x, y,z-coordinate system, the gradient in GND density can be written as

$$\vec{\nabla}\rho_{GND}^{\xi} = \frac{\Delta\rho_{GND}^{\xi}}{l}\vec{n}_{x}$$
(28)

for the interface regions with their normal in the *x*-direction. In this relation $\Delta \rho_{GND}$ is the difference in GND density between both sides of the region and *l* is the width of the region. No gradient in *y*- or *z*-direction is present in these regions.

[Insert Fig. 5 about here]

Further, the slip gradient is assumed to be accommodated by the interface regions only, which means that the total slip difference between the matrix γ and a precipitate γ' is distributed over the two interface regions in between both bulk regions. Moreover, it is assumed that the GND densities increase (or decrease) linearly from zero in the γ - and γ' -regions to a maximum (or minimum) value at the boundary between the constituents of the interface regions (see Figure 5). According to the equations (26) and (27) the GND density is proportional to the gradient in plastic slip. This gradient is based on the slip difference between the bulk γ - and γ' -regions. Due to the assumption of a linear variation of GND density inside a region, the GND density is the only relevant quantity whose distribution is not uniform inside a region. This assumption is necessary since only a *gradient* in GND density induces a back stress, but also physically more sound than a uniform GND density.

Finally, Figure 5 also shows that the two interface regions on either side of a matrix or precipitate region behave identically, both in terms of plastic deformation and in terms of GND density gradients (which determine the back stress). This motivates the reduction of the number of interface regions in the model that was mentioned in section 2.1.

4.3 Model summary

The complete model as described in sections 2, 3 and 4 is summarized in

Table 3.

 [Insert Table 3 about here]

Application

The framework described in the previous sections has been applied to the single crystal Ni-base superalloy CMSX-4 to demonstrate the effect of strain gradients on the mechanical response. First, the determination of the model parameters is discussed and simulated tensile and creep curves are compared to experimental results. Then, the contributions of the Orowan threshold and the strain gradient induced back stresses to the observed size effects are demonstrated and the simulated size effects due to a change in the microstructural dimensions are compared to experimental results. Finally, a real multi-scale analysis is performed, showing the effect of a change in microstructural dimensions on the creep strain accumulation in a gas turbine blade. The lattice constants of the γ and γ '-phase at 850 °C are 0.3590 nm and 0.3586 nm respectively, which leads to an unconstrained misfit of -1.1 x 10⁻³, see equation (18). The model parameters used for CMSX-4 are given in

Table 4. The parameters α , k, b and μ are physical quantities with a fixed value, obtained from [30,32]. The matrix phase parameters $\dot{\gamma}_0$ and *m* in the slip law, equation (7), and *c*, y_c , $\rho_{SSD,0}$, *K*, C_{soft} , *Q* and *p* in relations (12) to (17) for the slip resistance and the SSD density evolution, determine the mechanical behaviour for a fixed microstructure. Their values were obtained by calibrating the model to the experimental results [55] shown in Figure 6, using a least-squares fitting method. The parameters *n* and *R* and the relative width of the matrix phase interface layer determine the material size dependence. The value of n determines the relative strength of the Orowan threshold and the radius of the dislocation influence region R quantifies the magnitude of the back stress. The values for R and n were obtained by fitting the model to the two endpoints (only two points) of the experimentally determined size dependence curve in Figure 12, using a least-squares fitting method. The obtained value for the radius of the dislocation influence region R is significantly smaller than the rather large value of 3.16 µm that Evers et al. [37] obtained by fitting their model to results on pure copper. The value used here is more realistic for the present application, since it is in the same order as the dimensions of the matrix phase. Moreover, several studies [56-58] recently showed that R should be in the order of the dislocation spacing, which is equivalent to the inverse square root of the dislocation density. In our model, dislocation densities develop from an initial value of 5 x 10^{13} to values up to 10^{16} m⁻², which corresponds to *R*-values ranging from 30 to 140 nm. This is in the same order of magnitude as the resulting value for R. The width of the precipitate part of the interface layer does not affect the size dependence, because no plastic deformation occurs in the precipitate. Therefore this width can be chosen freely in between some limits, e.g. a physically acceptable fraction of the precipitate size. Increasing the width of the matrix interface layer decreases the slip gradients and the resulting back stress and therefore diminishes the size dependence. But on the other hand it increases the volume fraction of the interface regions, which results in stronger size effects. An interfacial width of 30 % of the matrix phase width proved to yield the best compromise between these two counteracting phenomena. This means that the interface effects are acting in a boundary zone with a characteristic size of 19% of the total channel width, located on each side of the channel. This is very close to the value of 23 % presented by Busso et al. [6] for the normalized channel width that contains the strain gradients in their FE unit cell analysis.

[Insert Table 4 about here]

5.1 Simulation results

In this subsection the model capabilities are demonstrated by comparing simulated tensile and creep curves to experimental results. The model has been implemented in a finite element (FE) code. Tensile tests at 800 and 850 $^{\circ}$ C at strain rates of 10⁻⁴, 10⁻³ and 10⁻² s⁻¹ and creep tests at 850 $^{\circ}$ C and 284, 345 and 393 MPa are simulated by using an FE model with only a single element. The results are shown in Figure 6, together with experimental results for CMSX-4 [55].

[Insert Fig. 6 about here]

The results in Figure 6 demonstrate that the present framework is able to simulate the real material response adequately. For the tensile curves, especially the steady-state stress levels correspond well to the experimental values, whereas the deviations are somewhat larger at the initial yielding stage of the curves. This is due to the use of the phenomenological description of the softening behaviour. The simulated creep curves describe the material behaviour quite well for the primary and secondary creep regime. The tertiary regime is associated with precipitate shearing and microstructural degradation. Since these mechanisms are not included in the present framework, the model is not able to accurately simulate the material response for this part of the creep curve.

To demonstrate the contributions of the individual unit cell regions to the macroscopic response, the evolution of the effective stresses and plastic strains on the micro-level during one of the tensile tests in Figure 6 is plotted in Figure 7 and Figure 8.

[Insert Fig. 7 about here]

Figure 7a shows that the regions have different starting values, which is caused by the misfit stress. In the precipitate (both bulk and interface) regions the tensile misfit stress increases the effective stress, while the compressive misfit stress in the matrix regions parallel to the applied load decreases the effective stress. As the misfit stresses only occur in the plane of the γ/γ' -interface, they do not affect the stresses in the load direction in the regions that are normal to the applied load. The figure also shows that the misfit stresses quickly disappear as soon as the plastic deformation starts. After that, the stresses in all bulk regions equal the macroscopic stress, as is required by the Sachs interaction law. Also, the average value of the matrix and precipitate interface regions

equals the macroscopic stress, but the strain gradient related back stresses cause a large difference between the two sides (matrix and precipitate) of the interface regions, especially for the regions parallel to the applied load. Finally, the results for the bulk and interface unit cell *regions* in Figure 7a are used to calculate the volume averaged values for the different *phases* (matrix and precipitate) in the material, as is shown in Figure 7b.

[Insert Fig. 8 about here]

Figure 8 shows the evolution of plastic strain in the different regions. There is a difference in plastic deformation rate between the matrix bulk regions parallel and normal to the applied load. This is caused by the different (initial) stress levels and the resulting differences in evolution rate of the slip resistance. The plastic flow in the interface regions is limited due to the development of strain gradient related back stresses that reduce the effective stress. The precipitate bulk and interface regions are absent in this figure, since they only deform elastically.

Finally, the evolution of the dislocation densities is illustrated in Figure 9, which compares the SSD and GND densities on a specific slip system in both bulk and interface regions at three stages during a tensile test. This shows that in the bulk regions, where no GNDs are present, the SSD density increases with a factor two during the test. In the interface regions strain gradients develop, which are accommodated by a rapidly increasing GND density. The resulting back stresses reduce the effective stress and therefore lower the slip rate. Consequently, the SSD density hardly increases in these regions.

[Insert Fig. 9 about here]

5.2 Strain gradient effects and size dependence

Nickel-base superalloys show a clear size dependence, which means that the mechanical behaviour changes when proportionally increasing or decreasing the microstructural dimensions while keeping all volume fractions constant. The present framework is able to simulate these microstructural size effects.

There are two essential contributions that make the model response size dependent. Firstly, the Orowan threshold stress is size dependent, since it is inversely proportional to the γ -channel width *h*. Secondly, the GND density is size dependent, because it is related to strain gradients. Reducing the microstructural dimensions will increase the strain gradients and consequently the GND densities. GND densities in their turn contribute to the

slip resistance and, through their gradients, govern the back stress. The Orowan threshold is incorporated in several existing superalloy models [30-35], whereas only strain gradient effects are present in the two FE unit cell approaches [6-8] discussed before. This section will demonstrate the necessity and possibility of including both ingredients in superalloy constitutive models.

<text><text><text>

Table 4 lead to an initial slip resistance (s^{α} = 98 MPa) which is lower than the Orowan stress (t^{or} = 255 MPa). This means that the Orowan threshold is the decisive threshold in this case. Downsizing the complete unit cell by a factor 2 or 4 increases the Orowan threshold by the same factor. The GND densities in the interface regions are proportional to the gradients in the plastic slip. Changing the interfacial width by increasing or decreasing the unit cell dimensions affects the gradients and hence the GND densities. Consequently, the material response changes since the GNDs contribute to the slip resistance and constitute the source of back stresses.

The unit cell dimensions were varied to quantify these size effects. Figure 10 shows the stress-strain curves at a rate of 10^{-3} s⁻¹ for the reference case, for which the microstructural dimensions used are L = 500 nm and h = 60 nm, and for three other cases with all unit cell dimensions multiplied by a factor 0.5, 0.75 and 2. In these simulations both the Orowan effect and the GND effects are included.

[Insert Fig. 10 about here]

To separate the effects of GNDs and the Orowan threshold, the internal stresses were removed from the model by setting all GND densities to zero. The resulting stress-strain curves are shown in Figure 11 for the reference case and for three other unit cell sizes, where the observed effects are now due to the change of the Orowan threshold only. This figure shows that the shape of the curves for the different unit cell sizes remains the same, while the maximum stress again shifts to a higher level with a decreasing matrix channel width.

[Insert Fig. 11 about here]

Comparison of the curves in Figure 10 and Figure 11 shows that their shape is identical for small strains (< 1.3 %), but quite different for larger strains. Also, the yield points for the curves in Figure 10 are higher than those in Figure 11. The increased slip resistance and back stresses that develop due to increasing internal strain gradients reduce the slip rates. Hence the material stress response is increasing. This effect is stronger when the microstructural dimensions decrease below the values of the reference case, i.e. smaller is stronger.

Finally, the simulated size effects were compared to experimental results (Figure 12). Duhl [59] measured the change of the steady-state flow stress at different precipitate sizes for PWA1480, a similar nickelbase superalloy with a high precipitate volume fraction. The steady-state flow stresses were normalised by the values for the reference cases to enable a direct comparison in Figure 12. Although the experimental results were determined at 760 °C and the present model was calibrated for 800 °C, the observed size effect could be simulated quite well. In the simulations, the steady-state flow stress was defined as the stress level at the end of the curve (at 5 % total strain). During the deformation, the slip resistance and back stress evolve until the plastic strain rate equals the externally applied strain rate. From that point on the stress has attained a steady-state value. In the majority of the simulations this point was reached before a strain level of 5 %.

Figure 12 also shows the simulated size dependence for the model without strain gradient effects, where the Orowan threshold is the only cause of size effects. For large microstructural dimensions, the curve is almost identical to the strain gradient curve, but for small dimensions there is a significant difference. At these dimensions the plastic strain gradients play an important role and the material size dependence cannot be described by the Orowan effect only.

Busso et al. [6] performed the same simulations with their gradient-dependent unit cell finite element model, consisting of about 500 finite elements. The present model with only 10 unit cell regions predicts the size effects at least as good as the model by Busso et al. [6], but with a considerably lower computational effort.

[Insert Fig. 12 about here]

5.3 Computational efficiency and multi-scale analysis

The present framework is developed specifically to be used in a multi-scale analysis on real gas turbine components. Therefore, it is essential that the model is computationally efficient. This efficiency is largely determined by the model's level of detail and the associated number of internal variables. Even though a direct comparison between different modelling approaches in terms of computational efficiency is difficult (in view of the many small or large differences in model capabilities and assumptions), an attempt is made in Table 5. The left-hand side of the table provides information about the model characteristics and capabilities, also classified by one or two + or – signs. In the right-hand side of the table the computational efficiency is quantified. The first column provides the number of degrees of freedom (d.o.f.) to be solved to obtain the local stress distribution for a given plastic strain distribution. For the analytical models this is the number of equations, for the FE models three (nodal d.o.f.) times the number of nodes, both for one material point. Then the number of internal variables per material point is specified and the time integration method is mentioned. For the present model, the time integration is fully explicit, both on the local (unit cell) and global (macro) level. Finally, the overall computational efficiency is classified by one or two + or – signs.

[Insert Table 5 about here]

Table 5 shows that the different approaches can be classified in three groups: traditional single phase models, analytical unit cell models and finite element unit cell models, requiring small, medium and very large computational effort, respectively. Within the groups the computational effort is comparable, but the level of detail and model capabilities differ considerably. The present modelling approach can be considered as the most extensive method amongst the analytical unit cell models, where it is the only model including strain gradient effects.

To clearly emphasize the computational efficiency of the present framework and to demonstrate the multi-scale capabilities, the proposed multi-scale model was applied to a finite element model of an aero-engine low pressure turbine blade discretized with 5668 hexagonal (8-noded) elements and 7302 nodes. The proposed unit cell model was implemented in a user-subroutine of the commercial finite element code MSC.Marc. During the analysis, it is solved for each integration point in the turbine blade model. A short-term creep analysis, divided into 32 time steps, was performed in only half an hour on a desktop PC. The temperature and stress distribution used in the creep analysis are shown in Figure 13 a and b respectively. Then the creep strain accumulation in a component with a reference microstructure (L = 500 nm, h = 60 nm) can be compared to the accumulation in a blade with a coarsened microstructure (L = 1000 nm, h = 120 nm). The results are shown in Figure 13 c and d. The evolution of the creep strain in time is plotted in Figure 14, which shows that the creep strain rate in the component with the coarsened microstructure is considerably higher than in the blade with the reference microstructure.

[Insert Fig. 13 about here]

[Insert Fig. 14 about here]

This analysis clearly demonstrates that the proposed framework can be used efficiently in a multi-scale approach. And it also reveals the relevance, for the engineering practice, of including strain-gradient effects in superalloy mechanical models.

6 Conclusions

Strain gradient effects are incorporated in a newly developed efficient crystal plasticity framework for nickelbase superalloys with the following innovative characteristics:

- The proposed unit cell contains special interface regions, in which the plastic strain gradients are located. In these interface regions strain gradient induced back stresses will develop as well as stresses due to the lattice misfit between the two phases.
- The limited size of the unit cell and the micromechanical simplifications, which condense the governing equations to 10 uniformly deforming regions, make the framework particularly efficient in a multi-scale approach. The unit cell response is determined numerically on a material point level within a macroscopic FE code, which is computationally much more efficient than a detailed FE-based unit cell discretization.
- The material constitutive behaviour is simulated by using an extension of an existing non-local strain gradient crystal plasticity model for the matrix material. In this model, non-uniform distributions of geometrically necessary dislocations (GNDs), induced by strain gradients in the interface regions, affect the hardening behaviour. Further, the model has been modified here for the present two-phase material by adding a threshold term related to the Orowan stress to the hardening law. Continuous dislocation densities and slip gradients, as typically used in the FE formulation, are approximated here by piecewise uniform fields for application in an efficient unit cell approach.

The model was applied to the Ni-base superalloy CMSX-4, where it proved to be capable of accurately simulating the experimentally observed change of the steady-state flow stress with varying microstructural dimensions. Further, the multi-scale capability was demonstrated by applying the model in a gas turbine blade finite element analysis. Therefore, it can be concluded that the proposed framework is able to describe the material response and size effects to a level of detail similar to complex FE unit cell models, while being computationally much more efficient.

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Tables

Table 1	List of indices and vec	ors for dislocation	n densities and slip	svstems in an F	CC metal.
rubic i		oro for albioballor	i dononioù de dina onp	by bionno in an r	oo mota.

Disloc	ation density	Slip system	Slip direction	Slip plane normal
ξ	type	α	\vec{s}	\vec{n}
1	edge	1	½√2 [ĪI0]	½√3 [III]
2	edge	2	½√2 [I0Ī]	¹ ∕₃√3 [III]
3	edge	3	½√2 [0ĪI]	½√3 [III]
4	edge	4	½√2 [110]	1∕₃√3 [I <u>I</u>]
5	edge	5	½√2 [I0I]	1∕₃√3 [I <mark></mark>]
6	edge	6	½√2 [0IĪ]	1∕₃√3 [I <u>I</u>]
7	edge	7	½√2 [II0]	½√3 [ĪIĪ]
8	edge	8	½√2 [Ī0I]	½√3 [ĪIĪ]
9	edge	9	½√2 [0]]	½√3 [ĪIĪ]
10	edge	10	½√2 [IĪ0]	½√3 []]
11	edge	11	½√2 [Ī0Ī]	½√3 [[]]
12	edge	12	½√2 [0II]	½√3 []]
13	screw	-4 or 7	½√2 [II0]	⅓√3 [IĪĪ] or ⅓√3 [ĪIĪ]
14	screw	5 or -11	½√2 [I0I]	⅓√3 [IĪĪ] or ⅓√3 [ĪĪI]
15	screw	-9 or 12	½√2 [0II]	⅓√3 [ĪIĪ] or ⅓√3 [ĪĪI]
16	screw	1 or -10	½√2 [ĪI0]	⅓√3 [III] or ⅓√3 [II I]
17	screw	2 or -8	½√2 [I0Ī]	⅓√3 [III] or ⅓√3 [ĪIĪ]
18	screw	3 or -6	½√2 [0ĪI]	⅓√3 [III] or ⅓√3 [I <mark>I</mark>]

Table 2 4 C elastic tensor components for CMSX-4 at 850 ${}^{\circ}$ C [6].

	γ-matrix	γ'-precipitate
C ₁₁₁₁ (GPa)	190.9	216.9
C ₁₁₂₂ (GPa)	127.3	144.6
C ₁₂₁₂ (GPa)	100.2	105.2

Table 3 Overview of mo	odel equations		
Fauilibrium	unit cell region(s	8)	eq.nr.
Equinorium			
Strain averaging	all	$\sum_{i} f^{i} \boldsymbol{\varepsilon}_{tot}^{i} = \boldsymbol{\varepsilon}_{tot}$	(1)
Sachs interaction	$\gamma', \gamma_1, \gamma_2, \gamma_3$	$\boldsymbol{\sigma}^{\gamma'} = \boldsymbol{\sigma}^{\gamma_1} = \boldsymbol{\sigma}^{\gamma_2} = \boldsymbol{\sigma}^{\gamma_3} = \boldsymbol{\sigma}_{tot}$	(3)
Modified Sachs interaction	$I_1^p, I_1^m, I_2^p, I_2^m, I_3^p, I_3^m$	$f^{I_k^p} \boldsymbol{\sigma}^{I_k^p} + f^{I_k^m} \boldsymbol{\sigma}^{I_k^m} = \left(f^{I_k^p} + f^{I_k^m} \right) \boldsymbol{\sigma}_{tot}$	(4)
Strain compatibility	$I_1^p, I_1^m, I_2^p,$ I_2^m, I_3^p, I_3^m	$\boldsymbol{\varepsilon}^{\mathbf{I}_{k}^{p}}\cdot\left(\mathbf{I}-\vec{n}^{k}\vec{n}^{k}\right)=\boldsymbol{\varepsilon}^{\mathbf{I}_{k}^{m}}\cdot\left(\mathbf{I}-\vec{n}^{k}\vec{n}^{k}\right)$	(5)
Traction continuity	$I_{1}^{p}, I_{1}^{m}, I_{2}^{p}, I_{2}^{m}, I_{3}^{p}, I_{3}^{m}$	$\boldsymbol{\sigma}^{\mathbf{I}_{k}^{\mathrm{p}}}\cdot\vec{n}^{k}=\boldsymbol{\sigma}^{\mathbf{I}_{k}^{\mathrm{m}}}\cdot\vec{n}^{k}$	(6)
Constitutive model	all	$\mathbf{\epsilon}^i \rightarrow \text{constitutive box} \rightarrow \mathbf{\sigma}^i$	(2)
Internal stresses			
Misfit	all	$\boldsymbol{\sigma}_{misfit}^{i} = {}^{4} \mathbf{B}_{misfit}^{i} : \boldsymbol{\varepsilon}_{misfit}^{i}$	(21)
		$\boldsymbol{\sigma}_{\mathbf{b}} = -\left(\boldsymbol{\sigma}_{e}^{\text{int}} + \boldsymbol{\sigma}_{s}^{\text{int}}\right)$	(23)
Back stress	$I_1^p, I_1^m, I_2^p,$	$\boldsymbol{\sigma}_{e}^{\text{int}} = \frac{\mu b R^2}{8(1-\nu)} \sum_{\xi=1}^{12} \vec{\nabla} \rho_{GND}^{\xi} \cdot \begin{pmatrix} 3\vec{n}^{\xi} \vec{s}^{\xi} \vec{s}^{\xi} - \vec{s}^{\xi} \vec{s}^{\xi} \vec{n}^{\xi} \\ -\vec{s}^{\xi} \vec{n}^{\xi} \vec{s}^{\xi} + \vec{n}^{\xi} \vec{n}^{\xi} \vec{n}^{\xi} + 4\nu \vec{n}^{\xi} \vec{p}^{\xi} \vec{p}^{\xi} \end{pmatrix}$	(24)
	I_2, I_3, I_3	$\boldsymbol{\sigma}_{s}^{\text{int}} = \frac{\mu b R^{2}}{4} \sum_{\xi=13}^{18} \vec{\nabla} \rho_{GND}^{\xi} \cdot \begin{pmatrix} -\vec{n}^{\xi} \vec{s}^{\xi} \vec{p}^{\xi} - \vec{n}^{\xi} \vec{p}^{\xi} \vec{s}^{\xi} \\ + \vec{p}^{\xi} \vec{s}^{\xi} \vec{n}^{\xi} + \vec{p}^{\xi} \vec{n}^{\xi} \vec{s}^{\xi} \end{pmatrix}$	(25)
Matrix constitutive mo	odel		
Effective stress	$\begin{array}{c} \gamma_1, \gamma_2, \gamma_3, \\ I_1^m, I_2^m, I_3^m \end{array}$	$\boldsymbol{\sigma}_{eff} = \boldsymbol{\sigma} + \boldsymbol{\sigma}_{misfit} - \boldsymbol{\sigma}_{b}$	(10)
Slip rate	$\gamma_1, \gamma_2, \gamma_3,$ I_1^m, I_2^m, I_3^m	$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left\{ \frac{\left \tau_{eff}^{\alpha} \right }{s^{\alpha}} \right\}^m \left\{ 1 - \exp\left(-\frac{\left \tau_{eff}^{\alpha} \right }{\tau^{or}} \right) \right\}^n \operatorname{sign}\left(\tau_{eff}^{\alpha} \right)$	(7)
Slip resistance	$\begin{split} &\gamma_1,\gamma_2,\gamma_3,\\ &I_1^m,I_2^m,I_3^m \end{split}$	$s^{\alpha} = \left\{ c \mu b \sqrt{\left \rho_{SSD}^{\alpha} \right + \left \rho_{GND}^{\alpha} \right } + C_{soft} \left(1 - \sqrt{\frac{\rho_{SSD}^{\alpha}}{\tilde{\rho}_{SSD}^{\alpha}}} \right)^{p} \right\} \exp\left[\frac{Q}{kT} \right]$	(12) (13) (16)
Precipitate constitutive	e model		
	$\boldsymbol{\gamma}', \mathbf{I}_1^p, \mathbf{I}_2^p, \mathbf{I}_3^p$	no plastic slip, purely elastic	-
Dislocation densities			
	$\mathbf{I}_{1}^{p}, \mathbf{I}_{2}^{m}, \mathbf{I}_{2}^{p}$	$\rho_{GND}^{\xi} = \rho_{GND,0}^{\xi} - \frac{1}{b} \vec{\nabla} \gamma^{\xi} \cdot \vec{s}^{\xi} \qquad (edge \ dislocations)$	(26)
GND densities	$\mathbf{I}_2^{\mathrm{m}}, \mathbf{I}_3^{\mathrm{p}}, \mathbf{I}_3^{\mathrm{m}}$	$\rho_{GND}^{\xi} = \rho_{GND,0}^{\xi} + \frac{1}{b} \left(\vec{\nabla} \gamma^{\alpha_1} \cdot \vec{p}^{\alpha_1} + \vec{\nabla} \gamma^{\alpha_2} \cdot \vec{p}^{\alpha_2} \right) (screw \ disl.)$	(27)
SSD evolution	$\gamma_1, \gamma_2, \gamma_3,$ I_1^m, I_2^m, I_3^m	$\dot{\rho}_{SSD}^{\alpha} = \frac{1}{b} \left(\frac{1}{L^{\alpha}} - 2y_c \rho_{SSD}^{\alpha} \right) \dot{\gamma}^{\alpha} \Big $	(14)

Table 4 Model	parameters	for the n	natrix pha	se of CMSX-4.
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Model parameter	Symbol	Value	Unit	Used in
				equation
Reference slip rate	$\dot{\gamma}_0$	6.5 x 10 ⁻¹⁰	s ⁻¹	(7)
Rate sensitivity exponent Orowan threshold	n	4		(7)
Rate sensitivity exponent slip resistance	m	11.7		(7)
Reference activation energy	Q	3.62 x 10 ⁻²⁰	J	(12)
Strength parameter	С	0.034		(13)
Shear modulus	μ	100.2	GPa	(13)
Burgers vector length	b	0.254	nm	(11),(13),(14)
Parameter in Orowan stress	α	0.85		(11)
Critical annihilation length	y_c	7.2	nm	(14)
Initial SSD density	$ ho_{SSD,0}$	$5.0 \ge 10^{13}$	m ⁻²	(14)
Material constant	K	7		(15)
Softening constant	C_{soft}	90	MPa	(16)
Softening exponent	p^{r}	0.7		(16)
Radius of dislocation influence region	R	8.3	nm	(24),(25)

Table 5 Comparison of different modelling approaches.

Author(s)	Characteristics / level of detail / capabilities		Computational efficiency			
			# d.o.f.	# int. vars	time integr.	
Traditional models	- single phase model		3 - 6	0		++
	- no microstructural details					
Svoboda and	- 4 regions unit cell	-	24	54	not specified	+
Lukas [35]	- analytic stress calculation					
	- dislocation based creep law in γ / γ'					
	- for <001> only					
	- isotropic elastic properties					
Fedelich [31]	- 8 regions unit cell	+	24, using 216	192	Runge-Kutta	+
	- Fourier series approach for stress		structural		-	
	calculation		tensor (Ω_{KI})			
	- dislocation based plasticity in γ / γ'		components			
Tinga et al.	- 10 regions unit cell	++	60	216	fully explicit	+
(present model)	- analytic stress calculation					
•	- dislocation based strain gradient					
	plasticity in γ / elastic precipitate					
Kuttner and Wahi	- 125 elm FE model	+	~ 1000	0	not specified	-
[34]	- Norton creep law for γ/γ'				-	
Busso et al. [6]	- 424 elm FE model	++	~ 4000	$\sim 10^{5}$	fully implicit	
	- dislocation based strain gradient					
	plasticity in γ / elastic precipitate					
Choi et al. [8]	- 424 elm FE model	++	~ 4000	$\sim 10^{5}$	combined	
	- phenomenological strain gradient				explicit /	
	plasticity in γ / elastic precipitate				implicit	

Figure captions

Figure 1 Micrograph of a superalloy microstructure showing the cube-like γ' -precipitates in a γ -matrix [9].

Figure 2 Schematic overview of the model, showing (a) the multi-scale character and (b) the multi-phase unit cell, consisting of one precipitate (γ '), three matrix (γ_i) and six double interface(I_i) regions.

Figure 3 Definition of the unit cell dimensions in the y-z plane cross section.

Figure 4 Overview of the interaction between the different levels of the multi-scale model. In the macroscopic FE analysis, the usual standard procedure to obtain the stress response for a given deformation is replaced by a mesoscopic calculation at the unit cell level. A crystal plasticity (CP) model yields the relation between the local stress and plastic strain rate for the matrix regions.

Figure 5 Overview of gradients in slip and GND density. The solid curved line represents the continuous plastic slip distribution that is expected in the real material and the series of straight solid lines the piecewise uniform approximation. The dashed line represents the GND density distribution.

Figure 6 Simulated curves (solid lines) compared to experimental results (markers) for CMSX-4; a) stressstrain curves at strain rates of 10^{-4} s⁻¹ at 850 °C and 10^{-3} and 10^{-2} s⁻¹ at 800 °C; b) creep curves at 284, 345 and 393 MPa at 850 °C.

Figure 7 Variation of micro-level effective stresses during a tensile test at 800 °C and a strain rate of 10^{-3} s^{-1} . a) stresses in individual unit cell regions; b) stresses in material phases, obtained from combining the results in a), compared to the macroscopic (unit cell averaged) stress. In all cases the stress component in the direction of the applied load is plotted. The symbols \perp and // denote the regions oriented normal and parallel to the applied load, respectively.

Figure 8 Plastic strain evolution in the unit cell regions during a tensile test at 800 $^{\circ}$ C and a strain rate of 10⁻³ s⁻¹. The strain component in the direction of the applied load is plotted. The macroscopic (unit cell averaged) stress and strain are plotted as a reference.

Figure 9 Evolution of the SSD and GND densities during a tensile test at 800 °C and a strain rate of 10^{-3} s^{-1} . Values are given for a bulk matrix region and an interface region at three stages of the tensile test.

Figure 10 Effect of changing microstructural dimensions on the stress-strain curve at a strain rate of 10^{-3} s^{-1} , including the effect of Geometrically Necessary Dislocations and resulting back stresses. The reference case is L = 500 nm and h = 60 nm.

Figure 11 Effect of changing microstructural dimensions on the stress-strain curve, using the model without Geometrically Necessary Dislocations. The reference case is L = 500 nm and h = 60 nm.

Figure 12 Simulated effect of changing microstructural dimensions on the steady-state flow stress for CMSX-4 at 800 °C. Results for simulations with Orowan effect only and with Orowan + strain gradient effects. Experimental data for PWA1480 at 760 °C obtained from [59].

Figure 13 Finite element analysis results on a gas turbine blade. a) temperature distribution, b) equivalent stress distribution, c) accumulated creep strain for reference microstructure, d) accumulated creep strain for coarsened microstructure.

Figure 14 Creep strain accumulation in time for a reference and a coarsened microstructure.

Figures



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