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Executive summary

Micro-mechanical modelling of the single crystal nickel-base superalloy CMSX-4

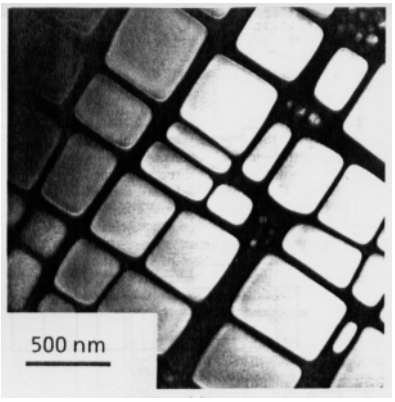

Fig.1 Superalloy microstructure

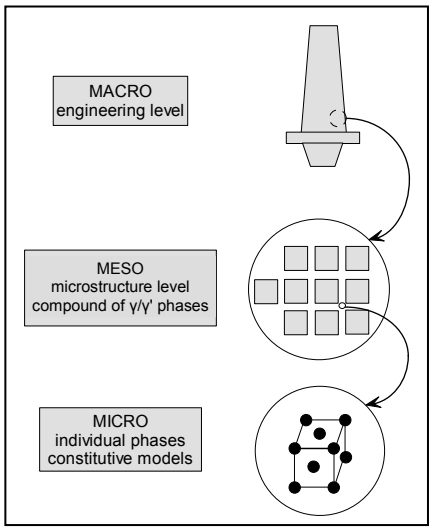

Fig.2 Overview of multi-scale model

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Problem area

Single crystal nickel-base superalloys are widely used as gas turbine blade materials because of their very high resistance against high temperature plastic deformation. The superior high temperature behavior is attributed to the two-phase composite microstructure, consisting of a γ matrix containing a large volume fraction of cuboidal γ' particles (Fig. 1). For both gas turbine component design and maintenance it is important to have the ability to perform a reliable life time assessment. However, to be able to accurately model the material behavior, the two-phase nature of the superalloy must be taken into account. Therefore, a lot of models have been developed that consider the microstructural morphology (shape, dimensions and properties of both phases) as a model parameter. But completely modeling a macroscopic component on a microscopic level would ask for an enormous computational effort.

Description of work

A multi-scale micromechanical model for a Ni-based superalloy is developed. The unit cell on the material point level incorporates the two-phase γ/γ'-microstructure of the material and the role of the γ/γ'-

This report is based on a presentation to be held at the 8th Liege Conference on Materials for Advanced Power Engineering, 18-20 September 2006, Liege, Belgium.

interfaces in the mechanical behavior is emphasized. A crystal plasticity framework is used to model the constitutive behavior of the γ-matrix phase. The limited number of unit cell constituents and the micromechanical simplifications make the framework particularly efficient in a multi-scale approach. The model is implemented in a commercial finite element code and can thus be applied to any FE model.

Results and conclusions

The model is applied to the commercial turbine blade alloy CMSX-4. The effect of microstructural changes on the mechanical response is demonstrated.

Applicability

The developed model can be applied to study the effect of microstructural changes on superalloy mechanical response. This is particularly interesting while performing life assessments on gas turbine components to determine inspection intervals or component service life.

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Micro-mechanical modelling of the single crystal nickel-base superalloy CMSX-4

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Summary

A multi-scale micromechanical model for a Ni-based superalloy is presented. The unit cell on the material point level incorporates the two-phase γ/γ'-microstructure of the material and the role of the γ/γ'-interfaces in the mechanical behavior is emphasized. A crystal plasticity framework is used to model the constitutive behavior of the γ-matrix phase. The limited number of unit cell constituents and the micromechanical simplifications make the framework particularly efficient in a multi-scale approach. The model is implemented in a commercial finite element code and adequately simulates the material response for the alloy CMSX-4. The effect of microstructural changes on the mechanical response is demonstrated.

Contents

5 Figures

(16 pages in total)

MICRO-MECHANICAL MODELLING OF THE SINGLE CRYSTAL NICKEL-BASE SUPERALLOY CMSX-4

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Abstract

A multi-scale micromechanical model for a Ni-based superalloy is presented. The unit cell on the material point level incorporates the two-phase γ/γ'-microstructure of the material and the role of the γ/γ'-interfaces in the mechanical behavior is emphasized. A crystal plasticity framework is used to model the constitutive behavior of the γ-matrix phase. The limited number of unit cell constituents and the micromechanical simplifications make the framework particularly efficient in a multi-scale approach. The model is implemented in a commercial finite element code and adequately simulates the material response for the alloy CMSX-4. The effect of microstructural changes on the mechanical response is demonstrated.

Keywords: Micromechanics; constitutive model; superalloy; crystal plasticity.

Introduction

The very high resistance against high temperature inelastic deformation is the main reason for the extensive use of single crystal nickel-based superalloys as gas turbine blade materials. This superior behavior 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 Ni_3Al (γ') precipitates, with a typical size of 0.5 μm, are more or less regularly distributed in a Ni-matrix (γ-phase). The typical size of the matrix channels in between the precipitates is only 60 nm.

For both gas turbine component design and maintenance it is important to have the ability to perform a reliable life time assessment. Therefore, a lot of models were developed to describe the superalloy mechanical behavior. The earlier models assumed the material to be a homogeneous single phase material [1-8]. In these approaches crystal plasticity theory was used to model the material response, which means that constitutive laws were defined on the slip system level. The formulation of the slip law ranges from purely phenomenological [1,5] to more physically based approaches [2-4,6]. Since these models are defined on a macroscopic level, they can easily be applied 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 accurately model the material behavior, the two-phase nature of the superalloy must be taken into account. Therefore, a lot of models have been developed that consider the microstructural morphology (shape, dimensions and properties of both phases) as a model parameter. But completely modeling a macroscopic component on a microscopic level would ask for an enormous computational effort.

There are two ways to reduce this effort. The first way is to use a multi-scale approach in which an appropriate homogenization method is applied to connect the microscopic to the macroscopic level [9-15]. The second way is to use microstructural models that predict the material response in a closed-form set of equations on the level of the material point [16-22]. The microstructural results are then used to develop constitutive descriptions that fit in traditional methods at the macroscopic level. All these microstructural models are based on a unit cell approach, in which a characteristic volume is defined that contains both γ and γ'-phase material with their respective properties and dimensions. The FE based unit cell models are detailed but usually too complex to be used efficiently in a multi-scale analysis of structural components.

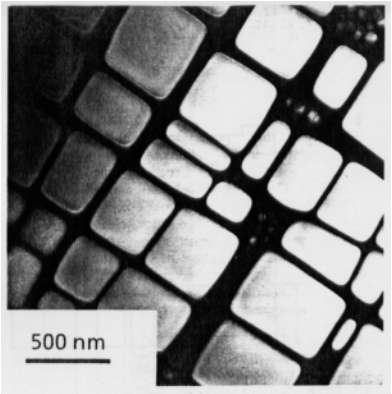

Figure 1 Micrograph of a superalloy microstructure showing the cube-like γ'-precipitates in a γ-matrix.

The model [23] described in this paper combines the merits of the previously mentioned models. The material response is described by a crystal plasticity formulation for the matrix material. Further, a new and efficient unit cell model is used, in which the role of the γ/γ'-interfaces is emphasized. The limited size of the unit cell and the micromechanical simplifications make the framework particularly efficient in a multi-scale approach.

The multi-scale model is described in the next section, providing definitions of the unit cell and the interaction laws. Then the constitutive models are described and the implementation in an FE code is discussed. Finally the model is applied to the Ni-based superalloy CMSX-4. Simulated stress-strain curves are compared to experimental results and the effect of changing microstructural dimensions is demonstrated.

Multi-scale approach

The multi-scale approach used for the prediction of the superalloy mechanical behaviour is shown schematically in Figure 2a . The *macroscopic* level is the engineering level on which a finite element (FE) model is commonly used to solve the governing equilibrium problem. The *mesoscopic* level is the level of the microstructure within a macroscopic material point. At this level the material is considered as a compound of two different phases: γ'-precipitates embedded in a γ-matrix. Finally, the crystallographic response of the individual material phases is described on the *microscopic* level, using a crystal plasticity framework.

Definition of the unit cell

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

- 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 behavior of the material. Therefore, special interface regions were included in the model to take into account the processes that take place at the γ/γ'-interfaces.

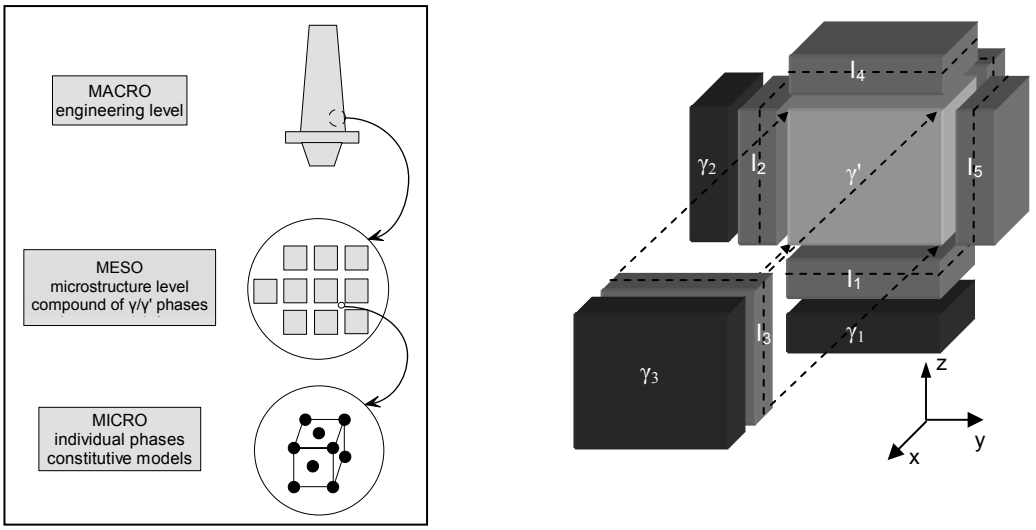

Figure 2 Schematic overview of the model, showing (a) the multi-scale character and (b) the multi-phase unit cell, consisting of one precipitate (γ'), three matrix (γ_i) and six double interface(I_i) regions.

Scale transitions and interaction law

In a conventional approach, 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. 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 ($\overline{\boldsymbol{\varepsilon}}$) and the mesoscopic average stress ($\overline{\boldsymbol{\sigma}}$). The stress tensor $\overline{\boldsymbol{\sigma}}$ is determined from the strain tensor $\overline{\boldsymbol{\varepsilon}}$ 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

$$\sum_{i=1}^{N} f^i \boldsymbol{\varepsilon}^i_{tot} = \overline{\boldsymbol{\varepsilon}}_{tot} \qquad i = \gamma', \gamma_1, \gamma_2, \gamma_3, \mathrm{I}^{\mathrm{p}}_1, \mathrm{I}^{\mathrm{m}}_1, \mathrm{I}^{\mathrm{p}}_2, \mathrm{I}^{\mathrm{m}}_2, \mathrm{I}^{\mathrm{p}}_3, \mathrm{I}^{\mathrm{m}}_3 \tag{1}$$

where f^i are the volume fractions, $\boldsymbol{\varepsilon}^i_{tot}$ the total strain tensors in the different regions and N indicates the effective number (10) of regions in the model.

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

$$\boldsymbol{\varepsilon}^i \quad \rightarrow \text{constitutive box} \rightarrow \quad \boldsymbol{\sigma}^i \qquad i = \gamma', \gamma_1, \gamma_2, \gamma_3, \mathrm{I}^{\mathrm{p}}_1, \mathrm{I}^{\mathrm{m}}_1, \mathrm{I}^{\mathrm{p}}_2, \mathrm{I}^{\mathrm{m}}_2, \mathrm{I}^{\mathrm{p}}_3, \mathrm{I}^{\mathrm{m}}_3 \tag{2}$$

The constitutive model on the micro level, for each phase, is based on a crystal plasticity theory and will be described in the next section.
Both stress and deformation are assumed to be uniform inside each of the different regions. To specify the coupling between the regions an interaction law has to be defined. For the present model a modified Sachs approach is used, which means that 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

$$\boldsymbol{\sigma}^{\gamma'} = \boldsymbol{\sigma}^{\gamma_1} = \boldsymbol{\sigma}^{\gamma_2} = \boldsymbol{\sigma}^{\gamma_3} = \overline{\boldsymbol{\sigma}} \tag{3}$$

- Modified Sachs interaction for the bi-crystal interfaces

$$f^{\mathrm{I}^{\mathrm{p}}_k} \boldsymbol{\sigma}^{\mathrm{I}^{\mathrm{p}}_k} + f^{\mathrm{I}^{\mathrm{m}}_k} \boldsymbol{\sigma}^{\mathrm{I}^{\mathrm{m}}_k} = \left(f^{\mathrm{I}^{\mathrm{p}}_k} + f^{\mathrm{I}^{\mathrm{m}}_k} \right) \overline{\boldsymbol{\sigma}} \qquad k = 1,2,3 \tag{4}$$

where $\boldsymbol{\sigma}^{\mathrm{i}}$ are the stress tensors in the different regions, $\overline{\boldsymbol{\sigma}}$ is the mesoscopic stress tensor and f^i are the volume fractions of the respective regions.

In the interface regions additional requirements are set. Both stress continuity (across the interface) and kinematical compatibility (in the plane of the interface) are required, resulting in the following equations:
- Compatibility between the matrix $(\mathrm{I}^{\mathrm{m}}_k)$ and the precipitate side $(\mathrm{I}^{\mathrm{p}}_k)$ of the k^{th} interface:

$$\boldsymbol{\varepsilon}^{\mathrm{I}^{\mathrm{p}}_k} \cdot \left(\mathbf{I} - \vec{n}^k \vec{n}^k \right) = \boldsymbol{\varepsilon}^{\mathrm{I}^{\mathrm{m}}_k} \cdot \left(\mathbf{I} - \vec{n}^k \vec{n}^k \right) \qquad k = 1,2,3 \tag{5}$$

- Stress continuity at the same interface:

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

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are the stress and strain tensors in the different regions and $\vec{n}^k$ is the unit normal vector on the k^{th} interface.

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. Equations (1) and (3) to (6) yield a total of 60 equations and the constitutive model (2) another 60 equations, which completes the system of equations.

Constitutive models

A crystal plasticity approach is used to model the constitutive behavior of the two phases. The elastic material behavior is described by a standard formulation for orthotropic materials with cubic symmetry. The three independent components of the elastic tensor $^4\mathbf{C}$ of both phases in CMSX-4 at 850 ^{o}C are given in Table 1 [24].

Table 1 $^4\mathbf{C}$ elastic tensor components for CMSX-4 at 850 ^{o}C [24].

	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

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 used:

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

where τ^{or} denotes the Orowan stress, s^α the actual slip resistance and τ^α_{eff} the effective stress on slip system α, defined as the combination of the resolved shear stress and the misfit stress.

$$\tau^\alpha_{eff} = \tau^\alpha + \tau^\alpha_{misfit} \qquad (8)$$

Recalling that the elastic properties of γ and γ' are very similar and assuming that the size of both phases is in the same order, it is assumed that the misfit is accommodated equally by both phases, leading to a misfit strain

$$\varepsilon_{misfit} = \frac{\frac{1}{2}\left(a_{\gamma'} - a_\gamma\right)}{a_\gamma} \qquad (9)$$

in the matrix (in the two directions in the plane of the interface) and the same strain with opposite sign in the precipitate. The lattice parameters $a_{\gamma'}$ and a_γ refer to the γ' and γ-phases respectively. The misfit stress and strain tensor are related to each other by a modified elastic stiffness tensor, which ensures that only the stress components parallel to the interface are non-zero.

The resolved shear stress τ^α is obtained from the Cauchy stress tensor $\boldsymbol{\sigma}$ by

$$\tau^{\alpha} = \boldsymbol{\sigma} : \mathbf{P}^{\alpha} \tag{10}$$

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

$$\mathbf{P}^{\alpha} = \tfrac{1}{2}\left(\vec{s}^{\alpha}\vec{n}^{\alpha} + \vec{n}^{\alpha}\vec{s}^{\alpha}\right) \tag{11}$$

The unit length vectors $\vec{n}^{\alpha}$ and $\vec{s}^{\alpha}$ are the slip plane normal and slip direction respectively. The (projected) misfit stress is obtained from the corresponding stress tensor in the same way.

The Orowan stress, which is the stress required to bow a dislocation line into the channel between two precipitates, is given by [25] as

$$\tau^{or} = \frac{\mu b}{2\pi d}\ln\left(\frac{d}{r_0}\right) = \alpha\frac{\mu b}{d} \tag{12}$$

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 α. A value of $\alpha = 0.80$ is taken here.

The slip resistance is related to the availability of mobile dislocations and the resistance of sessile / forest dislocations and therefore depends on the total dislocation density. The relation between the slip resistance and the dislocation density is defined according to

$$s^{\alpha} = c\mu b\sqrt{\left|\rho^{\alpha}\right|}\exp\left[\frac{Q}{kT}\right] \tag{13}$$

where ρ^{α} is the dislocation density on slip system α, c is a material constant, Q is an activation energy for overcoming the barriers, k is the Stefan-Boltzmann constant and T the absolute temperature.
The dislocation densities are calculated on the basis of an appropriate evolution equation [26], starting from their initial value ρ_0 :

$$\dot{\rho}^{\alpha} = \frac{1}{b}\left(\frac{1}{L^{\alpha}} - 2y_c\rho^{\alpha}\right)\left|\dot{\gamma}^{\alpha}\right| \quad , \quad \rho^{\alpha}\left(t=0\right) = \rho_0 \tag{14}$$

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

$$L^{\alpha} = \frac{K}{\sqrt{\left|\rho^{\alpha}\right|}} \tag{15}$$

where K is a material constant.

Precipitate constitutive model

In the present model, the precipitate in the superalloy is assumed to be elastic. 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 ^{o}C and moderate stress levels the simplification of an elastically deforming precipitate is justified. The development of an enhanced constitutive model that includes crystal plasticity in the precipitate for more extreme conditions, is subject of future work.

Application

The framework described in the previous sections was implemented, as a material subroutine, in the commercial finite element code MSC.Marc. The subroutine is called for every material point and a fully explicit time-integration is performed. An implicit method would be unconditionally stable, but would also require a significantly larger implementation effort. Therefore an explicit method was selected and limiting the time step yields accurate results within acceptable computation times. The local variables like dislocation densities and plastic strains in the individual regions are stored in state variables and updated at the end of each increment. The integration of the multi-scale model with an FE code in this way enables application of the material model to any structural component for which a FE model is available.

The model has been applied to simulate the mechanical response of the single crystal Ni-based superalloy CMSX-4, for which the model parameters are given in Table 2. In the remainder of this section, first the characteristics of the proposed slip law are demonstrated and then the influence of a change in the microstructural dimensions is shown.

Table 2 Model parameters for the matrix phase of CMSX-4.

Model parameter	Symbol	Value	Unit	Used in equation
Reference slip rate	$\dot{\gamma}_0$	1.4×10^{-4}	s^{-1}	(7)
Rate sensitivity Orowan threshold	n	3		(7)
Rate sensitivity exponent slip resistance	m	7		(7)
Lattice constant matrix	a_γ	0.3590	nm	(9)
Lattice constant precipitate	$a_{\gamma'}$	0.3586	nm	(9)
Boltzmann's constant	k	1.38×10^{-23}	$J\,K^{-1}$	(13)
Reference activation energy	Q	0.0	J	(13)
Strength parameter	c	0.426		(13)
Shear modulus	μ	100.2	GPa	(13)
Burgers vector length	b	0.25	nm	(12),(13),(14)
Parameter in Orowan stress	α	0.50		(12)
Critical annihilation length	y_c	2.31	nm	(14)
Initial SSD density	ρ_0	8.1×10^{14}	m^{-2}	(14)
Material constant	K	10		(15)

Slip law features

The slip law for the matrix material, equation (7), reflects that for each slip system two thresholds must be overcome before plastic slip can occur, associated with the slip resistance

and the Orowan stress. Plastic slip will only occur when both thresholds are exceeded by the effective resolved shear stress.

The slip rate as a function of the effective resolved shear stress was calculated for two cases to demonstrate the slip law characteristics. The results are shown in Figure 3 for the Orowan stress below (τ^{or} = 147 MPa) and above (τ^{or} = 368 MPa) the initial slip resistance (s^{α} = 305 MPa). The plots show that the slip rate in both cases reaches the reference slip rate $\dot{\gamma}_0$ when the resolved shear stress exceeds both thresholds.

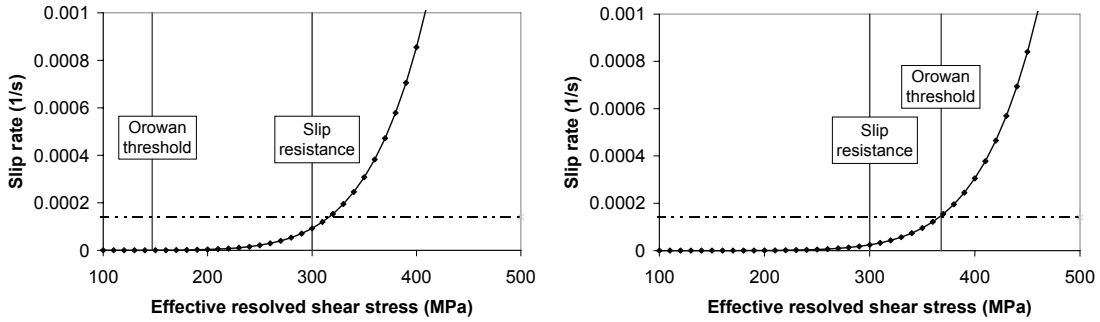

Figure 3 Activation of the proposed slip law for different values of the Orowan threshold.

Effect of microstructural changes

Nickel-based 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, since the Orowan threshold, which is inversely proportional to the γ-channel width h, is incorporated in the model. Before analysing the effects of microstructural changes, a reference case was studied by simulating a tensile test at 850 ^{o}C at a strain rate of 10^{-3} s^{-1}. The microstructural dimensions used are L = 500 nm and h = 60 nm. The result is shown in Figure 4, together with an experimentally determined stress-strain curve for CMSX-4 at the same conditions [24].

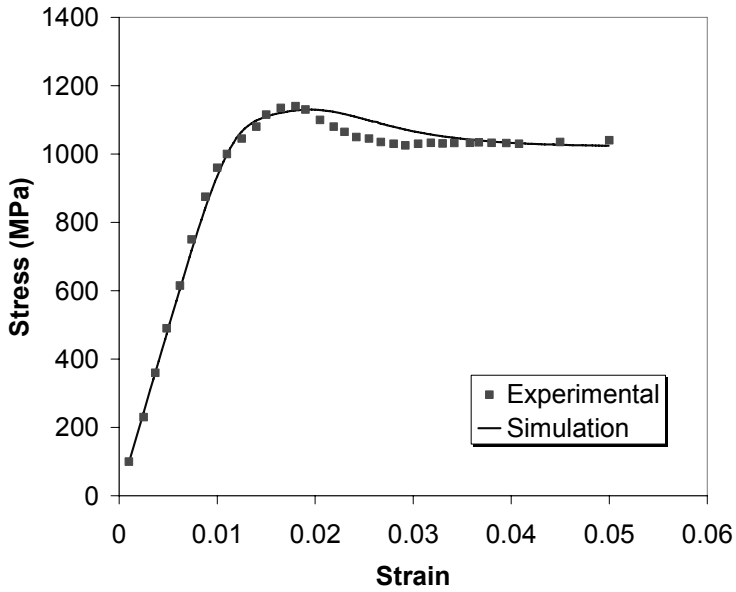

Figure 4 Simulated stress-strain curve for CMSX-4 at 850 ^{o}C at a strain rate of 10^{-3} s^{-1} compared to an experimentally determined curve.

The model parameters from Table 2 lead to an initial slip resistance (s^{α} = 305 MPa) which is considerably higher than the Orowan stress (τ^{or} = 147 MPa). This means that the slip resistance 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, which means that it approaches or even supersedes the slip resistance and becomes an active threshold. The unit cell dimensions were varied to quantify this size effect. Figure 5 shows the stress-strain curves for the reference case and for three other cases with all unit cell dimensions multiplied by a factor 0.5, 0.75 and 2. This figure shows that the shape of the curves for the different unit cell sizes remains the same, but the maximum stress shifts to a higher level with a decreasing matrix channel width, i.e. smaller is stronger.

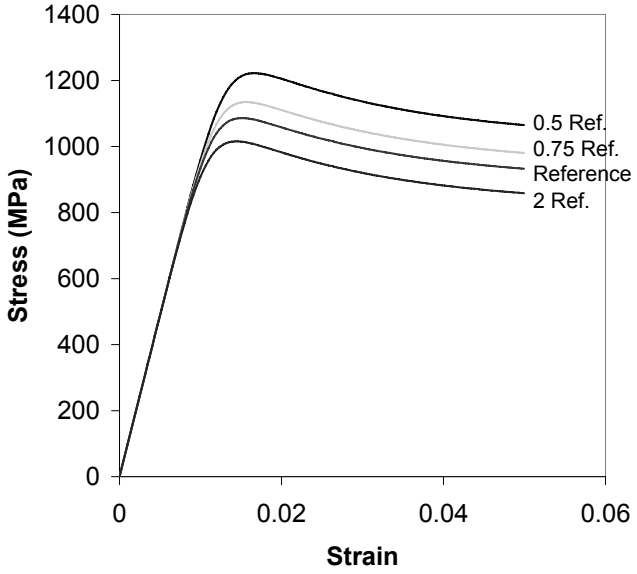

Figure 5 Effect of changing microstructural dimensions on the stress-strain curve. The reference case is L = 500 nm and h = 60 nm.

Conclusions

A physically motivated crystal plasticity framework is presented to describe the mechanical behaviour of the nickel-based superalloys. The framework has the following characteristics:

- The material response is predicted accurately by using a crystal plasticity model for the matrix material. A threshold term related to the Orowan stress is included, as well as the effect of lattice misfit between the two phases.
- The limited size of the unit cell and the micromechanical simplifications 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.
- Special interface regions have been included in the unit cell, since the role of the γ/γ'-interfaces is believed to play an important role in the material deformation behaviour. In the interface regions internal stresses will develop as a result of the lattice misfit between the two phases. Also conditions requiring stress continuity and strain compatibility across the γ/γ'-interfaces have been specified in these regions.

The model was implemented in the commercial FE code MSC.Marc and was applied to the Ni-based superalloy CMSX-4. It was shown to be capable of accurately describing the material stress-strain curve and the influence of changing microstructural dimensions was demonstrated. Therefore, it can be concluded that the present framework is able to accurately describe the material response, while being computationally much more efficient than complex FE unit cell models.

Acknowledgements

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