

COMPUTATIONAL MODELLING OF ANISOTROPIC MATERIALS UNDER CREEP CONDITIONS

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ABSTRACT. The modelling of the creep behaviour of single crystal superalloys is based on a non-linear rheological model, which describes the essential character of the uniaxial behaviour under different loadings, such as monotonous and cyclic creep (including damage) and LCF. A tensorial generalization of the governing differential equations, for uniaxial loading is derived by a projection method, which gives a general three-dimensional model obeying the crystal symmetries. A calibration of the material parameters for the single crystal superalloy CMSX-6 in the high temperature regime enables the model to describe the primary and secondary creep behaviour for tensile creep tests in different orientations.

Keywords : creep, anisotropic, superalloy, single crystal

1. INTRODUCTION

Experiments show that the three-dimensional inelastic behaviour of crystalline materials can be much more affected by the material anisotropy than the elastic properties [1]-[9]. The times to rupture under monotonous creep conditions can differ from one orientation to another by an order of two decimals. Therefore, any three-dimensional modelling must necessarily take into account the strong anisotropy of the behaviour.

Many authors model the anisotropic behaviour of single crystals by means of slip system theory [10]-[15]. They select classes of slip systems and formulate one-dimensional creep equations or, more generally, viscoplastic models for the relation between slip rate and resolved shear stress. The slip systems are then superposed. The advantage is that the one-dimensional (uniaxial) equations are much less complicated than three-dimensional ones, and the assemblage of all slip systems assures a three-dimensional law that automatically considers the symmetry of the crystal. The validity of this approach, however, is rather limited. Interactions between the different slip systems, although quite important, enter solely by the work-hardening law, namely by cross hardening parameters. In certain temperature regimes the creep behaviour is dominated by diffusional creep or phase transitions, which has little to do with slip system mechanisms. For this reason, slip system approaches turn out to be less adequate for creep modelling within these regimes [16]-[18].

The other approach, which is favoured in the present paper, makes use of representations by tensor functions, which are well known from linear algebra [19]-[23]. Our aim is the development of a three-dimensional constitutive model, that is calibrated solely by creep tests up to now, but is also applicable to other load conditions. The starting point is a

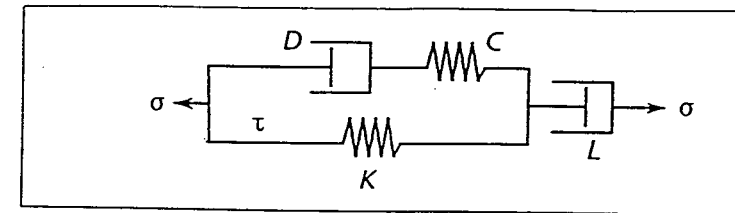


FIGURE 1. Rheological Creep Model

uniaxial model that has been successfully used to describe the creep behaviour of single crystal superalloys with $\langle 001 \rangle$ orientation [24], [25]. Its differential equation is derived from a four-parameter rheological model with two springs and two dampers. The non-linearity of the behaviour enters the constitutive equations by the assumption that the viscosities of the model depend on the applied stress.

The uniaxial model, however, has been successfully modified by a Kachanov-type damage parameter, which also describes tertiary creep till rupture [24],[26],[27]. Damage processes in three-dimensions, however, are rather complicated and not yet fully understood. Therefore, we will limit our considerations to the primary and secondary creep, excluding the tertiary creep phase. The uniaxial law has been generalized into three dimensions by an algebraic projection method, which has been especially developed for this purpose [28],[29]. The result is a set of first order tensorial differential equations, or evolution functions, which have been implemented into a finite element code for the computation of inhomogeneous processes such as torsion. The difficulty of this approach lies mainly in the task of giving the resulting constants and variables a physical interpretation. In some cases these can only be given in a rather implicit or complex way, which complicates the identification of the constants by experimental data.

For the identification procedure of the material constants, a least square fit of the calculated values to the measured ones has been performed. Mathematically, this leads to a problem of nonlinear optimization which has been solved by four different algorithms. The identification has been conducted by tensile creep tests at different loads and in different orientations for the single crystal superalloy CMSX-6 at 760°C. The results show the ability of the model to describe both the strong non-linearity of the creep with respect to the applied load, and the influence of the orientation. A calibration of this model for the superalloy SRR99 has been also made [30].

2. ONE-DIMENSIONAL MATERIAL MODEL

The starting point of our constitutive modelling is the rheological four-parameter BURGERS model (Fig. 1) which consists of two springs with elasticities C and K and two dampers with viscosities L and D (see [31]-[33]). All of these constants are assumed positive. The differential equations of the model are

$$\begin{aligned}\dot{\sigma} &= (C + K)\dot{\epsilon} - (C/L + C/D + K/L)\sigma + C/D\tau \\ \dot{\tau} &= K(\dot{\epsilon} - \dot{\sigma}/L)\end{aligned}\quad (1)$$

where σ denotes the stress, ϵ the strain, and τ an internal variable which corresponds to the stress in the spring K . The strong non-linearity of the creep behaviour is described by

the stress dependence of the viscosities

$$\begin{aligned} D &= D_0 \exp(-B|\sigma|) \\ L &= L_0 \exp(-B|\sigma|) \end{aligned} \quad (2)$$

with the material constants D_0 , L_0 , and B . If all of them are positive, higher stresses lead to lower viscosities and, hence, to higher creep rates. Note, that the viscosities remain constant during monotonous creep.

This one-dimensional model contains the five temperature-dependent parameters C , K , D_0 , L_0 , and B . It has been enlarged by a Kachanov-type damage variable and calibrated to monotonous and cyclic creep tests of the single crystals SRR99 and CMSX-6 in $\langle 001 \rangle$ near orientations. Experimental results and model calculations are presented in [24]- [27].

3. THREE-DIMENSIONAL GENERALIZATION

In the following section we derive a complete anisotropic generalization of the uniaxial model to three dimensions for cubic-face-centered crystals. We start again from the elementary laws of the springs and of the dashpots. The tensorial form of a linear elastic law can be represented by

$$\mathbf{S} = \mathbf{C}[\mathbf{E}] \text{ or } \sigma_{ij} = \sum_{kl} C_{ijkl} \epsilon_{kl} \quad (3)$$

with \mathbf{S} : stress tensor, \mathbf{E} : (infinitesimal) deformation tensor, \mathbf{C} : fourth rank elasticity tensor with cubic symmetry. With respect to a crystal base $\{ \mathbf{e}_i \}$ the cubic law can be brought into the following matricial form:

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = \frac{1}{3} C_1 \mathbf{e} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + C_2 \begin{bmatrix} \epsilon_{11-e} & 0 & 0 \\ 0 & \epsilon_{11-e} & 0 \\ 0 & 0 & \epsilon_{11-e} \end{bmatrix} + C_3 \begin{bmatrix} 0 & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & 0 & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & 0 \end{bmatrix} \quad (4)$$

$$[\mathbf{S}] = C_1[\mathbf{E}_1] + C_2[\mathbf{E}_2] + C_3[\mathbf{E}_3]$$

with $e := \text{tr}(\mathbf{E})$, the trace of the deformation tensor, and $C_{1,2,3}$ the elasticity constants. In this equation the strain tensor has been decomposed into (1) a spherical part $\mathbf{E}_1 := 1/3 \text{tr}(\mathbf{E})\mathbf{I}$; (2) a traceless diagonal part \mathbf{E}_2 ; (3) a diagonal-free part \mathbf{E}_3 . This can be formalized by three fourth-rank projection tensors

$$\begin{aligned} \mathbf{P}_1 &:= 1/3 \left(\sum_{i=1}^3 \mathbf{e}_i \otimes \mathbf{e}_i \right) \otimes \left(\sum_{j=1}^3 \mathbf{e}_j \otimes \mathbf{e}_j \right) \\ \mathbf{P}_2 &:= \left(\sum_{i=1}^3 \mathbf{e}_i \otimes \mathbf{e}_i \otimes \mathbf{e}_i \otimes \mathbf{e}_i \right) - \mathbf{P}_1 \\ \mathbf{P}_3 &:= \left(\sum_{i,j=1}^3 \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_i \otimes \mathbf{e}_j \right) - \mathbf{P}_1 - \mathbf{P}_2 \end{aligned} \quad (5)$$

such that

$$\mathbf{P}_i[\mathbf{E}] = \mathbf{E}_i \quad (6)$$

holds for $i = 1, 2, 3$. Here \otimes denotes the tensor product. The projection tensors depend only on the lattice directions indicated by the lattice base $\{ \mathbf{e}_i \}$. The compositions of the projections obey the following properties:

$$\mathbf{P}_i \mathbf{P}_j = \delta_{ij} \mathbf{P}_i \quad (7)$$

with Kronecker symbol δ_{ij} , i.e. they project into orthogonal subspaces of the 6-dimensional strain-space. The completeness of this set is demonstrated by the representation of the fourth-rank identity as the sum of these projections

$$\mathbf{I} = \mathbf{P}_1 + \mathbf{P}_2 + \mathbf{P}_3. \quad (8)$$

Now we can represent the f.c.c. elasticity tensor as a linear combination of the projections

$$\mathbf{C} = C_1 \mathbf{P}_1 + C_2 \mathbf{P}_2 + C_3 \mathbf{P}_3. \quad (9)$$

By assuming that the elementary constitutive laws of the springs and the dampers are f.c.c. with respect to the same lattice vectors, they have the same representations as linear combinations of the projection tensors, each of them determined by three real constants

$$\begin{aligned} \{K_1, K_2, K_3\} &\text{ for } \mathbf{K} = \sum_{i=1}^3 K_i \mathbf{P}_i \\ \{C_1, C_2, C_3\} &\text{ for } \mathbf{C} = \sum_{i=1}^3 C_i \mathbf{P}_i \\ \{D_1, D_2, D_3\} &\text{ for } \mathbf{D} = \sum_{i=1}^3 D_i \mathbf{P}_i \\ \{L_1, L_2, L_3\} &\text{ for } \mathbf{L} = \sum_{i=1}^3 L_i \mathbf{P}_i. \end{aligned} \quad (10)$$

The algebraic meaning of the three constants is that of (multiple) eigenvalues of the stiffness- or viscosity tensors. The eigenspaces are completely given by the lattice directions and do not depend on the material constants.

This fact is only assured in the case of isotropic and cubic materials. For other crystal classes the eigenspaces of the material fourth-rank tensors depend on the material constants and, thus, are not automatically equal for all elements of the rheological model.

In the present case the constitutive laws for the four elements of the rheological model are

$$\begin{aligned} \mathbf{S}_K &= \mathbf{K}[\mathbf{E}_K] = \sum_{i=1}^3 K_i \mathbf{P}_i[\mathbf{E}_K] = \sum_{i=1}^3 K_i \mathbf{E}_{K_i} \\ \mathbf{S}_C &= \mathbf{C}[\mathbf{E}_C] = \sum_{i=1}^3 C_i \mathbf{P}_i[\mathbf{E}_C] = \sum_{i=1}^3 C_i \mathbf{E}_{C_i} \\ \mathbf{S}_D &= \mathbf{D}[\mathbf{E}_D^*] = \sum_{i=1}^3 D_i \mathbf{P}_i[\mathbf{E}_D^*] = \sum_{i=1}^3 D_i \mathbf{E}_{D_i}^* \\ \mathbf{S}_L &= \mathbf{L}[\mathbf{E}_L^*] = \sum_{i=1}^3 L_i \mathbf{P}_i[\mathbf{E}_L^*] = \sum_{i=1}^3 L_i \mathbf{E}_{L_i}^* \end{aligned} \quad (11)$$

where $\mathbf{S}_{K,C,D,L}$ and $\mathbf{E}_{K,C,D,L}$ are the stresses and strains in the corresponding elements, respectively. If we apply a projector \mathbf{P}_j to these equations, we obtain the subspace formu-

lations

$$\begin{aligned} S_{K_j} &= K_j E_{K_j} \\ S_{C_j} &= C_j E_{C_j} \\ S_{D_j} &= D_j E_{D_j}^* \\ S_{L_j} &= L_j E_{L_j}^* \end{aligned} \quad (12)$$

The advantage of the projections is that we can reduce the algebraic operations of tensors to those of reals. For example, the sum of the two elasticity tensors can be evaluated as

$$K + C = \sum_{i=1}^3 (K_i + C_i) P_i \quad (13)$$

and the inverse of a viscosity tensor is

$$D^{-1} = \sum_{i=1}^3 (1/D_i) P_i \quad (14)$$

If these material tensors obey the usual symmetries, these are preserved under all algebraic operations between them because of their coaxiality. For example, they commute under composition

$$CD^{-1} = D^{-1}C = \sum_{i=1}^3 (C_i/D_i) P_i \quad (15)$$

These properties will be used for establishing the differential equations for the model in tensorial forms.

The kinematical conditions of the model are

$$E = E_K + E_L = E_C + E_D + E_L \quad (16)$$

whereas the equilibrium holds if

$$S = S_L = S_K + S_C = S_K + S_D \quad (17)$$

We introduce the tensor of the internal variable with dimension stress as before by

$$T := S_K \quad (18)$$

If we again apply the projection to these equations, we can work in the corresponding subspaces. As a result we obtain the differential equations

$$\begin{aligned} S_j^* &= (C_j + K_j) E_j^* - (C_j/D_j + C_j/L_j + K_j/L_j) S_j + C_j/D_j T_j \\ T_j^* &= C_j/(C_j + K_j) \{ E_j^* + (C_j/D_j + C_j/L_j + K_j/L_j) S_j \} \end{aligned} \quad (19)$$

If we superpose these equations by summation over j , we obtain the tensorial differential equations

$$\begin{aligned} S^* &= A_1 [E^*] + A_2 [S] + A_3 [T] \\ T^* &= A_4 [E^*] + A_5 [S] \end{aligned} \quad (20)$$

with the material fourth rank tensors A_i with cubic symmetry expressed as linear-combinations of the three structural tensors P_i

$$\begin{aligned} A_1 &= \sum_{j=1}^3 (C_j + K_j) P_j \\ A_2 &= \sum_{j=1}^3 -(C_j/D_j + C_j/L_j + K_j/L_j) P_j \\ A_3 &= \sum_{j=1}^3 (C_j/D_j) P_j \\ A_4 &= \sum_{j=1}^3 C_j/(C_j + K_j) P_j \\ A_5 &= \sum_{j=1}^3 C_j/(C_j + K_j) (C_j/D_j + C_j/L_j + K_j/L_j) P_j \end{aligned} \quad (21)$$

These equations present the complete generalization of eqns. (1) and (2). In this incremental form they can easily be implemented into a finite element program with user supplied material module.

Therefore, the advantage of this projection technique is that, within the subspaces, the tensorial equations can be handled as easily as real equations. We demonstrated this method for the rather simple, but non-trivial example of a four-parameter rheological model. However, it can be applied in the same way to any other (linear) rheological model or to evolution functions in form of linear differential equations. The resulting equations automatically fulfill the cubic symmetry and can be considered as complete generalizations of the one dimensional differential equations.

The task of generalizing from one to three dimensions, however, becomes non-unique and therefore much more complicated in the case of non-linear relations. Such a problem will be considered in the next section.

4. STRESS INTENSITIES

The non-linearity of our material model enters into the equations by the stress dependence of the viscosities. Under monotonous creep conditions, however, the stresses are constant and so are the viscosities. For any other load conditions the stresses will not be constant, nor are the viscosity tensors.

In the one-dimensional case the only natural stress intensity is the absolute value of the uniaxial stress. In three dimensions infinitely many equivalent stresses can be defined. The v. Mises equivalent stress is just one special choice, which is isotropic. In our case an isotropic invariant will not be sufficient, as an appropriate stress intensity should reflect the anisotropy of the material. A more general intensity can be introduced by means of

the cubic invariants which are listed below [34]

$$\begin{aligned}
J_1 &= \text{tr}(\mathbf{S}) \\
J_2 &= \sqrt{[\text{tr}^2(\mathbf{S}) + \text{tr}(\mathbf{S}^2)]} \\
J_3 &= \det(\mathbf{S}) \\
J_4 &= \sigma_{12}^2 + \sigma_{23}^2 + \sigma_{31}^2 \\
J_5 &= \sigma_{12}\sigma_{23}\sigma_{31} \\
J_6 &= (\sigma_{11} + \sigma_{22})\sigma_{12}^2 + (\sigma_{22} + \sigma_{33})\sigma_{23}^2 + (\sigma_{33} + \sigma_{11})\sigma_{31}^2 \\
J_7 &= \sigma_{12}^2\sigma_{23}^2 + \sigma_{23}^2\sigma_{31}^2 + \sigma_{31}^2\sigma_{12}^2 \\
J_8 &= \sigma_{11}\sigma_{12}^2\sigma_{31}^2 + \sigma_{22}\sigma_{23}^2\sigma_{12}^2 + \sigma_{33}\sigma_{31}^2\sigma_{23}^2 \\
J_9 &= \sigma_{11}\sigma_{22}\sigma_{12}^2 + \sigma_{22}\sigma_{33}\sigma_{23}^2 + \sigma_{33}\sigma_{11}\sigma_{31}^2.
\end{aligned} \tag{22}$$

The first three invariants are the isotropic ones, namely the pressure, the v. Mises stress, and the determinant. The remaining six invariants are anisotropic, as the formulas in this form hold only with respect to a lattice basis. This is a complete integrity base of this symmetry class, which means that any functional of the stress tensor which obeys the cubic symmetry can be expressed as a function of J_1, \dots, J_9 , and vice versa. In particular, any linear combination of these invariants can be used for our purpose to form a stress intensity. By testing different selections of these invariants, it turned out that the following ansatz-function up to third order invariants suffices to describe the non-linearity of the viscosities in the present model:

$$\begin{aligned}
D_j &= D_{0j} \exp(B_{j1}J_2 + B_{j2}J_4 + B_{j3}J_5 + B_{j4}J_6) \\
L_j &= L_{0j} \exp(B_{j1}J_2 + B_{j2}J_4 + B_{j3}J_5 + B_{j4}J_6)
\end{aligned} \tag{23}$$

with the material constants $B_{ji}, j = 1, 2, 3; i = 1, 2, 3, 4$, all of the assumed positive.

If we assume that creep deformations, or, more general, all inelastic deformations are volume preserving, then we can set

$$D_1^{-1} = L_1^{-1} = 0 = B_{1i}, i = 1, \dots, 4. \tag{24}$$

The identification of these constants B_{ji} is quite difficult, because they do not have a distinguished physical interpretation, nor can they be uncoupled under special conditions.

5. APPLICATION OF THE MODEL FOR CREEP MODELLING

One of the main difficulties of the present investigation results from limitation of appropriate experimental data for the identification. Production of specimens with prescribed orientations and experiments at high temperatures are complicated and costly. Moreover, the scatter of these tests is rather large. Therefore, any identification of the model has to be roughly average over these data. The calibration of the model has been made to the nickel-base single crystal superalloy CMSX-6 with standard two-stage heat-treatment. The used monotonous tensile creep test at three load levels in various orientations at 760°C have been performed by MTU (Munich) and Siemens KWU (Mülheim).

The identification has been made as follows. The experimental data have been reduced to the primary and secondary creep phase, which ends in a range of 2 to 5% creep strain depending on the specific experiment. The goal is to find material constants such that the creep curves calculated by the model fit to the measured experimental creep curves. This creates a problem of nonlinear optimization. The following methods have been applied: (1) a simplex-method, (2) an evolution strategy, (3) a gradient-method with parabolic line

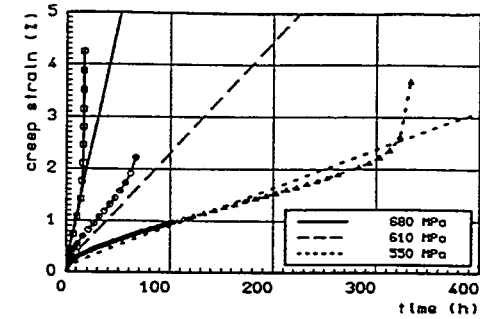


FIGURE 2. Monotonous Creep Tests ($\varphi_1 = 4^\circ, \varphi_2 = 43^\circ$)

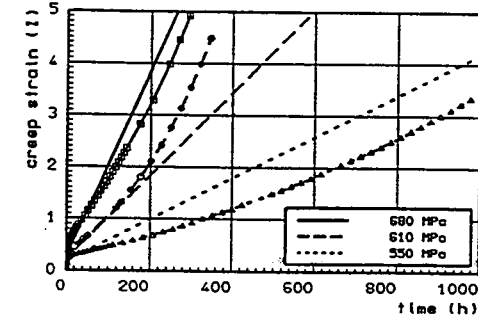


FIGURE 3. Monotonous Creep Tests ($\varphi_1 = 0^\circ, \varphi_2 = 2^\circ$)

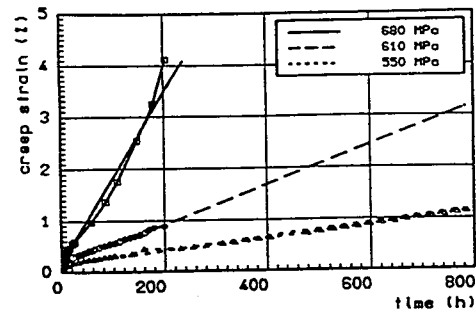
search, and (4) the Levenberg-Marquardt algorithm. Each of these has its advantages and shortcomings, so that no general preferences can be made so far.

With these constants the creep curves (without symbols) of Figs. 2, 3 and 4 have been calculated by the model and can be compared with the measured curves (with symbols at measuring-points). In all cases the deviation of calculated and measured data lies within the scatter band of such tests. φ_i are the Eulerian angles describing the orientation of the crystal with respect to the specimen. As all specimens exhibit rotational symmetry, the third Eulerian angle is unimportant. Orientations near $\langle 001 \rangle$ have a small Eulerian angle φ_2 . In that part of the orientation triangle the Eulerian angle φ_1 becomes less important than for the other orientations. The model has been implemented into a finite element code and can be used to predict the creep behaviour of structural elements such as bars, torsional shafts or turbine blades. The material model is general enough to give results for arbitrary deformation or stress processes. The reliability of such predictions, however, depends on the variety of experimental data available for the calibration of the material constants of the model. The presented model has to be considered as a first step towards a three-dimensional description of the general material behaviour, whose capabilities are still far from having been exhausted.

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FIGURE 4. Monotonous Creep Tests ($\varphi_1 = 43^\circ$, $\varphi_2 = 25^\circ$)

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