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Anisotropic continuum damage modeling for single crystals at high temperatures

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Abstract

In single crystals, the process of creep damage is generally anisotropic. Indeed, the damage evolution does not only depend on the loading conditions, but also on the lattice orientation. And the current state of damage has an anisotropic influence on the effective stress state, so that it is represented by a tensorial damage variable. Based on the continuum damage mechanics theory, a creep damage model for F.C.C. single crystals has been developed and implemented in a three-dimensional anisotropic creep model. It is shown that the resulting material model is capable of describing the orientation dependence of the creep and damage evolution of nickel-based superalloys in the high temperature regime. © 1999 Published by Elsevier Science Ltd. All rights reserved.

1. Introduction

It is well-known that the creep process of metals is accompanied by the nucleation, growth and coalescence of microcracks. In particular during the tertiary creep phase, this is the dominant mechanism, which causes the formation and coalescence of microcracks and finally leads to rupture. As a phenomenological approach to tertiary creep under uniaxial tensile loads, Kachanov (1958) and Rabotnov (1968) introduced a scalar damage parameter D to represent the loss of a load-carrying cross-section due to damage (see also Kachanov, 1986). In order to represent the

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effect of material damage (microcracks and microvoids) on the mechanical behavior of materials, it is convenient to define an *effective stress* $\tilde{\sigma}$ related to the surface that effectively resists the load, namely

$$\tilde{\sigma} = \frac{\sigma}{1 - D}, \tag{1}$$

where σ denotes the applied stress. By replacing the applied stress by the effective stress, the classical Norton's power law for steady creep stage can be extended to the tertiary creep stage:

$$\dot{\varepsilon}^c = A\sigma^n = A\frac{\sigma}{(1 - D)}^{n}, \tag{2}$$

where A and n are material constants. The corresponding damage evolution law is given by

$$\dot{D} = B\frac{\sigma^p}{(1 - D)^q}, \tag{3}$$

with the damage related material constants B, p, and q. This idea has resulted in the development of continuum damage mechanics and has found wide application.

Nickel-based single crystal superalloys are of increasing importance, especially in the turbine industry. Viscoplastic damage approaches and life-time prediction under multidimensional loading conditions are of great interest. Mechanical properties of single crystal superalloys are strongly anisotropic and nonlinear at elevated temperatures. For the description of the primary and secondary creep phases of cubic single crystals, a phenomenological anisotropic creep-model has been suggested by Bertram and Olschewski (1996). It is based on the 4-parameter Burgers-model which nicely reproduces the primary and secondary creep behavior. The nonlinearity between creep strains and applied stresses is incorporated into this model by taking the viscoelastic parameters as functions of the stresses being constant for monotonic creep processes. The generalization from this uniaxial model to a fully three-dimensional one is done by means of a projection technique, which gives general representations of tensor-functions identically satisfying the anisotropy of a cubic crystal. The nonlinearity with respect to the stresses is implemented in terms of an irreducible integrity base for the crystal class.

However, like other classical continuum mechanics modeling, this approach is restricted to the undamaged material behavior and converges to the steady-state creep behavior. For higher creep strains, it has to be extended to include the tertiary creep, i.e. the material damage inducing degradation of mechanical properties must be considered. Lemaitre (1971, 1992) proposed the *strain equivalence principle* which allows a modification of constitutive equations of an undamaged material to describe a damaged material. This is an extension of the effective stress formulation of Kachanov–Rabotnov and is usually called *effective stress concept*. According to this concept, the constitutive equations of any damaged material can be obtained by replacing the Cauchy stress in the constitutive equations of the corresponding undamaged material with an adequately defined *effective stress*. The constitutive model for the damaged material is then completed by the additional damage laws which describe the evolution of material damage variables. Microscopic investigations (see Ai et al., 1990; Schneider, 1993; Rumi et al., 1994; Portella, 1992) show that growth and coalescence of initial microcracks from casting pores are the main sources for material degradation in both single and polycrystalline superalloys. On the other hand, based on the continuum damage theory and the results of microscopic investigations, a multiaxial phenomenological damage model for the description of the anisotropic damage evolution and for the prediction of the life-time of cubic single crystals has been developed by Qi and Bertram (1997) and Qi (1998). In this paper, the anisotropic damage model is connected with the anisotropic creep model. Theoretical prediction of the creep behavior and damage development and their comparison with the experimental results for the f.c.c. single crystal superalloy CMSX-6 at 760°C are presented and discussed.

2. Damage representation and effective stress

Damage of materials is caused by progressive irreversible changes in internal structure of materials as an irreversible thermodynamical process. According to the principles of irreversible thermodynamics, internal variables (damage variables) for the description of the material damage must be introduced. These damage variables serve as a macroscopic approximation in describing the underlying micromechanical processes of microdefects. The predictive capabilities of a damage model depend strongly on its particular choice of damage variables. The selection of the damage variables is one of the most important and most contentious aspects of damage mechanics. Though damage mechanics theory has been developed with much effort in the last three decades, the selection of a damage variable is still widely a matter of taste or convenience. A study focused on this problem can be found in the work of Ju (1990) and Krajcinovic and Mastilovic (1995).

It is widely recognized that the damage process in metals is generally anisotropic, even if the material is initially isotropic. Briottet et al. (1998) studied the influence of ellipsoidal cavities in a viscoplastic material under axisymmetric loading. They found out that when the voids are significantly prolate or oblate, a strong damage-induced morphological anisotropy is observed even for low volume fractions. Therefore, for single crystals both the initial material anisotropy and the induced anisotropy due to damage must be taken into account. Because of this anisotropic nature, the damage influence can not be represented by a scalar variable alone. Experience has shown that it is advantageous to consider the internal structure and its orientation as a single entity and to use tensorial state variables for the representation of this entity (Onat and Leckie, 1988). An appropriate description of anisotropic damage generally requires a tensorial variable of order two or even higher order (see Lehmann, 1991). The latter probably capture the effects of damage more exactly than the lower ones, but it will also take much more effort for the identification and consumes more computational time. The geometrical properties of a given state of microcracks may be described, in a continuum sense, by a second-order symmetric tensor (Murakami and Ohno, 1981; Chaboche, 1990). Though this representation can not describe damage anisotropy more than orthotropy, it has been widely used to represent anisotropic damage state, e.g. in the anisotropic damage model proposed by Chow and Wang (1987a,b and 1988a,b), which has been successfully employed to predict the forming limit diagrams of VDIF steels (Chow et al., 1996), and of aluminum alloy 6111-T4 (Chow et al., 1997). In the present model, such a tensor **D** is also chosen as an internal variable to describe the anisotropic damage state.

According to the effective stress concept, the effect of material damage on the deformation behavior can be represented by an amplification of the stress called effective stress. This effective stress depends upon the damage and the stress state, and may also depend upon the current state of the material anisotropy. There are plenty suggestions on the formulation of effective stress related to a second-order symmetric damage tensor in the literature, e.g. in the work of Murakami and Ohno (1981), Codebois and Sidoroff (1982), Chow and Wang (1987a,b), Chow and Lu (1989), Voyiadjis and Park (1997). Motivated by other branches of material modeling, the effective stress $\mathbf{T}_e$ in the present model is defined similarly to the second Piola–Kirchhoff stress tensor by

$$\mathbf{T}_e = (\mathbf{I} - \mathbf{D})^{-1/2}\mathbf{T}(\mathbf{I} - \mathbf{D})^{-1/2T}, \tag{4}$$

I being the identity tensor of rank two, and **T** the Cauchy stress. The superscript T indicates transposition. This formulation is identical to the one suggested by Codebois and Sidoroff (1982) and by Chow and Wang (1987a,b).

3. Active and passive damage effects

Damage effects characterized by microvoids and microcracks can be both activated or deactivated according to the loading conditions, i.e. the damage may still exist but eventually does not effect the stiffness of the material (and also the development of the damage). However, the effective stress defined in Eq. (4) does not reflect the deactivation of damage. Many attempts have been made to model the crack closing phenomenon. Motivated by the mode I microcrack opening and closing mechanism, a phenomenological algorithm for the representation of the active and passive effects of material damage has been developed by Ortiz (1985), Ju (1989), and Hansen and Schreyer (1995). This strain-based representation theory introduces an active damage tensor deactivating the damage effects when the material damage is passive. The effective stress tensor including damage deactivation can still be defined by Eq. (4), only the damage tensor **D** is replaced by the *active damage tensor*. In the present model, this representation is chosen to obtain physically more realistic approximate solutions. The definition of the active damage tensor based on the work of Hansen and Schreyer (1995) is summarized in the following.

The basic idea of this approach can be simply demonstrated by considering one-dimensional elasticity coupled with damage. Suppose an elastic isotropic material having initial elastic stiffness E_0 is loaded tensely until a damage state $D > 0$ is reached. At this moment, the microcracks are open, i.e. the damage is active. The effective stress is as defined by the Eq. (1). The current elastic stiffness of the damaged material is given as $E_+ = (1 - D)E_0$ and the stress–strain response is

$$\varepsilon = \frac{\sigma}{E_+} = \frac{\sigma}{(1 - D)E_0} = \frac{\tilde{\sigma}}{E_0}. \tag{5a}$$

Now let us reverse the load to a compressive state. Although the damage still exists, it becomes inactive and does not effect the elastic stiffness. The current value of the elastic stiffness equals the initial one. The material behaves as if it were undamaged and the stress–strain response is

$$\sigma = E_0\varepsilon. \tag{5b}$$

By introducing an active damage variable D_a defined as

$$D_a = h(\varepsilon)D, \tag{6}$$

where $h()$ is the Heaviside function which equals unity for positive arguments and zero otherwise, the effective stress defined by (1) can be redefined as

$$\tilde{\sigma} = \frac{\sigma}{1 - D_a}. \tag{7}$$

Then the stress–strain responses (5a) and (5b) for the damaged material with respect to active and passive damage can be written as

$$\varepsilon = \frac{\tilde{\sigma}}{E_0} = \frac{\sigma}{(1 - D_a)E_0}. \tag{8}$$

Following this idea, for multidimensional elasticity, the active damage tensor $\mathbf{D}_a$, i.e. the portion of the damage tensor, $\mathbf{D}$, which remains active under arbitrary loading, is determined by the tensile strain projection of the damage tensor. A fourth-order positive spectral projection operator proposed by Ju (1989) is constructed in a series of steps as presented below. First we note the spectral decomposition of the total strain tensor $\mathbf{E}$ as:

$$\mathbf{E} = \sum_{i=1}^{3} \varepsilon_i \mathbf{n}_i^\varepsilon \otimes \mathbf{n}_i^\varepsilon, \tag{9}$$

where ε_i and $\mathbf{n}_i^\varepsilon$ are the ith eigenvalue and the corresponding ith eigenvector of $\mathbf{E}$, respectively, and the symbol $\otimes$ denotes the tensor product. Next a positive spectral tensor defined as

$$\mathbf{H} = \sum_{i=1}^{3} h(\varepsilon_i)\mathbf{n}_i^\varepsilon \otimes \mathbf{n}_i^\varepsilon \tag{10}$$

is introduced. The positive spectral projection operator (fourth-order tensors) is then constructed as

$$\overset{\langle 4\rangle}{\mathbf{P}}_e = \mathbf{H} \wedge \mathbf{H}, \tag{11}$$

where the composition of two second-order tensors, denoted by the wedge $\wedge$, is defined by $\mathbf{A} \wedge \mathbf{B} = a_{ij}b_{kl}(\mathbf{e}_i \otimes \mathbf{e}_k \otimes \mathbf{e}_j \otimes \mathbf{e}_l)$ for an orthonormal basis $\{\mathbf{e}_i\}$. The positive projection of the strain tensor is then given by

$$\mathbf{E}^+ = \overset{\langle 4\rangle}{\mathbf{P}}_e : \mathbf{E}, \tag{12}$$

where the symbol : denotes the double contraction. If all eigenvalues of $\mathbf{E}$ are negative (compressive), then $\overset{\langle 4\rangle}{\mathbf{P}}_e$ is the null tensor and, conversely, if all eigenvalues of $\mathbf{E}$ are positive (tensile), then $\overset{\langle 4\rangle}{\mathbf{P}}_e$ corresponds to the fourth-order identity tensor. Thus, the active damage tensor can be defined as

$$\mathbf{D}_a = \overset{\langle 4\rangle}{\mathbf{P}}_e : \mathbf{D}. \tag{13}$$

If inelastic strain occurs, the determination of the active damage is more complicated. In one-dimensional cases, the active damage can be represented by

$$D_a = \{1 - [1 - h(\varepsilon^e)][1 - h(\varepsilon)]\}D, \tag{14}$$

where ε^e and ε are the elastic and the total strain, respectively. This form is the result of a study of active/passive damage conditions for combinations of the elastic and inelastic strain. For more details see Hansen and Schreyer (1995).

For multidimensional elasto-viscoplasticity coupled with damage, we first consider the spectral decomposition of the elastic strain tensor $\mathbf{E}^e$ and the total strain tensor $\mathbf{E}$

$$\mathbf{E}^e = \sum_{i=1}^{3} \varepsilon_i^e \mathbf{n}_{ei}^\varepsilon \otimes \mathbf{n}_{ei}^\varepsilon, \tag{15a}$$

$$\mathbf{E} = \sum_{i=1}^{3} \varepsilon_i \mathbf{n}_i^\varepsilon \otimes \mathbf{n}_i^\varepsilon, \tag{15b}$$

where ε_i^e and ε_i are the ith eigenvalues, $\mathbf{n}_{ei}^\varepsilon$ and $\mathbf{n}_i^\varepsilon$ are the corresponding ith eigenvectors of $\mathbf{E}^e$ and $\mathbf{E}$, respectively. Next let the corresponding positive (tensile) spectral tensors be defined as

$$\mathbf{H}_{\varepsilon_e} = \sum_{i=1}^{3} h(\varepsilon_i^e) \mathbf{n}_{ei}^\varepsilon \otimes \mathbf{n}_{ei}^\varepsilon, \tag{16a}$$

$$\mathbf{H}_\varepsilon = \sum_{i=1}^{3} h(\varepsilon_i) \mathbf{n}_i^\varepsilon \otimes \mathbf{n}_i^\varepsilon. \tag{16b}$$

The positive spectral projection operators (fourth-order tensors) for the elastic and the total strains are then defined as

$$\overset{\langle 4\rangle}{\mathbf{P}}_{\varepsilon_e} = \mathbf{H}_{\varepsilon_e} \wedge \mathbf{H}_{\varepsilon_e}, \tag{17a}$$

$$\overset{\langle 4\rangle}{\mathbf{P}}_{\varepsilon} = \mathbf{H}_{\varepsilon} \wedge \mathbf{H}_{\varepsilon}, \tag{17b}$$

respectively. The positive projection of the elastic and the total strain tensors are then given by

$$\mathbf{E}^{e+} = \overset{\langle 4\rangle}{\mathbf{P}}_{\varepsilon_e} : \mathbf{E}^e, \tag{18a}$$

$$\mathbf{E}^{+} = \overset{\langle 4\rangle}{\mathbf{P}}_{\varepsilon} : \mathbf{E}, \tag{18b}$$

respectively. A positive projection operator based on the total strain is defined as follows

$$\overset{\langle 4\rangle}{\mathbf{T}} = \overset{\langle 4\rangle}{\mathbf{I}} - \left(\overset{\langle 4\rangle}{\mathbf{I}} - \overset{\langle 4\rangle}{\mathbf{P}}_{\varepsilon_e}\right) : \left(\overset{\langle 4\rangle}{\mathbf{I}} - \overset{\langle 4\rangle}{\mathbf{P}}_{\varepsilon}\right), \tag{19}$$

where $\overset{\langle 4\rangle}{\mathbf{I}}$ denotes the identity tensor of four. The active damage tensor is then given by

$$\mathbf{D}_a = \overset{\langle 4\rangle}{\mathbf{T}} : \mathbf{D}. \tag{20}$$

Under consideration of the active and passive damage effects, definition (4) of the effective stress tensor becomes therefore

$$\mathbf{T}_e = (\mathbf{I} - \mathbf{D}_a)^{-1/2}\mathbf{T}(\mathbf{I} - \mathbf{D}_a)^{-1/2T}, \tag{21}$$

In the coupled damage elasto-viscoplasticity formulation discussed above, the deactivation of the damage causes a discontinuity in the stress–strain response, as the projection operators are based on the Heaviside function which has a jump at zero strain. A way to avoid the discontinuity is to replace the Heaviside function by a smooth function, such as the one suggested by Hansen and Schreyer (1995):

$$\bar{h}(x) = \begin{cases} 0 & \text{for } x \leqslant x_m \\ \dfrac{1}{2}\left\{1 - \cos\left[\dfrac{\pi(x - x_m)}{x_p - x_m}\right]\right\} & \text{for } x_m < x < x_p\,, \\ 1 & \text{for } x \geqslant x_p \end{cases} \tag{22}$$

where x_m and x_p are material parameters.

4. Evolution law of damage

For simplicity, isothermal conditions are assumed so that the effect of temperature changes enters the constitutive equations only through the temperature dependence of the material parameters. As usual in classical continuum mechanics, we assume a decoupling of intrinsic and thermal dissipation. For practical purposes, we furthermore postulate that the dissipation due to damage processes and the dissipation associated with the other mechanisms, such as the plastic strain and the hardening process, are independent (see Lu and Chow, 1990).

In order to derive the damage constitutive equation without violating the second law of the thermodynamics, we first introduce a simple expression of the damage dissipation potential (Qi and Bertram, 1997; Qi, 1998)

$$\phi_D = \frac{1}{2}\mathbf{Y}_D : \overset{\langle 4\rangle}{\mathbf{S}} : \mathbf{Y}_D, \tag{23}$$

where $\mathbf{Y}_D$ is the thermodynamic force associated with damage, called *damage driving force*, and $\overset{\langle 4\rangle}{\mathbf{S}}$ is a fourth-order tensor, called *structure tensor*. The damage evolution law is then given by

$$\dot{\mathbf{D}} = \frac{\partial \phi_D}{\partial \mathbf{Y}_D} = \overset{\langle 4\rangle}{\mathbf{S}} : \mathbf{Y}_D. \tag{24}$$

If the fourth-order tensor $\overset{\langle 4\rangle}{\mathbf{S}}$ is symmetric and positive-definite, the thermodynamic restrictions will be automatically satisfied (Germain et al., 1983; Krajcinovic, 1983).

On the other hand, damage growth in a creep process generally depends on the current state of applied stress and damage, as well as on the material symmetry properties. Note that the effective stress concept assumes that the contribution of the damage to the strain rate can be represented by means of an effective stress which appears in the strain constitutive equation instead of applied stress and damage variable, i.e.,

$$\dot{\mathbf{E}} = \mathbf{F}(\mathbf{T}, \mathbf{D}, \ldots) = \tilde{\mathbf{F}}(\mathbf{T}_e, \ldots). \tag{25}$$

In analogy, it is assumed that the effect of the current state of damage on the damage growth can be represented by means of a so-called *damage active stress* $\mathbf{T}_a$ which appears in the damage evolution law instead of applied stress and damage variable

$$\dot{\mathbf{D}} = \mathbf{G}(\mathbf{T}, \mathbf{D}, \ldots) = \tilde{\mathbf{G}}(\mathbf{T}_a, \ldots). \tag{26}$$

As experimental investigations show, the creep rate is less sensitive to the damage state than the rate of void growth (see Murakami and Ohno, 1981). Particularly, the following definition of the damage active stress is chosen

$$\mathbf{T}_a = (\mathbf{I} - \mathbf{D}_a)^{-p}\mathbf{T}(\mathbf{I} - \mathbf{D}_a^T)^{-p}, \tag{27}$$

where the material parameter p is used to distinguish the effect of damage on the damage growth from that on the creep rate.

Experimental investigations of polycrystalline metals (Johnson and Henderson, 1962; Hayhurst, 1972; Dyson and McLean, 1977; Cocks and Ashby, 1982; Hayhurst and Leckie, 1990) indicate that the damage growth on grain boundaries with unit normal $\mathbf{n}$ takes place only when the normal stress σ_n acting on the plane is positive and may depend on the damage already present there (see also Onat and Leckie, 1988). Therefore, it is reasonable to assume that only the tensile damage active stresses are responsible for damage growth, and that for isotropic materials the anisotropy of the damage development only depends on the principal directions of damage active stress tensor. Consequently, motivated by these considerations and the uniaxial damage model of Kachanov and Rabotnov, the following expression for the damage driving force for isotropic materials is postulated

$$\mathbf{Y}_D = \langle \mathbf{T}_a \rangle^n = \sum_{i=1}^{3} \langle \hat{\sigma}_i \rangle^n \hat{\mathbf{n}}_i^\sigma \otimes \hat{\mathbf{n}}_i^\sigma, \tag{28}$$

where n is a material parameter, $\hat{\sigma}_i$ and $\hat{\mathbf{n}}_i^\sigma$ are the ith eigenvalue and eigenvector of the damage active stress $\mathbf{T}_a$, respectively, and $\langle . \rangle$ are McCauley brackets. It is easy to see that in the uniaxial case the Eqs. (24), (27) and (28) yield the Kachanov–Rabotnov formulation (3).

In order to consider the nonlinear directional influence of material anisotropy on the damage development, a *mapped damage active stress* $\mathbf{T}_m$

$$\mathbf{T}_m = \sum_{i=1}^{3} (\eta_i \hat{\sigma}_i) \hat{\mathbf{n}}_i^\sigma \otimes \hat{\mathbf{n}}_i^\sigma, \tag{29}$$

is introduced with help of an orientation function η_i. The orientation function η_i modifies the effect of the ith principal damage active stress $\hat{\sigma}_i$ depending on its orientation related to the material structure. The damage active stress acting in the direction where the material has weaker damage resistance will be magnified by the orientation function. Therefore, the orientation function must satisfy the material symmetry. For single crystals with cubic symmetry we suggest the following orientation function

$$\eta_i = \left[\sum_{j=1}^{3} (\hat{\mathbf{n}}_i^\sigma \mathbf{e}_j^k)^{2m} \right]^q = \left[(\hat{\mathbf{n}}_i^\sigma \mathbf{e}_1^k)^{2m} + (\hat{\mathbf{n}}_i^\sigma \mathbf{e}_2^k)^{2m} + (\hat{\mathbf{n}}_i^\sigma \mathbf{e}_3^k)^{2m} \right]^q, \tag{30}$$

where m and q are material parameters, and $\mathbf{e}_j^k$ ($j = 1, 2, 3$) are the lattice vectors. This orientation function satisfies the cubic symmetry and a graphic presentation for $m = 10.0$ and $q = -0.2$ is shown in Fig. 1. The anisotropic damage driving force is then given by

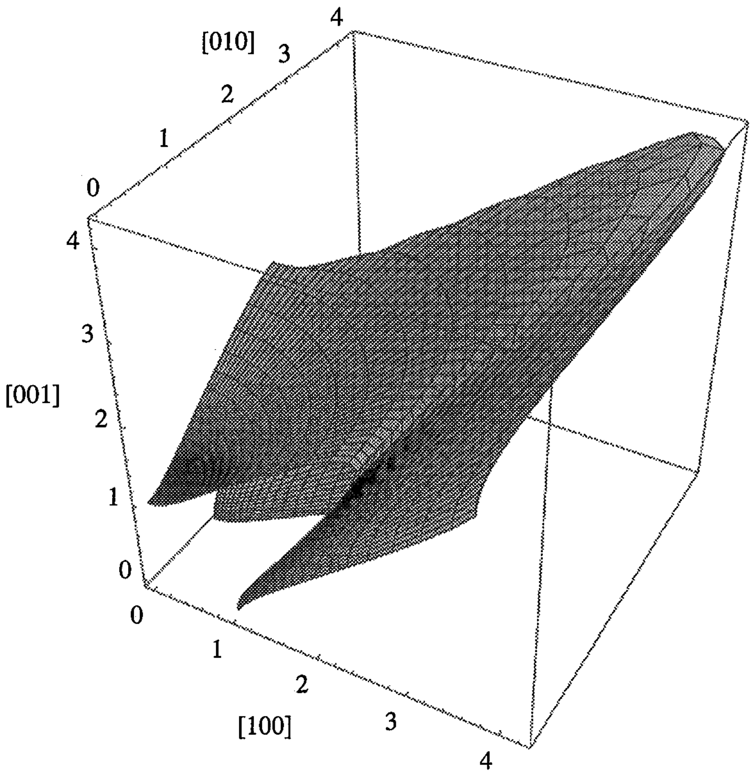


Fig. 1. Three-dimensional presentation of the orientation function (30) ($m = 10.0, q = -0.2$).

$$\mathbf{Y}_D = \sum_{i=1}^{3} \langle \eta_i \hat{\sigma}_i \rangle^n \hat{\mathbf{n}}_i^{\sigma} \otimes \hat{\mathbf{n}}_i^{\sigma}. \tag{31}$$

Under same damage active stress level, Eq. (28) shows that the damage driving force in an anisotropic material will be equally strong in all directions. In cubic single crystals, Eq. (31) says that the damage driving force in ⟨111⟩-orientation will be much stronger than that one in ⟨001⟩-orientation, if the material constants $m = 10.0$ and $q = -0.2$ (as shown in Fig. 1) are used.

Bertram and Olschewski (1993) use the following structure tensor in their creep model for cubic single crystals

$$\overset{\langle 4 \rangle}{\mathbf{S}} = \beta_1 \mathbf{I} \otimes \mathbf{I} + \beta_2 \overset{\langle 4 \rangle}{\mathbf{I}} + \beta_3 \overset{\langle 4 \rangle}{\mathbf{R}}, \tag{32}$$

with

$$\overset{\langle 4 \rangle}{\mathbf{R}} = \sum_{i=1}^{3} \mathbf{e}_i^k \otimes \mathbf{e}_i^k \otimes \mathbf{e}_i^k \otimes \mathbf{e}_i^k. \tag{33}$$

With this choice, we obtain the damage evolution law

$$\dot{\mathbf{D}} = \overset{\langle 4\rangle}{\mathbf{S}} : \mathbf{Y}_D = \left(\beta_1 \mathbf{I}\otimes\mathbf{I} + \beta_2 \overset{\langle 4\rangle}{\mathbf{I}} + \beta_3 \overset{\langle 4\rangle}{\mathbf{R}}\right) : \sum_{i=1}^{3} \langle \eta_i \hat{\sigma}_i \rangle^n \hat{\mathbf{n}}_i^\sigma \otimes \hat{\mathbf{n}}_i^\sigma, \tag{34}$$

or, alternatively

$$\dot{\mathbf{D}} = \left(\alpha_1 \mathbf{I}\otimes\mathbf{I} + \alpha_2 \overset{\langle 4\rangle}{\mathbf{I}} + \alpha_3 \overset{\langle 4\rangle}{\mathbf{R}}\right) : \sum_{i=1}^{3} \langle \frac{\eta_i \hat{\sigma}_i}{B} \rangle^n \hat{\mathbf{n}}_i^\sigma \otimes \hat{\mathbf{n}}_i^\sigma, \tag{35}$$

with $\alpha_1 + \alpha_2 + \alpha_3 = 1$. In the case of uniaxial loading in lattice direction, it is easy to see that the present model coincides with the Kachanov–Rabotnov model.

In order to predict the life-time, rupture criteria are needed. It is assumed that creep rupture occurs when

$$D_I = D_R, \tag{36}$$

where D_I denotes the first principal value of the damage tensor and D_R is a material parameter, i.e. the critical value of the damage parameter. The resulting material parameters of the present damage model are $\alpha_1, \alpha_2, (\alpha_3 = 1 - \alpha_1 - \alpha_2), B, n, p, m, q$, and D_R.

5. Constitutive modeling and experimental validation

The creep model proposed by Bertram and Olschewski has been applied to predict the anisotropic creep behavior of the nickel-based single crystal superalloys SRR99 (Bertram and Olschewski, 1996) and CMSX-6 (Bertram and Olschewski, in press) at 760°C. Implementing the derived damage model into this three-dimensional visco-plastic model, the constitutive equations coupled with material damage for cubic single crystal superalloys results in

$$\mathbf{E} = \overset{\langle 4\rangle}{\mathbf{A}}_1 : \dot{\mathbf{T}}_e + \overset{\langle 4\rangle}{\mathbf{A}}_2 : \mathbf{T}_e + \overset{\langle 4\rangle}{\mathbf{A}}_3 : \Omega, \tag{37}$$

$$\dot{\Omega} = \overset{\langle 4\rangle}{\mathbf{A}}_4 : \dot{\mathbf{T}}_e + \overset{\langle 4\rangle}{\mathbf{A}}_5 : (\mathbf{T}_e - \Omega), \tag{38}$$

with a tensor valued internal variable Ω and the following fourth-rank material tensors

$$\overset{\langle 4\rangle}{\mathbf{A}}_1 = \sum_{i=1}^{3} \frac{1}{C_i + K_i} \overset{\langle 4\rangle}{\mathbf{P}}_i, \tag{39a}$$

$$\overset{\langle 4\rangle}{\mathbf{A}}_2 = \sum_{i=1}^{3} \frac{1}{C_i + K_i}\left(\frac{C_i}{D_i} + \frac{C_i}{L_i} + \frac{K_i}{L_i}\right)\overset{\langle 4\rangle}{\mathbf{P}}_i, \tag{39b}$$

$$\overset{\langle 4\rangle}{\mathbf{A}}_3 = -\sum_{i=1}^{3} \frac{C_i}{C_i + K_i}\frac{1}{D_i}\overset{\langle 4\rangle}{\mathbf{P}}_i, \tag{39c}$$

$$\overset{\langle 4\rangle}{\mathbf{A}}_4 = \sum_{i=1}^{3} \frac{K_i}{C_i + K_i}\overset{\langle 4\rangle}{\mathbf{P}}_i, \tag{39d}$$

$$\overset{\langle 4\rangle}{\mathbf{A}}_5 = \sum_{i=1}^{3} \frac{K_i}{C_i + K_i}\frac{C_i}{D_i}\overset{\langle 4\rangle}{\mathbf{P}}_i, \tag{39e}$$

and the three structure tensors

$$\overset{\langle 4\rangle}{\mathbf{P}}_1 = \frac{1}{3}\mathbf{I}\otimes\mathbf{I}, \tag{40a}$$

$$\overset{\langle 4\rangle}{\mathbf{P}}_2 = \overset{\langle 4\rangle}{\mathbf{R}} - \overset{\langle 4\rangle}{\mathbf{P}}_1, \tag{40b}$$

$$\overset{\langle 4\rangle}{\mathbf{P}}_3 = \overset{\langle 4\rangle}{\mathbf{I}} - \overset{\langle 4\rangle}{\mathbf{P}}_1 - \overset{\langle 4\rangle}{\mathbf{P}}_2, \tag{40c}$$

where C_i, K_i, D_i, L_i $(i = 1, 2, 3)$ are material parameters.

The dependence of the viscosities D_i and L_i on the applied stress is expressed by the joint ansatz

$$D_i = D_{0i}\exp\left\{-\sum_j Z_{ij}J_j\right\}, \tag{41a}$$

$$L_i = L_{0i}\exp\left\{-\sum_j Z_{ij}J_j\right\}, \tag{41b}$$

with the material parameters Z_{ij} $(i = 1, 2, 3, 4; j = 1, 2, 3)$ and the following scalar invariants of cubic symmetry

$$J_1 = \sqrt{\tilde{\sigma}_{11}\tilde{\sigma}_{22} + \tilde{\sigma}_{22}\tilde{\sigma}_{33} + \tilde{\sigma}_{33}\tilde{\sigma}_{11}}, \tag{42a}$$

$$J_2 = \tilde{\sigma}_{12}^2 + \tilde{\sigma}_{23}^2 + \tilde{\sigma}_{31}^2, \tag{42b}$$

$$J_3 = \tilde{\sigma}_{11}\tilde{\sigma}_{22}\tilde{\sigma}_{33}, \tag{42c}$$

$$J_4 = \tilde{\sigma}_{11}(\tilde{\sigma}_{12}^2 + \tilde{\sigma}_{13}^2) + \tilde{\sigma}_{22}(\tilde{\sigma}_{23}^2 + \tilde{\sigma}_{21}^2) + \tilde{\sigma}_{33}(\tilde{\sigma}_{31}^2 + \tilde{\sigma}_{32}^2). \tag{42d}$$

From the assumption of incompressibility under creep, it follows

$$D_1^{-1} = 0, L_1^{-1} = 0 \text{ and } Z_{i1} = 0 \ (i = 1, 2, 3, 4). \tag{43}$$

The tensile creep tests at 760°C were performed at MTU Munich and at Siemens KWU. The crystal orientation of the specimen is characterized by the Eulerian angles φ_1 and φ_2, determining the orientation of the crystal relative to the load axis.

Table 1
Material parameters of damage model (CMSX-6 at 760°C)

α_1	α_2	α_3	B (MPa)	n	p	m	q	D_R
0.0	0.4	0.6	1244.3	15.096	0.40453	37.495	−0.19247	0.3
0.0	0.5	0.5	1234.4	15.349	0.41081	35.009	−0.20406	0.3
0.0	0.6	0.4	1232.9	15.199	0.33169	35.392	−0.19846	0.3

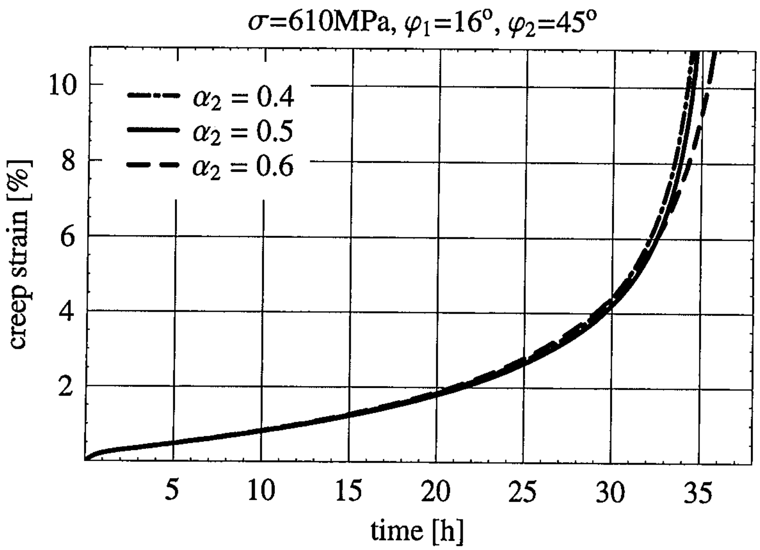


Fig. 2. Creep modeling by using the three different groups of damage material parameter in Table 1.

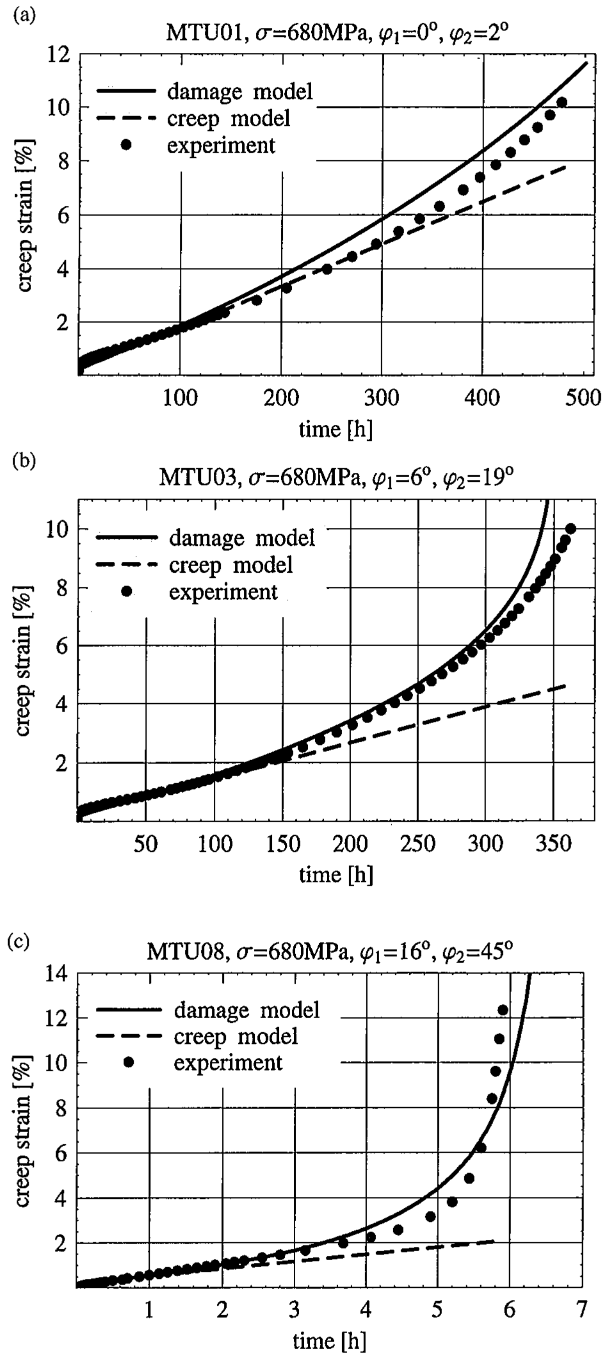


Fig. 3. Experiment and simulation for different orientations and loads (*continued on next page*).

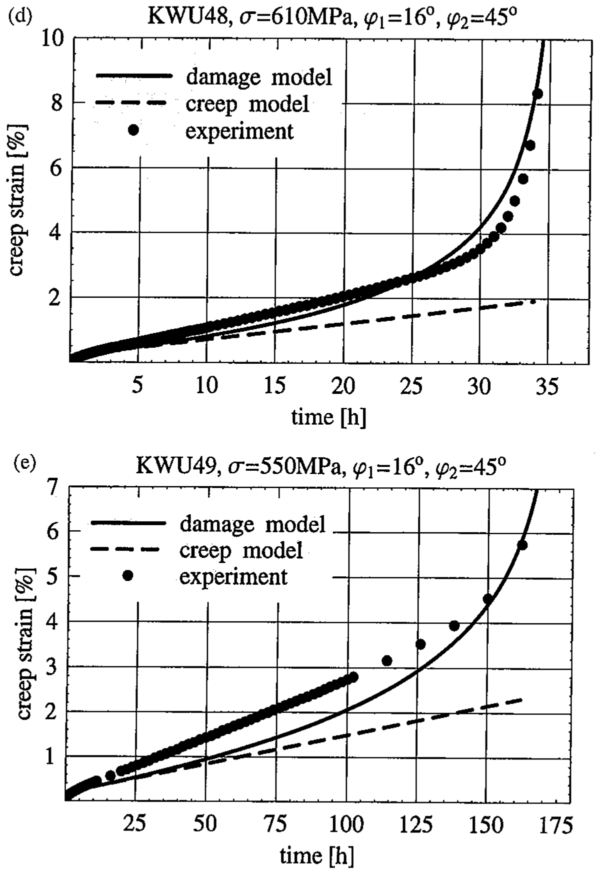
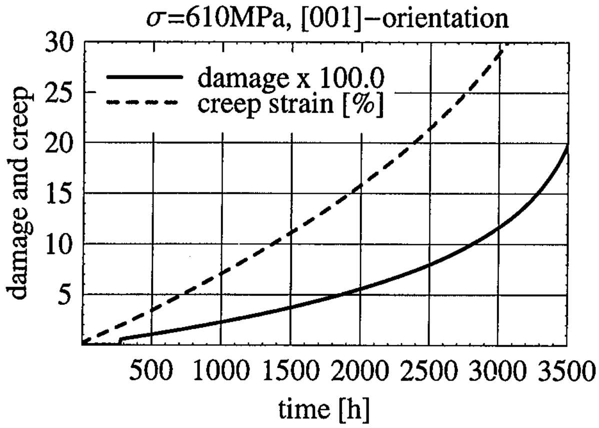
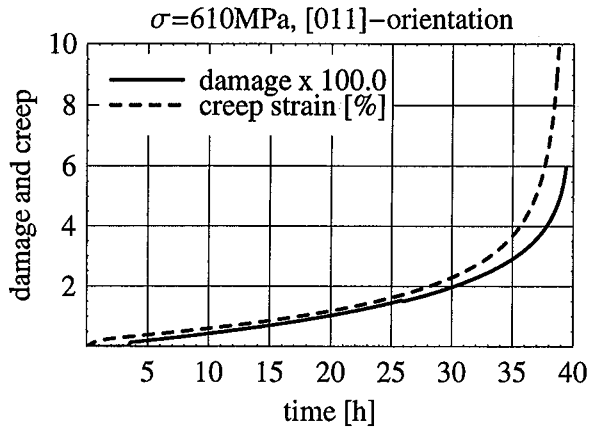


Fig. 3. (*continued*)

$\varphi_2 = 0$ characterizes the [001]-orientation, $\varphi_1 = 45°$ and $\varphi_2 = 54.73°$ characterizes the [111]-orientation. The creep material parameters of the creep model are adopted from the work of Bertram and Olschewski (in press). The corresponding damage material parameters of the damage model are obtained by calibrating the predicted creep curves with the test data, while the creep material parameters remain fixed (Qi, 1998). As there are only uniaxial tensile creep test data available, the parameter x_m and x_p for the description of active/passive damage mechanisms have been roughly estimated [one can use the Heaviside function instead of (22)], and the anisotropic character of damage process can not be completely studied, so that the relationship between α_1, α_2 and α_3 can not be uniquely identified. For $\alpha_2 = 0.4$, 0.5 and 0.6, the corresponding parameters fitted from the available uniaxial creep test data are shown in Table 1. A comparison of the creep behavior modeling with these three parameter groups are shown in Fig. 2 for three uniaxial loading conditions. It is to see that these three different parameter groups offer almost the same modeling results under uniaxial loading conditions.





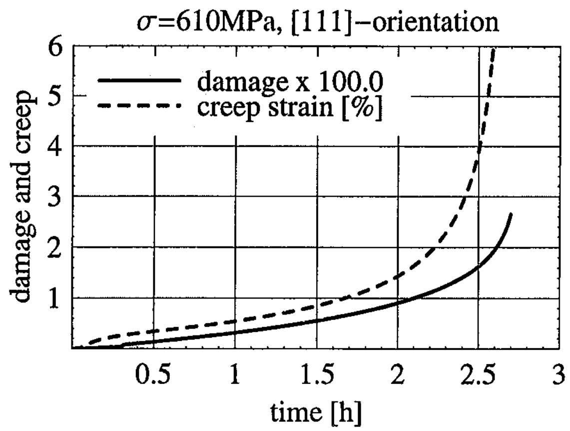


Fig. 4. Creep damage calculation for three ideal orientations.

The influence of the crystal orientation on the mechanical behavior was the most striking characteristic of single crystals. A comparison of the theoretical prediction with/without damage and the experimental results related to this character is shown in the Fig. 3. Here "creep model" means uncoupled with damage and "damage model" means the coupled model. Note that the time scale of the different figures differs widely. At the same stress level $\sigma = 680\,\text{MPa}$ Fig. 3a,b and c, [001]-orientation (MTU01) exhibits the longest creep rupture time. Three creep tests performed with the same oriented specimens ($\varphi_1 = 16°$ and $\varphi_2 = 45°$) but at different load levels, and the corresponding modeling are presented in Fig. 3c,d and e. It demonstrates that the present model is able to predict the strong nonlinearity of the stress-strain response of single crystal superalloys at high temperatures.

Comparing the results of the calculation by the model with and without damage shown in Fig. 3, it is to see that the creep rate calculated by the present model is always larger than the one calculated by the model without respect to material damage. As the material damage develops during the loading process, the effective stress increases and, therefore, the creep behavior till rupture can be simulated by the present model.

A prediction of the creep strain and the damage development for the three extreme orientations [001], [011] and [111] are presented in the Fig. 4.

6. Conclusions

A three-dimensional model for the description of creep-damage processes for single crystals has been suggested. It takes into account

- the initial anisotropy of the crystal in the evolution functions for the creep and damage variables,
- the damage-induced anisotropy by a tensorial damage variable,
- the crack-opening/closure behavior by an activation/deactivation mechanism of the damage.

The model has been applied to monotonous creep tests at high temperatures for single crystal superalloys in different orientations. It is capable to describe both the strong orientation dependence and the non-linearity with respect to the applied load of the entire creep process. It can, therefore, be used for the prediction of time to rupture for this class of materials and loads.

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