 CMES, vol.3, no.3, pp.313-320, 2002

Numerical Investigation of Creep Damage Development in the Ni-Based Superalloy IN738 LC at 850 ˚C

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Abstract: Results of a numerical study of creep damage development and its effect on the deformation behavior in the Ni-based superalloy IN 738 LC at 850 ˚C are reported. A continuum damage mechanics based anisotropic damage model has been coupled with the unified model of Chaboche, and is used for the present study. Numerical computations are performed on a plate containing a circular hole under tension. They show that the applied damage model does not cause damage localization and no significant mesh-dependence of the results are observed.

keyword: anisotropic damage, creep damage, damage localization, mesh-dependence.

1 Introduction

The design and analysis of engineering components and structures to operate at elevated temperatures and severe stress levels require an accurate prediction of the stress-strain-damage response encountered during loading processes. Many models have been developed and applied to the simulation of the viscoplastic behavior of metals, e.g. the unified models of Bodner-Partom [Bodner and Partom (1975), Kolkailah and McPhate (1990)], Chaboche [Chaboche (1977), Chaboche and Rousselier (1983)] and Ho [Ho (2001)]. The original formulations of these models, however, do not consider material damage, which can play an important role in engineering structures. Without considering damage, the respective models are not able to describe tertiary creep and to predict lifetime. Many efforts have therefore been put on extending the models to include material damage [Bodner (1984), Sherwood and Fay (1992), Olschewski, Haftaoglu and Noack (1996)]. Recently, a damage mechanics model for single crystals has been proposed by Qi and Bertram [Qi and Bertram (1997), Qi (1998), Qi and Bertram (1999)]. In this model, a second order symmetric tensor is used as a state variable to account for the anisotropy of material damage. Under the framework of thermodynamics of internal variables, the damage evolution law is established based on the results of micro-mechanical investigations. It is assumed that the dissipation due to the damage process and the dissipation associated with other mechanisms, such as plastic strain, are independent and only the current state of stress and damage effects the evolution of damage. A strain-based approach to the active/passive damage mechanism has also been used in this model. By ignoring the initial structural symmetry of single crystals, this damage model also applies to polycrystalline alloys [Qi and Brocks (2000a)].

Ni-based superalloys are specially developed for components operating at high temperature, severe stress and a hostile environment, such as gas turbine blades. The Chaboche model has been used to predict the material response of the Ni-based superalloy IN738 LC under creep and LCF loading conditions [Olschewski, Sievert, Qi and Bertram (1993), Olschewski, Haftaoglu and Noack (1996)]. According to the effective-stress concept of CDM, the Chaboche model can be coupled with the above mentioned anisotropic damage model by replacing the stress tensor in it by an adequately defined effective stress tensor. Thus, the Chaboche model is extended to include anisotropic damage.

Hayhurst and Leckie (1973) conducted a creep rupture test on a copper plate specimen (100 mm $\times$ 31 mm $\times$ 2.5 mm) containing a circular hole (radius 1.75 mm). It showed that widespread regions of material damage have been formed during the test. Numerical simulations using the conventional creep damage model of Kachanov-Rabotnov, however, as reported by Liu and Murakami (1998), lead to damage localization and mesh-dependent results. Although the proposed model of Liu and Murakami improves the results, the mesh-dependence of the results is still significant.

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The present paper displays the results of a numerical study of damage development and its effect on the deformation behavior in the Ni-based superalloy IN738 LC at 850 ° C. A square plate containing a circular hole of radius 0.5 mm undergoing creep load is used as the object of the study. FE-simulations using the original model of Chaboche and others using the extended model with anisotropic damage, respectively, are compared and discussed.

2 The Unified Model Coupled with Anisotropic Damage

2.1 The anisotropic damage model

Damage of material is an irreversible thermodynamic process, and damage generally develops anisotropically [Betten (1983), Kailasam, Aravas and Castañeda (2000)]. Experimental investigations [Hayhurst and Leckie (1990), Betten, El-Magd, Meydanli and Palmen (1995)] clearly show the strong influence of the anisotropic evolution of damage on the lifetime when the loading direction changes. As the stress state in engineering components changes in time, the damage anisotropy has to be considered. For describing the anisotropic character of material damage, tensorial variables are needed, see Lehmann (1991). When a second-order symmetric tensor **D** is employed [Murakami and Ohno (1981)], the effective-stress tensor $\tilde{\mathbf{S}}$ can be defined as [Cordebois and Sidoroff (1982)]:

$$\tilde{\mathbf{S}} = (\mathbf{I}-\mathbf{D})^{-\frac{1}{2}} \cdot \mathbf{S} \cdot (\mathbf{I}-\mathbf{D})^{-\frac{1}{2}} \tag{1}$$

where **S** and **I** denote the stress tensor and the identity tensor of rank two, respectively. Note that this definition is similar to the definition of the second Piola-Kirchhoff stress tensor in continuum mechanics.

From the linear irreversible thermodynamics point of view, the damage evolution law can be generally expressed as:

$$\dot{\mathbf{D}} = \overset{<4>}{\mathbf{S}} : \mathbf{Y}_D \tag{2}$$

where $\mathbf{Y}_D$ is the thermodynamic force conjugate to the damage tensor, and $\overset{<4>}{\mathbf{S}}$ is the damage characteristic tensor of rank four for a second-order damage tensor, respectively. If the fourth-order tensor $\overset{<4>}{\mathbf{S}}$ is symmetric and positive-definite, the thermodynamic restrictions will be automatically satisfied [Krajcinovic (1983), Germain, Nguyen and Suquet (1983), Yang, Zhou and Swoboda (1999)].

Remember that according to the effective stress concept of CDM, the effect of the stress and damage on the deformation behaviour can be represented by an adequately defined effective stress. Similarly, it is supposed that the contribution of the stress and damage to the damage development can be represented by a newly introduced damage-active stress $\tilde{\mathbf{S}}$. As experimental investigation show, the rate of cavity growth is more sensitive to the damage state than to the creep rate (see Murakami and Ohno (1981)). The damage-active stress hence is defined as

$$\hat{\mathbf{S}} = (\mathbf{I}-\mathbf{D})^{-q} \cdot \mathbf{S} \cdot (\mathbf{I}-\mathbf{D})^{-q} = \sum_{i=1}^{3} \hat{\sigma}_i \hat{\mathbf{n}}_i^{\sigma} \otimes \hat{\mathbf{n}}_i^{\sigma}, \tag{3}$$

using a material parameter, q, to distinguish the effect of damage on the damage growth from that on the creep rate in Eq. 1. $\hat{\sigma}_i$ and $\hat{\mathbf{n}}_i^{\sigma} (i = 1,2,3)$ are principal values and vectors of the damage-active stress tensor $\hat{\mathbf{S}}$, respectively. Motivated by the results of microscopic experimental investigations [Hayhurst and Leckie (1983), Hayhurst and Leckie (1990)] it is assumed that only the tensile principal damage-active stresses are responsible for the damage evolution and that the damage grows perpendicularly to the direction of the principal damage-active stresses. Thus, considering that damage may also develop partly isotropically, the damage law Eq. (2) takes the following particular form:

$$\dot{\mathbf{D}} = \overset{<4>}{\mathbf{S}} : \mathbf{Y}_D = \left(\beta_1 \mathbf{I} \otimes \mathbf{I} + \beta_2 \overset{<4>}{\mathbf{I}}\right) : \langle \hat{\mathbf{S}} \rangle^m \tag{4}$$

or:

$$\dot{\mathbf{D}} = \left(\beta \mathbf{I} \otimes \mathbf{I} + (1-\beta) \overset{<4>}{\mathbf{I}}\right) : \left\langle \frac{\hat{\mathbf{S}}}{B_0} \right\rangle^m = \left[\beta \mathbf{I} \otimes \mathbf{I} + (1-\beta) \overset{<4>}{\mathbf{I}}\right] : \sum_{i=1}^{3} \left\langle \frac{\hat{\sigma}_i}{B_0} \right\rangle^m \hat{\mathbf{n}}_i^{\sigma} \otimes \hat{\mathbf{n}}_i^{\sigma} \tag{5}$$

where β $(0 \le \beta \le 1)$, B_0, m are material parameters. $\overset{<4>}{\mathbf{I}}$ is the fourth-order identity tensor, and $\langle . \rangle$ denotes the McCauley bracket, which equals one for positive arguments and zero for others. Obviously, $\overset{<4>}{\mathbf{S}}$ is positive definite for $0 \le \beta \le 1$. The material parameter β

is called isotropy parameter.It is easy to see that $\beta = 1$ corresponds to totally isotropic damage, and for $\beta = 0$ the damage will develop perpendicularly to the principal damage-active stresses and there is no isotropic part of damage. Note that biaxial tests are needed for the determination of the isotropy parameter β. The creep rupture is assumed to take place when the maximum principal damageD_I reaches a critical value D_R.

2.2 Chaboche model coupled with the damage model

The unified model of Chaboche [Chaboche (1977)] did not consider the effect of material damage. According to the effective stress concept (also called principle of strain-equivalence), "any deformation behavior, whether uniaxial or multiaxial, of a damaged material is represented by the constitutive laws of the virgin material in which the usual stress is replaced by the effective stress" [Lemaitre and Chaboche (1990)]. Thus, replacing the stress tensor in the Chaboche model, we obtain a unified model of damaged material as follows:

- Flow rule:

$$\dot{\mathbf{E}} = \frac{3}{2}\dot{p}\frac{\tilde{\mathbf{S}}' - \mathbf{X}}{J_2(\tilde{\mathbf{S}}' - \mathbf{X})}, \quad \dot{p} = \left\langle \frac{J_2(\tilde{\mathbf{S}}' - \mathbf{X}) - R_y}{K} \right\rangle^n \quad (6)$$

with $J_2(.) = \sqrt{3/2|.|}$,

- Isotropic hardening rule:

$$\dot{R} = b(R_\infty - R)\dot{p}, \quad R(p=0) = R_0 \quad (7)$$

- Kinematic hardening rule:

$$\dot{\mathbf{X}} = c\left[\frac{3}{2}a\dot{\mathbf{E}} - \phi(p)\mathbf{X}\dot{p}\right] - d\left[\frac{J_2(\mathbf{X})}{a}\right]^r \frac{\mathbf{X}}{J_2(\mathbf{X})},$$
$$\phi(p) = \phi_\infty - (\phi_\infty - 1)e^{\omega p}. \quad (8)$$

The effective-stress tensor is defined in Eq. 1, and the evolution law of damage is described in Eq. 5. This coupled model has been implemented into the commercial finite-element-program ABAQUS by developing a user-supplied material subroutine UMAT, which is used for the present study. An explicit forward integration algorithm is applied for the numerical integration.

3 Material parameters of the IN 738 LC at 850 ˚C

Identification of the material parameters is the most important step for the practical application of any material model. From this point of view, a great advantage of the effective-stress concept is that the material parameters of the coupled model can be stepwise separately estimated. At first, the parameters of the original model without damage can be determined by fitting experimental data. The damage effects such as tertiary creep should be ignored in this step. After that, the coupled model will be used to fit the test data by varying the parameters in the damage law, while the previous obtained parameters are kept constant, so that the damage effects can be included. Finally, for refining the values of the material parameters by varying all the material parameters to fit the test data, the previously obtained values of the parameters will serve as starting values.

Table 1 : Material parameters of Chaboche model from Olschewski, Sievert, Meersmann and Ziebs (1990)

E	=	149650 MPa	a	=	311 MPa
ν	=	0.33	c	=	201
K	=	397 MPa·h$^{1/n}$	ϕ_∞	=	1.1
n	=	7.7	ω	=	0.04
R_0	=	153 MPa	d	=	81.72 MPa/h
R_∞	=	0.0 MPa	r	=	3.8
b	=	317			

The material parameters of the Chaboche model for IN 738 LC at 850 ˚C have been determined by Olschewski, Sievert, Meersmann and Ziebs (1990) as listed in Tab. 1 and used in the present study. The material parameters of the damage model are estimated by fitting the coupled model to the three creep curves presented in the work of Olschewski, Sievert, Meersmann and Ziebs (1990). Tab. 2 shows a set of estimated values of the parameters. For lack of biaxial test data, the isotropy parameter β can not be determined. As there are only three creep tests available, the final step of the identification process mentioned above has not been carried out.

Table 2 : Material parameters of damage model

β	q	B_0	m	D_I
0.0 ∼1.0	0.4	613 MPa·h$^{1/m}$	14	0.07

A comparison of the experimental data and the simulation results using original and coupled model, respectively, is shown in Fig. 1.

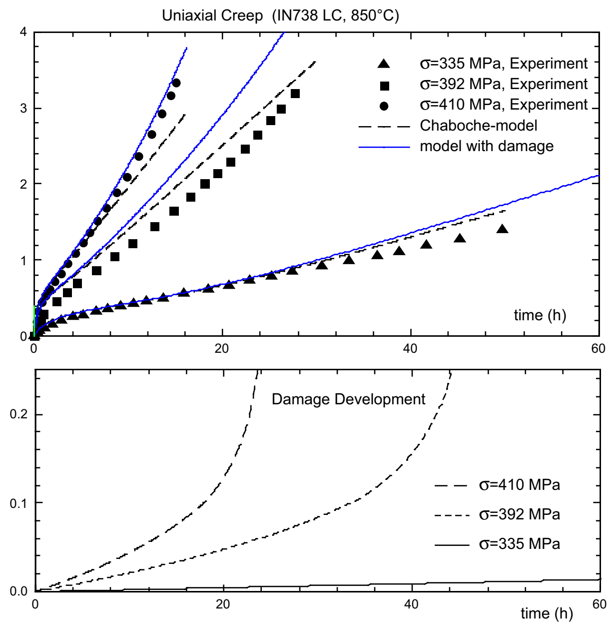

Figure 1 : Comparison of the model predictions and experiments

4 FE-investigation of anisotropic damage

The Ni-based superalloy IN738 LC is developed as high-temperature material for gas turbines. In advanced gas turbine blades with air cooling design, the typical stress concentration occurs due to the air cooling channels. Therefore, a square panel (10 mm × 10 mm × 0.5 mm) containing a circular hole (radius 0.5 mm) is chosen as an example representation of a blade's cross section where a cooling channel appears. The specimen is subjected to a constant tensile load of 200 MPa. Because of the symmetry, only 1/8 of the specimen is modeled in the finite element calculations. Fig. 2 shows the FE-mesh used for the computation. This mesh (created by I-DEAS) is characterized by r20-x12-y12-z5 (20 elements over radial direction, 12 over x-direction, 12 over y-direction and 5 over z-direction) with bias: r15-x5-y5-z3 (bias values are 15, 5, 5 and 3 in the radial, x, y and z direction, respectively). There are five elements over the half-thickness to consider the gradients of the stress, strain and damage fields over the thickness. As all the elements of the mesh have an approximately rectangular shape, three-dimensional incompatible solid elements C3D8I from the element library of ABAQUS are used for the calculations instead of second order compatible elements to save computation time. Geometrical non-linearity has been considered and the isotropy parameter β of the damage model is assumed to be 0.1 which represents a strong damage anisotropy.

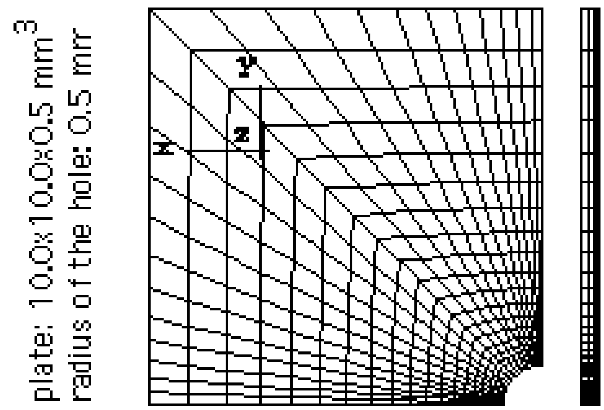

Figure 2 : FE-mesh (r20-x12-y12-z5)

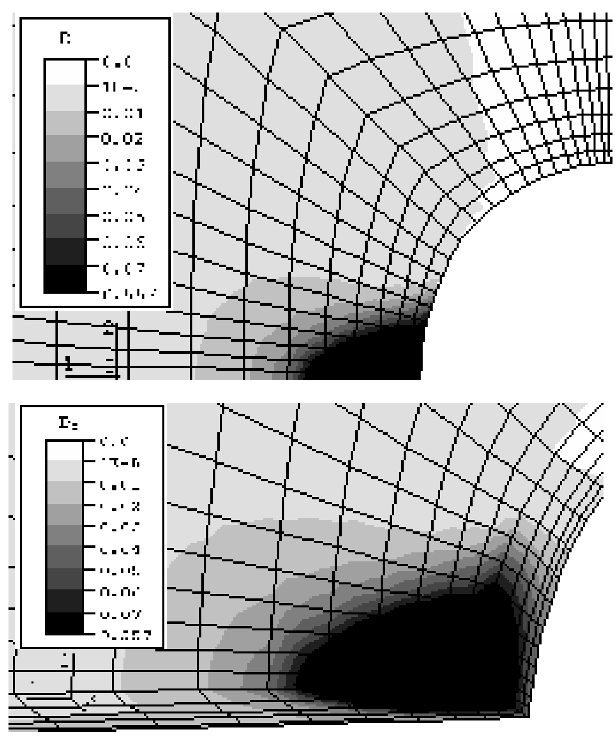

Figure 3 : Distribution of the maximum principal damage after 3788 hours.

For comparison, the calculations were performed using the Chaboche model with and without damage, respectively. The numerical results are shown in Figs. 3 to 7. Fig. 3 displays the distribution of the maximum principal damage after 3788 hours in the x-y plane and over the thickness, respectively. The in-plane and out-of-plane damage gradients are clearly to see. Note that the critical value of damage is D_R=0.07, which means that local fracture takes place when the damage value is larger. However, no limit value of the local damage was assumed in the calculations. The maximum damage has been found to occur beneath the surface of the hole, not directly on the surface. Though there is no experimental evidence available for this case, the experimental investigations on circumferentially notched bars [Kobayashi, Imada and Majima (1988)] showed that the maximum creep damage takes place beneath the notch surface. Results of notched tensile bar simulations using the coupled model agree well with the experimental observation [Qi and Brocks (2000b)].

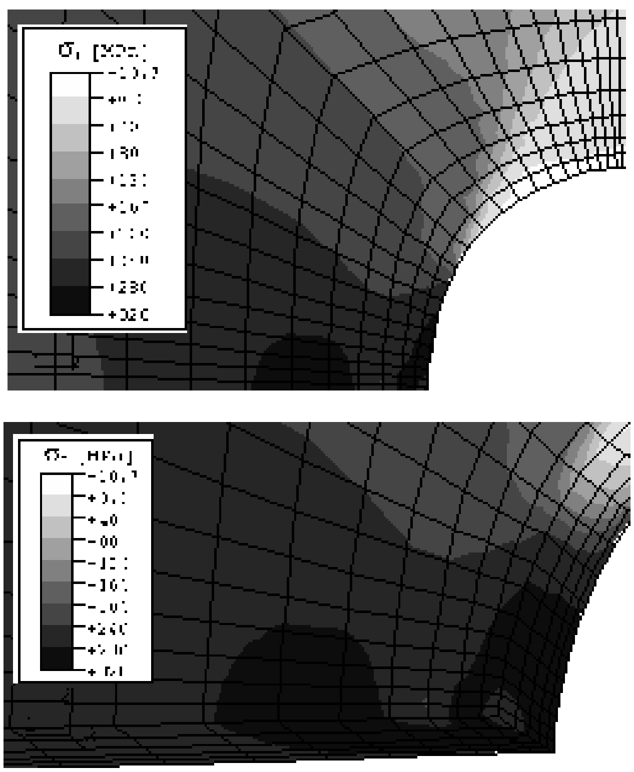

Figure 4 : Distribution of the maximum principal stress after 3788 hours.

Fig. 4 displays the distribution of the maximum principal stress after 3788 hours. For comparison, the distribution of the maximum principal stress at t = 3788 hours calculated with the Chaboche model without damage is shown in Fig. 5. The figures illustrate the stress redistribution due to damage at the hole. The deformed hole and the distribution of the maximum principal strain can be seen in Fig. 6. Finally, Fig. 7 shows the strain distribution calculated with the Chaboche model without damage for comparison, again.

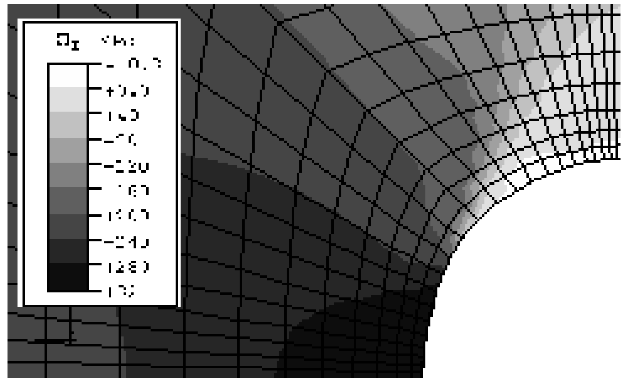

Figure 5 : Distribution of the maximum principle stress after 3788 hours. (CHABOCHE model without damage)

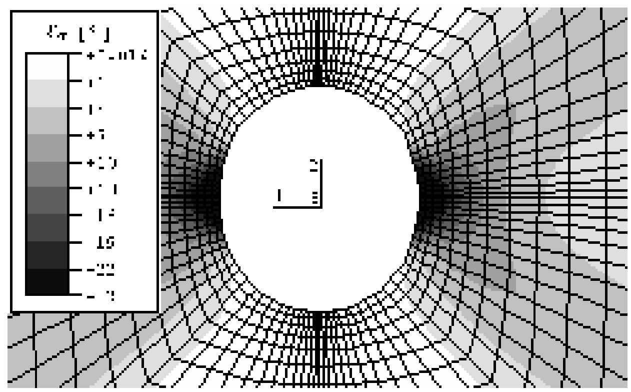

Figure 6 : Distribution of the maximum principle strain.

The same calculations have been repeated using two different meshes in order to check any mesh dependence. Fig. 8 gives the contour plot of the maximum damage estimated by using an FE-mesh characterized by r15-x6-y10-z4 with bias: r15-x1-y3-z1. The damage distribution calculated using a finer mesh (r24-x12-y16-z4 with bias: r18-x1-y2-z1) is shown in Fig. 9. Comparing Figs. 3, 8 and 9 display no significant differences between the three meshes.

In the above computations the gradients in the z-direction have been considered by five elements over the half-thickness. Liu and Murakami (1998) conducted numer-

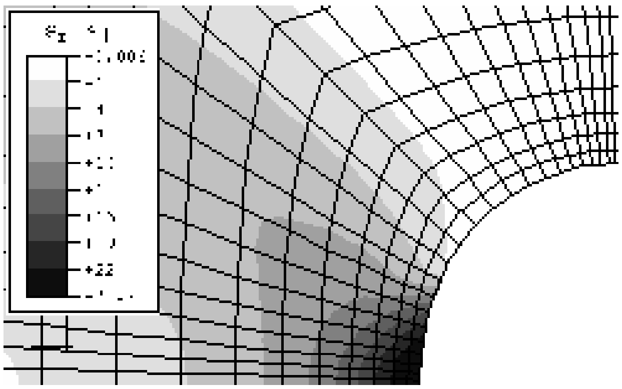

Figure 7 : Distribution of the maximum principle strain. (Chaboche model without damage)

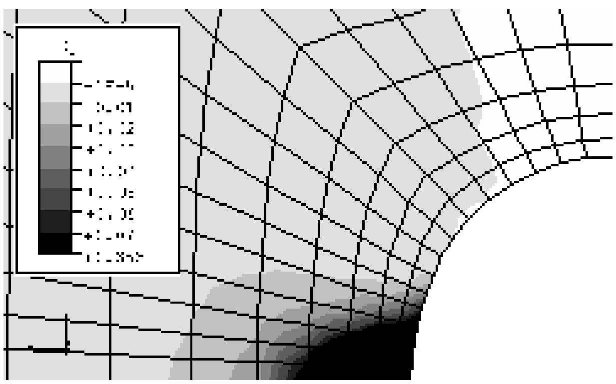

Figure 8 : Distribution of the maximum principal damage after 3788 hours; coarser mesh r15-x6-y10-z4.

ical computations for a thin copper plate (30 mm $\times$ 30 mm) containing a circular hole (radius 3 mm) under uniaxial tension and plane stress state. Their computations revealed a significant mesh dependence. As the present model is anisotropic and fully three-dimensional, the respective UMAT has been developed for this general case. For plane stress elements, a special UMAT formulation is required. Mesh dependence was investigated with a model having only one element in the thickness direction. A fine and a coarse mesh were applied. The geometrical non-linearity has not been considered and exactly the same time increment for the integration was used in both calculations. Fig. 10 shows the damage distribution for these two meshes (upper and lower half). There is no significant difference between the damaged zones obtained in the two calculations.

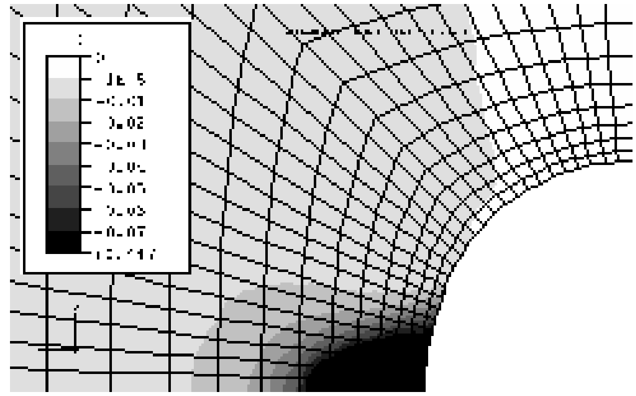

Figure 9 : Distribution of the maximum principal damage after 3788 hours, finer mesh r24-x12-y16-z4

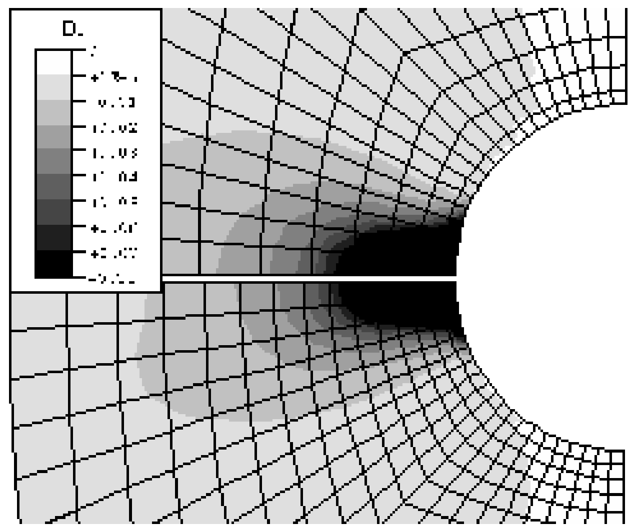

Figure 10 : Comparison of the distribution of the maximum principal damage after 6980 hours; upper half: coarse mesh, lower half: fine mesh.

5 Conclusions

A numerical study of damage evolution in a plate containing a circular hole subjected to uniaxial creep load has been presented. An anisotropic damage model coupled with the Chaboche model has been used for this purpose. The results show that the model predicts spread damage, no damage localization occurs and no significant mesh-dependence of the numerical results is observed. The direction of the principal damage can also be determined with the anisotropic model. If this direction is identified as the orientation of micro cracks, it opens perspectives for an experimental verification of the model. No numerical difficulties have been observed with this model so far. If isotropic damage is assumed (β=1), damage localization may occur in some cases. Under anisotropic conditions ($1 > \beta \geq 0$), damage localization is at least delayed if not even avoided. The mechanism of damage deactivation and reactivation, i.e. closing and opening of micro cracks, has not yet been considered, as it is not important for monotonic loading conditions. For further verification however, experimental investigations with multiaxial non-proportional and cyclic loading are needed to address all the various capabilities of the model.

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