

## Characterization of anisotropic damage by simulation of a microstructure with voids

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**Abstract:** Anisotropic damage is simulated by using the technique of the representative volume element. By doing so an internal length, which characterizes the microstructure of the material, is introduced. The boundary value problem of the RVE is calculated by a 3-dimensional finite element code for large deformations. For modelling the material behaviour elastic viscoplastic constitutive equations based on the theory of crystal plasticity are used. For the damage simulation the node doubling technique for modelling inter-crystalline cracks in the RVE is applied. A second internal length that characterizes the damaged parts of the material is introduced. In order to determine the macro-behaviour from the simulation of the micro-behaviour it is necessary to calculate the means of the local strains and stresses (homogenization). The calculations are carried out for an aluminum sample. The required material-parameters are determined by experimental results. A tensile test is performed for the RVE.

### 1. INTRODUCTION

The consideration of damage for the characterization of the material behaviour up to rupture, has gained more and more importance since the introduction of the continuum damage theory by Kachanov in 1958 [9]. In general one distinguishes between micromechanical concepts ([15], [16]) and the continuum damage theories ([11], [13]). In CDM the material inhomogeneities (voids) are smeared out and a damage variable is introduced. This can be defined as a scalar [9], a vector [10], a second order tensor [6], or higher order tensors [12].

Apart from continuum theories, several micromechanical concepts have been introduced. These concepts are based on the simulation of the physical behaviour of the damage evolution. They simulate the nucleation of voids (e.g. [3], [4]), the growth of voids (e.g. [7], [5]) and coalescence (e.g. [17]). Here a concept based on the micromechanical description of the material behaviour is presented. An internal length scale (the size of the voids) thus enters the modelling of damaged parts of the material. By using a suitable numerical homogenization the macroscopic material behaviour is obtained. Intercrystalline cracks are regarded. The morphology of the cracks and, thus, the introduced microstructure has been investigated in various forms. Starting from a single crack in a monocrystal, the procedure is extended to different arrangements of multiple cracks.

### 2. MATERIAL MODEL

The material behaviour is described in terms of crystal plasticity by an elasto-viscoplastic model based on overstresses. In order to take into account large deformations the right Cauchy-Green tensor  $C$  is used to measure the deformations. This tensor is power conjugated to the material stress

$\mathbf{S} = \mathbf{F}^{-1} \mathbf{T} \mathbf{F}^{-T}$  with the deformation gradient  $\mathbf{F}$  and the Cauchy-stress tensor  $\mathbf{T}$ . The material stress tensor is assumed to be determined by a linear elastic law

$$\mathbf{S} = \mathcal{K}_i [\mathbf{C} - \mathbf{C}_U]. \quad (1)$$

$\mathcal{K}_i$  is the current fourth order elasticity tensor and  $\mathbf{C}_U$  the stress free configuration. By using the concept of plastic transformation [2] the following equation is derived

$$\mathbf{S} = \mathbf{P} \mathcal{K}_0 [\mathbf{P}^T \mathbf{C} \mathbf{P} - \mathbf{C}_U] \mathbf{P}^T \quad (2)$$

with the initial elasticity tensor  $\mathcal{K}_0$ , where the inelastic transformation  $\mathbf{P}$  is an invertible non-symmetric tensor.

The inelastic deformations on the micromechanical level arise from the activation of slip systems ( $\mathbf{d}_i, \mathbf{n}_i$ ). By summing up all increments of all active slip systems the evolution equation for  $\mathbf{P}$

$$\dot{\mathbf{P}} \mathbf{P}^{-1} = - \sum_i \dot{\mu}_i \mathbf{d}_i \otimes \mathbf{n}_i \quad (3)$$

is obtained. In the case of cubic-face-centered materials, 12 octahedral slip systems are taken into account.

The shear rate for a particular slip system ( $\dot{\mu}_i$ ) is derived by the following equation

$$\dot{\mu}_i = \begin{cases} 0 & \text{for } |\tau_i - \alpha_i| \leq \tau_{cr_i} \\ \frac{1}{\eta} \text{sign}(\tau_i - \alpha_i) |\tau_i - \alpha_i - \tau_{cr_i}| & \text{for } |\tau_i - \alpha_i| > \tau_{cr_i} \end{cases} \quad (4)$$

If the resolved shear stress in a slip system  $\tau_i = \text{tr}(\mathbf{S} \mathbf{C} \mathbf{d}_{i0} \otimes \mathbf{n}_{i0})$  exceeds the critical value  $\tau_{cr_i}$ , it begins to glide with the shear viscosity  $\eta$ .

For the slip systems isotropic and kinematic hardening are considered

$$d\tau_{cr_i} = \sum_s h_{si} d\mu_s \quad (5)$$

$$d\alpha_i = \sum_s k_{si} d\mu_s \quad (6)$$

Both self ( $s = i$ ) and latent hardening ( $s \neq i$ ) of the slip systems are taken into account by different hardening coefficients  $h_{si}$  and  $k_{si}$ .

This model is used to simulate the deformations of single crystals.

### 3. HOMOGENIZATION

In order to determine the macro-behaviour by simulating the micro-behaviour it is necessary to calculate the means of the local strains and stresses (homogenization). This can be done by using different classical techniques (e.g. the Taylor model, the Sachs model, self consistent schemes and the representative volume element technique (RVE)).

The latter one turns out as the most realistic and versatile. The RVE, which is used here, is representative for the infinitesimal environment of the observed material point [8]. The complete solution of the boundary value problem assures compatibility and equilibrium within the RVE. For quantifying the RVE, two different length scales are necessary: the continuum- or macro-length scale (for measuring the infinitesimal environment) and the micro-length scale (for describing the microstructure). In order to obtain the macro behaviour of the material, the displacement field  $\mathbf{u} = (\bar{\mathbf{F}} - \mathbf{I})\mathbf{X} + \mathbf{w}$  is splitted into a global linear part  $(\bar{\mathbf{F}} - \mathbf{I})\mathbf{X}$  and the local inhomogeneous fluctuation  $\mathbf{w}$ . The Taylor model is included by setting  $\mathbf{w} = \mathbf{0}$ .

If the local fluctuation on the boundary is equal zero or periodic, the global deformation gradient  $\bar{\mathbf{F}}$  can be obtained from the local one  $\mathbf{F}$  as follows

$$\bar{\mathbf{F}} = \frac{1}{V_0} \int_{V_0} \mathbf{F} dV_0 \quad (7)$$

The global stress can be obtained by averaging over the first Piola-Kirchhoff-stress tensor ( $T^{iPK} = \det(\mathbf{F})\mathbf{T}\mathbf{F}^{-T}$ ).

$$\bar{\mathbf{T}}^{iPK} = \frac{1}{V_0} \int_{V_0} \mathbf{T}^{iPK} dV_0 \quad (8)$$

#### 4. NUMERICAL CALCULATIONS

The described constitutive model has been implemented in a finite element code to compute the RVE. To assure the representativity of this volume, it has been subjected to different test deformations. The RVE-technique allows to calculate the macro-behaviour of a sample and to compare it with experimental results. The concept has already been tested for different materials undergoing large deformations.

To simulate the damage, cracks are introduced into the mesh by doubling all nodes at the positions of the cracks (node doubling technique). These new nodes possess the same coordinates like the old nodes at the crack position. All elements, which contain these nodes, have to be checked to decide, if it is necessary to replace the old node number by the corresponding new one.

A tensile test for single crystal aluminum samples is simulated. The material parameters are taken as follows [1]:

$\nu_{\langle 100 \rangle}$	$G_{\langle 100 \rangle}$	$E_{\langle 100 \rangle}$	$\tau_{krit}$	$\eta$	$h_{\alpha\alpha}$	$h_{\alpha\beta}$
0.36	28 GPa	63 GPa	0.1 GPa	25 GPa s	0.01 GPa	0.014 GPa

The calculations simulate deformation-controlled tests by prescribing the global rate of deformation  $\mathbf{L}$ . An isochoric tension test is performed with

$$\mathbf{L} = \frac{10^{-4}}{273.3} \text{ s}^{-1} \begin{bmatrix} 8.16 & 0 & 0 \\ 0 & -4.10 & 0 \\ 0 & 0 & -4.10 \end{bmatrix}$$

The applied strain is about 25 %. The calculations are made for a undamaged 2mm×2mm×1mm sample and a sample with a single central crack. This sample is divided into 10×10×1 finite elements. For the computation of a single crystal the crystal axes in the initial coordinate frame have to be defined. The lattice vectors with respect to a cartesian frame are taken as  $G_1 = (0.5, 0, -0.866)$ ,  $G_2 = (0.75, 0.5, 0.433)$  and  $G_3 = (0.433, -0.866, 0.25)$ .

The first simulation is made for one doubled node couple (figure 1). The doubled node couple form a crack with a mode I load condition. By doubling a node, an inner length, which characterizes the load carrying cross section is introduced. Here the number of the doubled node couples is regarded. The simulation is also made for the undamaged material. In figure 2 the global equivalent Cauchy stress  $T_e$  in MPa is plotted over the equivalent value of the Green tensor  $E_{gv}$  for the two samples. This diagram shows that the difference between the damaged and the undamaged material is very remarkably high in the elastic part of the curve and in the transition from the elastic to the plastic part. At higher levels of deformation there is no aggravating difference between the cracked and the undamaged material. To obtain the measured curves, it is necessary to take crack growth into account. However, in a first approach this is neglected and the material behaviour in the elastic and

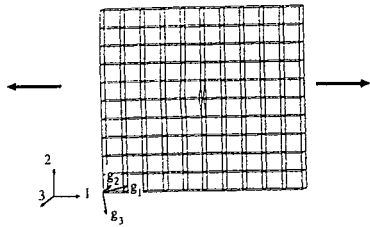


Figure 1: Sample with one doubled node couple

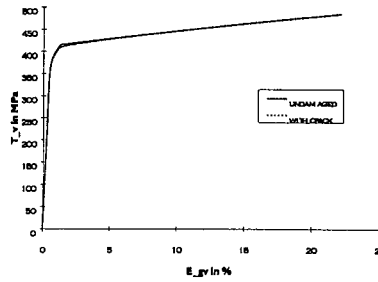


Figure 2:  $T_v - E_{gv}$ -diagram

the transition part is regarded.

In a test program more node couples are doubled. The calculations are made for one doubled node couple (V 1), two (V 2), three (V 3) and four (V 4). This is presented in figure 3. These samples

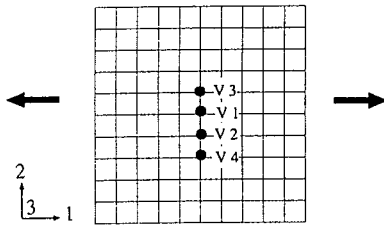


Figure 3: Mesh for calculations V1..V4

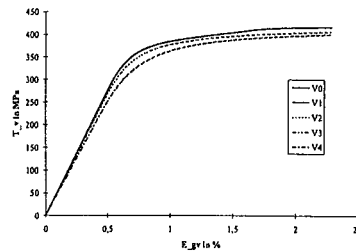


Figure 4:  $T_v - E_{gv}$ -diagram for calculations V1..V4

are submitted to a tensile strain of 0.7%, to investigate the elastic material behaviour and the transition to the plastic part. In figure 4 the equivalent Cauchy stress  $T_v$  in MPa is plotted over  $E_{gv}$ . Depending on the crack size, different Young's moduli are observed. This effect is most significant for the components of the tensile direction (figure 5).

The effective Young's modulus of the cracked material is smaller than the one of the undamaged material. The results can be compared with the equation [13]

$$D = 1 - \frac{E_{\text{damaged}}}{E_{\text{undamaged}}} \tag{9}$$

For the above simulations, the parameter is calculated as:

	V1	V2	V3	V4
D	0.03	0.09	0.16	0.25

The parameter  $D$  grows approximately with the square of the number of doubled node couples. The second difference between the curves is that the cracked material has a smaller range of elasticity

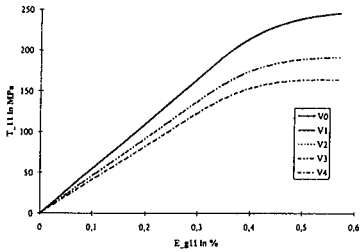


Figure 5:  $T_{11} - E_{g11}$ -diagram for calculations V1..V4

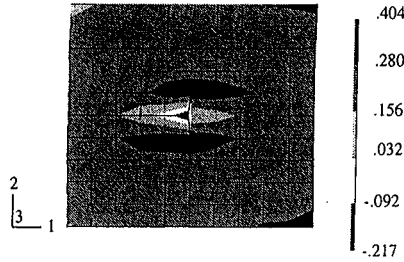


Figure 6: Distribution of  $T_{11}$  in GPa

and that the transition from elasticity to plasticity takes place more gradually at a higher degree of damage. This can be explained by the local higher stresses in the ligament (figure 6). The critical shear stresses in the slip systems are reached, the slip systems begin to glide, and local plastic behaviour in the vicinity of the crack is observed, whereas the material far away from the crack behaves elastically. The homogenization procedure gives the means over the total RVE, which leads to a more gradual transition.

In the following a microstructure is implemented (figure 7). In the center of the sample two node couples are doubled (S1). The next samples include more cracks caused by more doubled node couples. The local stress distribution for S4 is presented in figure 9.

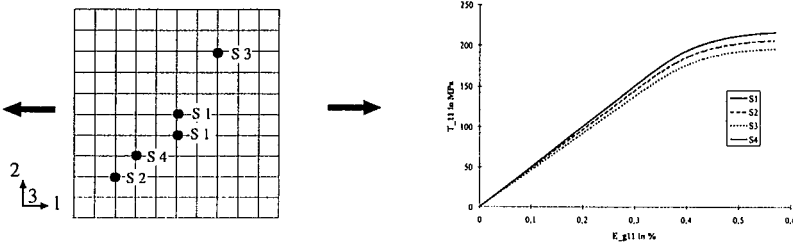


Figure 7: Mesh for S1..S4

The plastic zones at the crack tips are very large. In the region where no forces can be transferred, a local stress relief takes place. In order to obtain the global stress, the means over all this inhomogenities are taken. In figure 8 the global stress  $T_{11}$  is plotted over  $E_{g11}$ . The differences between the curves S1..S4 are less significant than for V1..V4.

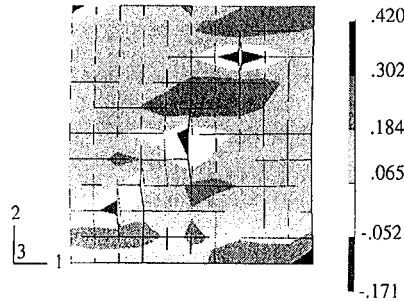


Figure 9: Stress distribution of  $T_{11}$  (in GPa) for S4

This is presented in the following by calculating the damage parameters.

	S1	S2	S3	S4
D	0.09	0.13	0.16	0.20

The calculation S2 is equal to V1. The damage parameter D here grows approximately linear by adding further cracks. A longer crack is more critical than several smaller cracks.

## 5. CONCLUSIONS

Tensile tests of different single crystal aluminum samples are investigated. The comparison of the global material behaviour for a cracked and a undamaged sample shows the expected differences in the Young's modulus. This is used to calculate the damage parameter  $D$ .

The damage influences the transition from the elastic behaviour to the plastic behaviour. For the damaged material the transition takes place more gradually because of the earlier activation of the slip systems in the vicinity of the crack tip and the local relief in the region of the crack.

The applied tests show that it is possible to model the macro-damage by adding cracks into the microstructure and using a suitable homogenization.

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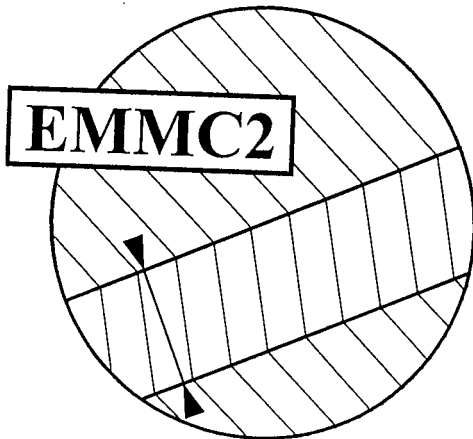
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