ON THE NUMERICAL VARIABILITIES IN APPLYING THE LOCAL CRITERION FOR CLEAVAGE FRACTURE

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ABSTRACT

To apply the local approach of rupture, with a fracture damage not coupled with plasticity, one has first to perform an elastic-plastic computation to calculate the stress and strain fields, and in a second step to calculate the local approach criterion, in introducing metallurgical material parameters. For cracked specimens, due to the strong stress and strain gradients, a very refined mesh is required, and usually the mesh size is chosen large enough to represent the microscopic phenomenon.

The damage criterion is calculated by integration on all plastified elements, but the effective number of elements, participating for more than 1% in the damage value, is limited to a few elements around the crack tip. Considering this very local calculation, the problem we looked to is to evaluate how the computed damage value can depend on the numerical hypothesis. To answer this question, a sensitivity study was carried out on an axisymmetric cracked specimen.

It was concluded that the damage value is not so dependent with the numerical parameters, but the mesh size and stress averaging technique must be well controlled.

1 INTRODUCTION

In a general point of view, the local approach of fracture is defined by the conjunction between:
- the calculation of the elastic-plastic stress-strain history at the most loaded location of a component,
- and the utilization of a physical process of fracture corresponding to a specific mecanism: cleavage, ductile tearing, fatigue, creep ...

For cleavage fracture, statistical models have been proposed for treating the scatter of the fracture toughness and the size effects.

The main problem, when applying these models to a crack tip situation, is that very steep stress gradients are present. This paper presents the numerical variability study carried out on an axisymmetric cracked specimen to analyse the influence of the numerical parameters, taken into account in the finite element computation, on the value of the local criterion.

2 THE WEIBULL STATISTICS

The Weibull statistical model, we considered in our sensitivity study, is briefly described below.
The cleavage fracture is modelled by a two-step process:
- formation of microcracks due to plastic deformation within the grains,
- propagation of these microcracks for a stress level higher than the critical value.
Introducing statistical considerations, the stressed volume is divided into elementary volumes \( V_0 \). \( V_0 \) is large enough so that the physical process described before can occur. The probability of rupture of each elementary volume is written as (Réf. [1]):

\[
P(\sigma_i) = \left( \frac{\sigma_i}{\sigma_u} \right)^m \]

\( \sigma_i \) is the maximum principal stress in the volume \( V_0 \), where the stress state is assumed homogeneous. \( m \) and \( \sigma_u \) are material constants.

For nonhomogeneously stressed specimens and for finite element calculations, the precedent expression is replaced by:

\[
P(\sigma_i) = \left( \frac{\sigma_i^i}{\sigma_u} \right)^m \frac{V_i}{V_0}
\]

where \( V_i \) is the volume of the \( i^{th} \) element experiencing the maximum stress \( \sigma_i \) (Réf. [1]).
The "Weibull stress" is introduced, noted \( \sigma_w \), and defined by:

\[
\sigma_w = \sqrt[m]{\sum_{i=1}^{n} \left( \frac{\sigma_i^i}{\sigma_u} \right)^m \frac{V_i}{V_0}}
\]

The cumulative probability of failure, \( P_R \), for the entire specimen is given by the expression:

\[
\ln(1 - P_R) = \sum_{i=1}^{n} \ln[1 - P(\sigma_i)]
\]

Since \( P(\sigma_i) \) is small, it can be written:

\[
\ln(1 - P_R) \approx \sum_{i=1}^{n} - P(\sigma_i)
\]

Then, the expression of \( P_R \) is given by:

\[
P_R = 1 - \exp \left[ - \left( \frac{\sigma_w}{\sigma_u} \right)^m \right]
\]

When large strains are needed for rupture, a correction of the Weibull stress must be introduced, to take into account the effect of plastic strain on cleavage fracture. The corrected expression for \( \sigma_w \) proposed in Réf. [1] is:
\[ \sigma_w = \sqrt{\sum_{i=1}^{n} \left( \sigma_i^4 \right)^m \frac{V_i}{V_o} \exp \left( - \frac{m \epsilon_i^4}{2} \right)} \]

The Weibull stress is computed in all the mesh elements \( i \) within the plastic zone.

3 IMPLANTATION IN A FINITE ELEMENT COMPUTER CODE

In a finite element calculation, the fracture analysis with such a damage model is performed in two steps:
- calculation of the elastic-plastic response of the structure subjected to the imposed loading conditions,
- calculation of the local approach criterion from the stress and strain fields previously determined, and in introducing metallurgical material parameters.

The value of the Weibull stress is obtained using the following procedure.

First, as it is assumed that in the elementary volumes the stress field is constant, we have to determine the mean stress tensor for each mesh element, by averaging the stresses, in each direction, over the Gauss points:

\[ \sigma_{ij} = \frac{\text{NBG}}{\sum_{k=1}^{\text{NBG}}} h_k \sigma_{ij}^k \]

\( \text{NBG} \) : number of plastified Gauss points,
\( h_k \) : weight of the Gauss point \( k \).

From the mean stress tensor, the principal stress tensor and then the maximal principal stress are determined:

\[ \sigma_1 = \max(\sigma_{11}, \sigma_{22}, \sigma_{33}) \]

In the same way, if the plastic strain correction is taken into account, we calculate the mean plastic strain, in each direction:

\[ \epsilon_{ijp} = \frac{\text{NBG}}{\sum_{k=1}^{\text{NBG}}} h_k \epsilon_{ijp}^k \]

and the projection of the so-determined \( \epsilon_p \) tensor in the direction of the maximal principal stress:

\[ \epsilon_1 = V_1^i \epsilon_p V_1 \]

where \( V_i \) is the normalized vector in the \( \sigma_1 \) direction.

Then, the \( \sigma_1 \) value is eventually multiplied by the corrective term function of \( \epsilon_1 \):

\[ \sigma_1 = \sigma_1 \exp \left( - \frac{\epsilon_1^4}{2} \right) \]

The plastic volume, in each mesh element, is calculated by integration of a function \( F \) equal to 1 (or \( 2 \pi R \) for axisymmetric case) for each plastified
Gauss point, and equal to 0 for other Gauss points:

\[ V_p = \sum_{k=1}^{NB} h_k F_k \text{JAC}, \]

where JAC is the Jacobian of the transformation.

Finally, the Weibull stress is obtained by summation on all mesh elements:

\[ \sigma_w = \left[ \sum_{i=1}^{NB} \left( \frac{\sigma_i^m}{V_o^m} \right) V_i^p \right]^{1/m}, \]

where NB is the number of mesh elements.

4 OBJECTIVE OF THE VARIABILITY STUDY

When applying the proposed criterion to a crack tip situation, the hypothesis made in the formulation, that the stress is homogeneous in a volume \( V_o \), falls through, since the stress field distribution is asymptotic near the crack tip. From a physical point of view, it is assumed, in Réf. [1], that below a certain distance - 1 or 2 grain sizes - the stress field will be constant. Numerically, this is done by inserting a fixed mesh size at the crack tip.

However, considering the steep stress gradients at the crack tip, a sensitivity study has been carried out, on an axisymmetric cracked specimen, to quantify the variation of the damage criterion value with the numerical hypothesis considered in the finite element calculation.

The variability analyses are relative to:
- the elastic-plastic calculation (convergence criterion used in the plastic algorithm, large displacement hypothesis, type of element and mesh discretization),
- the damage criterion calculation (stress averaging technique, plastic strain correction).

5 CRACKED TENSILE SPECIMEN CALCULATION USING STANDARD OPTIONS

5.1 Specimen geometry, material characteristics and loading conditions

The geometry of the axisymmetrically cracked type TA50 specimen, considered in this numerical study, is presented in Figure 1.

The uniaxial stress versus strain curve of the material at -100°C is plotted in Figure 2, and \((\sigma, \varepsilon)\) couples are tabulated in Table 1. Young's modulus is \( E = 210000 \) MPa, Poisson's coefficient is \( \nu = 0.3 \) and the yield stress in \( R_{0.002} = 580 \) MPa.

Material characteristics for the damage criterion calculation are respectively:

\[ V_o = (50 \ \mu m)^3 \quad m = 22 \quad \sigma_u = 2500 \) MPa

The specimen is subjected to an imposed axial displacement.
5.2 Finite element model

The cracked specimen is modelled with 8-node quadratic elements (figure 3). The refined zone at the crack tip (figure 4) is constituted of 24 x 8 square cells, the size of which is defined by the fixed elementary volume $V_0$, i.e. 50 x 50 $\mu$m$^2$.

5.3 Elastic-plastic resolution procedures used

For the stiffness matrix generation, a numeric integration with 3 x 3 Gauss points is used. The plasticity model is defined by a Von Mises initial yield surface and isotropic hardening with a multilinear modelling of the stress versus strain curve. The equilibrium iteration method is based upon the initial stress method, and the convergence is controlled by the residual forces, with a precision of 1/1000. Small displacements are assumed.

5.4 Weibull stress calculation procedures used

The Weibull stress calculation follows the procedure described in 3., and especially the first step corresponds to the average of the stresses, in each direction, over the Gauss points. The correction with the plastic strain is not taken into account.

5.5 Results of the elastic-plastic resolution

The incremental elastic-plastic calculation is conducted using 44 constant displacement increments, $u = 5\mu$m applied at distance L from the crack tip, up to $\Delta L = 0.22$ mm.

The specimen response becomes non-linear at $\Delta L = 0.1$ mm (figure 5). For this load step, plasticity starts to spread, from the crack tip, through the specimen (figure 6). But we can remark that, even at the last load step, the crack plane section of the specimen remains quite fully elastic. The evolution of the crack tip opening displacement (vertical displacement at 100 $\mu$m from the crack tip) as function of the load step shows up the modification in the crack tip loading condition, when plasticity spreads through the specimen: parabolic evolution before $\Delta L = 0.1$ mm corresponding to a load-controlled condition, linear evolution after that corresponds to a displacement-controlled condition (figure 7). The deformed shape at crack tip is visualised in figure 8. The cell behind the crack tip is largely deformed and supports a large part of the crack opening.

5.6 Results of the Weibull model application

The principal stresses which govern the Weibull criterion value are visualised in figure 9. This figure shows up that the maximal principal stresses are located in the cells ahead the crack tip, and are oriented in the traction direction. The maximal principal stress seems not so different from one element to another, but due to the high exponent taken into account in the damage formulation ($m = 22$), the number of elements which have an effective contribution in the Weibull criterion value are reduced to about 10 elements ahead the crack tip (figure 10). The evolutions of the Weibull stress and the cumulative probability of failure as function of the load step are plotted in figures 11 and 12: initiation is predicted at load step 35, i.e. for $\Delta L = 0.175$ mm.
6 VARIABILITY ANALYSES RELATIVE TO THE ELASTIC-PLASTIC RESOLUTION

6.1 Convergence criterion for the plasticity iterative algorithm

A first analysis consists to evaluate the influence of the precision and type of convergence criterion, used in the plasticity algorithm, on the probability of failure.

In a first step, for the same convergence criterion based upon the residual forces, we look to the influence of the precision value:

\[
\text{Convergence criterion } \quad \frac{\maxi (F_{\text{ext}} - F_{\text{int}})}{\sum F_{\text{ext}}} < \text{prec}
\]

Four calculations, with decreasing precision values, are performed: prec = 10^{-2}, 10^{-3}, 10^{-4} and 10^{-5}. The total plastified volumes obtained by all elastic-plastic calculations are almost similar (figure 13). But figure 14 shows up that the precision must be sufficiently low (< 10^{-4}) to obtain a correct Weibull stress, and even lower than 10^{-4} to have a monotonic evolution of the cumulative probability of failure (figure 15). With a bad precision, failure is predicted too early.

In a second step, we compare three different convergence criteria:

1. Convergence on the plastic forces between two successive iterations:

\[
\maxi \left( \frac{\sigma_n^{+1} - \sigma_n^*}{\sigma_n^*} \right) < 10^{-4}
\]

where \( \sigma_n^* \) is the equivalent Von Mises stress in one mesh element for the plasticity algorithm iteration n.

2. Convergence on the maximal value of the residual forces

\[
\maxi \left( \frac{F_{\text{ext}} - F_{\text{int}}}{\sum F_{\text{ext}}} \right) < 10^{-5}
\]

where \( F_{\text{ext}} \) and \( F_{\text{int}} \) are the external and internal forces in one mesh element.

3. Convergence on the norm of the residual forces

\[
\left\langle F_{\text{ext}} \cdot (F_{\text{ext}} - F_{\text{int}}) \right\rangle \left\langle F_{\text{ext}} \right\rangle < 10^{-5}
\]

These three criteria are largely different: the first one is very local, whereas the last one is global.

All calculations are conducted with the best precision in order to avoid error due to a bad convergence. Following this recommendation on the
precision value, figure 16 shows up that the damage value is independant of
the convergence criterion used in the plasticity algorithm: the evolutions
of the Weibull stress as function of the load step are almost similar.

6.2 Updated lagrangian algorithm

The local deformed shape of the specimen (figure 8) shows up large
displacements in the cells at the crack tip. The objective of this analysis
is to quantify the effect of geometry updating (at each elastic-plastic
iteration) in the resolution of the equilibrium equations.

An elastic-plastic calculation with an updated lagrangian algorithm was
performed and than the Weibull stress was evaluated using the post-processor
programm. Weibull stress evolutions, obtained without and with updating,
match well: the large displacement effect is not significant. This result
is not so surprising considering the fact that the most deformed element
behind the crack tip does not effectively participate in the damage
criterion calculation.

6.3 Kind of element

A first analysis is relative to the integration order for the quadratic
interpolation elements. In fact, due to the mesh refinement, the plastic
deformations at crack tip reach large values: \( \varepsilon^* = 30\% \) for \( \Delta L = 0.15 \) mm,
and, in such a case, a reduced gaussian integration is often recommended.

With \( 2 \times 2 \) integration, the number of mesh elements participating
effectively in the Weibull stress calculation is double than with a \( 3 \times 3 \)
integration: this is due to the smooth effect introduced by the reduced
integration. However the Weibull stress is not so much modified, difference
with the reference value being almost 1%.

The second analysis concerns the kind of elements: the four square
elements around the crack tip are replaced by triangular elements. On the
map, figure 18, we can see that only seven elements effectively participate
in the damage criterion evaluation. However the Weibull stress is again not
so much modified.

6.4 Mesh discretization

One principle of the local approach is that the mesh size can not be less
than the elementary volume \( V_0 \). However a coarser modelling can be used when
strain and stress gradients are not steep. In our case, it is interesting to
analyse the effect of the mesh refinement on the failure prediction. A new
mesh is built replacing the \( 24 \times 8 \) square cells by only \( 8 \times 50 \times 50 \) \( \mu m^2 \) in
size cells at the crack tip (figure 19). Whereas this mesh is refined very
locally, the Weibull stress prediction is similar with the reference one.

7 VARIABILITY ANALYSES RELATIVE TO THE WEIBULL MODEL APPLICATION

7.1 Averaging technique procedure

Another principle of the local approach is that the damage criterion must be
calculated from an average of the stresses stored at the Gauss points of the
elements. The question we want to answer is at what step this average must
be done.

In the standard version, the stress average is the first step of the
post-processor program. A mean stress tensor is obtained by averaging the
stresses in each direction. Two other tests are completed introducing the average later:
- average, over the Gauss points, of the maximal principal stress,
- average, over the Gauss points, of the maximal principal stress put to the power m.

A last test is done, without any average, by integration, over the plastified volume, of the values at each Gauss points.

The comparison of the four Weibull stress evolutions (figure 20) shows up that the stresses might be averaged either at the first step, or from the maximal principal stress values, but in any case before putting $\sigma$, to the power m, which leads to predict the failure too much early. This result is not so surprising: m is so high that averaging the stresses put to the power m is ineffective, when a stress gradient is present in one element.

7.2 Plastic strain correction

Due to the refined mesh at the crack tip, large strains are involved at rupture. In this case, a plastic strain correction term must be introduced in the Weibull stress formula. The corrected Weibull stress is plotted in figure 21. The correction term decreases the Weibull stress as the plastified volume increases, but the difference with the reference value is not so important, almost 5 % at the failure step.

8 CONCLUSION

A sensitivity study was carried out on an axisymmetric cracked specimen in order to quantify variabilities with numerical parameters, in applying to local approach to predict cleavage fracture.

Thus steep stress gradients are present at the crack tip, the local criterion is not so dependant upon:
- options used in the elastic-plastic resolution (convergence criterion, small or large displacement hypothesis, kind of elements),
- finite element evaluation of the Weibull stress.

Therefore the following recommendations must be respected:
- local refinement of the mesh at the crack tip with a few $V_o$ in size cells,
- verification of the equilibrium equations with a high precision,
- Weibull stress calculation performed with stresses averaged in each element before putting them to the power m.

A conservative effect on the failure prediction is noted if the plastic strain correction is not taken into account.

ACKNOWLEDGMENTS

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REFERENCE

Table 1 Stress versus plastic strain data

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<th>580</th>
<th>580</th>
<th>581</th>
<th>582</th>
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<th>593</th>
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<th>657</th>
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<th>711</th>
<th>738</th>
<th>758</th>
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<td>$\varepsilon_p$ (%)</td>
<td>0.1</td>
<td>0.29</td>
<td>0.49</td>
<td>0.69</td>
<td>1.18</td>
<td>1.67</td>
<td>2.63</td>
<td>3.58</td>
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<td>5.45</td>
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Table 1 (Continuation)

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<td>$\varepsilon_p$ (%)</td>
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Fig. 1: TA 50 specimen geometry

Fig. 2: Stress versus strain curve

Fig. 3: Finite element model

Fig. 4: Mesh refinement at the crack tip
Fig. 5: Load versus displacement response

Fig. 6: Plastic strain distribution at $\Delta L = 0.15$ mm

Fig. 7: Crack tip opening displacement versus load step

Fig. 8: Deformed shape at $\Delta L = 0.22$ mm

Fig. 9: Principal stresses at $\Delta L = 0.22$ mm

Fig. 10: $\sigma^R/\sigma_{\text{max}}^R$ isovales at $\Delta L = 0.15$ mm
Fig. 11: Weibull stress versus load step  
Fig. 12: Probability of failure versus load step

Fig. 13: Plastified volumes for different precision tests  
Fig. 14: Weibull stress for different precision tests

Fig. 15: Probability of failure for different precision tests  
Fig. 16: Weibull stress for different criterion tests
Fig. 17: $\sigma_1^m/\sigma_{1\text{max}}^m$ isovalues with reduced integration

Fig. 18: $\sigma_1^m/\sigma_{1\text{max}}^m$ isovalues with triangular elements

Fig. 19: Mesh refined locally

Fig. 20: Weibull stress for different averaging techniques

Fig. 21: Weibull stress with plastic deformation correction