MODELING DUCTILE DAMAGE OF STEEL IN AGGRESSIVE ENVIRONMENT

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Abstract: This paper is a proposition of a new damage model, extended to include the influence of the external environment, based on the Gurson yield function and a new damage evolution equation. The model also contains a mass transport equation based on Fick’s law. A comparison of experimental and numerical results is included.

Keywords: stress corrosion damage, reaction-diffusion equations, damage evolution equation, FEM

1. Introduction

In order to determine whether a material is damaged it may be necessary to study its cleavage, ductility, fracture, creep, fatigue and corrosion. Local models can be formulated for cleavage [1], creep [2–5] and low-cycle fatigue. Ductile fracture has received considerable attention since the initial study [6] that first recognized the formation and growth of microvoids as the governing mechanism of rupture. Since then, a number of papers have been published addressing both experimental and modeling issues. Ductile damage is described in terms of void volume fraction \( \omega \) that affects a material’s plastic potential at the macroscale by means of a softening term. The damage evolution law is developed from the study of a single isolated cavity in “virgin”, undamaged material. In this context Rice and Tracy [6] proposed their relation for the cavity growth rate. A modified yield criterion for ductile metals with increasing porosity was derived later in [7]. Void nucleation was incorporated into the Gurson model by Needleman [8] and adopted to creep damage by Bielecki [4]. Against this background, the author of this paper has decided to add the influence of the external environment to the well-known Gurson-Needelman model. Numerous experimental results have shown that aspect or external influence cannot be neglected and is one of the main factors resulting in material damage [9–13]. Similar results can be found in [14–16].

2. Governing equations of the general theory

The model consists of two parts: the mechanical and the diffusion-reaction part.
2.1. Mechanical

We confine ourselves to a situation in which the deformation rate, \( \dot{\varepsilon}_{ij} \), is a sum of the elastic and plastic parts:

\[
\dot{\varepsilon}_{ij} = \dot{\varepsilon}^{\text{el}}_{ij} + \dot{\varepsilon}^{\text{pl}}_{ij}. \tag{1}
\]

The elastic part of a strain tensor is defined as [6]:

\[
\dot{\varepsilon}^{\text{el}}_{ij} = 1 + \nu^{\text{eff}} \frac{E^{\text{eff}}}{\sigma_{ij}} - \nu^{\text{eff}} \frac{E^{\text{eff}}}{\sigma_{kk}} \delta_{ij}, \tag{2}
\]

where, as Robotnov has suggested [2]:

\[
E^{\text{eff}} = E_0 (1 - \omega), \quad \nu^{\text{eff}} = \nu_0 (1 - \omega), \tag{3}
\]

where \( \nu_0 \) and \( E_0 \) are respectively the Young and Poisson elastic moduli of a “virgin” material. The yield function depends on the linear invariant of \( \sigma_{ij} \) and the quadric invariant of \( \sigma_{ij} \). The model involves two variables of state: the equivalent microscopic plastic strain, \( \varepsilon_{\text{pl}} \), and \( \omega \), defined as volume fraction of voids. The yield surface is of the following form [7]:

\[
\Phi(q, p, \varepsilon_{\text{pl}}, \omega) = \left( \frac{q}{\sigma_y} \right)^2 - 2\omega \cosh \left( \frac{-3p}{2\sigma_y} \right) - (1 + \omega^2) = 0, \tag{4}
\]

where \( q = \sqrt{\frac{3}{2}} S_{ij} \) is the Huber-Mises equivalent stress, \( S_{ij} \) is the deviatoric part of \( \sigma_{ij} \), \( p = -\sigma_{kk}/3 \) is hydrostatic stress and \( \sigma_y \) is the flow stress of the matrix material. The yield function is used as the plastic potential, so that:

\[
\dot{\varepsilon}_{ij} = \lambda \frac{\partial \Phi}{\partial \sigma_{ij}} = \frac{\lambda}{\sigma_y} \left[ 3S_{ij} - \omega \sinh \left( \frac{3p}{2\sigma_y} \right) \delta_{ij} \right]. \tag{5}
\]

The evolution equation for variable \( \varepsilon_{\text{pl}} \) is based on the requirement that macroscopic plastic work \( \sigma_{ij} : \dot{\varepsilon}^{\text{pl}}_{ij} \) equals \( (1 - \omega) \sigma_y \varepsilon_{\text{pl}} \), so:

\[
\varepsilon_{\text{pl}} = \frac{\sigma_{ij} : \dot{\varepsilon}^{\text{pl}}_{ij}}{(1 - \omega)\sigma_y}. \tag{6}
\]

As a porous metal deforms plastically, its porosity may change due to the growth or closure of the existing voids or nucleation of new voids:

\[
\dot{\omega} = \dot{\omega}_{gr} + \dot{\omega}_{ini}. \tag{7}
\]

Assuming that the cristal material is plastically incompressible, it can readily be demonstrated that:

\[
\dot{\omega}_{gr} = (1 - \omega) \varepsilon_{\text{pl}}^{kk}. \tag{8}
\]

We consider plastic strain-controlled nucleation such that:

\[
\dot{\omega}_{ini} = \mathcal{A} \varepsilon_{\text{pl}}^{m}, \tag{9}
\]

where, as suggested in [17], parameter \( \mathcal{A} \) is so chosen that the nucleation strain follows a normal distribution with mean value \( \varepsilon_N \) and standard deviation \( S_N \):

\[
\mathcal{A} = \frac{f_N}{S_N \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\varepsilon_{\text{pl}}^m - \varepsilon_N}{S_N} \right)^2 \right], \tag{10}
\]

\( f_N \) being the volume fraction of void-nucleating particles.
2.2. *Mass transport in metal*

Let us formulate the general problem for chemical compound transport in metal as follows:

\[
\frac{dc^k}{dt} = \nabla \cdot (D^k \nabla c^k) + S^k, \tag{11}
\]

where \(c^k\) is a concentration of \(k\)th chemical compound in metal, \(D^k\) is the diffusion coefficient tensor of a given corrosive factor and \(S^k\) is the source. In our model the diffusion coefficient tensor is a function of total strain and local damage:

\[
D^k_{ij} = D^{k,0}_{ij} \exp \left( -\frac{Q^k}{RT} \right) A^{k,1}_{ij} \varepsilon_{tot}^{ij} + \omega D^{\omega,0}_{ij} \exp \left( -\frac{Q^\omega}{RT} \right) \delta_{ij}, \tag{12}
\]

where \(Q^k\) and \(Q^\omega\) are activation energies of a given chemical compound and damage, \(A^{k,1}\) is the material constant for steel and the chemical compound, \(T\) is temperature and \(R\) – the gas constant. Now the model includes an extension of the damage evolution equation (7):

\[
\dot{\omega} = \dot{\omega}_{gr} + \dot{\omega}_{ini} + \dot{\omega}_{chem}, \tag{13}
\]

where \(\dot{\omega}_{chem}\) is the source of damage due to the concentration of a given chemical compound:

\[
\dot{\omega}_{chem} = \sum_{k=1}^{n} A^k c_k \exp (c^{H_2O}), \tag{14}
\]

\(A^k\) being a material constant and \(c_k\) the concentration of a given chemical compound.

3. **Numerical examples**

The model contains many material constants, so the first step in their calibration should be a comparison of numerical and experimental data of steel samples under external mechanical force in ambient (e.g. air) and corrosion environment.

3.1. **Sample in air**

First, a comparison was made of experimental and numerical results for a sample in air.

| Table 1. Material constants for 34CrAlNi7 steel; \(q = 1.5\) value taken from [18] and [19] |
|---|---|---|---|---|---|---|
| \(n\) | \(b\) | \(f_N\) | \(\varepsilon_N\) | \(s_N\) | \(q\) |
| 4.03 | 501.3 | 0.003 | 0.29 | 0.09 | 1.5 |

Exemplary results of Huber-Mises stress taken from calibration tests are shown in Figures 1 and 2. A comparison of experimental and calculated strain-force curves for material parameters taken from Table 1 is presented in Figure 3 with quite good compatibility. In Figure 4, a normalized Huber-Mises stress and damage parameter \(\omega\) is presented versus global strain for five areas of the sample’s cross-section at half length; the value of stress decreases with increasing value of damage parameter. The same effect is presented in Figures 5 and 6, taken from point “D” in Figure 4.

3.2. **Sample in \(H_2SO_4\)**

Further calculations were performed for the same sample filled in \(H_2SO_4\), starting with calculations of the aggressive compound’s concentration. The initial
Figure 1. Example of calculations: Huber-Mises stress in a sample, point “B” in Figure 4

Figure 2. Example of calculations: Huber-Mises stress in a sample, point “D” in Figure 4

Figure 3. Results of comparison of numerical and experimental strain-force curves, sample in air
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Figure 4. Normalized stress and damage parameter versus strain, results of calculations

Figure 5. Huber-Mises stress at the sample’s cross-section at half length, at point “D” in Figure 4

Figure 6. Damage parameter $\omega$ at the sample’s cross-section at half length
concentration of hydrogen at the sample’s boundary surface can be calculated from the hydrolysis reaction of $\text{H}_2\text{SO}_4$:

$$0.01 \text{M} \xrightarrow{x} \frac{\text{H}_2\text{SO}_4}{\text{H}_2\text{O}} \xrightarrow{} 2\text{H}^+ + \text{SO}_4^{-4}, \quad \text{so} \quad x = 2.04 \cdot 10^{-4} \text{M}. \quad (15)$$

As in the previous case, comparison of experimental and numerical strain-force curves obtained for material parameters from Table 2 is presented in Figure 7. Normalized Huber-Mises stress versus strain is presented in Figure 8 and exhibits
Table 2. Model constants for 34CrAlNi8 steel; \( q = 1.5 \) value taken from [18, 19]

<table>
<thead>
<tr>
<th>( n )</th>
<th>( b )</th>
<th>( f_N )</th>
<th>( s_N )</th>
<th>( q )</th>
<th>( c_0 )</th>
<th>( A^{\text{tot}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.81</td>
<td>487.4</td>
<td>0.003</td>
<td>0.29</td>
<td>0.09</td>
<td>1.5</td>
<td>( 2.04 \cdot 10^{-4} )</td>
</tr>
</tbody>
</table>

Figure 9. Sample results of corrosive factor’s (H\(^+\)) penetration into metal (\( \varepsilon = 0.026 \))

Figure 10. Sample results of corrosive factor’s (H\(^+\)) penetration into metal (\( \varepsilon = 0.062 \))
the same effect as that presented in the previous subsection. Figures 9 and 10 present stress diffusion of hydrogen for two elongations $\varepsilon = 0.026$ and $\varepsilon = 0.062$.

4. Conclusions

- The present paper is a compilation of ideas of CDM (effective elastic moduli), Gurson’s yield function with Needleman extension and Fick’s law, and describes ductile damage of steel samples in an aggressive environment. A comparison of experimental and numerical $F - \varepsilon$ is presented in Figures 3 and 7.
- The proposed mechanism of coupling between the stress state and mass transport yields similar results as that given by Yokobori [20]. It means that the concentration of hydrogen in the place where the material is stressed is higher and it penetrates the metal more intensely (Figures 9 and 10).
- A simple form of the equation for damage from the presence of chemical compounds (Equation (14)) is good enough to describe the influence of a corrosive factor.

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References


