Numerical study to identify the material parameters of a damage model

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Abstract. In the continuous casting (CC) process, transversal cracks happen. This type of macroscopic damage is due to the process loading in the bending and unbending area of the CC line. In order to study this damage, a 2D model was developed. It simulates the intergranular crack at the mesoscopic level. Already validated for a microalloyed steel with C level < 0.1 wt%, this model must be extended to peritectic and stainless steels. The first step is to identify the model parameters for these grades. The type and the quantity of hot tensile tests required to identify a single set of parameters for the damage law must be determined. So, simulations of hot tensile tests of notched samples are needed. The computed stress and strain histories are applied on the representative mesoscopic cell and the moment of rupture is determined in function of the input parameters. Thanks to inverse modelling, the parameters of the damage law are adapted in order to get one single set of parameters with only two different geometries of notch.

Keywords: hot tensile test, continuous casting, steel, hot ductility, transverse cracking

1. Introduction

Continuous casting of steel became in recent years the first way to produce steel in large quantities. The technology and the production speed have quickly improved and the product quality has increased. So nowadays, to control this process in the best way, the comprehension of each step and each material grade must be studied.

A relevant problem in the production of low carbon steels and stainless steels by continuous casting is the appearance of transverse cracks. Actually, the temperatures of the steel during the process decreases from the liquidus temperature to the ambient passing by a very sensitive temperature range extending from 600°C to 1000°C (Brimacombe & Sorimachi, 1977; Suzuki et al., 1984) where a loss of ductility generates a weakness of the material. The material reaches in general this sensitive temperature range in the unbending area (Pascon et al., 2005) of the continuous casting mill. These cracks can be related to the steel grade but also to the mechanical and the thermal fields occurring during the process and to other factors such as the oscillations marks caused by the vertical oscillations of the mould.

The crack propagation for these steels in this temperature range is known to be intergranular and the damage mechanism occurring is a grain boundary sliding accompanied by creep controlled diffusion (Mintz et al., 1991). Thanks to a mesoscopic cell described in Castagne et al., 2003, which represents the microstructure of the material, it is possible to model this effect. The developed model needs thermomechanical histories from the macrosopic scale, which are available through a macroscopic finite element analysis of the continuous casting process like described in Pascon et al., 2005.
The identification method to determine the parameters of the damage law is described in section 2. The rest of the paper focuses on the parameters that have to be determined by the tensile tests (section 3). The results are presented in section 4.

2. Numerical study

In order to validate the damage model used in this study for stainless steels and peritectic grades, one must verify its prediction with experimental studies. In fact, it is important to get identical loading curves and fracture moments in the simulations and in the experimental studies. The damage study has to be achieved with only one set of material parameters. In order to reach this goal, different steps will be done. At first, tensile tests applied on samples with different shapes are performed in order to get different macroscopic stress-strain histories. A representative mesoscopic cell has to be designed that has the same microscopic properties than the true material. Then, the representative cell has to be loaded by the macroscopic history recovered from the macroscopic tensile test. Finally both curves, the one coming from the tensile test and the one coming from the mesoscopic simulation can be compared and the crack appearance is followed. All these different steps are described in the following chapters.

a. Tensile test modelling

Before doing expensive mechanical tests, the tensile test is simulated in order to know if the expected results will be there. In the real case, the test will be performed on a TREBEL hot tensile testing machine. This apparatus allows us to get temperature history close to the real case in the continuous casting mill. The sample shape (figure 1) presents a cylindrical section that is modelled only on ¼ of the whole sample.

To get the damage law parameters it is important to have a rich macroscopic history to load the cell. This will be obtained by notched samples providing different triaxialities, so most complete stress tensors with not only an axial loading but also circumferential stresses will be studied.
b. The mesoscopic representative cell

The creation of the representative cell is based on the one proposed by Castagne et al., 2006. It is composed of a central part that is the mesoscopic cell containing the grains with their grain boundaries and a surrounding part called the transition zone.

The transition zone serves to get a homogeneous stress and strain field around the cell. So it is possible to know quite precisely the stress and strain fields in the cell and to compare them to the real values occurring in the tensile test.

The grains and the transition zone are modelled with elements following a Norton-Hoff creep law given by equation [1].

\[
\sigma_e = \varepsilon_e^{p_1} \cdot \exp(-p_2 \varepsilon_e) \cdot p_3 \cdot \sqrt{\beta} \cdot (\sqrt{\beta} \cdot \dot{\varepsilon}_e)^{p_4}
\]  

[1]

The grain boundaries are modelled thanks 2D elements taking into account the cavitation and the sliding at the grain boundary. These elements are associated with the damage law which includes parameters linked to the presence of precipitates, voids, etc. In this law, a damage parameter explicitly defines the crack phenomenon. This law follows the cracking of the cell and determines the first crack appearance occurring through the mechanism of voids nucleation, growth and coalescence at high temperature. In this damage law \(a\) (cavity size) and \(b\) (distance between cavities) are the guiding parameters for the calculation of the different state variables occurring in the damage equations.

The design of the cell is based on a micrograph of an austenitic steel grade (figure 2) which presents a grain size of approximately 200µm.

![Figure 2: Metallographic inspection of sub surface, austenite grains and ferrite grain-boundary (Arcelor Research)](image)

The size of the cell (figure 3a) is calculated in order to have more or less 100 grains in the centre cell (figure 3b). So with a fast calculation the dimensions are the following:

- Cell = 2x2mm
- Cell + transition zone = 20x20mm
c. Loading of the cell

The cell is loaded by displacement in the z direction and forces in the x and y directions (figure 4). These displacements and forces are extracted from the macroscopic simulation of the tensile test. The displacements and the loading are taken from the critical area of the sample that is here the notched element. The coherence of the fields where verified by comparing the mean stress values of the elements of the transition zone in the mesoscopic cell to the critical element of the tensile test sample.

The simulations have been performed on two different shapes of tensile test samples. However both have low triaxialities, $\chi_1 = 0.335$ and $\chi_2 = 0.342$, they have been used to compare the sensibility of the different damage parameters subjected to changing triaxialities.

![Figure 3: Representative cell a) Transition zone + Cell, b) Cell](image)

![Figure 4: Loadings on the representative cell](image)

d. Loading curves and material damage

The chosen loading of the representative cell yields to identical mean forces in the elements of the transition area and in the notched element of the tensile test (figure 5). So the mechanical behaviour imposed to the representative cell (at the mesoscopic scale) is representative of the performed tensile test (at the macroscopic scale).

The loss of contact between two grains is identified by a damage parameter $a/b = 0.7$. If $a/b \geq 0.7$, a crack is appearing in the structure of the representative cell. The three first
cracks were noticed and the damage curve of the first cracking integration point was drawn as we can see it in figure 6.

![Figure 5: Comparison between forces extracted from the macroscopic tensile test and from the mesoscopic damage simulation](image)

The crack mechanism is divided into several stages. On the first hand the intergranular sliding (Ashby, 1972) is taken into account and on the other hand the nucleation, growth and coalescence of the cavities theory is used.

The damage curve shows the different stages in the damage evolution. The first step (I) shows a very slow damage increase due to the diffusion of voids and growth of those already present. Second step (II) presents a fast increasing of the damage. It indicates the beginning of nucleation, that is to say appearance of new cavities. Then the saturation state is reached (III), the growth of the damage slows down because no more cavities can be created. Step IV shows the crack appearance where $a/b = 0.7$.

![Figure 6: Damage parameter curve](image)
3. Law parameters and sensibility

The law used and described in Castagne et al., 2003 to determine the crack appearance in steel slabs is composed of different parameters (table 1) that have a particular role to play in the physical understanding of the rupture.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Description</th>
<th>Determination of the value</th>
<th>Literature</th>
</tr>
</thead>
<tbody>
<tr>
<td>d [mm]</td>
<td>Mean grain size</td>
<td>micrographic analyses</td>
<td></td>
</tr>
<tr>
<td>$D_{b0} \delta_b$ [mm$^3$s$^{-1}$]</td>
<td>Boundary diffusivity</td>
<td></td>
<td></td>
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<tr>
<td>$\Omega$ [mm$^3$]</td>
<td>Atomic volume</td>
<td></td>
<td>Needlemann and Rice (1980) data for austenite</td>
</tr>
<tr>
<td>$Q_b$ [N.mm/mol]</td>
<td>Activation energy</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\dot{\varepsilon}_c / \dot{\varepsilon}_B$</td>
<td>Grain viscosity parameter</td>
<td></td>
<td>Hot tensile test with different sample shapes (cylindrical, notched low, notched high) 973°K &lt; T &lt; 1173°K $\dot{\varepsilon} = 1x10^{-3}$ s$^{-1}$ or $5x10^{-4}$ s$^{-1}$ Validation of the parameters from simulations predicting cracking at the right time in regard with the experiment</td>
</tr>
<tr>
<td>$F_n$ [mm$^{-2}$]</td>
<td>Nucleation parameter</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$N_i$ [mm$^{-2}$]</td>
<td>Initial density of cavities</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\psi$ [°]</td>
<td>Cavities angle</td>
<td></td>
<td></td>
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<tr>
<td>a [mm]</td>
<td>Initial cavity size</td>
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<tr>
<td>b [mm]</td>
<td>Initial cavity distance</td>
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<tr>
<td>$N_{\text{max}}$</td>
<td>Nucleation threshold</td>
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<tr>
<td>a/b</td>
<td>Rupture criterion</td>
<td></td>
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<tr>
<td>n (T)</td>
<td>Creep exponent</td>
<td></td>
<td>Compression tests at constant T and $\dot{\varepsilon}$ T = 700, 800, 900, 1000, 1100 °C and $\dot{\varepsilon} = 0.01, 0.001, 0.0001$s$^{-1}$ Adjustment of the Norton-Hoff law parameters (equation [1])</td>
</tr>
<tr>
<td>$B$ (T) [MPa$^{-n}s^{-1}$]</td>
<td>Creep parameter</td>
<td></td>
<td>Maximal strain depending on the temperature $\varepsilon = 7%$ et $\dot{\varepsilon} = 10^{-3}$ s$^{-1}$</td>
</tr>
<tr>
<td>$\Sigma_0$ (T) [MPa]</td>
<td>Normalisation stress</td>
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<tr>
<td>$\Sigma_0$ (T) [MPa]</td>
<td>Normalisation stress</td>
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<tr>
<td>$k_n$ [MPa.mm$^{-1}$]</td>
<td>Penalty coefficient on the contact pressure</td>
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<tr>
<td>$k_s$ [MPa.mm$^{-1}$]</td>
<td>Penalty coefficient on the shear frictional stress</td>
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</table>

Table 1: Parameters entering the damage law and ways to identify of them

4. Results

Out of the seven parameters from the damage law that are determined by tensile tests, four will be studied. The first imposed parameter is $\psi$. This parameter stays constant during the whole test $\psi = 75^\circ$. The second imposed value is the rupture criterion $a/b$ that is imposed at 0.7. The third is the grain viscosity parameter and is imposed at a value of 10. The setting of these three parameters was made on the bases of results from Onck & van der Giessen (1999). We fixed also the parameter but the sensibility of this parameter should also be determined.

To study the sensibility of the damage law, the four modified parameters that have been are the nucleation parameter $F_n$, the initial cavity density $N_i$, the initial distance between cavities $b$ and the initial cavity size $a$.

- $F_n$ has a great influence in the nucleation phase of the damage evolution (figure 7). Indeed, when $F_n$ is important, the nucleation is faster and begins earlier. It is possible to take into account the microstructure gradient thanks different values of the nucleation parameter in the structure that implies a gradient of the precipitation according to any depth or the direction.
In the threshold calculation $N_I$ stands for the minimum cavity density from which the nucleation can be observed. It is a sort of incubator. If $N_I$ is great, the nucleation is delayed and so the end of the nucleation happens later. The crack appearance is very sensible to any modification of the parameter $N_I$.

- $b$ has an effect on the first phase of the damage evolution. If the value of $b$ is low, the nucleation start is delayed.

- A change in the value of $a$ can define an initial damage that could be used to put some weakened zones in the material.

Figure 7: Influence of the variation of the parameter a) $F_n$, b) $N_I$, c) $b$, and d) $a$ on the damage evolution for the case $\chi_1$.

Figure 8: Three first crack appearances for the variation of different parameters.
As shown in figure 8, it will be easy to determine the parameter $N_I$ from the tensile tests. The other parameters are not as sensible to a modification as $N_I$. In order to see if these parameters could have an influence, additional different shapes of sample will be used. Figure 8 shows the crack prediction for low values of triaxiality; it could be interesting to use greater triaxialities to improve that point.

5. Conclusions

Some fundamental parameters of the used damage model were analysed. How the model reacts to each parameter was studied. It has been seen that $a$ and $b$ are the guiding parameters and also thresholds for the nucleation. As soon as the ratio $a/b$ reaches the value of 0.7, a crack can appear in the structure and the grains are separating from each other. But all the parameters described in the paragraph 3 are relevant for the calculation of the damage. And that's why it is important to notice that the determination of all these parameters has to be done in the best way in order to get the most accurate values for these parameters. The current chosen experimental test (hot tensile test) has almost the same properties and the same characteristics that the real case of the continuous casting.

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