Development of a Microscopic Damage Model for Steel at High Temperature

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1 Introduction

Transverse cracking is recognized as a problem in continuous casting (CC) of steel. Experimental studies have demonstrated the existence of an embrittlement of steel in the temperature range from 600 to 1000°C. This loss of ductility is responsible for the appearance of cracks during the bending and unbending operations of the strand.

The research aims to model the damage process at elevated temperature using a microscopic approach. In the studied temperature range, creep has to be considered. Experimentally, cracks have been shown to be intergranular.

The first step in the development of the damage model is the construction of a 2D cellular model representative of the material. As the microstructure influences damage and creep, it has to be introduced in the model if we want to determine the predominant factors for crack initiation. Diffusion of voids and grain boundary sliding are taken into account. The cell, which includes grains and their boundaries, will be submitted to stress and strain fields determined by macroscopic experiments.

The damage law will be implemented in the finite element code LAGAMINE developed in the MSM Department and it will be applied to model CC of steel. The final goal of the research is a parametrical study of various microscopic factors such as grain size, precipitation state or oscillation marks on the initiation of transverse cracking during the CC process.

2 Crack appearance in CC

The importance of two zones of low ductility in steels has been demonstrated [1]: the first one exists above 1340°C and probably accounts for the formation of all internal cracks and surface longitudinal cracks while the other one lies between 600 and 1000°C and is related to the appearance of transverse cracks in slabs that is the particular point we want to study. To minimise crack formation, the control of the steel chemistry is absolutely essential. A lot of research work is done in this domain by the metallurgical community. Nevertheless, the measures to prevent transverse cracks are divided into two parts: certainly the control of the steel chemistry but also the prevention of the crack initiation and propagation due to the mechanical solicitations during the process. This second point is the principal objective of our study.

Mintz realised a large review on the hot ductility of steels and its relationship to the problem of transverse cracking during CC [2], [3]. The four most important variables that control ductility are strain rate, grain size, precipitation and inclusion content. Increasing the strain rate and refining the grain size give rise to improved ductility: the former by reducing the amount of grain boundary sliding and the latter by making it more difficult for crack to propagate along the boundaries. On the other hand, when the particles at the boundaries are finer, they are closer to each other and it is easier for cracks to interlink.

According to Harada *et al.* [4], the origin of cracks is the microsegregation. The formation mechanism of the surface segregation, particularly of phosphorous, has a close relation with that of oscillation marks which are caused by the vertical oscillations of the mould during the CC. When an oscillation mark is formed, the partially solidified shell is deformed and the dirty segregated liquid steel between dendrite arms is squeezed out to the surface. The degree of segregation depends on the depth of the oscillation marks. Internal cracks may be formed at the subsurface below an oscillation mark. When the surface temperature along the mark reaches the low ductility temperature zone, cracks sensitivity increases.

Suzuki *et al.* [5] propose to reproduce experimentally the oscillation marks and to study their in-

fluence. One of their most important conclusion is that the oscillation marks have to be reduced in order to enhance the resistance to transverse cracking but the shape of these oscillation marks seems to have no effect on the sensibility to crack, only the depth has an influence. The effect of the Nb content is also exposed, the conclusions are that the trough of the ductility curve go deeper and wider as the Nb content is incremented and that the combination of Nb and Al is very detrimental due to the precipitation of nitrides and carbonides. Also, the effect of strain rate was studied, it has been shown that the embrittlement decreases when the strain rate increases.

3 Creep damage modelling

3.1 State-of-the-art

Since the pioneering works of Kachanov, 1958, and Robotnov, 1959, quite a large number of papers on modelling of creep damage for polycrystalline materials have been published (see [6] for references). Most of the research work for damage at elevated temperature focus on the computation of the life time of a structure in service. Usually fatigue and creep are incorporated into the models in which time is an important variable. Models specially dedicated to creep are not very accurate to reproduce the damage phenomenon in CC where time scale is quite small. Another point is that continuum damage mechanics (CDM) enables to compute damage evolution in complex structure ; nevertheless, a more accurate physical description of microscopic process involving damage is necessary to improve the existing models. Indeed, it is difficult to account for all the physics of the phenomena only with macroscopic descriptions. Moreover, continuum damage models suffer from a lack of mesh independence and from localisation phenomenon. The introduction of a material length scale is necessary to overcome this problem.

In the framework of micro-macro modelling, Liu *et al.* [7] propose a new approach where they introduce a continuum damage variable and calculate its evolution on the basis of polycrystal microstructures simulated by Voronoi tessalation and models of cavity nucleation and growth. This approach to creep-cavitation damage is developed by combining the basic features of the CDM approach and microscopic mechanisms. First, an anisotropic continuum damage variable is defined directly based on the microcrack system of the simulated microstructure. Then, its evolution is given applying the mechanism-based equations of cavity nucleation and growth to each grain boundary in a Voronoi microstructure. This damage variable is then coupled with constitutive equations of continuum damage mechanics to analyse creep damage. Finally, macroscopic creep deformation coupled with this damage variable is calculated by CDM equations. Another scientific team, Onck *et al.* [8], proposes a multiscale study of polycrystalline materials at elevated temperature under creep conditions which are subject to intergranular cracking. The relevant damage mechanisms at the microscale, i.e. viscous grain boundary sliding, nucleation, growth and coalescence of cavities leading to microcracks are taken into account. The zone around the crack tip is modelled with special grain elements linked with boundary element while the surrounding material, far from the crack tip, is represented by a classical creep law. Actually, the grains surrounding the propagating crack are represented individually. Cavitation and sliding along all grain boundaries in this zone are described by a set of constitutive equations based on micromechanical studies at smaller scales. Grain elements account for creep deformation of individual grains and are connected by interface elements that incorporate physical mechanisms active at grain boundaries.

As far as intergranular failure is concerned, the microstructure has to be reproduced. Voronoi tessallation is used by various authors in order to have a certain randomness of the grain disposition while keeping the specific characteristics of the studied material [7], [9].

3.2 Development of a new microscopic representative cell and its exploitation for CC

The material used for the study is a microalloyed steel with C level < 0.1 wt%. The elaboration of the model requires lots of microscopic and macroscopic experiments. A metallographical analysis will determine the size and the shape of the grains. The chemical composition of the material will inform us on the nature of the precipitates which could be present at grain boundaries. Hot traction and compression tests on healthy or not material will help to identify the damage and creep laws and to validate the damage model. Non-destructive damage tests are also planed [10], they use an acoustic technique to determine the moment of initiation and the localisation of the first cracking. The CC conditions should be reproduced in the experiments, that is why the samples will be heated up to 1350°C before testing and then cooled down to the test temperature.

In order to represent intergranular creep fracture, the developed model contains grain elements and grain boundary elements (see also [8]). The laws governing our model are described here after, the grain contains an elastoviscoplastic law without damage and the boundary a law with damage.

3.2.1 Solid finite elements and grain representation

The grain is modelled by thermomechanical solid elements available in LAGAMINE code. Figure 1 shows an example of the microscopic representative cell. On the rigth part, a zoom on three grains allows to visualise the meshing of these grains and their interfaces.

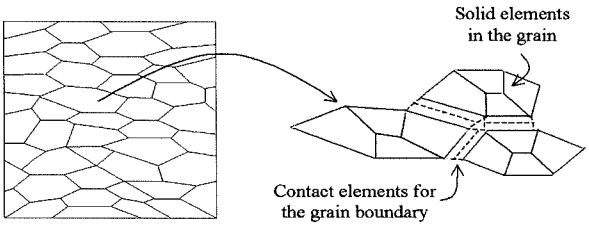

Figure 1: Microscopic representative cell

The creep behavior inside the grain can be represented by Norton Hoff law (1):

$$(1) \qquad \overline{\sigma} = \overline{\varepsilon}^{p_4}.\exp\left(-p_1\overline{\varepsilon}\right).p_2.\sqrt{3}.\left(\sqrt{3}\dot{\overline{\varepsilon}}\right)^{p_3}$$

where p_1 to p_4 are parameters that depend on temperature. These parameters will be identified thanks to the macroscopic experiments on the healthy material.

The number of grains in the microscopic cell as well as the density of the mesh inside the grains have to be tested to define a cell which gives accurate results with a reduced CPU time.

The shape and size of grains will be determined from results of the microscopic analysis.

3.2.2 Contact finite elements and grain boundary representation

As the thickness of the grain boundary is small compared to the grain size, we represent the grain boundary by a one-dimensional element (cohesive zone). This element will be associated with a constitutive law which includes parameters linked to the presence of precipitates, voids, etc. The damage variable will appear explicitly in this law.

We want to follow the initiation and the propagation of cracks by coalescence of micro-voids in the grain boundary, so we propose to use interface elements to represent the cohesive zone. This type of elements is available in the LAGAMINE code, it has been used by Charlier [11] for the study of shear bands localisation. Here follows a brief description. For the interface element the stress tensor has only two components $\Sigma^T = [p, \tau] = [\sigma_{11}, \sigma_{12}]$. Let $\underline{u}$ be the distance between the two faces of the cohesive zone, if the strain is constant on the thickness e of the cohesive zone, we have:

$$(2) \qquad \dot{\varepsilon}_{11} = \frac{\dot{u}_1}{e} \qquad \text{and} \qquad \dot{\varepsilon}_{12} = \frac{\dot{u}_2}{e}$$

The assumption that the strain rate along the element can be neglected gives the last component $\dot{\varepsilon}_{22}$ equal to zero. If we consider, to simplify the explanation, an elastic constitutive law for the interface element, we have the following relation:

$$(3) \quad \underline{\dot{\sigma}} = \begin{bmatrix} \dot{p} & \dot{\tau} \\ \dot{\tau} & z \end{bmatrix} = \underline{\underline{C}}\,\underline{\dot{\varepsilon}} = \frac{1}{e}\,\underline{\underline{C}} \begin{bmatrix} \dot{u}_1 & \dot{u}_2 \\ \dot{u}_2 & 0 \end{bmatrix}$$

The elastic tensor divided by the thickness e is equivalent to a penalty matrix in contact finite elements based on penalty approach. The elastic law will obviously be replaced by a constitutive law with damage in our model. This work is in progress.

3.2.3 Application to CC

Figure 2 shows a schematic representation of the CC process. Figures 3 and 4 illustrate the CC problem at different scales: first at the slab scale (figure 3) where the possible sections for the two-dimensional representation are shown in relation with the oscillation marks orientation ; then a section (figure 4 left) on which the solicitations, issued from a macroscopic model developed at the present time in the MSM Department, will be applied to be transfered to the microscopic cell ; and finally (figure 4 right), the microscopic cell surrounded by a transition zone, it is at this scale that oscillation marks can appear.

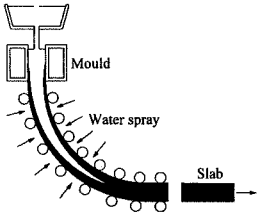

Figure 2: CC process

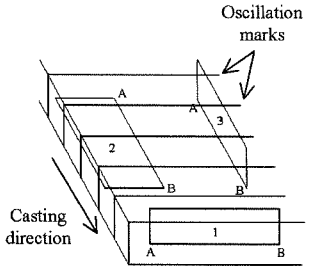

Figure 3: Slab: studied sections

If we want to take account of oscillation marks, only planes 2 and 3 on figure 3 are useful, this remark is important to choose the good orientation for tensile and compression tests and for metallographic observations. Moreover, due to the solidification process, we supose that grains are not equiaxe.

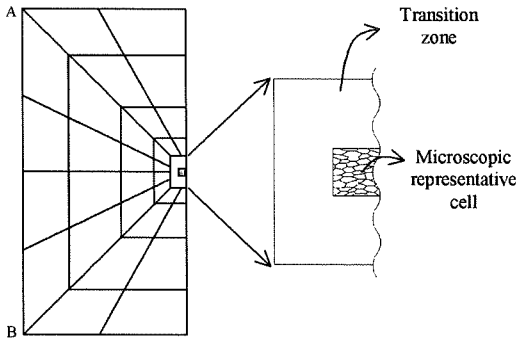

Figure 4: Embedded cell

4 Conclusions and further work

The research is dedicated to a microscopic study of damage at elevated temperature of a microalloyed steel for CC. With our 2D model, we will be able to determine the initiation of a crack and its depth but not directly its propagation in the transverse direction.

Our aim is to develop a model predicting fracture for a specific steel during the CC process ; nevertheless a bibliographical study concerning the factors influencing transverse cracking in CC as well as the creep damage modelling was useful to understand the scope of the study. At present, this work comes to end. It has given rise to a wide reflection which allows us to begin efficiently the development of the damage model in parallel with convenient experimental tests.

5 References

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