

## NUMERICAL STUDY TO IDENTIFY THE MATERIAL PARAMETERS OF A DAMAGE MODEL

RENÉE SCHWARTZ<sup>1</sup>, SYLVIE CASTAGNE<sup>2</sup>, ANNE MARIE HABRAKEN<sup>1</sup>

<sup>1</sup>University of Liège, ArGenCo Department, MS2F Division,  
Chemin des Chevreuils, 1 4000 Liège, Belgium

<sup>2</sup>UNSW Asia, Tanglin Campus, 1 Kay Siang Road, Singapore 248922

### 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.

**Key words:** 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 macroscopic 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.

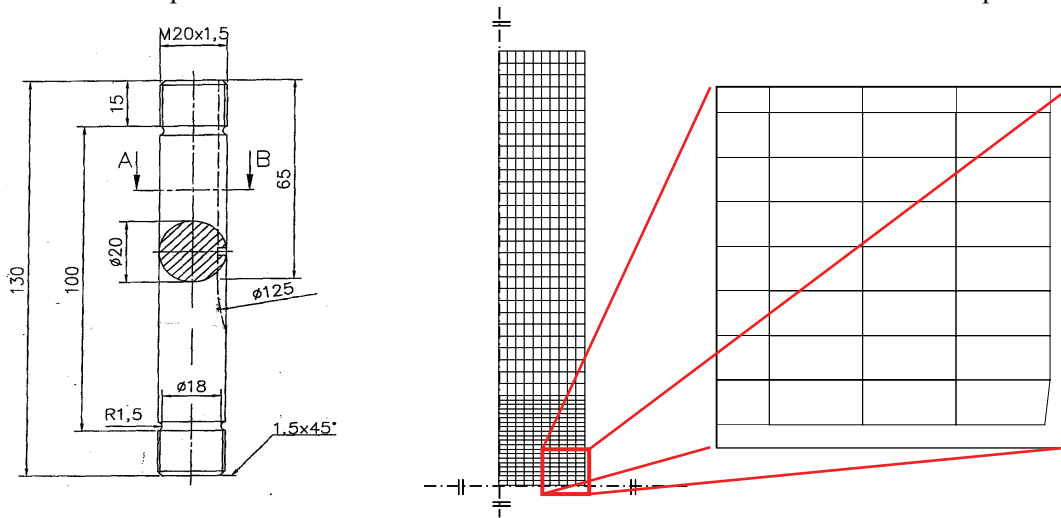


Fig. 1. Modelling of the sample.

## 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.

### 2.1. 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  $\frac{1}{4}$  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.

### 2.2. 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). It represents the Von Mises equivalent stress  $\sigma_e$  as a function of the equivalent strain  $\varepsilon_e$  and the equivalent strain rate  $\dot{\varepsilon}_e$  ( $p_1$  to  $p_4$  are non dimensional functions of temperature).

$$\sigma_e = \varepsilon_e^{p_1} \cdot \exp(-p_1 \varepsilon_e) \cdot p_2 \cdot \sqrt{3} \cdot (\sqrt{3} \cdot \dot{\varepsilon}_e)^{p_3} \quad (1)$$

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  $200\mu\text{m}$ .

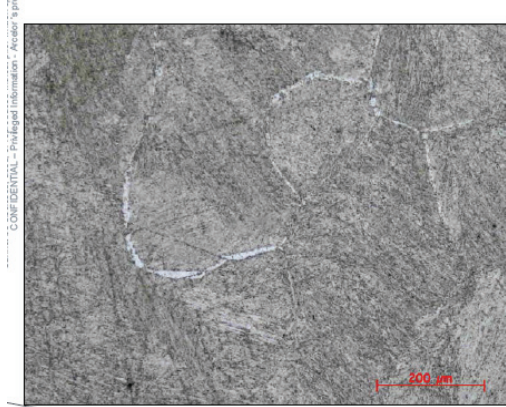


Fig. 2. Metallographic inspection of sub surface, austenite grains and ferrite grain-boundary (Arcelor Research).

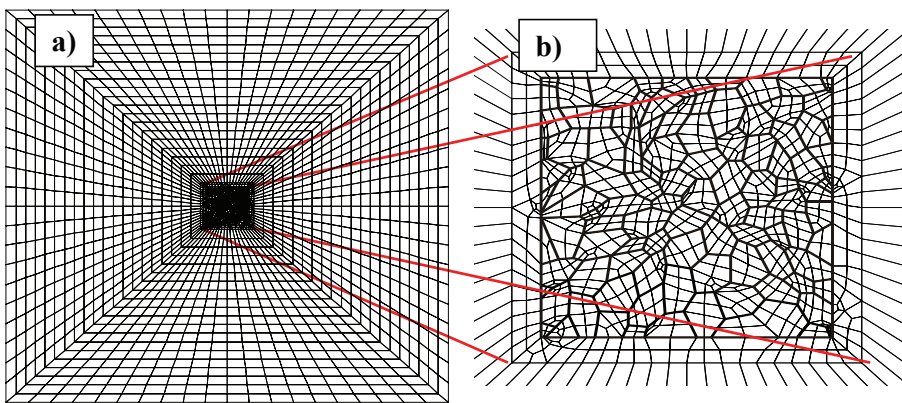


Fig. 3. Representative cell a) Transition zone + Cell, b) Cell.

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:

$$\text{Cell} = 2 \times 2 \text{ mm}$$

$$\text{Cell} + \text{transition zone} = 20 \times 20 \text{ mm}$$

### 2.3. 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 displacement and the loadings 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.

### 2.4. 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. 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.

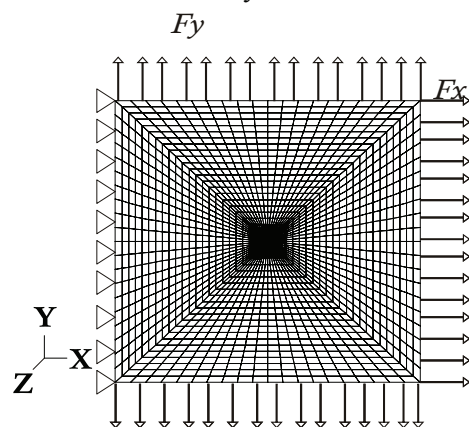


Fig. 4. Loadings on the representative cell.

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  $a/b = 0.7$ .

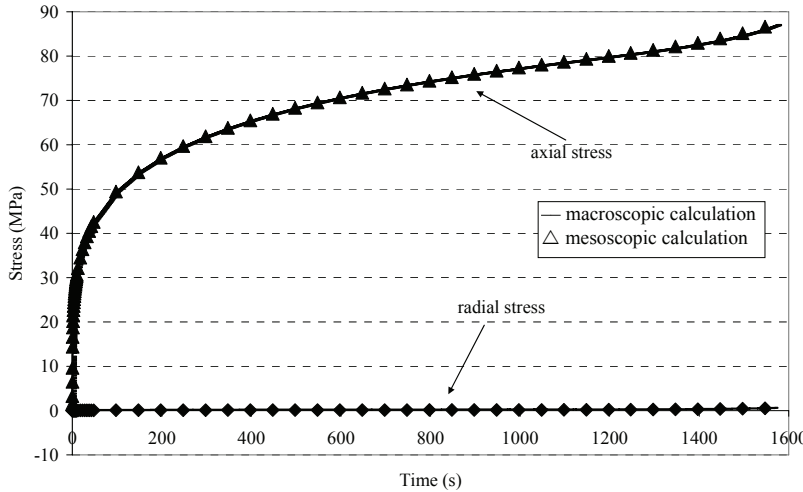


Fig. 5. Comparison between forces extracted from the macroscopic tensile test and from the mesoscopic damage simulation.

#### 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  $N_{max} = 40N_I$  but the sensibility of this parameter should also be determined.

To study the sensibility of the damage law, the four modified parameters 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 evo-

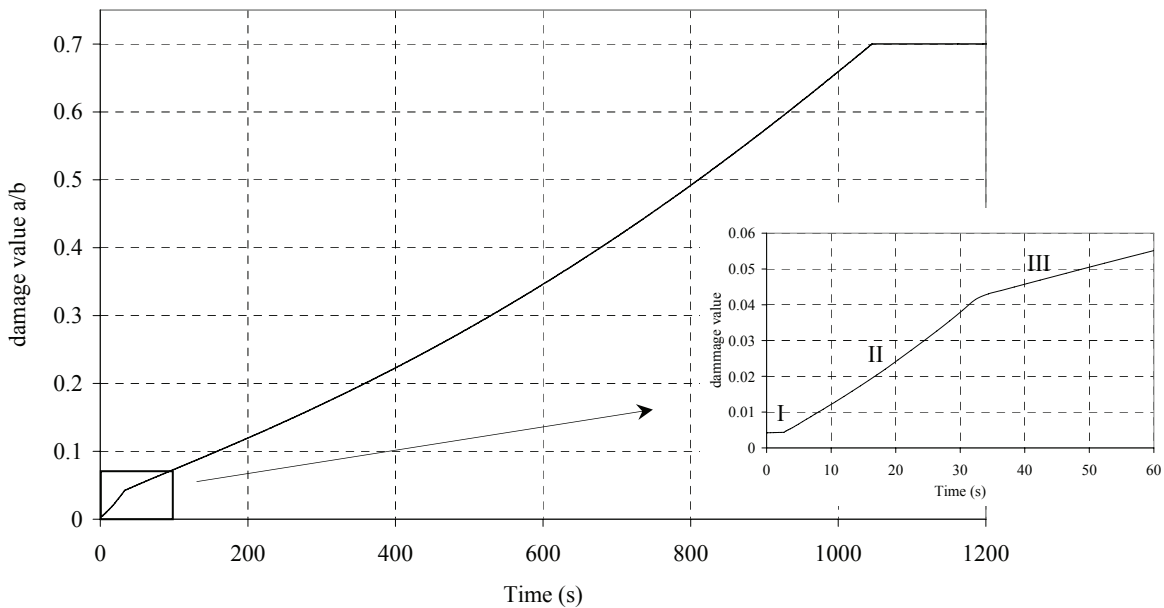


Fig. 6. Damage parameter curve.

#### 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.

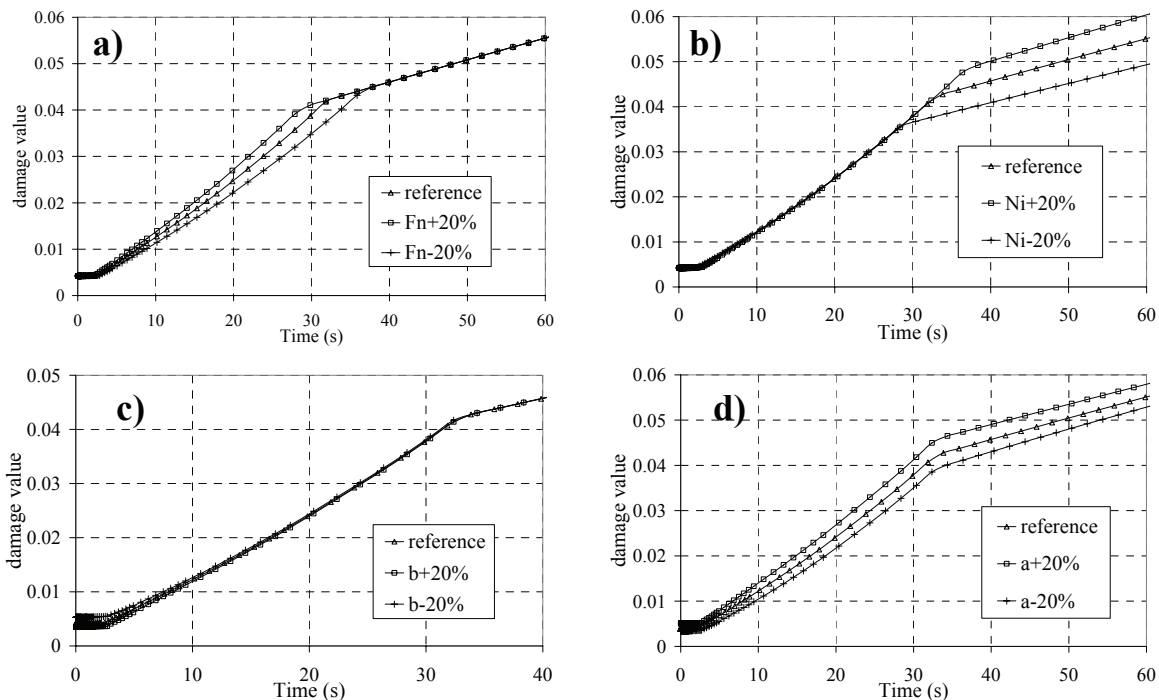
lution (figure 7). Indeed, when  $F_n$  is important, the nucleation is faster and begins earlier. It is possible to take into account the microstructure gradient thanks different values of the nucleation parameter in the structure that implies a gradient of the precipitation according to any depth or the direction.





**Table 1.** Parameters of the damage law and ways to identify them.

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


**Fig. 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  $\chi_1$ .

- 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.



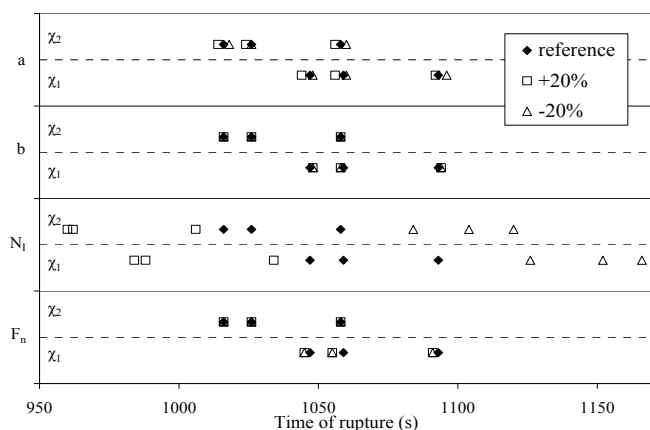


Fig. 8. Three first crack appearances for the variation of different parameters.

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

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.

#### 4. 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. In fact all the parameters described in the paragraph 3 are relevant for the calculation of the damage. 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.

**Acknowledgements.** The authors express their gratitude to the industrial partner: Arcelor, Industeel, Carinox and IEHK. The Walloon Region is also acknowledged.

As Research Director of the Fund for Scientific Research (FNRS), Anne-Marie Habraken thanks this institution.

#### REFERENCES

- Ashby, M.F., 1972, Boundary defects and atomistic aspects of boundary sliding and diffusional creep, *Surf. Sci.*, 31, 498-542
- Brimacombe, J.K., Sorimachi, K., 1977, Crack formation in the continuous casting of steels, *Metallurgical Transactions B*, 8 (3), 489-505
- Castagne, S., Remy, M., Habraken, A.M., 2003, Development of a mesoscopic cell modelling the damage process in steel at elevated temperature, *Key. Eng. Mater.*, 223, 145-150
- Castagne, S., Talamona, D., Habraken, A.M., 2006, A damage constitutive law for steel at elevated temperature, *IJFP*, accepted
- Mintz, B., Yue, S., Jonas, J.J., 1991, Hot ductility of steels and its relationship to the problem of transverse cracking during continuous casting, *Int. Mater. Review*, 36(5), 187-217
- Needleman, A., Rice, J.R., 1980, Plastic Creep Flow Effects in the Diffusive Cavitation of Grain Boundaries, *Acta Metallurgica*, 28, 1315-1332
- Onck, P., van des Giessen, E., 1999, Growth of initially sharp crack by grain boundary cavitation, *J. Mech. Phys. Solids*, 47(1), 99-139
- Pascon, F., Cescotto, S., Habraken, A.M., 2005, A 2.5D finite element model for bending and straightening in continuous casting of steel slabs, *Int. J. Numer. Meth. Engng*, 1, 1-34
- Suzuki, H., Hishimura, S., Imamura, J. and Nakamura, Y., 1984; Embrittlement of steels occurring in the temperature range from 1000 degrees-C to 600 degrees-C, *Transaction ISIJ*, 24 (3), 169-177
- Tvergaard, V., 1984, On the creep constrained diffusive cavitation of grain boundary facets, *J. Mech. Phys. Solids*, 32(5), 373-393

#### IDENTYFIKACJA PARAMETRÓW MODELU PĘKANIA W OPARCIU O ANALIZĘ NUMERYCZNĄ

Streszczenie

W wyniku obciążenia i gięcia materiału w procesie ciągłego odlewania pojawiają się defekty makroskopowe w formie poprzecznych pęknięć. W celu symulacji procesu pęknięcia międzyziarnowego opracowano model 2D w mezoskali dla stali mikroscopowych, gdzie zawartość węgla nie przekracza 0.1% wagi. Celem niniejszej pracy jest rozszerzenie możliwości modelu w celu uwzględnienia stali perytektycznych i nierdzewnych. Aby określić parametry reologiczne dla poszczególnych materiałów przeprowadzono testy rozciągania na gorąco. W pracy wykorzystano symulacje MES z podłączoną komórką reprezentującą materiał w skali mezo. Do określenia parametrów modelu pęknięcia posłużyła metoda analizy odwrotnej inverse.

Submitted: November 22, 2006

Submitted in a revised form: November 30, 2006

Accepted: December 1, 2006

