POLYCRYSTALLINE PLASTICITY AND LOCAL APPROACH OF INTERGRANULAR BRITTLE FRACTURE IN A508 STEEL

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The use of Beremin model based on Weibull's statistics for the assessment of critical tensile stresses for brittle fracture initiation in embrittled A508 steel showed that the lower values are not correctly described and that their scatter was larger than for the higher values. This work aims at investigating the evolution of the plastic strain inhomogeneities and the stress redistribution in such polycrystalline materials and to determine if there is an effect on intergranular brittle fracture. For this we use a polycrystalline model in which the local stresses in the grains are determined from macroscopic stress and plastic strain by mean of a plastic accommodation rule at the level of grains. The model has already shown good prediction capabilities for complex monotonic and cyclic loadings.

INTRODUCTION

Brittle fracture in ferritic steels normally occurs by cleavage at low temperature. However, segregation of impurities such as phosphorus and antimony to grain boundaries can change the brittle fracture mode to intergranular (Mc Mahon (1)), Guttmann et al. (2), Kantidis (3)). The material investigated is a low alloy steel. It is used in nuclear industry and its chemical composition was : 0.16 C, 1.33 Mn, 0.22 Si, 0.23 Cr, 0.49 Mo, 0.72 Ni, 0.010 P, 0.0036 S, 0.012 Al, 0.006 Cu, 0.002 V, 0.022 As. It was austenitized at 1150°C for one hour, and after oil quenching, tempered at 630°C for two hours, and then embrittled by a step cooling heat treatment (Borit et al (4)). Tensile tests on axisymmetric notched specimens and smooth specimens at low temperatures from -196°C to -30°C were carried out.
The use of Beremin criterion (Beremin (5)) for intergranular brittle fracture showed that the scatter is larger for the lower values than for the higher values of fracture stress (4) . The Weibull modulus, m, for intergranular fracture was found

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to be equal to 11, which is a value much lower than for cleavage where m~20. Recently (3), an iterative procedure to determine the Weibull modulus, m, for embrittled A 533 B Cl 1 steel showed a bilinear behaviour between lnln(1/(1-Pr)) and ln(σ_w) (where Pr is the fracture probability and σ_w is the Weibull stress) which could be perfectly fitted by two straight lines with two values of m and σ_u, m=8.7 for the low values and m=29 for the higher values. Low fracture stresses could be connected with a second initiation mechanism involving an easier microcrack propagation from cracked or decohered MnS inclusions on grain boundaries after the embrittlement (see figure 1). A modified Beremin model taking into account the temperature effect was proposed. It gives a better prediction of the scatter and temperature dependance of fracture toughness (Kantidis et al (6)). On the other hand, the low values of the Weibull stress are associated with small plastic strains at which the inhomogeneity of plastic deformation could be important because the plasticity takes place firstly in the favourably oriented grains from a cristallographic point of view.

THE POLYCRYSTALLINE MODEL

This approach is based on a simple representation of microstructure of the material orientation distribution function and slip systems. The model is expressed in the framework of viscoplasticity in order to improve the efficiency of the numerical treatment but in our case there is an evidence of viscoplastic behaviour perceptible on relaxation tests at low temperature. The main specificity of the present model is the introduction of transgranular internal variables able to model the cyclic behaviour (Cailletaud (7)). The model is summarized in table 1. A supplementary variable for each grain, $\underline{\beta}^g$, (Eq.1), is introduced in order to have the inelastic accommodation of the intergranular incompatibilities (Pilvin (8)), the rule of which is similar with Zaoui-Berveiller's (9) for monotonic loading. The kinematic hardening variable, x_s, accounts for internal heterogeneities inside the grain (Eq. 5-8). The isotropic part of the hardening, r_s, is modelled by a nonlinear relations with a saturation versus accumulated shear strain at the slip system level (Eq. 6). The resolved shear stress for the slip system s, τ_s, is expressed as a function of the local stress in the grain g, $\underline{\sigma}^g$, by means of the orientation tensor $\underline{m}_s$ (Eq. 4) which is also used to obtain the plastic grain strain rate (Eq. 11), $\dot{\underline{\varepsilon}}^g$, from the knowledge of all the shear strain rates γ_s on each slip system.
Due to the strength differential effect in such martensitic steels which are stronger in compression than in tension, a local criterion was modified by adding a linear term of the normal stress to the slip plan σ_{nn} (Eq. 7) to describe this phenomenon. It is assumed that each grain presents the same elasticity than the aggregate, so that the macroscopic plastic strain is the average on the grain plastic strains (Eq. 13-14). The coefficient D and δ characterize the plastic accommodation, c and d are for intragranular kinematic hardening, Q and b are the coefficients for intragranular isotropic hardening, n and K deal with the flow rule are the viscosity

coefficients, A describes the strength differential effect.

TABLE 1 - Equations of the polycrystalline model

¤ **Localisation rule**

$$\underline{\underline{\sigma}}^g = \underline{\underline{\Sigma}} + \mu(\underline{\underline{B}} - \underline{\underline{\beta}}^g) \ldots\ldots(1) \qquad \underline{\underline{B}} = \sum_{g \in G} f_g \underline{\underline{\beta}}^g \ldots\ldots (2)$$

¤ **Constitutive equations for each grain**

$$\tau_s = \underline{\underline{\sigma}}^g : \underline{\underline{m}}_s \ldots\ldots(3) \qquad \underline{\underline{m}}_s = \frac{1}{2}(\underline{l}_s \otimes \underline{n}_s + \underline{n}_s \otimes \underline{l}_s) \ldots\ldots(4)$$

$$x_s = c\alpha_s \ldots(5) \qquad r_s = Qq_s \ , \ \dot{q}_s = (1 - bq_s)\dot{v}_s \ldots (6)$$

$$F_s = |\tau_s - x_s| - \tau_0 - r_s - A\sigma_{nn} + \frac{1}{2}\frac{d}{c}x_s^2 \ , \ \sigma_{nn} = \underline{\underline{\sigma}}^g : (\underline{n}_s \otimes \underline{n}_s) \ldots(7)$$

$$\dot{\alpha} = \dot{\gamma}_s - \frac{d}{c}x_s\dot{v}_s \ldots\ldots(8) \qquad \dot{\gamma}_s = \dot{v}_s \, \mathrm{sgn}(\tau_s - x_s) \ldots\ldots(9)$$

$$\dot{v}_s = \left\langle \frac{F_s}{K} \right\rangle^n \ldots\ldots(10)$$

$$\dot{\underline{\underline{\varepsilon}}}_p^g = \sum_{g \in G} \underline{\underline{m}}_s \dot{\gamma}_s \ldots\ldots(11) \qquad \dot{\underline{\underline{\beta}}}^g = \dot{\underline{\underline{\varepsilon}}}_p^g - D[\underline{\underline{\beta}}^g - \delta \underline{\underline{\varepsilon}}_p^g]\sqrt{\frac{2}{3}\dot{\underline{\underline{\varepsilon}}}_p^g : \dot{\underline{\underline{\varepsilon}}}_p^g} \ldots\ldots(12)$$

¤ **Homogenization**

$$\underline{\underline{E}}^p = \sum_{g \in G} f_g \underline{\underline{\varepsilon}}^g \ldots\ldots(13) \qquad \underline{\underline{E}}^e = \frac{1}{2\mu}[\underline{\underline{\Sigma}} - \frac{\nu}{1+\nu}\mathrm{tr}(\underline{\underline{\Sigma}})\underline{\underline{1}}] \ldots\ldots(14)$$

APPLICATION TO THE EMBRITTLED A508 Cl 3

The method used consists in considering one dimensional cyclic and monotonic experimental tests and performing a simultaneous identification of all coefficients based on experimental data and also to give the same behaviour between the present localisation rule and the Berveiller-Zaoui's for monotonic loading. As far as body centered cubic steel is concerned, at low temperature only slip on {110}<111> system is allowed. We can now simulate tension tests with the identified coefficients (see table 2) using the experimental orientation distribution function in order to calculate the average of mechanical fields for each grain.
Figure 3 shows the grain equivalent plastic strain versus axial grain stress for some loading level from 0.5% to 4.5% of macroscopic plastic strain. The width of the grain strain distribution spread with the macroscopic plastic strain but its ratio to the latter decreases (see figure 2). This means that the absolute value of the inhomogeneity, defined as the difference between maximum and mean grain

equivalent plastic strain, increases with the macroscopic strain but its relative value decreases. These results are in accordance with local measurements performed by the fiducial grids method on an iron body centered cubic polycrystal (Bretheau et al. (10)).

TABLE 2 -. The identified coefficients on experimental data. (Units : MPa, s).

D	δ	K	n	c	d	Q	b	τ_0	A
183	0.06	7.5	5.2	35300	352	-15700	172	430	-0.028

The grains stresses increase at the beginning of plasticity and then decrease slightly in the most loaded ones (see figure 3) due to the isotropic softening(Q<0). The inverse pole figure (above) gives the orientations of loading axis with respect to the grains. The maximum value of grain stress does not remain in the same grain. The intergranular plastic strain heterogeneities performed with the present model show that the plastic inhomogeneities are less pronounced at low plastic strain and do not explain the discrepancy between the experimental scatter and the one given by the Weibull statistics. However, the polycrystalline model enables the use of local variables to make statistical investigations such as Monte-Carlo simulations. This work is under development.
The weakest link models assume that fracture is controlled by the largest or most favorably located particle. The fact that the Weibull statistics does not describe very well the scatter of the intergranular brittle fracture indicates that the implicit size defect distribution which involves only one population of defects is not satisfactory. The MnS inclusions are usually not considered as crack inducers in cleavage fracture but the grain boundaries embrittlement brings down their resistance and could make easier propagation beyond cracked or decohered MnS inclusions on grain boundaries (see figure 1). In this case, modelling the scatter of intergranular brittle fracture implies to take into account two populations of defects in the flaws distribution : carbides involved in cleavage fracture and intergranular MnS inclusions.

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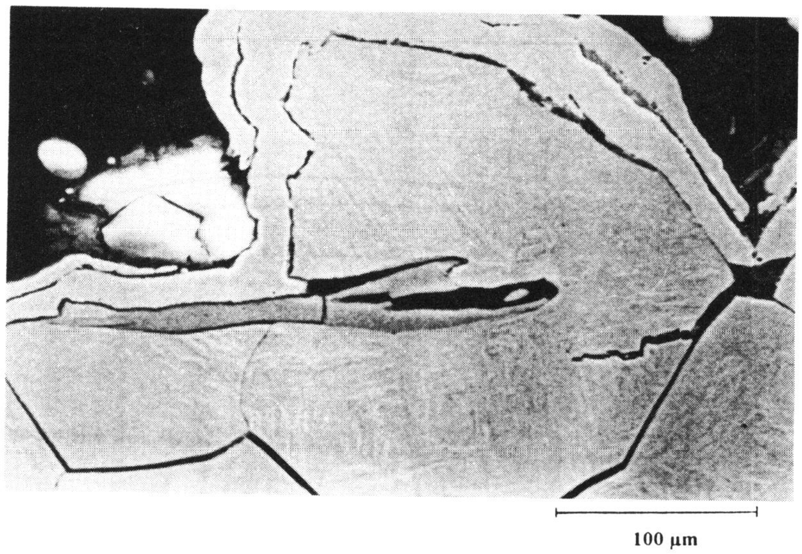

Figure 1. Fracture surface recovered by a thin Nickel layer. The crack takes place firstly in the MnS inclusion and can propagate in the embrittled grain boundaries.

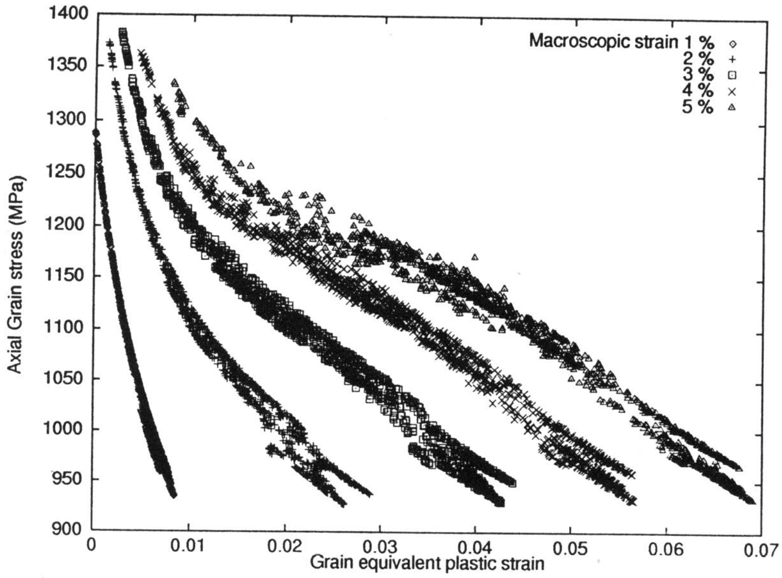

Figure 2. The evolution of the grains fields with increasing macroscopic strain

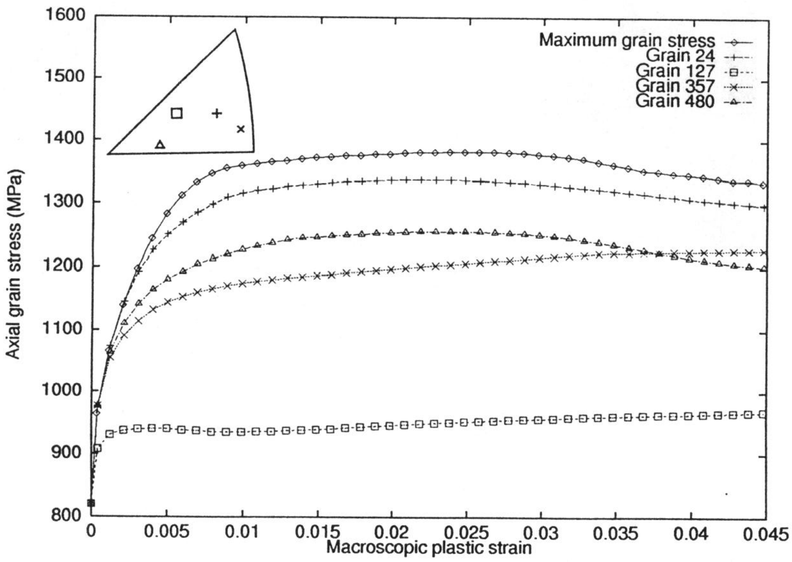

Figure 3. Maximum grain stress vs macroscopic plastic strain and the evolution of the grain stress for different cristallographic orientations.