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Prediction of crack initiation in low-cycle fatigue in an austenitic stainless steel

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Abstract :

The initiation of damage in low cycle fatigue in metal alloys is strongly linked to the crystal orientations of grains at the surface. In order to predict its occurrence, the elastoplastic behavior of an austenitic stainless steel is first simulated with a polycrystalline model. A specific localization law is used to determine stresses in grains at the surface, and a criterion based on the physical mechanisms allows to predict the number of cycles to damage initiation.

Résumé :

L'amorçage en fatigue oligocyclique dans les alliages métalliques est fortement lié aux orientations cristallines des grains de surface. Afin de prédire son apparition, le comportement élastoplastique d'un acier inoxydable austénitique est tout d'abord simulé à l'aide d'un modèle polycristallin, les paramètres sont identifiés par méthode inverse. Une loi de localisation spécifique est utilisée pour déterminer les contraintes dans les grains de surface, un critère d'amorçage basé sur les mécanismes physiques permet alors de prédire le nombre de cycles à l'amorçage.

Key words: low-cycle fatigue, austenitic stainless steel, polycrystalline model, initiation criterion

1 Introduction

The level of cyclic plastic strain is very high in low-cycle fatigue. In metallic materials, their accumulation leads to crack initiation in grains at the surface, usually at the interface between a persistent slip band (PSB) and the matrix, as described by Essmann, Gösele and Mughrabi [1]. These observations have also been made by Hunsche and Neumann [2] and Ma and Laird [3, 4]. Crack initiation is therefore strongly connected to the orientation of surface grains. The prediction of this initiation depends then on the plastic behavior of these grains and their orientation. The objective of the present work is to propose a model of crack initiation in low-cycle fatigue based on these physical observations.

In a first step, the material studied is presented, with the experimental procedure used for the mechanical tests. In a second step, a polycrystalline model is described, and the way surface grains are taken into account is presented. The choice of an appropriate criterion for crack initiation is then discussed.

2 Material

Because of their excellent anticorrosion properties, stainless steels are widely used nowadays in large fields of industry like automotive industry, water and construction industries. Among the large stainless steel family, austenitic stainless steels represent about 70% of the annual stainless steel production. The material studied is an austenitic stainless steel, AISI 316L. It is supplied in sheets of 14 mm in thickness, it was solution treated for an hour and then water-quenched. The microstructure obtained after an electrochemical attack is shown in Figure 1.



FIG. 1 – Microstructure of AISI 316L stainless steel studied.

3 Mechanical tests

Mechanical tests were done with a tension-compression servo-hydraulic machine INSTRON (Figure 2a). The specimens were cylindrical and button-headed, with a useful part of 10 mm in diameter and 25 mm in length (Figure 2b). An axial extensometer with a 10 mm gauge length was fixed on the specimen. Three cyclic tests were carried out under total strain control, with a strain rate of 6.6×10^{-4} and strain amplitudes of 0.3%, 0.5% and 0.8%. All the tests were carried out at room temperature. Load and strain were simultaneously recorded during the cycling.

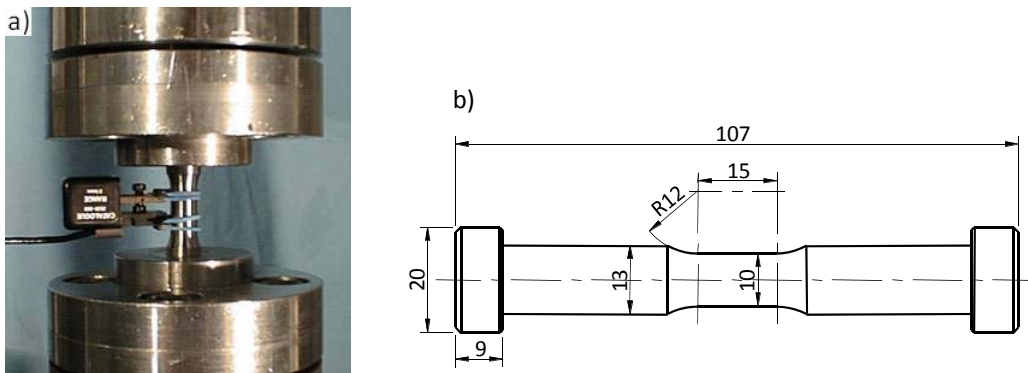


FIG. 2 – a) Uniaxial machine: servo-hydraulic INSTRON of type 8501; b) plan of specimen (mm)

4 Presentation of the model developed

As crack initiation depends on grain orientation, it is necessary to take into account crystal plasticity in the modeling. The model is composed of two parts. The first part aims at simulating the elastoplastic behavior of the steel, and the second part is concerned by crack initiation prediction in surface grains.

4.1 Polycrystalline model

The first part of the model is based on a polycrystalline model proposed by Evrard [5]. According to the microstructure of the material, a single grain scale is considered; a one site self-consistent scheme is then used. In this model, a spherical inclusion is placed in a so-called Equivalent Homogeneous Medium (EHM), and this inclusion (or phase) represents all the grains of the same orientation. The material being isotropic and not textured, an isotropic distribution of 40 crystal orientations is chosen [6-8]. The localization law proposed by Cailletaud [6] and Pilvin [7] is used to link macroscopic and microscopic mechanical fields. The following hypotheses are considered: (i) elasticity is isotropic and is considered at the macroscopic scale, (ii) the grains are spherical and (iii) the plastic behavior of the homogeneous equivalent medium is isotropic. The localization law takes the following form:

$$\underline{\sigma}^g = \underline{\Sigma} + \mu(\underline{B} - \underline{\beta}^g) \quad \text{with} \quad \underline{B} = \sum_g^{N_g} f^g \underline{\beta}^g \quad (1)$$

where $\underline{\beta}^g$ is an internal variable representing the intergranular accommodation of each grain in the matrix, \underline{B} is the average of $\underline{\beta}^g$ and f^g is the volume fraction of each grain (1/40). On the contrary to the localization law

proposed by Berveiller and Zaoui [9] limited to monotonous proportional loadings, this localization law allows the simulation of cyclic and/or non-proportional loadings. The evolution of variable β^g is written with an Armstrong-Frederick [10] type kinematic hardening law:

$$\dot{\underline{\beta}}^g = \underline{\dot{\epsilon}}^{pg} - D \left(\underline{\beta}^g - \delta \underline{\epsilon}^{pg} \right) \left\| \underline{\dot{\epsilon}}^{pg} \right\| \quad (2)$$

where D and δ are two material parameters to be identified.

On the grain scale, the plastic behavior is due to the dislocation slip on crystallographic planes. For FCC materials like austenitic stainless steels, 12 slip systems, $\{111\} \langle 110 \rangle$, are considered. The resolved shear stress on each slip system is then calculated by:

$$\tau^s = \underline{\underline{\sigma}}^g : \underline{\underline{m}}_g^s = \underline{\underline{\sigma}}^g : \frac{1}{2} \left(\underline{\underline{n}}^s \otimes \underline{\underline{b}}^s + \underline{\underline{b}}^s \otimes \underline{\underline{n}}^s \right) \quad (3)$$

where $\underline{\underline{n}}^s$ and $\underline{\underline{b}}^s$ define respectively the slip direction and the direction normal to slip plane s . The single crystal law is that proposed in [5]. It is based on the description of dislocation density evolution on each slip plane, and needs 8 material parameters.

The plastic strain rate being calculated in each grain, the macroscopic plastic strain rate is obtained through a homogenization procedure:

$$\underline{\underline{\dot{E}}}^D = \sum_g f^g \underline{\underline{\dot{\epsilon}}}^{pg} \quad (4)$$

4.2 Identification of material parameters of the polycrystalline model

The identification of material parameters of the polycrystalline model was carried out in two steps. In the first step, elasticity and crystal law parameters were identified. Some parameters were measured (elasticity parameters) or fixed according to the literature (Burgers vector, initial dislocation density, viscosity parameters, mean free path). The other parameters (initial shear stress τ^0 , interaction matrix parameter h , and annihilation distance of dislocation dipoles y_c) were identified using automatic optimization software SiDoLo which compares experimental data and simulation results. Only a monotonous tension test is used for this identification. The loading being monotonous, the Berveiller-Zaoui localization law was used.

In the second step, material parameters of Cailletaud-Pilvin interaction law (D and δ) were identified with the same procedure. The identification database is composed of the monotonous test simulated with Berveiller-Zaoui localization law (the self-consistency condition is then guaranteed) and the first hysteresis loop with a strain amplitude of 0.5%.

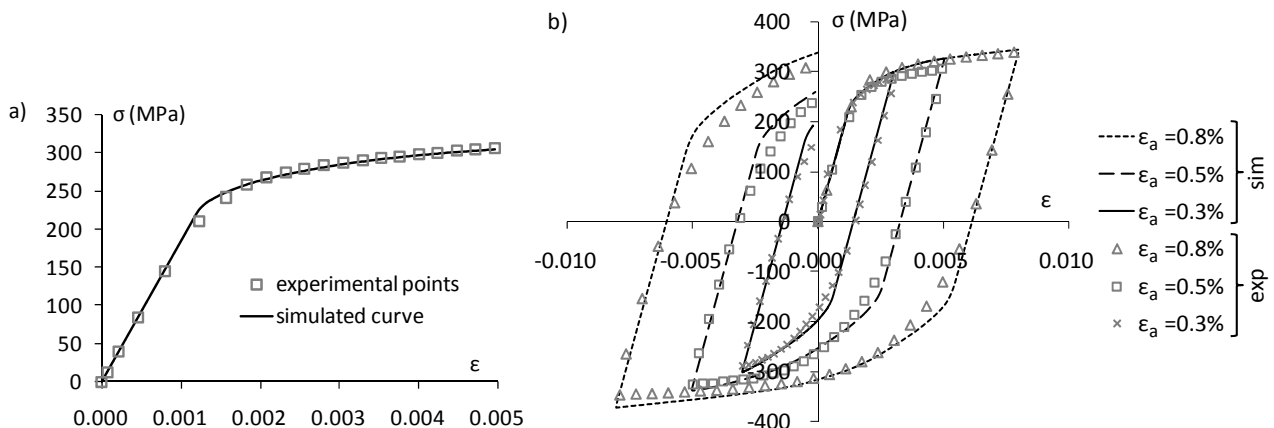


FIG. 3 – Comparison between experimental results and numerical simulation.

a) Monotonous tension test; b) First hysteresis loop.

In Figure 3, the simulated monotonous test and the first hysteresis loops inside ($\epsilon_a = 0.5\%$) and outside ($\epsilon_a = 0.3\%$ and 0.8%) identification base are compared to experimental results. It can be seen that the model is able to predict accurately the Bauschinger effect and the amplitude effect. The parameter values obtained are given in Table 1.

Step	1			2	
Parameter	τ^0 (MPa)	h	y_c (m)	D (MPa)	δ
Value identified	50.7	0.55	2.2×10^{-9}	-30	0.62

TAB. 1 Values of identified parameters

4.3 Grain at the surface and its localization and crystal laws

The second part of the model focuses on grains where crack initiation takes place, which means, surface grains (as shown in Figure 5a). In this case, the self-consistent model introduced above can no longer be applied. Because grains at the surface, on the contrary to internal grains, are not completely surrounded by other grains. Furthermore, for a given stress level and a crystallographic orientation, plastic slip could be much larger in grains at the surface than in the bulk because they are less constrained by neighbor grains. So a new localization law is needed to correctly reflect the mechanical behavior of grains at the surface.

The plastic behavior of the grain is based on simple gliding, characteristic of low-cycle fatigue. Grains most favorably oriented for the gliding have the highest Schmid factor. The Schmid factor is however not sufficient to predict the risk of crack initiation. It is necessary to consider the possibility to create intrusions-extrusions at the surface on a given slip system. Among slip systems good oriented to simple gliding, two slip systems have a particular orientation toward the surface: systems A and B (Miller [11]). In both cases, slip planes make an angle of 45° to the direction of loading, but the slip direction changes. For system A, the slip direction is parallel to the free surface, and no intrusion-extrusion is created during the gliding (Figure 5b). On the contrary, for system B, the slip direction makes an angle of 45° to the free surface, and the gliding along this slip system will create steps at the free surface (Figure 5c), where micro cracks initiate.

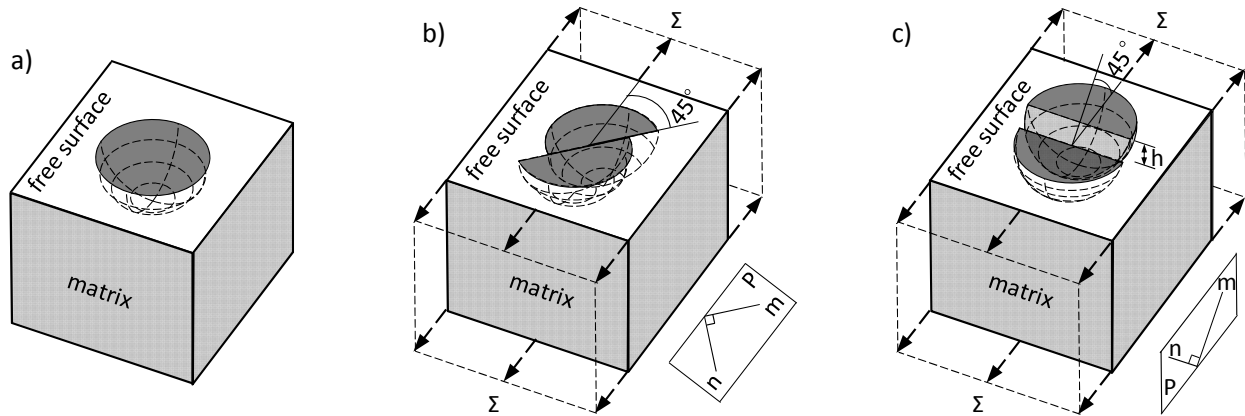


FIG. 5 – a) Grain at the surface; b) System A; c) System B
(m, slip direction; n, normal of slip plan; h, step height)

Maxime Sauzay [12] calculated stresses and strains in a hemispheric grain at the surface of a matrix. The matrix is considered isotropic elastic and the grain elastoplastic. As the grain behavior is elastoplastic, stresses are not uniform in the grain. Both analytical method and finite element calculation allows to evaluate stress and strain in the surface inclusion. Through a decomposition of the plastic strain in a 5 dimension space, a localization law is obtained in the form:

$$\underline{\underline{\sigma}}^g(\mathbf{x}) = \underline{\underline{\Sigma}} + \underline{\underline{\underline{M}}}(\mathbf{x}) : \underline{\underline{\varepsilon}}^p \quad (5)$$

where $\underline{\underline{\underline{M}}}(\mathbf{x})$ is the localization tensor for a grain at the surface, $\underline{\underline{\underline{M}}}(\mathbf{x})$ is not uniform in the surface grain and depends on the point $\mathbf{M}(\mathbf{x})$ where it is calculated.

The average value of stresses in a grain at the surface can be calculated in the simple form:

$$\begin{aligned} \sigma_{11} &= \Sigma_{11} + M_{1111}\varepsilon_{11}^p + M_{1122}\varepsilon_{22}^p & \sigma_{12} &= \Sigma_{12} + M_{1212}2\varepsilon_{12}^p \\ \sigma_{22} &= \Sigma_{22} + M_{1122}\varepsilon_{11}^p + M_{1111}\varepsilon_{22}^p & \sigma_{23} &= M_{1313}2\varepsilon_{23}^p \\ \sigma_{33} &= M_{3311}(\varepsilon_{11}^p + \varepsilon_{22}^p) & \sigma_{13} &= M_{1313}2\varepsilon_{13}^p \end{aligned} \quad (6)$$

In fatigue, the surface effect is characterized by the ratio r , defined by:

$$r = \frac{\Delta\gamma_{\text{surf}}^p}{\Delta\gamma_{\text{vol}}^p} \quad (7)$$

where $\Delta\gamma_{\text{surf}}^p$ and $\Delta\gamma_{\text{vol}}^p$ are the amplitude of shear strain in a grain of the same orientation respectively at the surface and in the volume. The surface effect is maximal if a slip system has orientation B and if the contrast between matrix and inclusion behaviors is the highest. This means that the plastic strain in a surface grain will be higher, compared to the same grain totally surrounded by the matrix, if the kinematic hardening modulus is lower. In these conditions, $\Delta\gamma_{\text{surf}}^p$ reaches 155% of $\Delta\gamma_{\text{vol}}^p$. Although the hypothesis of an elastic behavior of the matrix is not verified in low-cycle fatigue, the localization law obtained by Sauzay was used in this study in order to maximize the shear strain in surface grains. In a second step, a more precise evaluation of the localization law for low-cycle fatigue hypothesis will be done.

The crystal plasticity law used for surface grains is the law defined above for the polycrystalline model.

4.4 Prediction of crack initiation

This present work uses the fatigue crack initiation criterion proposed by Mura [13]. This law is based on Gibbs' free energy, which is considered to be in charge of the evolution of dislocation structures. The author shows that there exists a critical fatigue cycle number beyond which the local accumulated energy will be larger than the surface energy necessary for creating a decohesion surface, when the initial state of dislocation dipole accumulation becomes energetically unstable and the dislocation dipoles are annihilated to form a crack. The length of an initiated crack is supposed to be the same as the grain size. The cycle number for crack initiation, N , is expressed by:

$$N = C \frac{\mu \gamma_{\text{surf}}}{\bar{d} p^2 (1-\nu)^2} \frac{1}{(\max|\tau_i| - \tau_{\text{PSB}})^2} \quad (8)$$

with C a material parameter, μ the shear modulus, ν the Poisson's ratio, γ_{surf} the specific energy of surface creation, \bar{d} the grain size, p a factor of irreversibility of slip, τ_i the shear stress in slip system i ($i = 1 \sim 12$) and τ_{PSB} the critical shear stress for the appearance of slip bands.

For the material studied here, the first part of formula (8), $k = C \frac{\mu \gamma_{\text{surf}}}{\bar{d} p^2 (1-\nu)^2}$, as τ_{PSB} are two constants and can be obtained by inverse method. So, for a given material, N depends only on the value of $\max|\tau_i|$, which is linked to the amplitude of stress and slip system orientation.

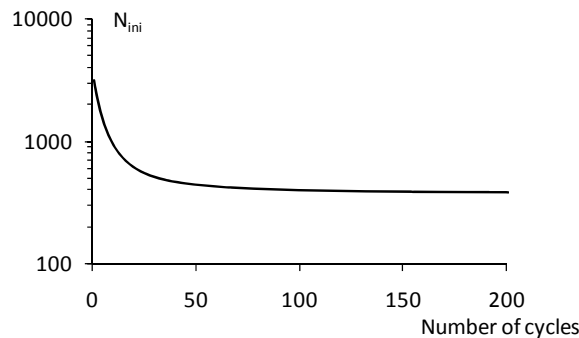


FIG. 6 –Number of cycles for crack initiation calculated for grain B during the first 200 cycles with a strain amplitude of 0.5%

First predictions of the number of cycles to crack initiation have been done, using $k = 4.0 \times 10^6$ and $\tau_{\text{PSB}} = 80$ MPa. Figure 6 shows the number of cycles N_{ini} predicted by Mura's model for grain B during the first 200 cycles with a strain amplitude of 0.5%. Because of the cyclic hardening, N_{ini} decreases and then stabilizes.

It should be mentioned that the values of k and τ_{PSB} here are chosen arbitrary and cannot reflect the real behavior of this material. The exact values of these two parameters have to be identified through fatigue tests.

5 Conclusion and prospect

In order to predict crack initiation in low-cycle fatigue, a model is developed in this paper. It consists of, on one side, a polycrystalline model to predict the mechanical behavior and, on the other side, the calculation of stresses in the grains at the surface where initiation occurs. The parameters of the polycrystalline model were identified through an optimization procedure. Several cyclic tests were simulated and the results were compared to experimental data. Concerning the grains at the surface, a specific localization law is chosen and allows the calculation of stresses and strains in these grains. The model proposed by Mura allows the prediction of the number of cycles for crack initiation. Fatigue tests have still to be done in order to validate the prediction of crack initiation and identify some parameters of the model.

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