Micromechanical investigation of the influence of defects on the high cycle fatigue strength

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ABSTRACT. *The aim of this study is to analyse the influence of notches on the fatigue behaviour of an electrolytic copper using finite element simulations of polycrystalline aggregates. In these simulations, in which the grains are explicitly modelled, the anisotropic behavior of each FCC crystal is described by the generalized Hooke's law with a cubic elasticity tensor and by a single crystal visco-plastic model. The numerical analysis is done using several smooth and notched microstructures composed of about 200 grains. The cyclic mechanical responses of the grains are then studied for different defect sizes and the ability of three fatigue criteria to predict the defect size effect on the fatigue strength is evaluated thanks to the comparison with experimental data [1].*

INTRODUCTION

The scatter encountered in the high cycle fatigue (HCF) behavior of metallic materials is often explained by the anisotropic elasto-plastic behavior of individual grains leading to a highly heterogeneous distribution of plastic slip. Since fatigue crack initiation is a local phenomenon, intimately related to the plastic activity at the crystal scale, it seems relevant to evaluate the mesoscopic mechanical quantities (i.e. the average mechanical quantities at the grain scale). Localization schemes [8] encounter difficulties when estimating the local mechanical fields in the presence of defects whose size is comparable to the characteristic length of the microstructure (i.e. the mean grain size). An alternative way to estimate these mechanical fields is to perform finite element analysis of explicitly modeled polycrystalline aggregates. This kind of approach has already been applied to investigate the HCF behavior of metallic material [2-4] and more precisely in the case of notched microstructures [3]. The present study fits into this framework and attempts to provide additional results to these previous works. In particular, fatigue tests performed by Lukáš et al. [1] are numerically investigated and the results of these FE analyses are used to predict fatigue limits for different defect sizes. These predictions are then compared to the experimental fatigue limits.

MODELLING APPROACH

Material constitutive laws

Three material constitutive models are investigated in this study: linear elasticity, cubic elasticity and crystal plasticity in addition to the cubic elasticity. In the first case, elastic properties of each grain are isotropic and are defined with the Young's modulus and the Poisson's ratio. In the second and third case, cubic elasticity, which corresponds to the elastic anisotropic behaviour of FCC crystals, is characterized, in the crystal coordinate system, by 3 coefficients: C_{1111}, C_{1122} and C_{1212}. The orientation of each crystal with respect to the reference frame is then defined by a triplet of Euler angles.

The crystal plasticity is described by the constitutive model proposed by Méric and Cailletaud [5] using a viscoplastic framework. In this model, the plastic slip rate $\dot{\gamma}_s$ on a slip system s is governed by a Norton-type flow rule involving the resolved shear stress τ_s acting on s (Eq. 1). The relations linking the stress tensor $\underline{\underline{\sigma}}$ to the resolved shear stress τ_s acting on s and the plastic slip rate $\dot{\gamma}_s$ to the plastic strain rate tensor $\underline{\underline{\dot{\varepsilon}}}^p$ are given in Eq. 2. These equations involve the orientation tensor $\underline{\underline{m}}_s$ which is defined as a function of the slip plane unit normal vector $\underline{n}_s$ and the slip direction unit vector $\underline{l}_s$ (Eq. 3). The evolution law of the isotropic hardening r_s introduced in the flow rule is described by Eq. 4. In this equation, the influence of the accumulated plastic slip on the slip system r on the hardening of the slip system s is taken into account thanks to the interaction matrix h_{sr}.

$$\dot{\gamma}_s = \left\langle \left(|\tau_s| - r_s\right)/K \right\rangle_+^n sign\left(\tau_s\right) = \dot{v}_s \ sign\left(\tau_s\right) \tag{1}$$

$$\tau_s = \underline{\underline{m}}_s : \underline{\underline{\sigma}} \quad and \quad \underline{\underline{\dot{\varepsilon}}}^p = \sum_s \dot{\gamma}_s \underline{\underline{m}}_s \tag{2}$$

$$\underline{\underline{m}}_s = \left(\underline{n}_s \otimes \underline{l}_s + \underline{l}_s \otimes \underline{n}_s\right)/2 \tag{3}$$

$$r_s = r_0 + Q \sum_r h_{sr} \left(1 - \exp(-b\, v_r)\right) \tag{4}$$

Table 1. Material parameters for an annealed electrolytic copper

Isotropic elasticity		Cubic elasticity [5]		
E $[GPa]$	ν	C_{1111} $[GPa]$	C_{1122} $[GPa]$	C_{1212} $[GPa]$
118	0.344	159.3	122.0	81.0159

Crystal plasticity [6]										
K $[MPa.s^{1/n}]$	n	r_0 $[MPa]$	Q $[MPa]$	b	h_0	h_1	h_2	h_3	h_4	h_5
8	20	4	7	9	1	1	0.2	90	3	2.5

Finite element model

In order to reproduce numerically, in a reasonable computation time, the fatigue tests conducted by Lukáš et al. [1] using finite element simulations of polycrystalline aggregates, a simplified geometry of the specimen is modelled (cf. Fig. 1). The first simplification is the use of 2-dimensional geometries. The second one consists in explicitly modelling the microstructure only in the area near one of the notches. A homogeneous matrix which embeds the polycrystal is added so that the ratio between the half-width of the specimen used by Lukáš et al. [1] and the notch radius is respected for all geometries. The dimensions presented in Fig. 1 have been chosen such as the smooth polycrystalline aggregate contains 200 grains for a mean grain size of 50 µm.

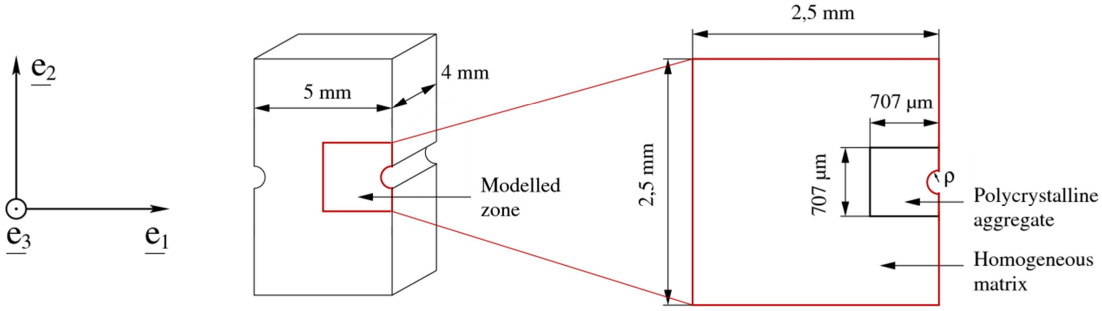


Figure 1. Specimen geometry and modelled zone

The process used to generate the 2-dimensional polycrystalline aggregates geometries is described in [4]. Both smooth and notched microstructures are used. The notches considered in this work are semi-circular and 3 notch radii ρ are studied: 40, 80 and 120 µm. Finally, the finite element mesh of the CAD of the microstructure is generated using Gmsh [7]. The grains are meshed in average with 100 linear three-node triangular finite elements.

For each defect size studied, three geometries containing approximately 200 equiaxed grains and ten orientations sets are used. Orientation sets are composed by triplet of Euler angles chosen such as to represent an isotropic texture. As a result, the response of 30 different microstructures is investigated per defect size.

When the crystal plasticity model is assigned to the grains, an isotropic elasto-plastic model with non-linear kinematic and isotropic hardenings (resp. Armstrong-Frederick and Voce relations) is applied to the matrix and 10 cycles are computed so that the aggregates reach a stabilized behaviour. In the case of purely elastic models used for the grains, an isotropic elastic law is assigned to the matrix and, thanks to the linearity of these behaviours, only one cycle is applied. Computations are performed to simulate fully reversed load control fatigue tests. Such loading cases are modelled by imposing a displacement $U_2 = 0$ to the lower edge and a cyclic macroscopic stress Σ_{22} to the upper edge of the matrix. A displacement $U_1 = 0$ is imposed on the left edge to model the specimen symmetry. A generalized plane strain hypothesis is used for the simulations.

The numerical simulations are conducted with ZeBuLoN FE software developed by Mines ParisTech, Northwest Numerics and ONERA.

Fatigue criteria

The predictions of three different fatigue criteria are studied in this work. Their expressions are inspired from multiaxial HCF fatigue criteria based on a mesoscopic approach and proposed by Dang Van [8], Papadopoulos [9] and Huyen and Morel [10]. The main change made on these reference criteria is the replacement of the macroscopic quantities by mesoscopic quantities, i.e. the quantities computed from the average stress tensors per grain $\langle \underline{\underline{\sigma}} \rangle_g$ which are obtained from the last cycle of the FE simulations.

Critical plane-based criterion

The criterion, inspired from the one proposed by Dang Van, checks that no crack initiates in each slip plane contained in the polycrystal (Eq. 5). In this relation, the fatigue failure is prevented as long as the inequality is satisfied.

$$\sigma_{DV} = \max_{\underline{n}} \left(\max_t \left[\left\| \underline{\tau}(\underline{n},t) - \underline{\tau}_m(\underline{n}) \right\| + \alpha_{DV} \sigma_h(t) \right] \right) \leq \beta_{DV} \tag{5}$$

$\underline{\tau}(\underline{n},t)$ and $\sigma_h(t)$ correspond respectively to the mesoscopic shear stress vector acting on the slip plane of normal $\underline{n}$ and to the mesoscopic hydrostatic stress. The mesoscopic mean shear stress vector $\underline{\tau}_m(\underline{n})$, in Eq. 1, is defined as the centre of the smallest circle circumscribing the path described by $\underline{\tau}(\underline{n},t)$ during the last loading cycle.

Integral criterion

Papadopoulos proposed a criterion based on the quadratic mean, along every slip systems in the polycrystal, of the macroscopic resolved shear stress amplitude $\mathrm{T}_{s,a}$ and the average, along every slip planes in the polycrystal, of the macroscopic normal stress Σ_n. In this work, the form of this criterion is preserved (Eq. 6) but mesoscopic quantities are used instead of the macroscopic ones: $\tau_{s,a}$ and σ_n replace respectively $\mathrm{T}_{s,a}$ and Σ_n.

$$\sigma_P = \sqrt{\left\langle \tau^2_{s,a} \right\rangle} + \alpha_P \sqrt{\sigma_n} \leq \beta_P \tag{6}$$

Probabilistic criterion

Huyen and Morel have proposed a criterion based on the assumption that the fatigue crack initiation threshold at the grain scale follows Weibull distribution which led them to define a failure probability for each grain. In order to estimate the failure probability of a polycrystal, the authors then applied the weakest-link hypothesis. This approach is summarized in the following.

First, a fatigue crack is assumed to initiate in a slip plane of normal $\underline{n}$ if the amplitude of the shear stress τ_a acting on this plane exceeds a threshold τ_a^{th}. This threshold is then supposed to be a random variable following a Weibull distribution characterized by a shape parameter m and a scale parameter τ_0. Thus, the failure probability of the slip plane can be expressed by:

$$P_{Fn} = P(\tau_a \geq \tau_a^{th}) = 1 - \exp\left[-\left(\frac{\tau_a}{\tau_0} \right)^m \right] \tag{7}$$

The normal stress effect on fatigue strength is taken into account by considering that τ_0 depends on the normal stress amplitude $\sigma_{n,a}$ and on the mean normal stress $\sigma_{n,m}$ acting on the slip plane of normal $\underline{n}$ (Eq. 8).

$$\tau_0 = \tau_0' \frac{1 - \gamma\sigma_{n,m}}{1 + \alpha\left(\sigma_{n,a} / \tau_a\right)} \tag{8}$$

The failure probability P_{Fg} of a grain g is supposed to correspond to the maximum among the failure probabilities of its slip planes. Finally the failure probability of the polycrystal P_{Fa} is determined with the use of the weakest-link hypothesis (Eq. 9).

$$1 - P_{Fa} = \prod_{g=1}^{Ng} \left(1 - P_{Fg}\right) \tag{9}$$

Identification of the criteria parameters

For each constitutive models assigned to the grains, the parameters of the criteria are identified thanks to results of the numerical simulation of polycrystalline aggregates loaded, at the average fatigue limit level, in fully reversed tension and in fully reversed shear. Moreover, as the probabilistic criterion has a parameter which defined the sensitivity to the mean normal stress, the results obtained from a third loading case are needed. The loading case chosen is cyclic tension with a stress ratio $R = 0$.

The average fatigue limits in fully reversed tension and in fully reversed torsion, for an electrolytic copper, has been determined respectively by Lukáš [1] and Ravilly (reported in [11]) and are $s_{-1} = 73\,MPa$ and $t_{-1} = 44.3\,MPa$. The fatigue limit in tension with $R = 0$ has been estimated with the Gerber's relationship which gives $s_0 = 66.4\,MPa$ for $R_m = 220\,MPa$.

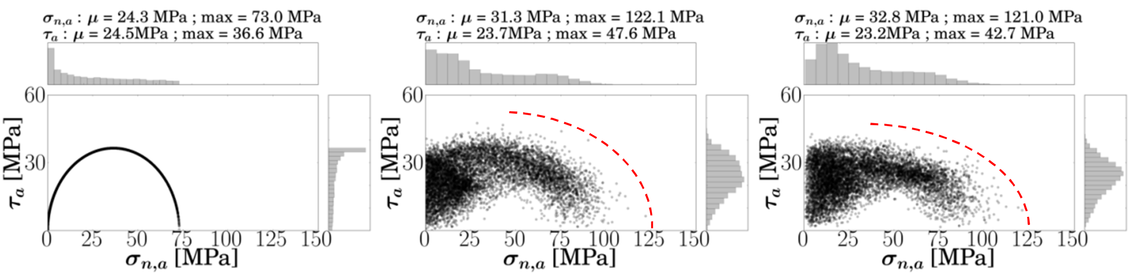
For the integral and the critical plane-based criteria, the parameters are identified such that σ_{DV} / β_{DV} and σ_P / β_P are, in average on the 30 realisations, equal to 1 in fully reversed tension on the one hand and in fully reversed shear on the other hand. Regarding the probabilistic criterion, the procedure is similar excepted that the shape parameter m is imposed and two values are chosen: 5 and 20. The other parameters are identified such that P_{Fa} is, in average, equal to 50% for each of the three loading cases.

RESULTS AND DISCUSSIONS

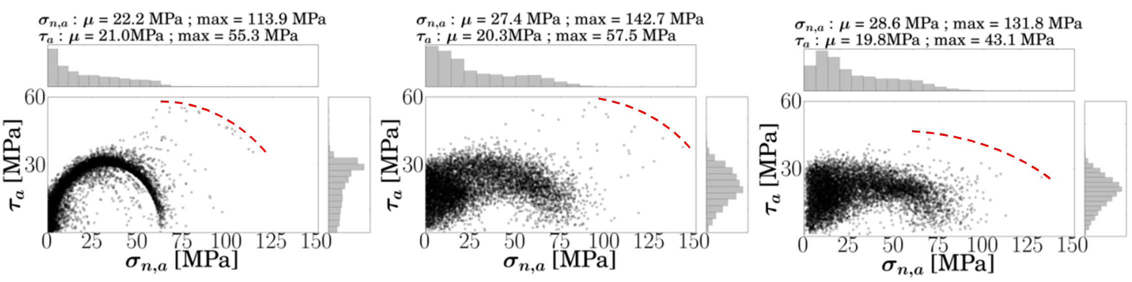
Effect of the constitutive models on the mechanical response of the smooth and notched polycrystalline aggregates

The mesoscopic mechanical response during the last loading cycle of the smooth and notched microstructures is investigated for the three constitutive models studied. For each defect size, the polycrystalline aggregates are loaded in fully reversed tension at the fatigue limit level. In each subfigure of Fig. 2, the response of each slip plane of the polycrystalline aggregates, in terms of τ_a-$\sigma_{n,a}$ is reported. On this figure, the results obtained with the isotropic elastic behavior (Figs 2.a and 2.d), the cubic elastic behavior (Figs 2.b and 2.e) and the combination of the cubic elasticity and the crystal plasticity (Figs 2.c and 2.f) are presented. Figs 2.a, 2.b and 2.c concern the results obtained on the smooth microstructures while Figs 2.d, 2.e and 2.f present the results from the FE computations on the notched microstructures with ρ=80µm. The dashed curves represent a partial estimate of the convex envelopes of the sets of points.

From these figures, it can be observed that the cubic elasticity affects more significantly than the crystal plasticity the distributions, obtained with the isotropic case, of the two considered mechanical quantities. Moreover, this constitutive model leads to an important increase of the amplitude of the normal stresses. Nevertheless, it has to be noted that the plasticity reduces the maximum values of the shear stress amplitude and especially in the cases of notched microstructures in which some grains near the defect are highly stressed. Similar conclusions were proposed by Robert et al. [4].



(a) Isotropic elasticity, ρ=0µm **(b) Cubic elasticity, ρ=0µm** **(c) Cubic elasticity and crystal plasticity, ρ=0µm**



(d) Isotropic elasticity, ρ=80µm **(e) Cubic elasticity, ρ=80µm** **(f) Cubic elasticity and crystal plasticity, ρ=80µm**

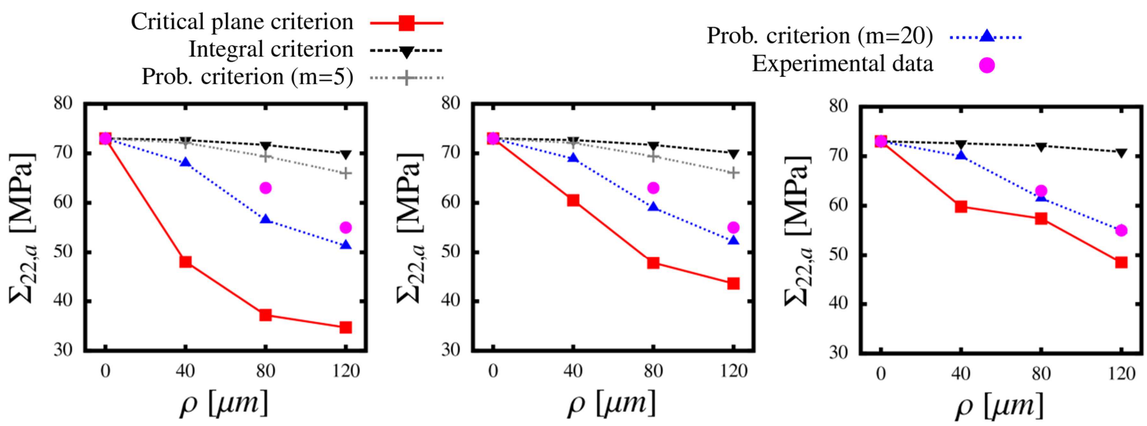
Figure 2. Mesoscopic response, in terms of τ_a-$\sigma_{n,a}$, of each slip planes obtained from the FE simulations of the polycrystalline aggregates

Predictions of the fatigue criteria for the different constitutive models

The determination of the predicted average fatigue limit in fully reversed tension, for a given defect size, consists to search $\Sigma_{22,a}$ which have to be applied to the polycrystalline aggregates such that $\sigma_{DV}/\beta_{DV}=1$ in average for the critical plane criterion, $\sigma_P/\beta_P=1$ in average for the integral criterion and $P_{F_a}=50\%$ in average for the probabilistic criterion. The predictions obtained for each criterion and each constitutive models assigned to the grains are presented in Fig. 3. When the crystal plasticity is used, the predicted fatigue limits are iteratively searched and thus a significant computation time is required. For this reason, only the predictions of the most promising case ($m=20$) are determined for the probabilistic fatigue criterion.

Whatever constitutive model is applied at the grain scale, it can be observed in Fig. 4 that the critical plane-based criterion provides the most conservatives results whereas the predictions of the integral criterion overestimates the fatigue limit of the notched microstructures. It has to be noted that the predictions of this last criterion highly depend of the number of grains considered in the vicinity of the notch. Indeed, the grains farthest from the notch, which are less stressed, reduced the notch effect on the predicted fatigue limits.

Furthermore, it has to be noted that the probabilistic fatigue criterion, for $m=20$, provides good estimations of the experimental fatigue limits. This criterion can be seen as a good compromise between the local approach of the critical plane-based criterion and the global approach of the integral criterion. Indeed, all the grains in the aggregate are considered to predict the failure of the polycrystal but the contribution of each grain to the fatigue failure is driven by the parameters of the fatigue crack initiation threshold distribution. The lower the standard deviation of the distribution (high m value and low τ_0 value), the more the most stressed grains contribute effectively to the failure whereas the less stressed grains have a negligible effect.



(a) Isotropic elasticity **(b) Cubic elasticity** **(c) Cubic elasticity with crystal plasticity**

Figure 3. Comparison between the predictions of the criteria and the experimental results for each constitutive material model assigned to grains

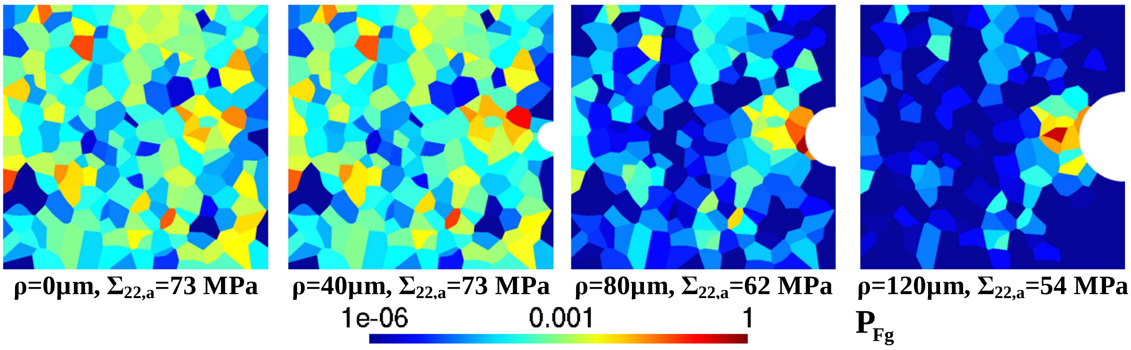


Figure 4. Failure probabilities of the grains, predicted by the probabilistic criterion (m=20) in the case of cubic elasticity with crystal plasticity, for different defect sizes

Finally, it can be observed in Fig. 4, which represents the predicted P_{Fg} for the same microstructure with different defect sizes and loaded approximately at the fatigue limit level, that the more the notch radius, the more heterogeneous are the failure probabilities and that the maximum values are localised near the notch.

CONCLUSIONS

In this work, the significant role of the cubic elasticity on the distributions of the amplitudes of the shear and normal stresses has been shown whereas the crystal plasticity mainly affects the maximum values of the shear stress amplitude.

On the other hand, the ability of a fatigue criterion based on a probabilistic approach to predict the fatigue limit in the presence of notches has been demonstrated in the case of fully reversed tension and for some defect sizes.

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