A new interpretation of the loading path effect in high cycle fatigue via numerical simulation of polycrystalline aggregates

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Abstract. In this work, an analysis of a high cycle multiaxial fatigue criterion is undertaken via the simulation of polycrystalline aggregates. The metallic material chosen for investigation is pure copper with a FCC crystalline structure. Three material models are investigated: isotropic elasticity, cubic elasticity and combination of cubic elasticity and crystal plasticity. Two-dimensional polycrystalline aggregates, which are composed of 300 randomly orientated equiaxed grains, are loaded at the median fatigue strength defined at 10^7 cycles. The aim is to calculate the mechanical quantities at the grain scale. In order to analyse the effect of the loading path on the local mechanical response, combined tension-torsion loads, in-phase and out-of-phase, with different biaxial ratios, are applied to each polycrystalline aggregate. An analysis of the Huyen and Morel fatigue criterion is conducted, using mechanical quantities computed at the grain scale.

Introduction

Fatigue crack initiation in metallic materials is a local phenomenon intimately related to the plastic activity at the grain scale. Thus, it seems relevant to try to evaluate the mesoscopic mechanical quantities (i.e. the average values per grain) in order to study the high cycle fatigue (HCF) strength. Unfortunately, due to the complex anisotropic elasto-plastic behavior of the crystals constituting a metal, no simple method exists to precisely estimate these quantities.

Localization schemes are a common way to estimate the mechanical response of each grain knowing the macroscopic loading applied to a polycrystal. This approach has been successfully used in the development of well-known HCF criteria [1,2]. Nevertheless, simplifying assumptions on the local behavior are usually needed to obtain simple analytical expressions of HCF criteria. Moreover some aspects like neighborhood or free surface effects can hardly be taken into account.

A promising approach consists in computing, by finite elements (FE) method, the mechanical response of explicitly modeled polycrystalline aggregates. In recent years, several works have involved this kind of numerical simulations in the fatigue domain [3,4]. Our study falls within this framework and is divided into two parts:

- An investigation of the role of the material behavior on the mesoscopic mechanical response of pure copper polycrystals cyclically loaded at levels close to the median fatigue strength at 10^7 cycles ;
- An analysis of the predictions of a probabilistic fatigue criterion, in the cases of combined tension-torsion loads with different biaxial ratios and phase differences, considering several material behaviors.

Modeling approach

Material behavior models. Three material behaviors have been investigated in this study:

- Linear isotropic elasticity ;
- Linear cubic elasticity;
- Linear cubic elasticity with crystal plasticity.

In the first case, elastic properties of each grain are identical in all directions and are completely defined by the Young's modulus and the Poisson's ratio. In the second and third cases, cubic elasticity, which corresponds to the elastic anisotropic behavior of FFC grains, is characterized, in the crystal coordinate system, by three coefficients: C_{1111}, C_{1122} and C_{1212}. The orientation of each crystal with respect to the coordinate system of the aggregate is then defined by three Euler angles which are randomly generated according to an equiprobable distribution. Finally, crystal plasticity is described by the material behavior model introduced by Méric and Cailletaud [5]. In order to deal with the crystal plasticity problem, two mechanical quantities are used: the plastic slip γ^s and the resolved shear stress τ^s on the slip system s. Linking relations between, on one hand, the plastic strain rate tensor $\underline{\underline{\dot{\varepsilon}}}^p$ and the plastic slip rates $\dot{\gamma}^s$ and on the other hand, the stress tensor $\underline{\underline{\sigma}}$ and the resolved shear stress τ^s acting on the slip system s are respectively:

$$\tau^s = \underline{\underline{m}}^s : \underline{\underline{\sigma}} \quad and \quad \underline{\underline{\dot{\varepsilon}}}^p = \sum_s \dot{\gamma}^s \underline{\underline{m}}^s \tag{1}$$

where the orientation tensor m^s is defined by:

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

with $\underline{n}^s$ and $\underline{l}^s$ corresponding respectively to the slip plane unit normal vector and to the slip system s orientation vector. The plastic slip rate on a slip system s is described by the following flow rule:

$$\dot{\gamma}^s = \left\langle \frac{\left|\tau^s - x^s\right| - r^s}{K} \right\rangle_+^n sign\left(\tau^s - x^s\right) = \dot{v}^s \; sign\left(\tau^s - x^s\right) \tag{3}$$

The isotropic and kinematic hardening laws, respectively r^s and x^s, are defined by:

$$r^s = r_0 + Q\sum_r h^{sr}\left(1 - \exp\left(-b\,v^r\right)\right) \quad and \quad x^s = c\alpha^s \quad with \quad \dot{\alpha}^s = \dot{\gamma}^s - d\,\dot{v}^s\alpha^s \tag{4}$$

with h^{sr} the interaction matrix proposed by Franciosi [6].

Table 1. Material parameters values for a pure copper

Isotropic elasticity		Cubic elasticity [5]		
$E\,[GPa]$	ν	$C_{1111}[GPa]$	$C_{1122}[GPa]$	$C_{1212}[GPa]$
83	0.3	159	122	81

Crystal plasticity [6]												
$K\left[MPa.s^{1/n}\right]$	n	$r_0\,[MPa]$	$Q\,[MPa]$	b	c	d	h_0	h_1	h_2	h_3	h_4	h_5
8	20	15	4	12	32000	900	1	1	0.2	90	3	2.5

Numerical model. Polycrystalline aggregates morphologies are generated by randomly positioning and orienting ellipses, without superimposition, in a square. A watershed algorithm is then used to extend each water source, i.e. ellipse, and build barriers when different sources are meeting. These barriers, which constitute the grain boundaries of the microstructure, are approximated with Bézier curves to form the CAD model of the polycrystalline aggregate. Finally, the finite element mesh is generated using Gmsh software [7].
Three-node triangular finite elements, with linear interpolation and generalized plane strain hypothesis, are used. Each grain is discretized in average with 400 elements. An overview of the meshed microstructure is showed in Fig. 1.

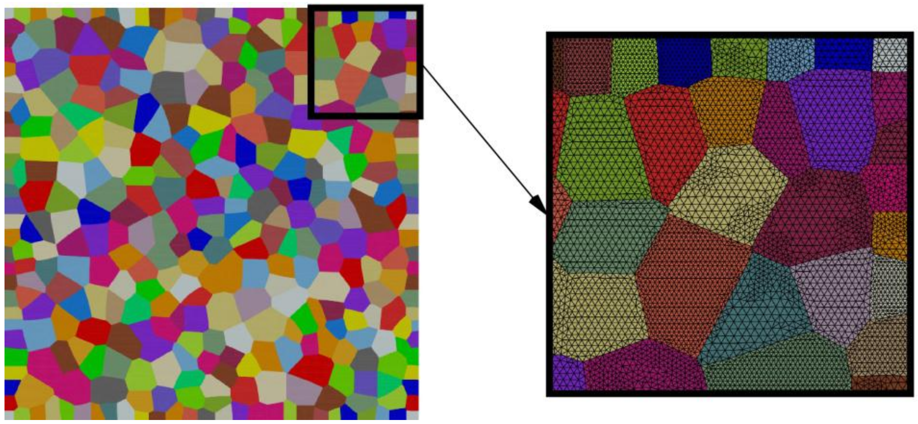


Fig.1. Geometry and finite element mesh of a periodic 2-dimensional polycrystalline aggregate with 300 grains and approximately 120,000 elements.

For each studied loading condition, three microstructures containing 300 equiaxed grains have been generated. Moreover, three different sets of random triplets of Euler angles are associated for each microstructure. As a result, nine configurations, per loading condition, are used.
Thanks to the linearity of the elastic behaviors, only one loading cycle is simulated when no plasticity is assigned to grains. In the case where crystal plasticity is used, 10 cycles are performed so that aggregates tend to a plastic shakedown state at the local scale. Periodic displacement conditions are imposed at the edge of the aggregate in addition to an applied average stress tensor $\underline{\underline{\Sigma}}$. The numerical simulations are conducted using the ZéBuLoN FE software developed by Mines ParisTech, Northwest Numerics and ONERA.

Loading conditions. Polycrystalline aggregates are loaded in combined tension-shear representative of the stress state encounter in tension-torsion fatigue tests. The applied macroscopic stress tensor $\underline{\underline{\Sigma}}$ can be expressed, in the aggregate coordinate system, by

$$\underline{\underline{\Sigma}} = \begin{bmatrix} \Sigma_{11,a}\sin(\omega t) & \Sigma_{12,a}\sin(\omega t - \varphi) & 0 \\ \Sigma_{12,a}\sin(\omega t - \varphi) & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (5)$$

Several biaxiality ratio k and phase difference φ have been selected for this study (Table 2).

Table 2. Biaxiality ratio and phase angle studied

$k = \Sigma_{12,a} / \Sigma_{11,a}$							φ [°]				
0	0.25	0.5	0.75	1	2	∞	0	30	45	60	90

Loading amplitudes $\Sigma_{11,a}$ and $\Sigma_{12,a}$ have been chosen so that the polycrystalline aggregates are loaded at the median fatigue limits at 10^7 cycles of a pure copper. These limits under fully reversed tension s_{-1} and under fully reversed torsion t_{-1} are approximated ($s_{-1} = 56MPa$ and $t_{-1} = 36MPa$) from experimental results [8]. In the case of combined tension-torsion, endurance limits are estimated with the Huyen and Morel fatigue criterion (defined in the next section).

Probabilistic HCF crack initiation criterion

The criterion described here is a slightly modified version of the criterion proposed by Morel and Huyen [9]. Here, we supposed that fatigue crack initiation in a crystal does not occur if the shear stress amplitude τ_a acting on a slip plane p belonging to the considered grain does not exceed a threshold value τ_a^{th}. In addition to the scatter of the mesoscopic mechanical quantities, characterized by the FE computations, the heterogeneity of the crack initiation threshold at the grain scale is taken into account thanks to the assumption that τ_a^{th} follows a Weibull distribution. In that way, the probability that a crack initiates in a slip plane p can be expressed by:

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

The normal stress effect on fatigue strength is taken into account by postulating an expression (Eq. 8) of the scale parameter τ_0 depending of the normal stress amplitude $\sigma_{n,a}$ and the mean normal stress $\sigma_{n,m}$ acting on the slip plane p:

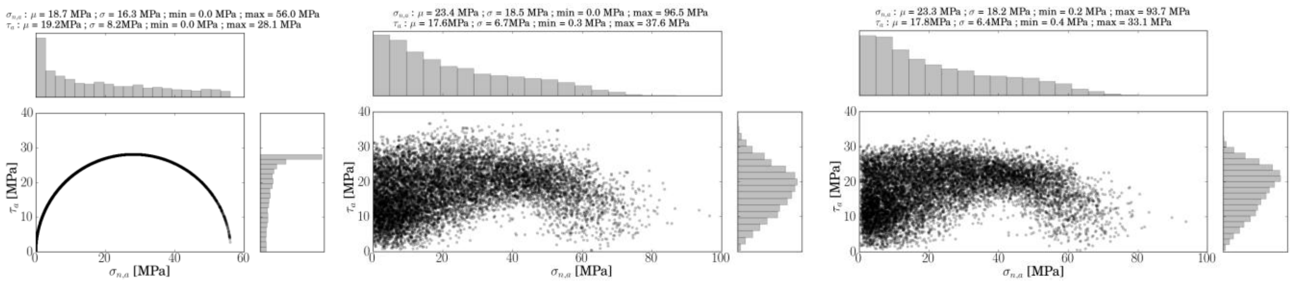
$$\tau_0 = \tau_0' \frac{1 - \gamma \sigma_{n,m}}{1 + \alpha \left(\sigma_{n,a} / \tau_a \right)} \quad (8)$$

The failure probability P_{Fg} of a grain g is supposed to be equal to the maximum among the failure probabilities of its slip planes (FCC crystal structure has 4 slip planes). Finally, the weakest-link hypothesis [9] is used to determine the failure probability of a polycrystalline aggregate P_{Fa} (Eq. 9) where ng is the number of grains constituting this aggregate.

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

Simulations results

Effect of the material behavior on the mechanical response of the polycrystalline aggregates. The mechanical response of the polycrystalline aggregates is studied at the grain scale through the mesoscopic mechanical quantities (i.e. average mechanical quantities in the grains) for the three material behaviors chosen. This analysis is focused on the mechanical quantities used in the Huyen and Morel criterion: the shear stress amplitude τ_a and the normal stress amplitude $\sigma_{n,a}$. For each slip plane of the nine configurations studied (3 microstructures $\times$ 3 orientations sets), the couple (τ_a, $\sigma_{n,a}$) is reported on each subfigures of Fig. 2. On this figure, the results obtained with the isotropic elastic behavior (Fig. 2.a), the cubic elastic behavior (Fig. 2.b) and the combination of the cubic elasticity and the crystal plasticity (Fig. 2.c) in the case of fully reversed tension are presented. The loading amplitude applied on the aggregates corresponds to the median fatigue limit s_{-1}.



(a) Isotropic elasticity (b) Cubic elasticity (c) Cubic elasticity and crystal plasticity

Fig.2. Mesoscopic mechanical response of the 9 aggregates under fully reversed tension.

It can be observed that the distributions of the considered mechanical quantities are strongly affected when the isotropic elasticity is replaced by the cubic elastic behavior. Indeed, compared to the isotropic elastic behavior (Fig. 2.a), the cubic elasticity (Fig. 2.b) causes a significant increase of the maximum and the mean values of the normal stress amplitude. Conclusions about the shear stress amplitude are slightly different. Indeed, even though an increase of the maximum value of τ_a is observed, a slight decrease of its mean value is found. It should be noted that the use of cubic elasticity instead of linear elasticity symmetrizes significantly the shear stress amplitude distributions. This leads to a decrease in the number of slip planes exhibiting high shear stress level. The trends described here for tensile loading have also been observed for the other studied loading cases.

When compared to the cubic elastic behavior alone, it appears that the addition of crystal plasticity affects slightly the distributions of the two considered mechanical quantities. Indeed, its effect on the normal stress amplitude distribution is negligible. Furthermore, the distribution of τ_a becomes a slightly more asymmetric which leads to maintain the mean value while the maximum value decreases.

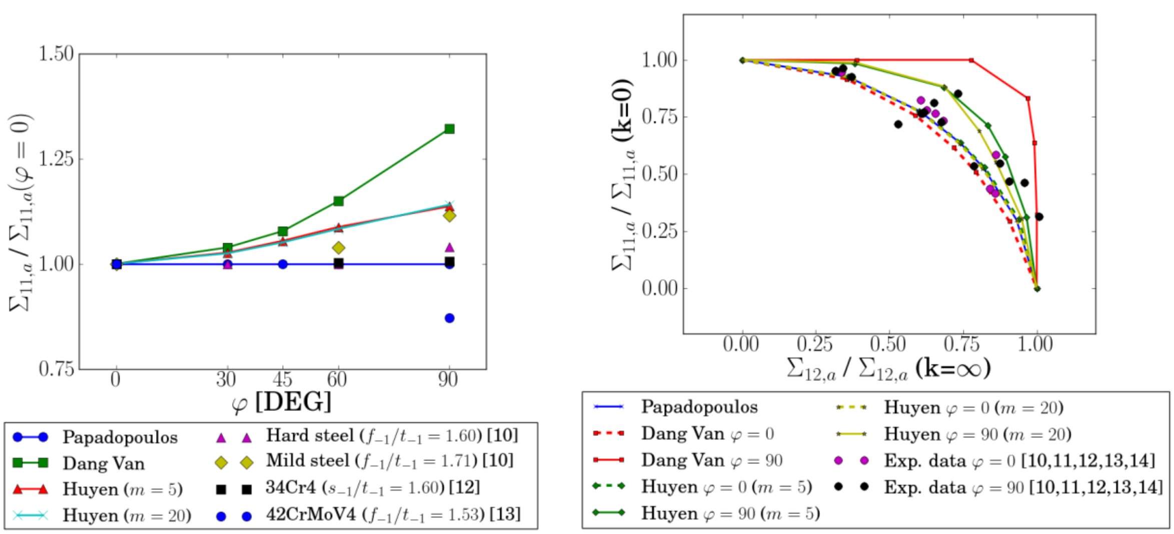
For reasons of computation times and because its effect on the mesoscopic mechanical response seems to be moderate at the fatigue limit level compared to the influence of the cubic elasticity, the crystal plasticity will be neglected in the following discussion.

Identification of the Huyen and Morel criterion parameters. The identification of the Huyen and Morel criterion parameters uses the results of the numerical simulations of polycrystalline aggregates which are loaded at the median fatigue limits in fully reversed torsion and in fully reversed tension. These parameters are then identified so that the failure probabilities of the 9 studied aggregates are in average equal to 50% both in tension and in torsion. Moreover, the identifications are performed separately for each material behavior assigned to grains. Finally, the shape parameter m, which characterizes the fatigue strength scatter, is arbitrarily chosen in this study because of the lack of experimental results about the fatigue limit standard deviation of pure copper. Two m values have been considered (5 and 20) which correspond to standard deviations of s_{-1} of about 13 MPa and 3.5 MPa respectively. The identified parameters are summarized in Table 3.

Table 3. Parameters of the Huyen and Morel criterion identified for the studied copper

Material behavior assumption	m	$\tau_0'\ [MPa]$	α
Isotropic elasticity	5	110.9	0.219
Cubic elasticity		114.6	0.281
Isotropic elasticity	20	47.0	0.248
Cubic elasticity		51.1	0.272

Predictions of the proposed criterion for the isotropic elastic behavior. To determine the fatigue limits with the Huyen and Morel criterion, loading amplitudes are iteratively searched so that the mean value of P_{Fa} (for the 9 configurations studied) is equal to 50%. The predictions of this criterion are studied for the isotropic elastic behavior and are compared to experimental results found in the literature and to the fatigue limits predicted by two other classical multiaxial HCF criteria based on a multi-scale approach: Dang Van [1] and Papadopoulos [2]. Otherwise, the fatigue test data have been chosen so that the tested materials have a ratio s_{-1}/t_{-1} close to the one of copper. According to the Papadopoulos criterion, phase difference for tension-torsion loading conditions does not affect the fatigue limits of the material while the Dang Van criterion predicts a beneficial effect of an increasing φ (from 0° to 90°) on the fatigue strength (Fig. 3.a and 3.b). In the case of in-phase tension-torsion, the Huyen and Morel criterion gives predictions similar to those of the Papadopoulos criterion and slightly more optimistic than those of the Dang Van criterion (Fig. 3.b). Otherwise, in the case of high phase differences ($\varphi > 45°$), fatigue limits estimated with the proposed criterion lies between those predicted by the Papadopoulos criterion and the Dang Van criterion. Finally, it is worth noting that the value of the shape parameter m does not strongly affect the average fatigue limits predicted by the Huyen and Morel criterion. The maximum difference encountered, occurring for $\varphi = 90°$ and $k = 1$, results in an increase of about 4% of the predicted fatigue limits for m ranging from 20 to 5.



(a) (b)

Fig.3. Comparison between the predictions of the criteria and the experimental results: a) Effect of φ on the tensile mean fatigue strength at 10^7 cycles for $k = 0.5$; b) Effect of the biaxiality on the tensile and torsional fatigue limits for $\varphi = 0°$ and $\varphi = 90°$.

Concerning the experimental results, no clear trend can be observed. Indeed, in some cases [10], an increase in phase difference (for $\varphi \in [0°;90°]$) has a beneficial effect on the fatigue strength while in other cases, it can have a negligible [11,12] or even a detrimental influence [13,14].
It appears that the fatigue limits predicted by all the considered criteria are in good agreement with experimental results for in-phase tensile and torsion fully reversed loading conditions. On the contrary, in the case of high phase difference, the Dang Van criterion mostly overestimates the fatigue limits while the Papadopoulos criterion generally provides conservative predictions. Finally, the Huyen and Morel criterion seems to be a good alternative to the Papadopoulos criterion only for materials showing a significant fatigue strength improvement due to phase difference.

Effect of the constitutive law on the predictions of the Huyen and Morel criterion. The identification being performed for the two considered material behaviors, the predictions of the proposed criterion will now be studied. It appears that the average fatigue limits predicted by the Huyen and Morel criterion for a cubic elastic behavior are surprisingly close to those obtained in the case of the isotropic elasticity. Indeed, when $\varphi = 0°$, the maximum difference, relative to the case of the isotropic elastic behavior, observed is lower than 1%. Differences between fatigue limits predicted for the two material behaviors are more pronounced in the case where $\varphi = 90°$ but they never exceed 5% regardless of the considered m value.
Thus, despite the fact that the mesoscopic mechanical quantities of the criterion are misestimated (especially concerning the normal stresses acting on the slip planes) when the hypothesis that grains have an isotropic elastic behavior is made, the proposed criterion provides almost identical predictions, at least for the cases of in-phase and out-of-phase combined tension-torsion.

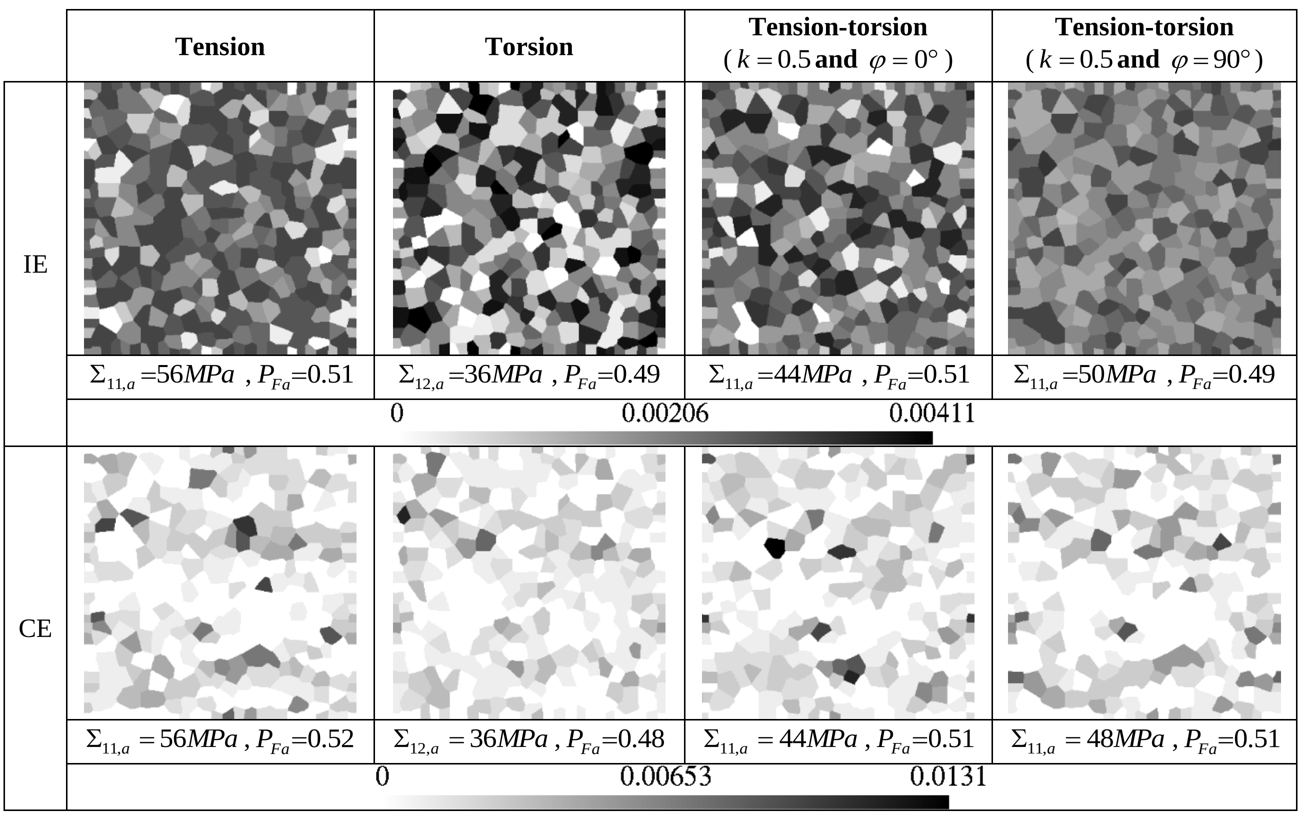


Fig.4. Grain failure probability fields of one microstructure and one orientation set for $m = 5$ (IE: isotropic elasticity, CE: cubic elasticity).

In order to look at the criterion predictions in a polycrystalline aggregate, the grain failure probability P_{Fg} fields of one microstructure and one orientation set are represented in Fig. 4. These fields have been plotted for the two elastic behaviors and for four loading conditions: tension, torsion, tension-torsion with $k = 0.5$ and $\varphi = 0°$ and tension-torsion with $k = 0.5$ and $\varphi = 90°$. In the case of isotropic elasticity, it can be observed that the torsional loading leads to the largest scatter of P_{Fg} in the polycrystalline aggregate while the combined loading with $k = 0.5$ and $\varphi = 90°$ give the most homogeneous field. Regarding the cubic elasticity, the grain failure probability fields are far more heterogeneous compared to those obtained with the isotropic elastic behavior, regardless of the loading case considered. Finally, the most critical grains for the anisotropic elastic case do not correspond to those predicted for the isotropic elastic case due to neighboring effects on the local stress state in the case of cubic elasticity.

Summary

Thanks to numerical simulations of polycrystalline aggregates, it appears that, for loading amplitudes at the fatigue limits levels, the anisotropic elastic behavior is the main factor responsible for the scattering of the mesoscopic mechanical quantities for the studied material while crystal plasticity only affects slightly the distribution of the shear stress amplitude.

Moreover, the analysis of the Huyen and Morel criterion shows that its predictions are close to those provided by the Papadopoulos criterion in the case of in-phase combined tension-torsion. For high phase differences ($\varphi \in [45°;90°]$), the fatigue limits estimated by the proposed criterion are between those predicted by the Papadopoulos and Dang Van criteria. Furthermore, this criterion approximately predicts the same fatigue limits regardless the elastic behavior used at the grain scale.

Only fully reversed combined tension-torsion loads have been considered in this work. In order to verify the validity of the conclusions for a wider range of loading paths, an investigation of biaxial tensile loading will be performed in a forthcoming study together with mean stress effect.

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