Competition between microstructure and defect in multiaxial high cycle fatigue

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ABSTRACT. This study aims at providing a better understanding of the effects of both microstructure and defect on the high cycle fatigue behavior of metallic alloys using finite element simulations of polycrystalline aggregates. It is well known that the microstructure strongly affects the average fatigue strength and when the cyclic stress level is close to the fatigue limit, it is often seen as the main source of the huge scatter generally observed in this fatigue regime. The presence of geometrical defects in a material can also strongly alter the fatigue behavior. Nonetheless, when the defect size is small enough, i.e. under a critical value, the fatigue strength is no more affected by the defect. The so-called Kitagawa effect can be interpreted as a competition between the crack initiation mechanisms governed either by the microstructure or by the defect. Surprisingly, only few studies have been done to date to explain the Kitagawa effect from the point of view of this competition, even though this effect has been extensively investigated in the literature. The primary focus of this paper is hence on the use of both FE simulations and explicit descriptions of the microstructure to get insight into how the competition between defect and microstructure operates in HCF.

In order to account for the variability of the microstructure in the predictions of the macroscopic fatigue limits, several configurations of crystalline orientations, crystal aggregates and defects are studied. The results of each individual FE simulation are used to assess the response at the macroscopic scale thanks to a probabilistic fatigue criterion proposed by the authors in previous works. The ability of this criterion to predict the influence of defects on the average and the scatter of macroscopic fatigue limits is evaluated. In this paper, particular emphasis is also placed on the effect of different loading modes (pure tension, pure torsion and combined tension and torsion) on the experimental and predicted fatigue strength of a 316 stainless steel containing artificial defect.

KEYWORDS. High cycle fatigue; Multiaxial loading; Defect; Polycrystalline aggregate; Probabilistic fatigue criterion.

INTRODUCTION

Traditionally, the fatigue design of components submitted to complex loading modes during service life is based on extensive material property databases. The relationship between microstructure and the resulting fatigue strength is primarily qualitative. This is all the more true in the presence of geometrical defects inducing stress and strain concentrations and hence affecting the strength. Several authors have established fatigue criteria taking into account accurately the detrimental influence of defects on the fatigue limits in tension [1], in torsion [2] and in combined tension and torsion [3]. However, although the practical interest of these approaches is undeniable, they often involve a material characteristic length whose physical meaning is unclear.

Moreover, these methods neglect the variability of the microstructure in the vicinity of the defect and thus cannot correctly reflect the scatter observed in the HCF strength of metallic materials. This scatter is often explained by the anisotropic elasto-plastic behaviour 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 and use the mesoscopic mechanical quantities (i.e. the average mechanical quantities at the grain scale) to assess the macroscopic fatigue response. To get access to them, localization schemes are sometimes used, for instance by Dang Van [4], Papadopoulos [5], Monchiet [6] and Morel [7]. Despite the qualities of these criteria (ease of application, fairly accurate predictions), some simplifying assumptions (e.g. same elastic behaviour at the grain scale and the macroscopic scale) lead at most to a first order approximation of the fatigue problem. In particular, the free surface effects and the influence of the neighbouring grains are ignored.

A promising approach, consisting in computing, by FE method, the mechanical response of explicitly modelled polycrystalline aggregates, allows to take into account microstructural details generally neglected in the homogenisation schemes and to deepen the analysis of the mesoscopic mechanical responses of metals under cyclic multiaxial loading. In recent years, several works have involved this kind of numerical simulations to contribute to the study of the HCF behaviour [8-12].

The present study falls within this framework and a specific effort is made to quantify the multiaxial fatigue performance of metals in the presence of defects through statistical modeling of the microstructure.

The practical implications of such a work are numerous. Commercial alloys are indeed composed of various microstructural heterogeneities depending on the type of material and the manufacturing process used. For instance the shrinkage or gas pores which are most of the time present in cast alloys are known as the main source of crack initiation in such materials [13]. In some forged steels, the presence of non-metallic inclusions can be at the origin of a fatigue anisotropy caused by a change of fatigue damage mechanisms depending on the fibering orientation to the loading axis [14]. These two examples have one thing in common: the defects responsible for the crack initiation are often of the same size as the microstructure.

This paper is hence focused on the specific case where the defect size is of the order of the grain size. More exactly, the purpose is to analyze the competition existing between the stress concentration induced, on one hand, by a small defect and, on the other hand, by the most highly stressed regions of the microstructure caused by the anisotropic behavior of the grains. This work contributes to a better understanding of the Kitagawa effect characterized by the existence of a critical defect size under which the fatigue strength is no more affected by the defect.

MODELLING APPROACH AND PROBABILISTIC FATIGUE CRITERION

Finite Element modelling

Finite Element simulation of polycrystalline aggregate requires most of the time simplified geometries in particular to get reasonable computation time. In the present study, most of the FE models are of 2D type and the microstructure is explicitly modelled only in the immediate vicinity of the geometrical defect. A few 3D hemispherical notches are also modelled but only for the smallest defect size. For both 2D and 3D models, an homogeneous isotropic matrix embeds the polycrystal. The process used to generate the 2D polycrystalline geometries is described in [10]. Both smooth and notched microstructures are studied. The finite element mesh of the CAD of the microstructure is generated using Gmsh [15]. Three-node triangular finite elements with linear interpolation and generalised plane strain hypothesis are employed for the 2D simulations. Each crystal is distretized with an average of 75 elements. A finite element mesh illustration of a microstructure embedded in a matrix in shown in Fig. 1. In the absence

of the central defect, 3265 grains are contained in the "smooth" polycrystalline aggregate. 5 defect diameters are considered : 0, 50, 95, 365 and 510 μm.

For each defect size investigated, one geometry of the polycrystalline aggregate and ten orientation sets are used. Orientation sets are composed by triplet of Euler angles such as to represent the anisotropic texture. The numerical simulations are conducted with the ZeBuLoN FE software [9].
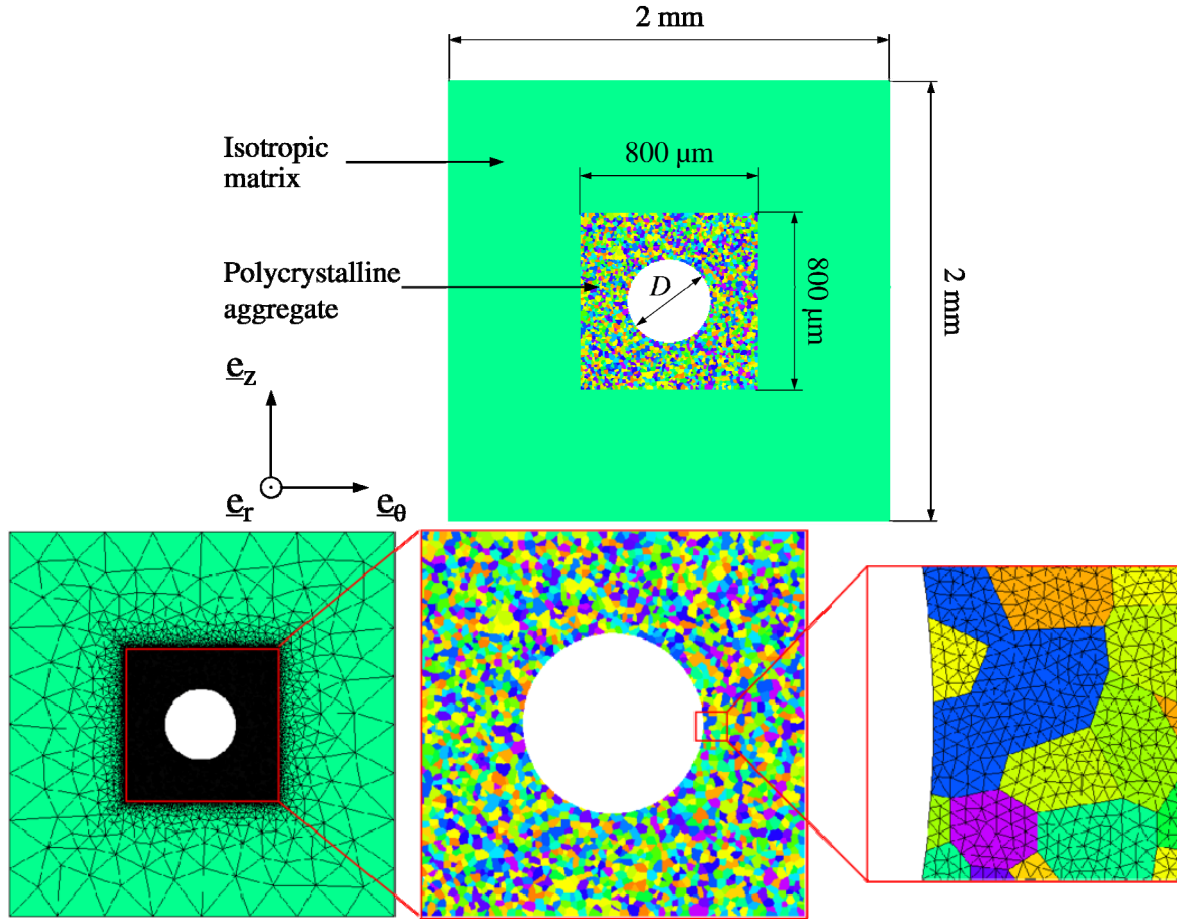

Figure 1: Shape and dimensions of the polycrystalline aggregate and the matrix used in the 2D finite element model.

Constitutive material models at the mesoscopic (grain) scale and probabilistic criterion

To represent the behavior of each individual grain of the 316L polycrystalline aggregate, an elasto-visco-plastic constitutive material model is used. For the FCC structure under interest, the elastic behavior is cubic and the plastic slip occurs along the closed-packed planes {1 1 1} and directions <1 1 0>. Cubic elasticity is assigned to each grain and is characterized by three coefficients defined in the crystal coordinate system: C_{1111}, C_{1122} and C_{1212}. A phenomenological single crystal visco-plastic model proposed by Méric et al. [9] is employed for the crystal plasticity.

The slip rate $\dot{\gamma}_s$ on a slip system s is governed by a Norton-type flow rule making appear the resolved shear stress τ_s acting on s and the isotropic and kinematic hardening variables, respectively r_s and x_s, related to s :

$$\dot{\gamma}_s = \left\langle \frac{\left| \tau_s - x_s \right| - r_0 - r_s}{K} \right\rangle_+^n \operatorname{sgn}\left(\tau_s - x_s \right) = \dot{v}_s \operatorname{sgn}\left(\tau_s - x_s \right) \tag{1}$$

K and n are the parameters controlling the viscosity and r_0 is the critical resolved shear stress.

The resolved shear stress τ_s is computed from the stress tensor by means of an orientation tensor.

In the evolution laws of the hardening variables r_s and x_s, the influence of the accumulated plastic slip v_r of the slip system r on the hardening of the slip system s is taken into account thanks to the components h_{sr} of an interaction matrix [16]. Q and b are the other isotropic hardening parameters and c and d are the kinematic hardening parameters.

$$\dot{x}_s = c\dot{\gamma}_s - d\dot{v}_s x_s \tag{2}$$

$$r_s = Q\sum_r h_{sr}\left(1 - e^{-bv_r}\right) \tag{3}$$

All the material parameter values used in the FE simulations are identified by means of an optimization procedure (Levenberg-Marquardt algorithm) applied to an important experimental database built by the authors and pertaining to the multiaxial cyclic elasto-visco-plastic behavior of the 316L.

Even though the material constitutive model is found to give good predictions of the macroscopic cyclic response under different loading modes, its capability to clearly capture the different sources of the mesocrack initiation scatter is questionable. To the authors' mind, the description by the FE model of the polycrystalline microstructure is too partial to get access to all the actual causes of crack initiation at the scale of the grain. In particular, the phenomenological crystal visco-plastic model cannot account for all the transgranular heterogeneities (for instance the formation of dislocation structures leading to the localization of the plastic strain in slip bands is ignored). To reflect this variability that can appear from grain to grain (and independent of the grain orientation and position within the aggregate), it has been proposed, as done by Morel et al. [7], to introduce a statistical distribution of the mesoscopic fatigue crack initiation threshold and to use it in a global probabilistic approach. More exactly, the formation of a fatigue crack at the scale of a single grain is assumed to be governed not only by the mesocopic shear and normal stresses on a slip plane (deduced from the FE computations) but also affected by a statistical distribution of the crack initiation threshold representative of the local microstructural heterogeneities.

In all the fatigue analyses proposed from now on, the mesoscopic mechanical quantities used in the criterion are computed from the stress tensors averaged per grain which are obtained thanks to the finite element simulations of polycrystalline aggregates.

A crack is hence supposed to initiate at the grain scale when the shear stress amplitude τ_a acting on the most stressed plane exceeds a threshold τ_a^{th}. The latter is supposed to be a random variable following a Weibull distribution characterized by a shape parameter m and a scale parameter τ_0. The probability for a crack to initiate on a slip plane is then given by

$$P_{Fn} = P\left(\tau_a \geq \tau_a^{th}\right) = 1 - \exp\left[-\left(\frac{\tau_a}{\tau_0}\right)^m\right] \tag{4}$$

The mesoscopic normal stress acting on the slip plane is assumed to change the initiation conditions by affecting the scale parameter. The choice is made to make appear a dependence of τ_0 on the mesoscopic normal stress amplitude $\sigma_{n,a}$ (more exactly on the triaxiality factor $\sigma_{n,a}/\tau_a$) and the mesoscopic mean normal stress $\sigma_{n,m}$:

$$\tau_0 = \tau_0 {}'\frac{1 - \gamma\,\sigma_{n,m}}{1 + \alpha\left(\sigma_{n,a}/\tau_a\right)} \tag{5}$$

The failure probability of a grain P_{Fg} is chosen as the maximum among the failure probabilities P_{Fn} of its slip planes. Finally the failure probability of the polycrystalline aggregate P_{Fa} is computed according to the weakest-link hypothesis:

$$1 - P_{Fa} = \prod_{g=1}^{Ng}\left(1 - P_{Fg}\right) \tag{6}$$

Where N_g is the number of grain in the whole aggregate. The use of the weakest-link concept seems reasonable in the HCF regime because the failure is most of the time governed by the initiation and the propagation of a single crack rather than the initiation and the coalescence of a large set of cracks. The interactions between the different cracks are disregarded here.

In a previous paper [16], the authors have investigated the influence of geometrical defects on the high cycle fatigue behavior of an electrolytic copper. In order to better understand the role of each source of local anisotropy on the macroscopic response, three different material constitutive models were assigned to the grains: isotropic elasticity, cubic elasticity, crystal plasticity in addition to the cubic elasticity. Some 2D finite element simulations on synthetic microstructures have proved the predominant influence of the elastic anisotropy of the grains. In the presence of notches, the influence of the plasticity increases with the notch size. In order to get the macroscopic response from the local stress and strain distributions, three different fatigue criteria (Dang Van [4], Papadopoulos [5], Morel [7]) were used. It was found that the predictions of the critical plane criterion (Dang Van) are too conservatives as only the most critical slip plane in the polycrystal is hold responsible for the entire macroscopic response. The integral criterion (Papadopoulos) overestimated the fatigue strength and the probabilistic fatigue criterion (Morel) was a good alternative to these two criteria. The predictions of this probabilistic criterion in fully reversed tension and fully reversed shear were in good agreement with most of the experimental trends. In particular, it has been numerically found that the fatigue strength is less sensitive to the shear mode than to the tension mode when the defect size increases.

The present study deals with the fatigue strength of another metallic material: 316L stainless steel. The experimental and numerical works concern the case of polycrystalline aggregates containing small hemispherical defects.

EXPERIMENTAL MULTIAXIAL FATIGUE BEHAVIOR OF A 316L STEEL IN THE PRESENCE OF DEFECTS

Material and fatigue test conditions

The austenitic stainless steel AISI 316L produced by Aubert & Duval and commercially named 316L M25W is provided in the form of round bars for this study. The grain morphology is roughly equiaxed with a mean grain size around 14 μm. Fatigue tests are carried out on tubular specimens at room temperature, in air environment at a frequency of 10 Hz on an Instron 8850 servohydraulic multiaxial fatigue testing machine. The latter can apply to the gauge length of the specimens combined axial load and torque. Three loading conditions are applied: uniaxial tension with a load ratio R=-1, torsion with a load ratio R=-1, in-phase uniaxial tension and torsion with a load ratio R=-1 and a biaxiality ratio $k_{\theta z}$=0.5. Some artificial hemispherical defects are introduced at the surface of the gauge length by sinker electric discharge machining. Defect diameters ranging from 95 to 510 μm are considered. Both smooth specimens and specimens containing defects are tested under the different loading modes. Three specimens are used per configuration (defect size and loading mode) to estimate the fatigue strength defined at 2.10^6 cycles.

Results and discussion of the fatigue tests

All the fatigue test results under fully-reversed loading conditions are gathered in a Kitagawa-type diagram in Fig. 2. The macroscopic stress amplitude $\Sigma_{ij,a}$ corresponds to $\Sigma_{zz,a}$ in the cases of fully-reversed tension and fully-reversed combined tension and torsion whereas it corresponds to $\Sigma_{\theta z,a}$ in the case of fully-reversed torsion. The dashed lines give the experimental evolution of the fatigue strength at 2.10^6 cycles as a function of the defect diameter D.

It is clearly observed a decrease of the fatigue strength with the biaxiality ratio $k_{\theta z}$ increase for any defect size. The case of the combined tension and torsion loading with a biaxiality ratio $k_{\theta z}$=0.5 lies between the pure tension and the pure shear cases for any defect size.

A striking feature of the fatigue behavior in the presence of defect is the evolution of the experimental ratio $\varphi= t_{-1}/ s_{-1}$ between the fatigue limits under fully reversed torsion denoted as t_{-1} and fully reversed tension denoted as s_{-1} with respect to the defect size (Fig. 6). Using the geometrical parameter $\sqrt{area}$, it appears that the defects are more detrimental in fully-reversed tension than in fully-reversed torsion. The ratio φ shows indeed an increase with the defect size. This is coherent with the trends observed in the literature by Endo et al. [18] and Billaudeau et al. [19] on other steels and represented in Fig. 6.

Some observations of the crack initiation mechanisms for all the test configurations (with and without defects) show the predominant role played by the defects and the microstructure. When the surface is defect-free, the microcracks generally initiate along slip bands even though some inter-granular cracks are sometimes observed. In the presence of defect, the initiation always takes place at the surface of the defect (for any defect size). In that case, it is not possible to identify the initiation site which seems to be homogeneously distributed at the periphery of the defect. The nucleated crack propagates on the plane(s) perpendicular to the maximum principal stress direction for all the loading cases.
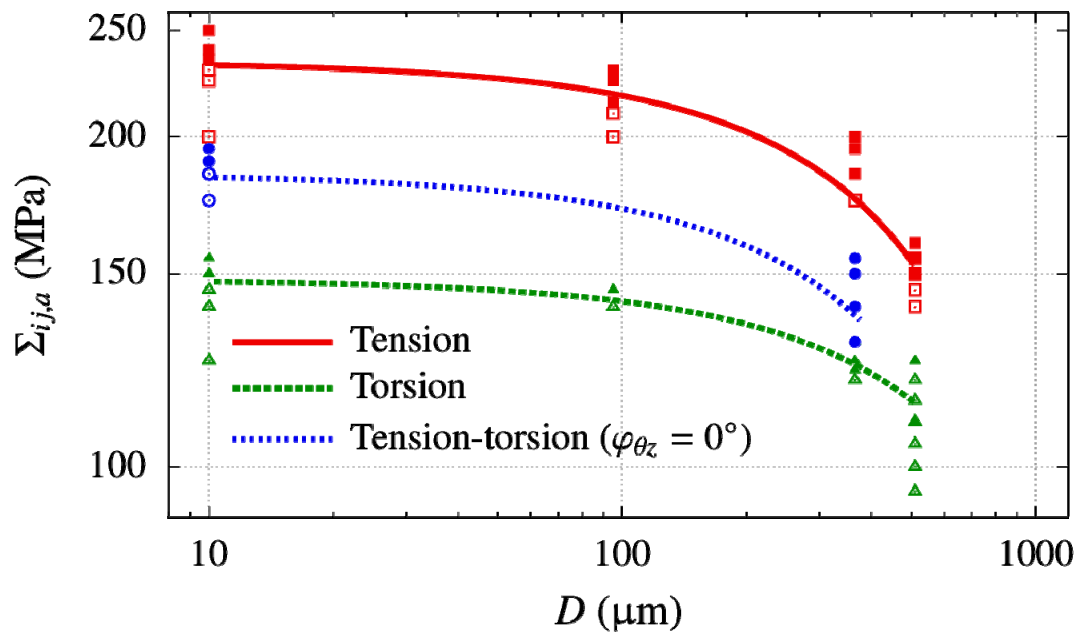
Figure 2: Results of the fatigue tests conducted on the 316L steel in uniaxial tension, torsion and combined tension and torsion (with a biaxiality ratio $k_{\theta z}=0.5$) with a load ratio R=-1 as a function of the defect diameter D.

RESULTS AND DISCUSSIONS

Distribution of the local stress fields in the presence of defects

Before going into the details of the analysis of the macroscopic response under different loading modes, it is useful to look more closely at the way stresses and strains are distributed within the aggregate. For each loading mode and defect size investigated, the mechanical response at the mesoscopic scale is depicted in the plane $\tau_a - \sigma_{n,a}$, where τ_a is the shear stress amplitude and $\sigma_{n,a}$ is the normal stress amplitude acting on all the slip planes of the 10 configurations simulated (Fig. 3). For each combination loading mode - defect size, the distribution, the mean value and the maximum value are given. The most striking feature of the graphs is the big range of the mesoscopic stress values. It can be shown that both the grain orientation to the loading axis and the (elastic and visco-plastic) anisotropic behavior are responsible for this huge scatter. As expected, it is also observed that the loading mode strongly affects the average distribution. When a hole defect is introduced into the aggregate, it occurs that the average distribution is not strongly affected but the maximum can increase significantly. This is a consequence of the stress concentration due to the defect that affects the mechanical response of a few grains.

Distribution of crack initiation and predictions of the average fatigue limits

The Morel probabilistic criterion is now used to derive the macroscopic failure probability from the mesoscopic stress fields. In order to illustrate the way the failure probability is derived, the distributions of the failure probability per grain are given for different loading mode – defect configurations. The results with two different shape parameters m (5 and 20) are given as well. For the two loading modes, fully reversed uniaxial tension and fully-reversed torsion, analysed in Fig. 4, the role of the exponent m is very clear. The heterogeneity of the crack initiation mechanism is much higher with the m value of 20 than with 5. This is true for the two loading modes used for the illustration but for the combined loading as well.

The shape factor m can hence be seen as the parameter that governs the way the crack initiation is heterogeneously distributed within the aggregate. It is important to note that both the grain orientation and the crystal anisotropic behavior affect the local mechanical response distribution. Their contributions to the crack initiation mechanisms are important and unquestionable. Nonetheless, the numerical model to compute them is partial by nature and does not allow to reflect all the potential microstructural heterogeneities within a grain. The simple probabilistic criterion proposed here helps to bridge the gap between the actual crack initiation mechanisms (and the related scatter) and the results of the EF simulations of polycrystalline aggregate.
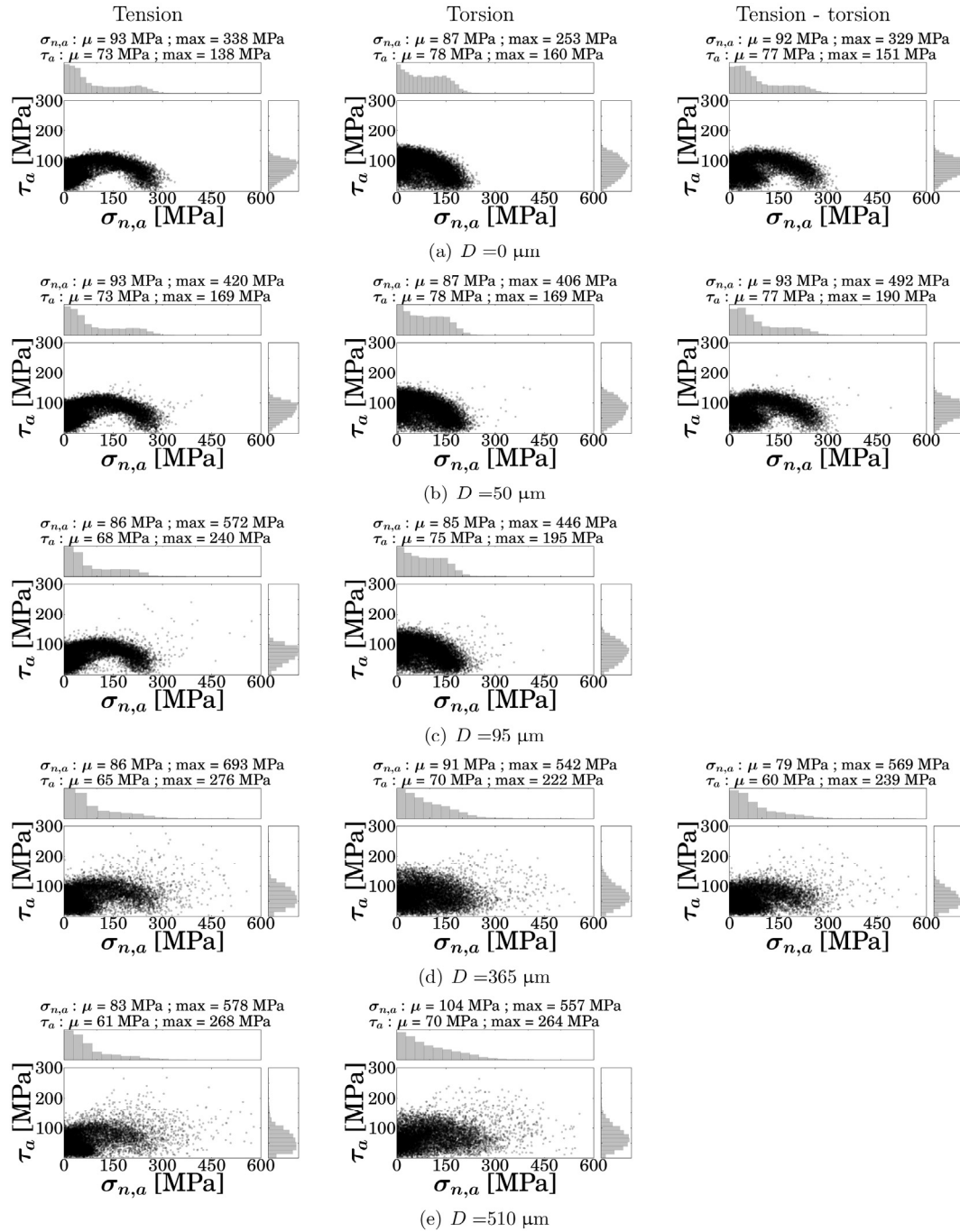
Figure 3: Mesoscopic response in the plane $\tau_a - \sigma_{n,a}$ for different defect diameter D. Evolution of the average and maximum values for three loading modes (tension, torsion, tension-torsion) and 5 defect sizes a) D=0 μm, b) D=50 μm, c) D=95 μm, d) D=365 μm, e) D=510 μm.

About the holed structure and as expected, the stress concentration induced by the defect leads to a sharp increase of the granular failure probability. The way the failure probability is distributed around the defect strongly depends on the m parameter. For the highest value of the shape factor (m=20), the crack initiation is more likely to occur in a few grains located in the most stressed region. For the smallest value (m=5), much more grains around the defect are prone to make appear a crack. In other words, even though all the grains in the microstructure are considered to predict the failure

probability of the aggregate, the contribution of each grain to the initiation mechanism is driven by the parameters of the statistical distribution defining the crack initiation threshold.

This short analysis aims at proving that the shape factor m of the probabilistic criterion proposed plays a role similar as a material characteristic length for the crack initiation mechanism ; this length being very small (of the order of the grain) for the highest value of m. In the presence of a defect, this criterion allows to know how localized is the crack initiation mechanism at the notch root.
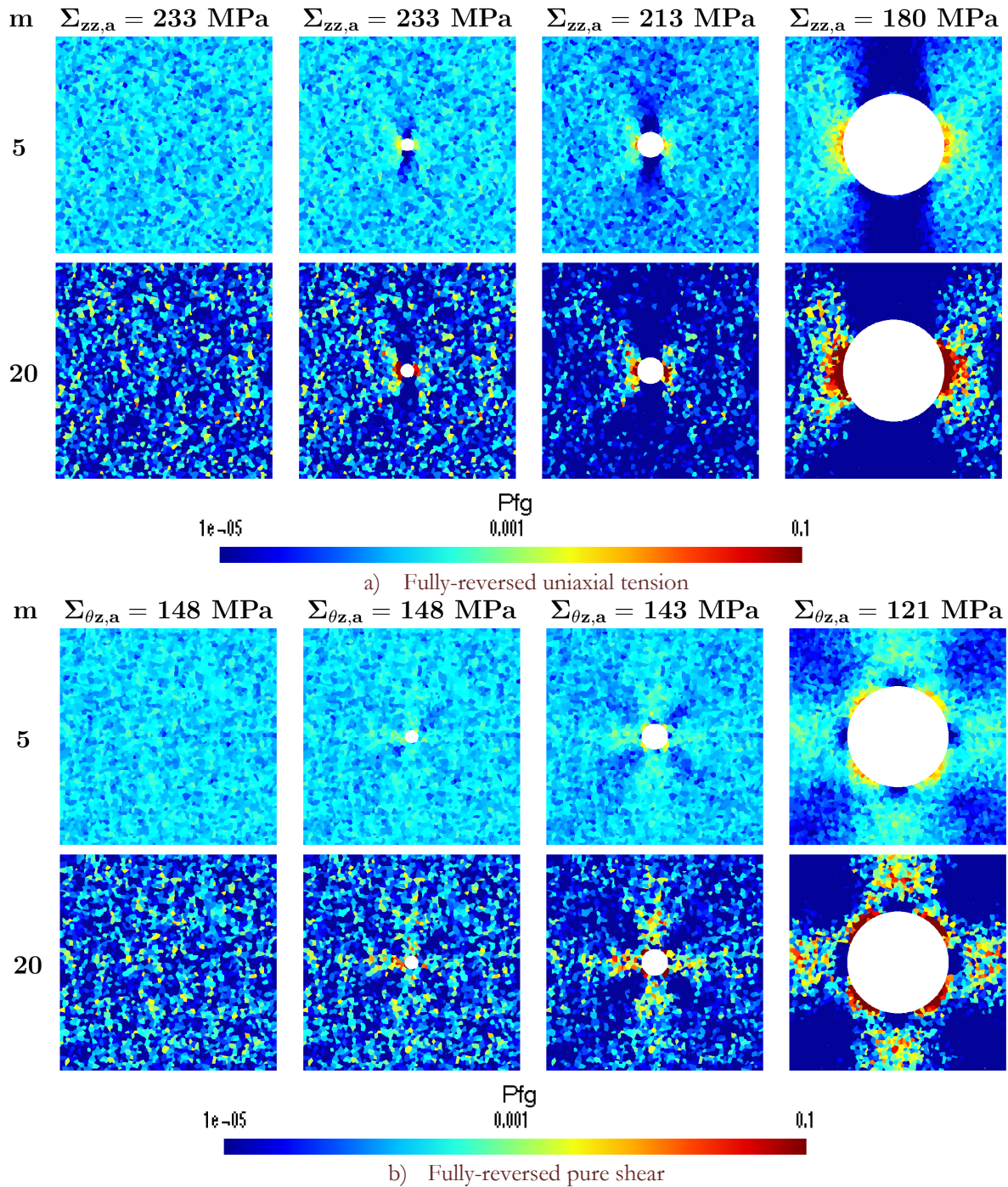

Figure 4: Distributions of the failure probability per grain for a synthetic microstructure of 316L steel loaded in a) fully-reversed uniaxial tension and b) fully-reversed pure shear at the experimental average fatigue limit level. Effect of the defect diameter D (from 0 to 365 μm) and the shape parameter m (5 or 20).

The average macroscopic fatigue limits $\Sigma_{ij,a}$ (represented by $\Sigma_{\theta z,a}$ for the torsion loading mode and $\Sigma_{zz,a}$ for the other loading modes) predicted by the probabilistic criterion are presented along with those derived from the experimental fatigue tests in a diagram $\Sigma_{ij,a}$ –D in Fig. 5. In the absence of defect, the predictions of the probabilistic fatigue criterion are in very good agreement with the experimental fatigue limits. In the presence of defect, the criterion is found to reflect the Kitagawa effect for all the loading modes. More exactly, when the defect size is small enough, the fatigue strength is no more affected by the defect. The so-called Kitagawa effect can be interpreted as a competition between the crack initiation mechanisms governed either by the microstructure or by the defect (Fig. 4). When the defect size is big enough, the fatigue strength is less sensitive to the local microstructure since the highly loaded zone is large compared to the microstructure. It is also important to notice that there is no need to introduce an extra material parameter so that the criterion applied to the data from the EF simulations predicts the decrease of the fatigue strength with the defect size increase.
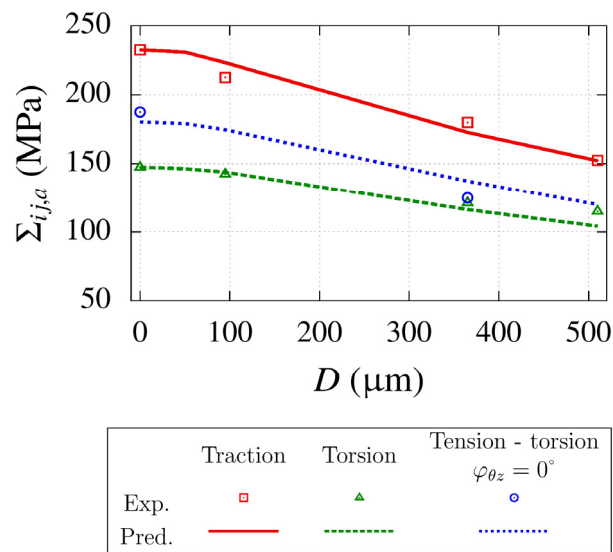

Figure 5: Predictions of the probabilistic model in a Kitagawa type diagram. Comparison with the multiaxial fatigue experimental data for the 316L steel.
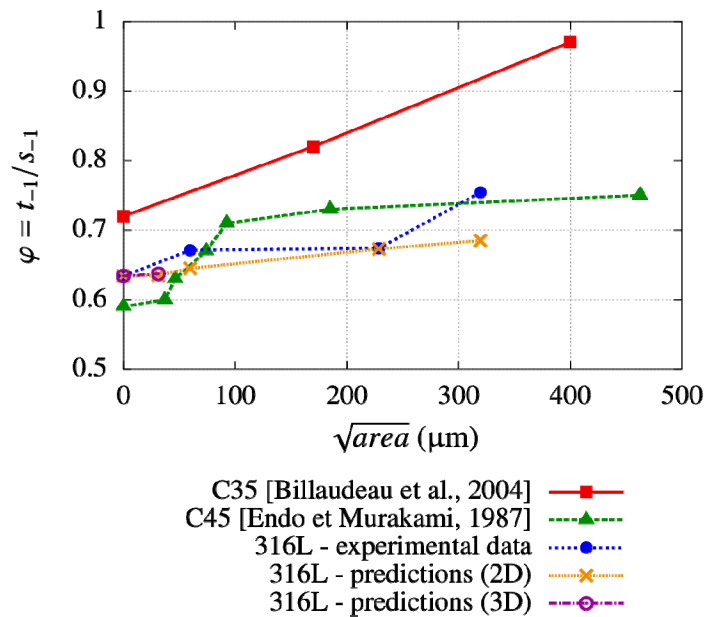

Figure 6: Comparison between the experimental and the predicted ratios of the fatigue limits under fully-reversed torsion t_{-1} and fully reversed tension s_{-1}: t_{-1}/s_{-1}

CONCLUSIONS

The purpose of this study has been to investigate the multiaxial fatigue performance of metals in the presence of defects through statistical modeling of the microstructure. More exactly, the goal has been to analyze the competition existing between the stress concentration induced, on one hand, by a small defect and, on the other hand, by the most highly stressed regions of the microstructure caused by the anisotropic behavior of the grains.

In a first phase, the cyclic mechanical responses of polycrystalline aggregates, obtained from finite element simulations, have been analysed for various loading modes and in the presence of geometrical defects. It has been shown the local stress field is highly scattered and differs significantly from the macroscopic response of the polycrystalline aggregate.

In a second phase, an experimental campaign conducted on an austenitic steel 316L has shown the influence of hemispherical defect on the fatigue strength. The role of the loading modes for different defect sizes has been clearly established. It has been observed an evolution of the experimental ratio between the fatigue limits under fully reversed torsion and fully reversed tension with respect to the defect size.

The predictions reached from a probabilistic criterion (originally proposed by Morel) using the FE computations appear to be in good agreement with most of the experimental results. The role of the shape factor m of the probabilistic criterion is discussed and it is shown to play a role similar as a material characteristic length for the crack initiation mechanism. The Kitagawa effect is perfectly reflected by means of the model proposed and the related loading mode influence is also adequately accounted for.

The simulations discussed in this paper are of 2D types but some extra 3D EF simulations have been conducted for the smallest defect size (50 μm) and the same trends have been observed. In particular, both 2D and 3D simulations together with the probabilistic criterion show an increase of the ratio between the fatigue limits under fully reversed torsion and fully reversed tension with respect to the defect size (Fig. 6).

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