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Micromechanical investigation of the influence of defects in high cycle fatigue

R. Guerchais [a,b,*], N. Saintier [b], F. Morel [a], C. Robert [a]

[a] Arts et Metiers ParisTech, LAMPA, 2 bd du Ronceray, 49035 Angers Cedex, France
[b] Arts et Metiers ParisTech, I2M – UMR CNRS 5295, Université Bordeaux 1, Esplanade des Arts et Métiers, 33405 Talence Cedex, France

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ABSTRACT

This study aims to analyse the influence of geometrical defects (notches and holes) on the high cycle fatigue behaviour of an electrolytic copper based on finite element simulations of 2D polycrystalline aggregates. In order to investigate the role of each source of anisotropy on the mechanical response at the grain scale, three different material constitutive models are assigned successively to the grains: isotropic elasticity, cubic elasticity and crystal plasticity in addition to the cubic elasticity. The significant influence of the elastic anisotropy on the mechanical response of the grains is highlighted. When considering smooth microstructures, the crystal plasticity have has a slight effect in comparison with the cubic elasticity influence. However, in the case of notched microstructures, it has been shown that the influence of the plasticity is no more negligible. Finally, the predictions of three fatigue criteria are analysed. Their ability to predict the defect size effect on the fatigue strength is evaluated thanks to a comparison with experimental data from the literature.

1. Introduction

The ability to assess the effects of small defects on the high cycle fatigue (HCF) strength appears to be crucial from the design point of view as the stress concentrations induced by these defects favour fatigue crack initiation. 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. Besides, some of them do not allow to account for a complex defect geometry. Moreover, these methods neglect the variabilities of the microstructure in the vicinity of the defect and thus cannot 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 the mesoscopic mechanical quantities (i.e. the average mechanical quantities at the grain scale) the HCF behaviour of metallic materials. Unfortunately no simple method exists to precisely estimate these quantities due to the complexity of the morphology and of the behaviour of the grains constituting a metal. Localisation schemes are a common way to relate the mechanical response of each grain to the macroscopic loading applied to a polycrystal. However, they 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 (FE) analysis of explicitly modelled polycrystalline aggregates. This promising approach allows to take into account microstructural features generally neglected in the localisation schemes and to deepen the analysis of the mesoscopic mechanical responses of metals under cyclic loading. In recent years, several works have involved this kind of numerical simulations to contribute to the study of the HCF behaviour. For instance, Bennett and McDowell [4] have analysed the distribution of fatigue crack initiation parameters inspired from well-known HCF criteria. This study was enriched by the work of Guilhem et al. [5] in which the mechanical response of the grains is studied according to their positions in the aggregate (for instance at the free surface or in the core), their orientations and those of the neighbouring grains. Some studies have highlighted the important role played by the anisotropic elasticity on the mechanical responses at the grain scale in several metallic materials with a face-centred cubic (FCC) structure [6–8] and a body-centred cubic (BCC) structure [9]. Moreover, FE simulations of polycrystalline aggregates have

* Corresponding author at: Arts et Metiers ParisTech, LAMPA, 2 bd du Ronceray, 49035 Angers Cedex, France. Tel.: +33 (0)2 41 20 73 27; fax: +33 (0)2 41 20 73 20.
E-mail address: raphael.guerchais@ensam.eu (R. Guerchais).

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Nomenclature

γ_s	plastic slip on the slip system, s
v_s	accumulated plastic slip on the slip system, s
τ_s	resolved shear stress on the slip system, s
r_s	isotropic hardening variable on the slip system, s
x_s	kinematic hardening variable on the slip system, s
$\boldsymbol{\sigma}$	stress tensor
$\boldsymbol{\varepsilon}^p$	plastic strain tensor
$\underline{n}_s$	unit vector normal to the slip plane (Fig. 1)
$\underline{l}_s$	unit vector in the slip direction (Fig. 1a)
$\boldsymbol{m}_s$	orientation tensor of the slip system, s
$\langle\bullet\rangle_a$	volume-weighted average over the aggregate
$\langle\bullet\rangle_g$	volume-weighted average over the grain, g
$\boldsymbol{\Sigma} = \langle\boldsymbol{\sigma}\rangle_a$	macroscopic stress tensor
$\langle\boldsymbol{\sigma}\rangle_g$	mesoscopic stress tensor
$\underline{\sigma}(\underline{n})$	mesoscopic stress vector across the plane of unit normal vector $\underline{n}$ (Fig. 1b)
$\underline{\tau}$	mesoscopic shear stress vector (Fig. 1b)
τ_a	mesoscopic shear stress amplitude (Fig. 1b)
τ_m	mesoscopic mean shear stress (Fig. 1b)
$T_{s,a}$	macroscopic resolved shear stress amplitude on the slip system, s
$\tau_{s,a}$	mesoscopic resolved shear stress amplitude on the slip system, s (Fig. 1b)
Σ_n	macroscopic normal stress acting on the plane $\underline{n}$
σ_n	mesoscopic normal stress acting on the plane $\underline{n}$ (Fig. 1b)
$\sigma_{n,a}$	mesoscopic normal stress amplitude acting on the plane $\underline{n}$
$\sigma_{n,m}$	mesoscopic mean normal stress acting on the plane $\underline{n}$
σ_h	mesoscopic hydrostatic stress
P_{Fn}	failure probability of a slip plane
P_{Fg}	failure probability of a grain
P_{Fa}	failure probability of an aggregate

recently been used to analyse the influence of defects on the high cycle fatigue strength. For example, the effect of a rough surface has been investigated in [10,11] and the influence of the crystallographic orientations and of the defect size and acuity have been extensively studied by Owolabi et al. [12] in the case of semicircular notches. In the present work, which falls within this framework, two points are addressed:

- A numerical analysis is conducted on notched microstructures, based on push–pull fatigue limits determined by Lukàš et al. [1] thanks to notched specimens made of electrolytic copper. In a first step, the objective is to analyse the mechanical responses of the grains in microstructures cyclically loaded at a stress amplitude corresponding to the macroscopic average fatigue limit. This analysis focuses more specifically on the effects of the constitutive model used at the grain scale and the notch on the mesoscopic mechanical responses. In a second step, a comparison is carried out between the predictions provided by three different criteria with the experimental average fatigue limits.
- A qualitative numerical study is made on holed microstructure, in order to compare the influence of a defect on the mesoscopic mechanical response for different loading conditions: fully reversed tension and fully reversed shear. The fatigue limits predicted by one of the studied criterion are determined and compared to experimental trends.

2. Modelling approach

2.1. Constitutive material models at the grain scale

The anisotropic behaviour of the grains is due, on the one hand, to the elastic behaviour and, on the other hand, to the crystallographic nature of the plastic slip. In FCC structure, as for pure copper, the elastic behaviour is cubic and the plastic slip occurs along the {1 1 1} planes in the ⟨1 1 0⟩ directions which correspond respectively to the closed-packed planes and directions of this crystal structure. In order to dissociate the effect of each sources of anisotropy on the mesoscopic mechanical responses, three constitutive models, assigned to the grains, are investigated:

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

In each case, a Hooke's law is used to describe the elastic behaviour. In the first case, an isotropic elastic behaviour is considered and is defined by the Young's Modulus $E$and the Poisson's ratio ν. In the second and third cases, cubic elasticity is considered and completely characterised by three coefficients defined in the crystal coordinate system: C_{1111}, C_{1122} and C_{1212}. After homogenisation, when considering an isotropic texture, the cubic elastic model is equivalent to the isotropic elastic model at the macroscopic scale.

Finally, crystal plasticity is described by a single crystal viscoplastic model proposed by Méric et al. [13]. In this constitutive model, the plastic slip rate $\dot{\gamma}_s$ on a slip system s is governed by a Norton-type flow rule (Eq. (1)) involving the resolved shear stress τ_s acting on s and an isotropic hardening variable r_s associated to the slip system s.

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

where K and n are the parameters defining the viscosity and r_0 corresponds to the critical resolved shear stress. In this equation, $\langle x \rangle_+ = \max(x, 0)$. The resolved shear stress τ_s acting on s is

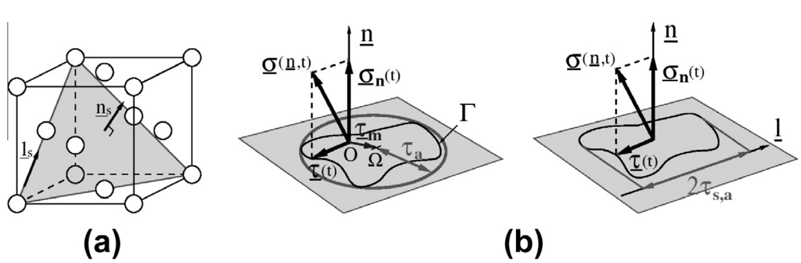

Fig. 1. Representation of some mechanical quantities and vectors in (a) a FCC unit cell and (b) a slip plane.