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DISSIPATION ESTIMATION IN A MULTISCALE MODEL

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ABSTRACT

This paper is devoted to the study of fatigue of metallic alloys by a multiscale approach. It proposes a scale transition rule taking into account non uniform elasticity, and introduces a crystal plasticity model valid for cyclic loading in order to estimate the heat dissipation and calculate the temperature elevation in a material element submitted to HCF loadings. The relation between dissipation and a few candidate models for predicting crack initiation is discussed.The cases of both FCC and HCP alloys are addressed.

MOTIVATION

The estimation of the fatigue limit from temperature measurements is now a well established technique. After pioneering studies during the 90's, it has been fully characterized in France by a series of groups. Among other, the interested reader will find one of the first expression in [1]. The same group has then precised the description, specifically the link between dissipation and temperature rise [2; 3; 4], and applied to more and more complex cases (see for instance [5] for multiaxial loadings). A similar track has been followed by [6], who shed the light on the various regimes generated by fatigue loadings in grains. In both cases, the dissipation calculation is based on a classical thermodynamical formulation of the model, assuming that plastic flow occurs only in an inclusion (a grain representing the cristallographic phase with the most favorable orientation). The stress redistribution is defined for instance by means of a Kröner model [5] for multiaxial loadings). A similar track has been followed by [6], so that the stress in the grain $\underset{\sim}{\sigma}^g$ can be obtained by correcting the macroscopic stress $\underset{\sim}{\sigma}$ by means of a term depending on the local $\underset{\sim}{\varepsilon}^{pg}$ and macroscopic $\underset{\sim}{\varepsilon}^{p}$ plastic strain :

$$\underset{\sim}{\sigma}^g = \underset{\sim}{\sigma} + \alpha\mu(\underset{\sim}{\varepsilon}^p - \underset{\sim}{\varepsilon}^{pg}) \tag{1}$$

where μ is the elastic shear modulus and α a parameter coming from the solution of the auxiliary inclusion problem. The macroscopic plastic strain is neglected in Doudard et al's work. In both cases, the following limitations are introduced :

— Uniform elastic strain.
— A heuristic rule to determine the volume fraction of the plastic grain. In [6], this volume fraction is adjusted after a previous experimental study [7], meanwhile the other papers select a probabilistic model to generate the critical sites and to describe the progressive activation of the microplasticity.

The main motivation of the present paper is then to evaluate the effect of these assumptions by introducing a scale transition rule accounting for non uniform elasticity, and crystal plasticity at the grain scale to naturally activate more and more grains for increasing load levels. This solution has been already adopted in the literature. In [8], a quasi-physical crystal plasticity model based on dislocation densities is used, together with a translated field solution for the scale transition [9; 10]. In [11; 12], the crystal plasticity model adopted is Méric-Cailletaud's [13; 14], as in the present paper, and the scale transition is obtained either by FFT, Finite Element, or a self-consistent approach.

SCALE TRANSITION WITH THE β–rule

The self-consistent approach is the classical reference for the homogenization of polycrystals. Introducing self-explanatory notations where the superscript g stands for the local phase behaviour, Table 1 regroups the equations needed for modeling an elastic heterogeneous medium in this framework. According to Hill [15], the same relations hold in rate form for the case of time independent plasticity, provided $\underset{\approx}{C}$ and $\underset{\approx}{C}^g$ are replaced by the tangent operators $\underset{\approx}{L}$ and $\underset{\approx}{L}^g$. Specifically, Eq.5 writes :

$$\dot{\underset{\sim}{\sigma}}^g = \dot{\underset{\sim}{\sigma}} + \underset{\approx}{L} : (\underset{\approx}{S}^{-1} - \underset{\approx}{I}) : (\dot{\underset{\sim}{\varepsilon}} - \dot{\underset{\sim}{\varepsilon}}^g) \tag{7}$$

Elastic behaviour :	$\underset{\sim}{\sigma} = \underset{\approx}{C} : \underset{\sim}{\varepsilon} \qquad \underset{\sim}{\sigma}^g = \underset{\approx}{C}^g : \underset{\sim}{\varepsilon}^g$	(2)
Strain concentration :	$\underset{\sim}{\varepsilon}^g = \underset{\approx}{A}^g : \underset{\sim}{\varepsilon} \quad \text{with} \quad \underset{\approx}{A}^{g\,-1} = \underset{\approx}{I} - \underset{\approx}{S} : \underset{\approx}{C}^{-1} : (\underset{\approx}{C} - \underset{\approx}{C}^g)$	(3)
Stress concentration :	$\underset{\sim}{\sigma}^g = \underset{\approx}{B}^g : \underset{\sim}{\sigma} \quad \text{with} \quad \underset{\approx}{B}^{g\,-1} = \underset{\approx}{C} : \underset{\approx}{C}^{g\,-1} - \underset{\approx}{C} : \underset{\approx}{S} : (\underset{\approx}{C}^{-1} - \underset{\approx}{C}^{g\,-1})$	(4)
Scale transition rule :	$\underset{\sim}{\sigma}^g = \underset{\sim}{\sigma} + \underset{\approx}{C}^{\dagger} : (\underset{\sim}{\varepsilon} - \underset{\sim}{\varepsilon}^g) \quad \text{with} \quad \underset{\approx}{C}^{\dagger} = \underset{\approx}{C} : (\underset{\approx}{S}^{-1} - \underset{\approx}{I})$	(5)
Averaging operations :	$\underset{\approx}{C} = \langle \underset{\approx}{C}^g : \underset{\approx}{A}^g \rangle = \langle \underset{\approx}{C}^{g\,-1} : \underset{\approx}{B}^g \rangle^{-1} \qquad \langle \underset{\approx}{A}^g \rangle = \langle \underset{\approx}{B}^g \rangle = \underset{\approx}{I}$	(6)

TABLE 1: Definition of the scale transition for an heterogeneous elastic medium. The symmetric second order and fourth order tensors are underlined by a single or a double tilde, and a double dot indicates a double subscript contraction. $\langle - \rangle$ stands for the averaging operation on the representative material element ; Eshelby's tensor is denoted by $\underset{\approx}{S}$.

Multipying each term of Eq.7 by $\underset{\approx}{C} : \underset{\approx}{S} : \underset{\approx}{L}^{-1}$ and expressing the strain as a sum of elastic, plastic strain and thermal dilatation, it comes :

$$\dot{\underset{\sim}{\sigma}}^g = \underset{\approx}{B}^{g*} : \left(\underset{\approx}{B}^{*\,-1} : \dot{\underset{\sim}{\sigma}} + \underset{\approx}{C}^* : (\dot{\underset{\sim}{\varepsilon}}^p - \dot{\underset{\sim}{\varepsilon}}^{pg}) + \underset{\approx}{C}^* : (\dot{\underset{\sim}{\varepsilon}}^{th} - \dot{\underset{\sim}{\varepsilon}}^{thg}) \right) \tag{8}$$

$$\underset{\approx}{B}^{*\,-1} = \underset{\approx}{I} + \underset{\approx}{C} : \underset{\approx}{S} : (\underset{\approx}{L}^{-1} - \underset{\approx}{C}^{-1}) \qquad \underset{\approx}{C}^* = \underset{\approx}{C} : (\underset{\approx}{I} - \underset{\approx}{S}) \tag{9}$$

$$\underset{\approx}{B}^{g*\,-1} = \underset{\approx}{C} : \underset{\approx}{C}^{g\,-1} + \underset{\approx}{C} : \underset{\approx}{S} : (\underset{\approx}{L}^{-1} - \underset{\approx}{C}^{g\,-1}) \tag{10}$$

The non linearity of the relation defined by Eq.7 is depicted by two tensors :

— $\underset{\approx}{B}^*$, accounting for the difference between the macroscopic tangent operator $\underset{\approx}{L}$ and the macroscopic elastic operator $\underset{\approx}{C}$,

— $\underset{\approx}{B}^{g*}$, accounting for the difference between $\underset{\approx}{L}$ and the local elastic behaviour, described by $\underset{\approx}{C}^g$.

If $\underset{\approx}{L}$ is assumed to remain equal to $\underset{\approx}{C}$, which is justified at the onset of plastic flow, $\underset{\approx}{B}^*$ is nothing but identity, and $\underset{\approx}{B}^{g*}$ is equal to $\underset{\approx}{B}^g$, a tensor which remains constant during the loading. The resulting expression after integration is the Kröner-Budianski-Wu (KBW) model, where the stress concentration tensor $\underset{\approx}{B}^g$ operates on the macroscopic stress tensor and on additional residual stress terms originating from the heterogeneity of the plastic strain and of the thermal dilatation (the initial value of which is taken equal to zero) :

$$\underset{\sim}{\sigma}^g = \underset{\approx}{B}^g : \left(\underset{\sim}{\sigma} + \underset{\approx}{C}^* : (\underset{\sim}{\varepsilon}^p - \underset{\sim}{\varepsilon}^{pg}) + \underset{\approx}{C}^* : (\underset{\sim}{\alpha} - \underset{\sim}{\alpha}^g) \Delta T \right) \tag{11}$$

$$\underset{\approx}{B}^{g\,-1} = \underset{\approx}{C} : \underset{\approx}{C}^{g\,-1} + \underset{\approx}{C} : \underset{\approx}{S} : (\underset{\approx}{C}^{-1} - \underset{\approx}{C}^{g\,-1}) \tag{12}$$

Two equivalent expressions can be found for the macroscopic plastic strain and for the macroscopic coefficient of thermal expansion (CTE). They are obtained either from Eq.11, by means of an averaging operation, and accounting for the fact that the macroscopic stress is the average of the local stresses, or by deducing from this equation the corresponding equation in terms of total strain, then averaging it, knowing that the macroscopic strain is the average of the local strains :

$$\underset{\sim}{\varepsilon}^p = \underset{\approx}{C}^{*\,-1} : \langle \underset{\approx}{B}^g : \underset{\approx}{C}^* : \underset{\sim}{\varepsilon}^{pg} \rangle = \langle \underset{\sim}{\varepsilon}^{pg} \rangle + \langle (\underset{\approx}{C}^{-1} - \underset{\approx}{C}^{g\,-1}) : \underset{\approx}{B}^g : \underset{\approx}{C}^* : \underset{\sim}{\varepsilon}^{pg} \rangle \tag{13}$$

$$\underset{\sim}{\alpha} = \underset{\approx}{C}^{*\,-1} : \langle \underset{\approx}{B}^g : \underset{\approx}{C}^* : \underset{\sim}{\alpha}^g \rangle = \langle \underset{\sim}{\alpha}^g \rangle + \langle (\underset{\approx}{C}^{-1} - \underset{\approx}{C}^{g\,-1}) : \underset{\approx}{B}^g : \underset{\approx}{C}^* : \underset{\sim}{\alpha}^g \rangle \tag{14}$$

As mentioned by many authors (see for instance [16]), this model is known to provide far too large internal stresses, due to the elastic accomodation which replaces the plastic accomodation. A solution to preserve the ease of use of expression 11 (namely integrated form, explicit scale transition) while limiting the internal stresses, consists in replacing plastic strain by a state variable, the evolution of which is bounded for large plastic strain values [17; 18; 19].

The equations of the model are summarized in Table2. The new scale transition rule is expressed by Eq.15. Equation 16 provides a possible evolution of the accommodation variable β^g, which depends on material behaviour. The expression introduces two fading memory terms, in order to represent the strain dependent dynamic recovery (with an Armstrong–Frederick expression [20]) and also the time dependent recovery. An application to Directionnally Solidified alloys can be found in [21; 22]. The scale transition parameters ($\underset{\sim}{D}$, M, m) have to be characterized by comparing the results of the model with full field Crystal Plasticity computations, performed by Finite Element or FFT method [18]. As shown by Eq.15, the variable β^g plays now the role that was taken by $\underset{\sim}{\varepsilon}^g$ in the KBW model (Eq.11). This is why the evaluation of β (Eq.17) has the shape taken by $\underset{\sim}{\varepsilon}$ in the KBW model (Eq.13). An other consequence is that the corrective term needed to evaluate the macroscopic plastic strain in Eq.18 depends on β^g.

As shown by Eq.14, a non uniform CTE is a source of residual stresses inside the material element, for instance in a two-phase material with two different CTE. In polycrystal materials were the phase is just characterized by its crystallographic orientation, the grains have a cubic symmetry so that $\underset{\sim}{\alpha}^g$ is a spherical tensor, and the CTE is uniform. For HCP materials, the local CTE is transverse orthotropic, unlike the macroscopic CTE, which is isotropic, at least in absence of texture. The latter will then develop residual stresses due to temperature change.

Scale transition rule :	$\underset{\sim}{\sigma}^g = \underset{\approx}{B}^g : \left(\underset{\sim}{\sigma} + \underset{\approx}{C}^* : (\underset{\sim}{\beta} - \underset{\sim}{\beta}^g) + \underset{\approx}{C}^* : (\underset{\sim}{\alpha} - \underset{\sim}{\alpha}^g)\Delta T \right)$	(15)
Evolution of $\underset{\sim}{\beta}^g$:	$\dot{\underset{\sim}{\beta}}^g = \dot{\underset{\sim}{\varepsilon}}^{pg} - \underset{\approx}{D} : \underset{\sim}{\beta}^g \lVert \dot{\underset{\sim}{\varepsilon}}^{pg} \rVert - \left(\frac{\lVert \underset{\sim}{\beta}^g \rVert}{M} \right)^m \frac{\underset{\sim}{\beta}^g}{\lVert \underset{\sim}{\beta}^g \rVert}$	(16)
Definition of $\underset{\sim}{\beta}$:	$\underset{\sim}{\beta} = \underset{\approx}{C}^{*-1} : \langle \underset{\approx}{B}^g : \underset{\approx}{C}^* : \underset{\sim}{\beta}^g \rangle$	(17)
Definition of $\underset{\sim}{\varepsilon}^p$:	$\underset{\sim}{\varepsilon}^p = \langle \underset{\sim}{\varepsilon}^{pg} \rangle + \langle (\underset{\approx}{C}^{-1} - \underset{\approx}{C}^{g-1}) : \underset{\approx}{B}^g : \underset{\approx}{C}^* : \underset{\sim}{\beta}^g \rangle$	(18)

TABLE 2: Expression of the beta–rule for a material element with non uniform elasticity. $\underset{\approx}{B}^g$ is taken from Eq.12.

As for CTE, the macroscopic plastic strain defined in Eq.18 is computed by adding a corrective term to the average of the local plastic strain tensors. If the local plastic strain is deviatoric, the variables $\underset{\sim}{\beta}^g$ are also deviatoric. For the case of a polycrystalline material with a cubic symmetry, the spherical terms are the same in $\underset{\approx}{C}$ and $\underset{\approx}{C}^g$, so that this additional term is also deviatoric. On the contrary, this additional term will create a volume change at the macroscale for a HCP polycrystal.

GRAIN BEHAVIOUR

For a given scale transition framework, the behaviour of the phases can be either described by models deduced from a single potential (with criteria like von Mises, Hill, etc.) or by crystal plasticity models, which derive from several potentials. Having in view fatigue damage, the latter is the most desirable. The model used, which has been already presented [14; 23], refers to the classical thermodynamical framework [24], which is not recalled here for the sake of brevity. For a grain g with N slip systems, three terms are introduced in the free energy, depending on the elastic strain $\underset{\sim}{\varepsilon}^{eg}$, and on the state variables defining kinematic hardening, $\alpha^s, s = 1..N$ or isotropic hardening, $\rho^s, s = 1..N$. The partial derivatives provide the associated variables, namely the stress in the grain, $\underset{\sim}{\sigma}^g$, the kinematic and isotropic variables x^s and r^s :

$$\rho\Psi(\underset{\sim}{\varepsilon}^{eg}, \alpha^s, \rho^s) = \frac{1}{2}\, \underset{\sim}{\varepsilon}^{eg} : \underset{\approx}{C}^g : \underset{\sim}{\varepsilon}^{eg} + \frac{1}{2}\, c \sum_s \alpha^{s2} + \frac{1}{2}\, bQ \sum_s \sum_r h_{rs} \rho^r \rho^s \tag{19}$$

$$\underset{\sim}{\sigma}^g = \underset{\approx}{C}^g : \underset{\sim}{\varepsilon}^{eg} \qquad x^s = c\alpha^s \qquad r^s = bQ \sum_r h_{rs} \rho^r \tag{20}$$

A viscoplastic potential, $\Omega = \sum_s \Omega^s$ allows to determine the evolution of the state variable. It is built as a sum of the individual potentials for each slip system s, which depend on the yield criterion for each system, f^s :

$$\Omega = \frac{n+1}{K} \sum_s \left(\frac{f^s}{K} \right)^{n+1} \quad \text{with} \quad f^s(\underset{\sim}{\sigma}^g, x^s, r^s) = |\underset{\sim}{\sigma}^g : \underset{\sim}{m}^s - x^s| - r^s - \tau_y = |\tau^s - x^s| - r^s - \tau_y \tag{21}$$

$$\dot{\underset{\sim}{\varepsilon}}^{pg} = \frac{\partial \Omega}{\partial \underset{\sim}{\sigma}^g} = \sum_s \frac{\partial \Omega}{\partial f^s} \frac{\partial f^s}{\partial \underset{\sim}{\sigma}^g} = \sum_s \eta^s \dot{v}^s \underset{\sim}{m}^s \quad \text{with} \quad \dot{v}^s = \frac{\partial \Omega}{\partial f^s} \quad \text{and} \quad \eta^s = \text{sign}(\tau^s - x^s) \tag{22}$$

The evolution of the hardening variables is deduced from a second potential, $\Omega^* = \sum_s \Omega^{*s}(f^{*s})$:

$$\Omega^* = \frac{n+1}{K} \sum_s \left(\frac{f^{*s}}{K} \right)^{n+1} \qquad f^{*s} = f^s + \frac{dx^{s2}}{2c} + \frac{b\rho^{s2}}{2} \tag{23}$$

$$\dot{\alpha}^s = -\frac{\partial \Omega^{*s}}{\partial x^s} = (\eta^s - \frac{dx^s}{c})\dot{v}^s \qquad \dot{\rho}^s = -\frac{\partial \Omega^{*s}}{\partial r^s} = (1 - b\rho^s)\dot{v}^s \tag{24}$$

The dissipation in one grain writes :

$$\mathcal{D}^g = \underset{\sim}{\sigma}^g : \dot{\underset{\sim}{\varepsilon}}^{pg} - \rho\dot{\Psi} = \underset{\sim}{\sigma}^g : \sum_s \eta^s \dot{v}^s \underset{\sim}{m}^s - \sum_s \eta^s x^s \dot{\alpha}^s - \sum_s r^s \dot{\rho}^s \tag{25}$$

$$= \sum_s \left(|\tau^s - x^s| - r^s + \frac{d}{c} x^{s2} + bQ \sum_r h_{rs} \rho^r \rho^s \right) \dot{v}^s \tag{26}$$

$$= \sum_s f^s \dot{v}^s + \sum_s \tau_y \dot{v}^s + \sum_s \left(\frac{d}{c} x^{s2} + bQ \sum_r h_{rs} \rho^r \rho^s \right) \dot{v}^s \tag{27}$$

As demonstrated by Eq.27, it contains three terms :

— the first is the dissipation due to viscosity, that can be dropped for the case of a time independent behaviour,
— the second is produced by internal friction, depending on the initial critical resolved shear stress,
— the third is linked to the non linearity of the hardening.

DISCUSSION

The questions that are to be treated are the following :

— The approach proposed in the scale transition model is valid in an infinite medium. The justification for using such an approach comes from the fact that the temperature change during a fatigue test is generated by the dissipation inside the material element. Nevertheless, it can be interesting to implement the computation of the dissipation in a full field calculation, and to compare the results obtained in a material element with various boundary conditions, specifically periodic, or with a free surface.
— Equation 27 has to be implemented in a micromechanical model (beta-rule), in order to evaluate the effect of the heterogeneous elasticity on the calculated dissipation. This will offer an opportunity to improve the existing models used for the estimation of the yield limit.

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