ASSESSMENT OF THE CONTRIBUTION OF PLASTIC STRAIN GRADIENT EFFECTS TO THE FATIGUE THRESHOLD OF DUCTILE MATERIALS

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ABSTRACT

The decreasing size of the plastic zone of a large crack growing by fatigue as the applied stress intensity factor range ΔK decreases implies a concomitant increase of the plastic strain gradient there. In a ductile, crystalline material, a plastic gradient must be resolved by storing a density of Geometrically Necessary Dislocations (GND) proportional to it. Such density represents an extra amount of dislocations superposed to the dislocation density that would locally accumulate without the presence of gradients for the same local plastic deformation in any volume element of the plastic zone (the size-independent Statistically Stored Dislocations (SSD) density). The net effect of the gradients is to progressively hinder the plasticity at the crack tip as ΔK decreases. For materials where the crack advance per cycle Δa can be assumed proportional to the crack tip opening displacement $\Delta a \propto$ CTOD, the sole effect of the plastic gradients leads to predict a fatigue threshold effect.

In this paper such contribution to the fatigue threshold has been quantified for ferritic steels by performing FEM calculations (ABAQUS[®] code) using a gradient-dependent continuum plasticity model based on the storage of GND and an appropriate constitutive equation of the Voce type. Further refinements of the model can easily be proposed.

INTRODUCTION

Conventional plasticity ignores the existence of size effects without any trouble for most macroscopic engineering purposes [1]. However, several observed plasticity phenomena display a size effect whereby the smaller is the size the stronger is the response. Plastic strain gradients appear either because of the geometry of loading or because the material itself is plastically inhomogeneous [2]. The existence of plastic size effects in the low scale, as attested by experimental evidence, leads to the conclusion that any continuum theory based solely on strain hardening, with no strain gradient dependence, would necessarily predict an absence of any such size effect [3]. In the present paper, the contribution of the plastic strain gradient effects not only to the fatigue threshold for crack propagation but also to the flow stress in ductile materials are analised. The steep gradients of plastic strain that appear in the plastic zone at the crack tip can be predicted if we include size effects in the constitutive law postulating that the yield stress depends both upon strain and strain gradient.

As a point of departure, we will discuss the specific relation between flow stress and dislocation density that is in common usage. According to the experimental observations carried out by Narutani and Takamura [4] and other investigators [5-7], the flow stress is proportional to the square root of dislocation density ρ irrespective of the grain size, amount of strain and test temperature. For a coarse-grained, single-phase material, which can be regarded as "structureless", the flow stress at zero temperature is set equal to

$$\sigma = M\alpha G b \sqrt{\rho}$$
(1)
$$\sigma = \hat{\alpha} G b \sqrt{\rho}$$

Here, *M* is the average Taylor factor, which evolves in the process of straining (in what follows, *M* will be considered constant for simplicity), *b* is the magnitude of the Burgers vector, *G* is an appropriate shear modulus and $\hat{\alpha}$ is a constant of order unity which depends, in part, on the strength of the dislocation/dislocation interaction [8]. Thermal activation may lower this effective obstacle strength so that the flow stress at a finite temperature and strain rate becomes

$$\sigma = s(\dot{\varepsilon}, T)\,\hat{\alpha}Gb\sqrt{\rho} \tag{2}$$

where $s(\dot{\varepsilon}, T)$ is a function that goes to 1 as $T \rightarrow 0$. From eq (2) it is apparent that the flow stress is a product of a rate sensitivity term and a structure sensitive term. The flow stress, as given by Eqs. (1) and (2), relates only to the impediment to dislocation motion that is provided by other dislocations. In most materials, there are other contributions to the plastic resistance. In some cases (e.g., lattice resistance, solution hardening, some grain size effects), these are additive to the contributions discussed above [8]

$$\sigma = \sigma_0(\dot{\varepsilon}, T) + \hat{\alpha}(\dot{\varepsilon}, T) G b \sqrt{\rho^T}$$
(3)

Here, the rate dependence of σ_o may be more important than that of $\hat{\alpha}$ (or *s*), or it may be negligible; the less rate sensitive term (contained into the σ_o term) is often called an "internal stress" (Pierls or friction stress). The total dislocation density ρ^T is defined by Ashby [7] as the sum of geometrically necessary dislocations ρ^G and statistically stored dislocations ρ^S . The statistically stored dislocations are accumulated in pure crystals during straining and are responsible for the normal 3-stage [7]. Plastic strain gradients are caused by the geometry of deformation, by local boundary conditions (this case) or by the microstructure [2]. These strain gradients require, for compatibility reasons, the presence of geometrically necessary dislocations of density ρ^G , which are introduced to accommodate the incompatibility of deformation between neighbouring grains.

Dislocation density-related constitutive modelling

The step of translating from the simple dislocation equations to a continuum formulation is not obvious. The statistically stored dislocations, ρ^{S} , are assumed to be dependent on the plastic strain ε^{p} , while the geometrically necessary dislocations, ρ^{G} , are assumed to be dependent on strain gradient $\partial \varepsilon^{p} / \partial x$ [9] or in a linear manner with the reciprocal of the grain size [4, 7].

In its present state, dislocation density-related constitutive modelling is considered mature enough to be broadly used in finite element codes including viscoplasticity [10]. In order to formulate the grain-size or local boundary conditions dependence of the total dislocation density, it is necessary to derive an equation to describe the accumulation of dislocations during deformation, but the constitutive equation to describe the work hardening process in polycrystalline materials has not been well established. The flow stress dependence on a rate sensitivity term and on a structure sensitive term (including lattice resistance and solution hardening) is accounted for Eq. (3). For the purpose of this paper, we assume that σ identifies only the dislocation/dislocation interaction component of the flow stress through the evolution of the ρ term. Lattice resistance and solution hardening are accounted for the σ_0 term.

$$\sigma = \sigma_0 + M\alpha G b \sqrt{\rho^T} \tag{4}$$

To describe the work-hardening process in polycristalline ferrite, the following model constructed in the basis of Kocks-Mecking model (Voce type constitutive equation) is proposed:

$$\sigma = \sigma_0 + M\alpha G b \sqrt{\rho^s + \rho^G}$$
⁽⁵⁾

$$\rho^{S} = \left[\frac{K_{1}}{K_{2}}\left(1 - e^{\frac{-MK_{2}\varepsilon}{2}}\right) + \sqrt{\rho_{0}} e^{\frac{-MK_{2}\varepsilon}{2}}\right]^{2}$$
(6)

$$\rho^{G} = C \frac{\chi_{eq}}{b} \tag{7}$$

Here, M, ρ^{G} , ρ^{S} , and others were defined in the preceding, C is a constant ranging from 1 to 2, χ_{eq} represents the magnitude of the curvature tensor χ used as the scalar measure of the density of geometrically necessary dislocations ρ^{G} [2]

$$\chi_{eq} = \sqrt{\frac{2}{3}\chi_{ij}\chi_{ij}}$$

 $\chi_{ni} = e_{nkj} \varepsilon_{ij,k}$ $e_{nkj} =$ the alternating tensor $\varepsilon_{ij,k} =$ the strain gradient tensor $\rho_o =$ the initial dislocation density (present in the undeformed crystal).

 K_1 and K_2 characterise the processes of dislocation storage and concurrent dislocation annihilation by dynamic recovery, respectively [11]. The process of dislocation storage is athermal, so that K_1 is a constant. By contrast, the coefficient K_2 represents a thermally activated process of dynamic recovery by dislocation cross-slip (low temperature case) or dislocation climb (high temperature case). The boundary between the two temperature regimes lies at approximately two thirds of the melting temperature. In both cases, the strain rate and temperature dependence of K_2 can be expressed as [11]:

$$K_{2} = K_{20} \left(\frac{\dot{\varepsilon}^{p}}{\dot{\varepsilon}_{0}^{*}} \right)^{-1/n}$$
(8)

where K_{20} is a constant. The temperature dependence is contained either in *n* (in the low-temperature case when *n* is inversely proportional to temperature *T*, while $\dot{\varepsilon}_0^*$ can be considered constant) or in $\dot{\varepsilon}_0^*$ (in the high-temperature case when it is given by an Arrhenius-type equations, *n* being a constant ranging from 3 to 5).

In the present work we do not consider the temperature and strain rate dependence in K_2 , and then the term associated with the dynamic recovery is assumed to be a constant. The identification of constants K_1 and K_2 are explained below.

Parameter Identification

For a coarse-grained (or monocrystalline) single-phase material which can be regarded as "structureless", the evolution equation in the form of Eq. (9) describes materials where dislocation storage is controlled by the total dislocation density

$$\frac{d\rho}{d\varepsilon} = M(K_1\sqrt{\rho} - K_2\rho) \tag{9}$$

Differentiation of Eq. (1) gives

$$\frac{d\sigma}{d\varepsilon} = \frac{1}{2} M \alpha G b \frac{1}{\sqrt{\rho}} \frac{d\rho}{d\varepsilon}$$
(10)

Combining Eqs. (1), (9) and (10), the following equation can be derived

$$\sigma \frac{d\sigma}{d\varepsilon} = \frac{1}{2} M^2 \alpha G b K_1 \sigma - \frac{1}{2} M K_2 \sigma^2$$
(11)

or
$$\sigma \frac{d\sigma}{d\varepsilon} = \theta_{II} \sigma - \frac{1}{2} M K_2 \sigma^2$$
 (12)

where $\theta_{II} = \frac{1}{2} M^2 \alpha Gb K_1$ is the stage II hardening rate, i.e., the slope of the stress-strain curve in stage II

It is recognized that θ_{II} is the limit value of the strain hardening rate for $\sigma \to 0$. On the other hand, when σ approaches its saturation value σ_s , the strain hardening coefficient $\theta = (d\sigma / d\varepsilon)_{\varepsilon} \to 0$. So, from Eq. (11)

$$\sigma_s = \alpha GbM \, \frac{K_1}{K_2} \tag{13}$$

and Eq. (12) can also be expresed in the form

$$\theta = \theta_{II} \left(1 - \frac{\sigma}{\sigma_s} \right) \tag{14}$$

The constants K_1 and K_2 for a polycristalline material can be calculated if the value of the stage II hardening rate, θ_L , and the value of the saturation stress σ_s are estimated. In references [12,13] it is established that σ_s is independent of strain rate and varies from 0.6 to 3 x 10⁻² *G* for different materials, the higher values being those for materials with a lower Stacking Fault Energy (SFE). According to Refs. [11,12], the work hardening rate θ_{II} which is almost independent of temperature or strain rate, ranges from 1/15 to 1/30 of the shear modulus *G*. In Ref. [14], the following expressions are documented:

$$\theta_{II} = \left(\frac{d\sigma}{d\varepsilon}\right)_{\sigma = \sigma_0 \cdot \frac{M_i}{M}} = 4.5 \ M_i^2 \frac{G}{1000}$$
(15)

$$\sigma_{s} = \sigma_{0} \frac{M_{i}}{M} + 213.M_{i} = \sigma_{y} + 213.M_{i}$$
(16)

In absence of other expressions, the constants K_1 and K_2 calculated from a coarse-grained single-phase material basis, can be used in polycristalline materials

$$K_1 = \frac{2\theta_{II}}{M_i^2 \alpha G b} = \frac{0.009}{\alpha b}$$
(17)

$$K_{2} = \frac{2\theta_{II}}{\sigma_{s}M_{i}} = \frac{0.009 \, G \, M}{\sigma_{0} + 213 \, M} \tag{18}$$

Finite Element Modelling

The asymptotic crack tip geometry has been modelled by means of a finite element mesh using plane strain elements CPE8R (Figure 1).



Figure 1: Finite element mesh for crack tip problem using element CPE8R.

Pure mode I is considered with asymptotic displacements $u_1(r, \theta)$ and $u_2(r, \theta)$ applied on the outer boundary of the mesh

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \frac{K_I}{2G} \sqrt{\frac{2r}{\pi}} \begin{bmatrix} \cos\frac{\theta}{2} \left(\frac{(3-4\nu)-1}{2} + sen^2\frac{\theta}{2} \right) \\ sen\frac{\theta}{2} \left(\frac{(3-4\nu)+1}{2} - \cos^2\frac{\theta}{2} \right) \end{bmatrix}$$
(19)

Here, K_I is the stress intensity factor in the crack-opening mode (mode I), G and v are the shear and the Poisson modulus respectively, r is the radius of the mesh, and θ is the angle that defines a node localised in the outer boundary (Figure 1).

The simplest model of cyclic crack propagation in ductile materials links the crack advance per cycle, da/dN, either to the CTOD range (the crack tip opening displacement range) or to the advance of the plastic zone (*L*) in the symmetry plane side (Figure 1), by assuming geometrical similarity of the blunting-sharpening sequence at the tip during the fatigue life [1].

To model a gradient plasticity theory using ABAQUS, we use the URDFIL subroutine to read the quantities that output in the results file. In particular, we read the strains at each Gauss integration point at the end of an increment, and calculate the strain gradient function from the previous increment (not current strain gradients). For further calculations, the strain gradients are passed into UMAT routine through a common block.

RESULTS AND DISCUSSIONS

The fatigue threshold has been quantified for ferritic steels by performing FEM calculations (ABAQUS[®] code) using a gradient-dependent continuum plasticity model based on the storage of GND and an appropriate constitutive equation of the Voce type (Eqs. (5) to (7)). For maximum K_I values above 10 MPa m^{0.5}, no differences in the CTOD or in the size of the plastic zone, *L*, are obtained from the application of the conventional theory or the gradient dependent theory. In both cases the usual proportionality of size with K_I^2 is predicted, i.e., a Paris's regime on the blunting - resharpening model of fatigue crack advance.



(a)

(b)



. 201 - H Î . HIC- D I

+3.80-01 +4.20-01

45,30-01

+0.00-01

+6.52-81

(e)

11,0040

-1.80-0

+1.80+00

ab mint

(**f**)

Figure 2: Equivalent plastic strain contours for increasing values of K_I : (a,c,e) Conventional plasticity; (b,d,f) Strain gradient plasticity. Note the differences in plastic zone size. For $K_I < 10$ MPa m^{1/2}, the plastic zone taking into account the strain gradient effect is significantly smaller than the plastic zone calculated using conventional plasticity ($L \propto K_I^2$). Note differences in scale.

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To observe the size effect which cannot be predicted with conventional plasticity theories, Fig. 2 compares the equivalent plastic strain contours for different values of K_I (2.27, 7.43 and 10 MPa m^{1/2}). In all cases, differences in contour values are observed. These differences are due to the strain gradient term introduced into the constitutive law via Eq. (7). By comparing the results observed in Fig. 2, it is clear that strain gradient plasticity predicts smaller and narrow plastic zone sizes at the crack tip, for stress intensity factor values smaller than 10 MPa m^{1/2}.

CONCLUSIONS

Inclusion of the influence of the plastic strain gradient in the flow stress ("strain gradient dependent plasticity") predicts a fatigue threshold of the correct order of magnitude ($\Delta K_{th} < 10 \text{ MPam}^{1/2}$ for steel) without recourse to any other possible contributon to deviatons from the Paris' law at low ΔK_I values (crack closure, etc.).

REFERENCES

- 1. Ocaña, I. and Gil Sevillano, J. (1998). J. Phys. IV France 8, 129.
- 2. Fleck N. A., Muller G. M., Ashby M. F. and Hutchinson J. W. (1994) Acta Metall. Mater. 42, 475.
- 3. Fleck, N.A. and Hutchinson, J.W. (1997). Advances in Appl. Mech. 33, 295.
- 4. Narutani, T. and Takamura, J. (1991). Acta Metall. Mater. **39**, 2037.
- 5. Meakin J. D. and Petch N. J. (1974). *Phil. Mag.* **30**, 1149.
- 6. Dingley D. J. and McLean D. (1967). Acta Metallurgica, 15, 885.
- 7. Ashby M.F. (1970). *Phil. Mag.* **21**, 399.
- 8. Mecking H. and Kocks U.F. (1981). Acta Metallurgica 29, 1865.
- 9. Hutchinson J.W. (2000). Int. J. Solids Structures 37, 225.
- 10. Estrin Y, (1996). In: *Unified Constitutive Laws of Plastic Deformation*, pp. 69-106, Krausz A.S. and Krausz K. (Eds.), Academic Press, New York.
- 11. Estrin Y. (1998). Journal of Materials Processing Technology 80-81, 33.
- 12. Gil Sevillano J., Van Houtte, P. and Aernoudt, E. (1980). Prog. Mat. Sci. 25, 69.
- 13. Kocks, U.F. (1976). J. Engng. Mater. Tech. 98, 76.
- 14. Modelling of mechanical properties and local deformation of high strength multi-phase steels. *ECSC Steel RTD Annual Report*, March 2000.