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MODELING THE ANISOTROPIC BEHAVIOR OF POLYCRYSTALS WITH VOIDS

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Abstract. *The viscoplastic selfconsistent (VPSC) formulation is by now a well established approach for simulating texture development and constitutive response during plastic forming of high and low-symmetry aggregates. In this work we consider the presence of voids of anisotropic shape inside 3D polycrystals submitted to large strain deformation. For this purpose, the originally incompressible VPSC formulation has been extended to deal with compressible polycrystals. In doing this, both the deviatoric and the spherical components of strain-rate and stress are accounted for. As a consequence, the extended model provides now a relationship between the void growth rate and the hydrostatic pressure, which in turn can be used to keep track of the porosity evolution in the polycrystal. The model is applicable to the stage of void growth but does not account for void nucleation or coalescence. The extended VPSC model is used here to study the role of voids (and their evolution) in texture evolution. In addition, we also study the coupling between texture, void shape, crystal symmetry and strain rate on both, mechanical response and void growth.*

1 INTRODUCTION

The evolution of porosity is of relevance for assessing damage during both quasi-static and high-strain-rate deformation of metallic aggregates[1]. The Gurson criterion[2], which provides a constitutive description of yield stress and porosity evolution, is widely used in simulations of metal deformation. The Gurson model applies to an isotropic, rate-independent medium with spherical voids. Extensions of the Gurson model have been proposed to address issues like void shape[3,4], matrix anisotropy[5] and rate-sensitivity[3,6]. In this work we present a 3D viscoplastic selfconsistent (VPSC) model for polycrystal with prexisiting voids, which allows consideration of the full anisotropy associated with mophologic evolution of voids and grains and with crystallographic texture development in the aggregate, as well as rate effects. With an appropriate fitting of one parameter that determines the local linearized behavior in the grains, this model reproduces Gurson's results for the case of low rate-sensitivity isotropic aggregates with spherical voids. In addition, it accounts for the effect of porosity and texture evolution on the mechanical response of the polycrystal. Our formulation is a generalization of the tangent incompressible fully anisotropic VPSC formulation developed by Lebensohn and Tomé[7]. This model treats each grain as a viscoplastic ellipsoidal inclusion embedded in a Homogeneous Effective Medium (HEM). Both, the inclusion and the HEM are anisotropic and incompressible. The cavities are also assumed to be ellipsoidal inclusions, but the assumption of incompressibility does not apply neither to the pores nor to the HEM (the inclusions representing grains, however, remain incompressible).

2 MODEL

2.1 Compressible VPSC formulation (CVPSC)

The deviatoric part of the constitutive behavior of the material at local level is described by means of the non-linear rate-sensitivity equation:

$$\dot{\varepsilon}'_{ij}(\bar{x}) = \dot{\gamma}_o \sum_s m^s_{ij} \left(\frac{m^s_{kl} : \sigma'_{kl}(\bar{x})}{\tau^s} \right)^n \tag{1}$$

where $\dot{\varepsilon}'(\bar{x})$ and $\sigma'(\bar{x})$ are the deviatoric strain-rate and stress fields; m^s_{ij} and τ^s are the Schmid tensor and the threshold stress of slip (s); $\dot{\gamma}_o$ is a normalization factor and n is the rate-sensitivity exponent. Linearizing equation (1) inside the domain of a grain and adding the spherical local relation gives:

$$\left| \begin{array}{l} \dot{\varepsilon}'_{ij} = M_{ijkl}\, \sigma'_{kl} + \dot{\varepsilon}'^{o}_{ij} \\ \dot{\varepsilon}_{kk} = \sigma^m / K \end{array} \right. \tag{2}$$

where $\dot{\varepsilon}'$ and σ' are the average local quantities in the grains; M_{ijkl} and $\dot{\varepsilon}'^{o}_{ij}$ are the local compliance and the back extrapolated term and $\dot{\varepsilon}_{kk}$, σ^m and K are average local dilatation-rate, mean stress ($\sigma^m = \sigma_{kk}/3$) and viscoplastic bulk modulus, respectively. For the infinitely compliant void phase, we can write expressions formally equivalent to (2), taking $M_{ijkl} \to \infty$ and $K = 0$. Assuming a constitutive relation analogous to (2) at polycrystal level:

$$\left| \begin{array}{l} \dot{E}'_{ij} = \overline{M}_{ijkl}\, \Sigma'_{kl} + \dot{E}'^{o}_{ij} \\ \dot{E}_{kk} = \Sigma^m / \overline{K} \end{array} \right. \tag{3}$$

where, by comparison with (2), the meaning of the macroscopic state variables and moduli becomes aparent. Using the equivalent inclusion method[8] the local (heterogeneous) constitutive behavior can be rewritten in terms of the (homogeneous) macroscopic moduli as:

$$\left| \begin{array}{l} \dot{\varepsilon}'_{ij} = \overline{M}_{ijkl}\, \sigma'_{kl} + \dot{E}'^{o}_{ij} + \dot{\varepsilon}^{*}_{ij} \\ \dot{\varepsilon}_{kk} = \sigma^m / \overline{K} + \dot{\varepsilon}^{\#} \end{array} \right. \tag{4}$$

where $\dot{\varepsilon}^{*}_{ij}$ and $\dot{\varepsilon}^{\#}$ are the deviatoric eigen-strain-rate and the eigen-dilatation-rate, respectively. Rearranging and subtracting (3) from (4) gives:

$$\left| \begin{array}{l} \tilde{\sigma}'_{ij} = \overline{L}_{ijkl} \left(\tilde{\dot{\varepsilon}}'_{kl} - \dot{\varepsilon}^{*}_{kl} \right) \\ \tilde{\sigma}^m = \overline{K} \left(\tilde{\dot{\varepsilon}}_{kk} - \dot{\varepsilon}^{\#} \right) \end{array} \right. \tag{5}$$

where the "~" quantities are local deviations from macroscopic values and $\overline{L}_{ijkl} = \overline{M}^{-1}_{ijkl}$. Separating the deviatoric and hydrostatic components of the stress and using the equilibrium condition:

$$\sigma_{ij,j} = \tilde{\sigma}_{ij,j} = \tilde{\sigma}'_{ij,j} - \tilde{\sigma}^m_{,i} \tag{6}$$

gives:

$$\left| \begin{array}{l} \overline{L}_{ijkl}\, \tilde{\dot{u}}_{k,lj} + \tilde{\sigma}^m_{,i} + f_i = 0 \\ \overline{K}\, \tilde{\dot{u}}_{k,k} - \tilde{\sigma}^m + F = 0 \end{array} \right. \tag{7}$$

where the heterogeneity terms explicitly are:

$$\begin{cases} f_i = -\overline{L}_{ijkl}\dot{\varepsilon}^*_{kl,j} \\ F = -\overline{K}\dot{\varepsilon}^{\#} \end{cases} \tag{8}$$

Equation (8) represents a system of 4 differential equations with 4 unknowns (3 components of the deviation in velocity $\tilde{\dot{u}}_i$ and one deviation in the mean stress $\tilde{\sigma}^m$). After solving these differential equations using Green functions and Fourier transforms[9] we obtain:

$$\begin{cases} \tilde{\dot{\varepsilon}}'_{ij} = S_{ijmn}\dot{\varepsilon}^*_{mn} + \beta_{ij}\tilde{\dot{\varepsilon}}_{kk} \\ \tilde{\dot{\varepsilon}}_{kk} = S_{kkmn}\dot{\varepsilon}^*_{mn} + \Psi\ \dot{\varepsilon}^{\#} \end{cases} \tag{9}$$

where S_{ijkl} is the fourth order viscoplastic deviatoric Eshelby tensor, $\Psi = S^s_{kk}$ (Ψ and S^s_{ij} are the viscoplastic spherical Eshelby factor and tensor, respectively) and $\beta_{ij} = S^s_{ij}/\Psi - \frac{1}{3}\delta_{ij}$. Inverting (9):

$$\begin{cases} \dot{\varepsilon}^*_{ij} = S^{-1}_{ijmn}\tilde{\dot{\varepsilon}}'_{mn} - S^{-1}_{ijmn}\beta_{mn}\tilde{\dot{\varepsilon}}_{kk} \\ \dot{\varepsilon}^{\#} = \tilde{\dot{\varepsilon}}_{kk}/\Psi \end{cases} \tag{10}$$

Replacing (10) in (5) we obtain the interaction equations:

$$\begin{cases} \tilde{\dot{\varepsilon}}'_{ij} = -\tilde{M}_{ijkl}\tilde{\sigma}'_{kl} - \tilde{\beta}_{kl} \\ \tilde{\dot{\varepsilon}}_{kk} = -\tilde{\sigma}^m/\tilde{K} \end{cases} \tag{11}$$

where:

$$\tilde{\mathbf{M}} = (\mathbf{I}-\mathbf{S}):\mathbf{S}^{-1}:\overline{\mathbf{M}} \tag{12a}$$

$$\tilde{\boldsymbol{\beta}} = -\mathbf{S}^{-1}:\boldsymbol{\beta}\,\tilde{\dot{\boldsymbol{\varepsilon}}}_{\mathbf{kk}} \tag{12b}$$

$$\tilde{K} = (1-\Psi)\Psi^{-1}\overline{K} \tag{12c}$$

Replacing the constitutive relations (2) and (3) in (11) gives the following self-consistent equations for the macroscopic moduli:

$$\overline{\mathbf{M}} = \langle \mathbf{B} \rangle^{-1} : \langle \mathbf{M}:\mathbf{B} \rangle \tag{13a}$$

$$\dot{\mathbf{E}}'^{\mathbf{0}} = \left\langle \mathbf{M} : \mathbf{\Phi} + \dot{\varepsilon}'^{\mathbf{0}} \right\rangle - \left\langle \mathbf{M} : \mathbf{B} \right\rangle : \left\langle \mathbf{B} \right\rangle^{-\mathbf{1}} : \left\langle \mathbf{\Phi} \right\rangle \tag{13b}$$

$$\overline{\mathrm{K}} = \frac{1-\phi}{\Psi_v} \frac{1-\Psi_g}{\phi} \overline{\mathrm{K}} \tag{13c}$$

where <.> indicates spatial average. The localization tensors are functions of the local and macroscopic moduli, i.e.:

$$\mathbf{B} = \left(\mathbf{M} + \tilde{\mathbf{M}}\right)^{-\mathbf{1}} : \left(\overline{\mathbf{M}} + \tilde{\mathbf{M}}\right) \tag{14a}$$

$$\mathbf{\Phi} = \left(\mathbf{M} + \tilde{\mathbf{M}}\right)^{-\mathbf{1}} : \left(\dot{\varepsilon}'^{\mathbf{0}} - \dot{\mathbf{E}}'^{\mathbf{0}} + \tilde{\boldsymbol{\beta}}\right) \tag{14b}$$

and Ψ_g and Ψ_v are the Eshelby factors of grains and voids and ϕ is the porosity. Equations (14) allow obtaining improved estimates of the macroscopic moduli $\overline{\mathbf{M}}, \dot{\mathbf{E}}'^{\mathbf{0}}$ and $\overline{\mathrm{K}}$. Once $\overline{\mathrm{K}}$ is adjusted, the macroscopic dilatation-rate is given by: $\dot{\mathrm{E}}_{kk} = \Sigma^m / \overline{\mathrm{K}}$ and the porosity-rate can be calculated by means of the following kinematic relation:

$$\dot{\phi} = (1-\phi)\,\dot{\mathrm{E}}_{kk} \tag{15}$$

2.2 Local linearization for voided polycrystals

The deviatoric local constitutive behavior (1) can be linearized in different ways. The macroscopic response resulting of the selfconsistent formulation will eventually depend on the choice made for that local linearization. For instance, if the back-extrapolated term $\dot{\varepsilon}'^{o}_{ij}$ is a priori set to zero, the resulting model is a secant one, which has been proved to be in general too stiff, leading to close-to-upper-bound result. On the other hand, if $\mathrm{M}_{ijkl} = \partial\dot{\varepsilon}'_{ij}(\sigma')/\partial\sigma'_{kl}$, the model is tangent, a less stiff approach. However, any homogenization scheme whose local linearization depends only on the average of local states in the phases (or grains) fails in reproducing Gurson's results at high triaxialities, leading to completely rigid response in the pure hydrostatic limit[10]. This result is connected to the high deformation gradients that physically appear inside the grains, in the vicinities of a void, when high hydrostatic pressure is applied to the aggregate. These strong gradients make the effective response of the grains softer than the one that would be obtain by linearization using just the average local states. For these reasons, a good matching between the present theory (in its isotropic and rate-insensitive limit) and the Gurson model at high triaxialities requires the following linearization for the local compliance:

$$\mathrm{M}_{ijkl}\left(\hat{\sigma}'_{kl} - \sigma'_{kl}\right) = \left(\hat{\dot{\varepsilon}}'_{ij} - \dot{\varepsilon}'_{ij}\right) \tag{16}$$

with:

$$\hat{\sigma}'_{kl} = \left(1 + \alpha(X,\phi)|X|\right)\sigma'_{kl} \tag{17}$$

where X is the stress triaxiality: $X = \Sigma^m / \Sigma^e$, with $\Sigma^e = \left(\frac{3}{2}\Sigma'_{ij}\Sigma'_{ij}\right)^{1/2}$, and $\alpha(X,\phi)$ is an adjustable parameter whose dependence with X and ϕ should been adjusted to match the predictions of the selfconsistent formulation, in its isotropic and rate-insensitive numeric limit, with Gurson's results. Defined in this way, the local tensors $\hat{\sigma}'_{kl}$ are evidently related with second order stress moments but, rather than estimate them directly, we make use of the parameter $\alpha(X,\phi)$ and of the Gurson model to tune the value of α for different triaxialities and porosities. Details of the adjustment of $\alpha(X,\phi)$ are given elsewhere[9]

3 RESULTS

In order to isolate the effects of void morphology from the full anisotropy evolution due to morphologic and crystallographic texture development, Fig. 1 shows the CVPSC predictions of porosity evolution for a initially random fcc polycrystal, deforming in tension by (111)<110> slip in the cases of: a) different initial void morphologies when no texture or morphology evolution were allowed and b) initial spherical voids with evolving texture and morphology, for triaxialities 1/3 and 1. In all cases, the initial porosity is 1% and the total longitudinal strain is 0.5. It is seen that oblate voids (ellipsoid's ratios 5:5:1) tends to grow faster than prolate ones (ellipsoid's ratios 1:1:5) and that texture evolution favors porosity growth, even if the voids become prolate as deformation proceeds.

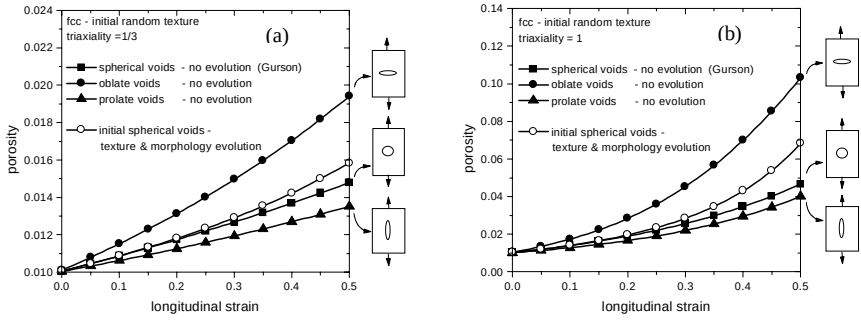

Figure 1: CVPSC predictions of porosity evolution for different void morphologies and no texture or morphology evolution (solid symbols) and for initial spherical voids with evolving texture and morphology (open symbols). Initial porosity: 1%, total longitudinal strain: 0.5. Cases of: a) triaxiality 1/3, b) triaxiality 1.

The next example concerns an hcp aggregate and reveals a strong coupling between texture and porosity evolution. In this case we consider an aggregate of 500 grains with easy basal and prismatic slip (τ^s =1) and hard pyramidal <c+a> slip (τ^s =4), and an initial strong texture

consisting of a basal component along the axis x_1 (see Fig. 2b). Tension was imposed parallel to the axis x_1 or perpendicular to it (along axis x_2), triaxialities of 1/3 and 1 were enforced, and an initial concentration ϕ=0.01 of spherical voids was considered. Texture evolution is not very sensitive to triaxiality, and rather depends on the relative orientation of the initial texture and the tensile axis (see Fig. 2b). The porosity evolution, instead, is strongly influenced by the texture, especially at high triaxialities (Fig. 2a). Indeed, the cases of tension along x_1 (i.e.: most crystals with their <c>-axis aligned in tensile direction and therefore hard to deform) exhibit a faster void growth than the cases of tension along x_2, which final porosities for triaxialities 1/3 and 1 do not differ substantially.

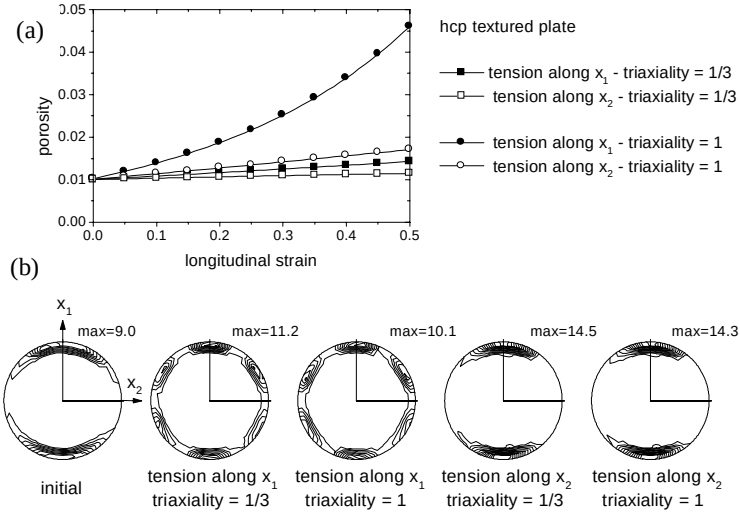

Figure 2: Interplay between texture and porosity. CVPSC predictions of: a) porosity evolution in an initially textured hcp polycrystal, deformed in tension along x_1 and x_2, for triaxialities 1/3 and 1. Initial porosity: 1%. Slip modes: prismatic and basal slip (τ^s=1) and pyramidal <c+a> slip (τ^s=4). Total longitudinal strain: 0.5. b) initial and final (0001) basal poles figures for the four cases shown above.

4 CONCLUSIONS

We propose a compressible VPSC polycrystal model which accounts for porosity and texture, and its evolution, during plastic forming. The model is tuned to give the same response as Gurson when the material has low rate-sensitivity, is isotropic and the cavities are spherical. Such tunning is done through a single parameter, as a function of triaxiality.

We may say that, in much the same way as VPSC represents an improvement over the limited isotropic Von Mises plastic formulation, CVPSC represents an improvement over the simple isotropic Gurson formulation.

Concerning the interplay between porosity and texture, the above results show that: a) the void shape has a major effect on porosity evolution, oblate voids tends to grow faster than prolate voids under tensile stress; b) porosity evolution does not affect substantially texture evolution by comparison with an aggregate without voids deformed to the same strain; c) texture changes substantially the porosity evolution in the case of a textured and highly anisotropic hexagonal aggregate tested along and across the main texture component.

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