Mecánica Computacional Vol. XXIII, pp. 161-177
G.Buscaglia, E.Dari, O.Zamonsky (Eds.)
Bariloche, Argentina, November 2004

CALCULATION AND USE OF INTRAGRANULAR FIELD FLUCTUATIONS IN NON-LINEAR HOMOGENIZATION SCHEMES FOR THE PREDICTION OF THE MECHANICAL BEHAVIOR OF VISCOPLASTIC POLYCRYSTALS

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Key Words: polycrystal, viscoplasticity, non-linear homogenization, second-order moments, self-consistent model, average field fluctuations

Abstract. *In this contribution we present an implementation of the calculation of the average field fluctuations inside the grains of a thermoelastic aggregate, in terms of the derivatives of the stress potential given by the self-consistent (SC) approximation for linear polycrystals. Similar expressions are applicable to non-linear viscoplastic polycrystals, whose behavior can be estimated by means of the different non-linear homogenization schemes, which require linearization of the constitutive behavior at grain level. These statistical indicators are in turn used to calculate the standard deviations (SD) of the mechanical fields, considering both intergranular and intragranular fluctuations. The SDs corresponding to different first-order non-linear SC extensions are then compared, for the case of a non-linear hcp polycrystal. Finally, we show how to use the above statistical information to generate more refined non-linear SC estimates, taking into account both first- and second-order moments to define the local linearized behavior of the grains.*

1 INTRODUCTION

The self-consistent (SC) approximation, originally proposed by Kroner[1] for linear elastic materials, is by far the most commonly used method for estimating the macroscopic behavior of polycrystalline aggregates or composites. For non-linear polycrystalline systems deforming by dislocation glide, many different extensions of the standard linear SC approximation have been proposed in the literature. These various approximations, which are all based in adopting a particular linearization scheme to approximate the actual non-linear local constitutive behavior, generally provide improvements on the Taylor and Sachs bounds and reduce to the standard linear SC estimate for linearly viscous behavior. However, they give widely diverging predictions for materials with low rate-sensitivity and/or high contrast in local properties.

On the one hand, the classical non-linear SC formulations are based on information of the first-order moments (averages) of the mechanical fields inside the grains, to define the local linearized behavior. For instance, the 'incremental' method of Hill[2] and Hutchinson[3] becomes close to the Taylor upper bound estimate for low rate-sensitivity materials, while the 'tangent' procedure of Molinari et al.[4] and Lebensohn and Tomé[5] leads to estimates that are close to the Sachs lower bound estimate in that case. On the other hand, the 'affine' formulation of Masson et al.[6], which makes use of general linearization, yields results in between the 'incremental' and the 'tangent' estimates. For single-phase polycrystals with large grain anisotropy or for multiphase polycrystals with high contrast in phase properties, these first-order approaches can lead to large differences in the predicted behavior and microstructural evolution.

On the other hand, recent extensions of the SC approximation make use of rigorous non-linear homogenization methods to express the effective potential of a non-linear viscoplastic polycrystal in terms of that of a linearly viscous polycrystal with properties that are determined from suitably-designed variational principles. The most recent of these variational approaches is the new 'second-order' (SO) method of Ponte Castañeda[7], which combines the advantages of two earlier versions, i.e. the 'variational' method[8] and the old 'second-order'[9] procedure. The first of these methods has the advantage that it incorporates into the linear comparison polycrystal information not only on the field averages in the grains, but also on the average field fluctuations. On the other hand, the old 'second-order' method was the first one to yield estimates capable of reproducing exactly to second-order in the contrast the asymptotic expansions of Suquet and Ponte Castañeda[10] but did not contain information of second-order moments.

In this work, we first present how to implement the calculation of average field fluctuations inside the grains of a thermoelastic aggregate in terms of the derivatives of the stress potential, which has to be determined by means of the standard SC model for linear polycrystals. The above methodology can be extended to non-linear viscoplastic polycrystals whose behavior is estimated by means of the different SC non-linear extensions. These statistical indicators are in turn used to calculate standard deviations (SD) of the mechanical fields over the entire polycrystal, considering both intergranular and intragranular fluctuations. The SDs corresponding to different non-linear first-order SC extensions are then compared for the case

of a non-linear hcp polycrystal. Finally, we show how the above statistical information can be used to generate more refined estimates for non-linear viscoplastic polycrystals that take into account both first- and second-order moments of the mechanical fields in the grains, using the variational second-order method of Ponte Castañeda[7].

In what follows, all the tensors are symmetric and represent incompressible magnitudes or properties. Therefore, they can be represented in the so-called "b-basis" convention[11]. Under this convention the 2nd and 4th rank tensors are represented by 5-dim vectors and 5x5 matrices, respectively, vg: $\sigma_{ij} \leftrightarrow \sigma_k$ (ij=1,3; k=1,5) and $M^{(r)}_{ijkl} \leftrightarrow M^{(r)}_{mn}$ (ijkl=1,3; mn=1,5). Moreover, the contraction of two or four indices between Cartesian tensors corresponds to the contraction of one and two indices in b-basis convention, v.g. $M^{(r)}_{ijkl}\sigma_{kl} \leftrightarrow M^{(r)}_{pq}\sigma_q$ or, in implicit notation, the cartesian product $M^{(r)} : \sigma$ is equivalent to the b-basis product $M^{(r)} \cdot \sigma$, also $\sigma_{ij}M^{(r)}_{ijkl}\sigma_{kl} \leftrightarrow \sigma_p M^{(r)}_{pq}\sigma_q$ or, implicitly, the cartesian product $M^{(r)} :: (\sigma \otimes \sigma)$ is equivalent to the b-basis product $M^{(r)} : (\sigma \otimes \sigma)$.

2 SELF-CONSISTENT APPROXIMATION FOR LINEAR POLYCRYSTALS

The effective behavior of a generalized linear "thermoelastic" polycrystal is characterized by a stress potential $\tilde{U}_T$ that may be written in the form[12]

$$\tilde{U}_T = \frac{1}{2}\tilde{M} : (\Sigma \otimes \Sigma) + \tilde{e} \cdot \Sigma + \frac{1}{2}\tilde{g} \tag{1}$$

such that

$$E = \tilde{M} \cdot \Sigma + \tilde{e} \tag{2}$$

where Σ is the macroscopic stress, and E should be interpreted as the macroscopic strain (in the case of an actual thermoelastic material) or strain-rate (for a linearly viscous material), and where $\tilde{M}$, $\tilde{e}$ and $\tilde{g}$ are the effective compliance, back-extrapolated strain (or strain-rate) and energy under zero applied stress, defined (in the case all grains have the same shape) by

$$\tilde{M} = \sum_r c^{(r)} M^{(r)} \cdot B^{(r)} \tag{3}$$

$$\tilde{e} = \sum_r c^{(r)} e^{(r)} \cdot B^{(r)} \tag{4}$$

$$\tilde{g} = \sum_r c^{(r)} e^{(r)} \cdot b^{(r)} \tag{5}$$

where $c^{(r)}$ is the volume fraction associated with grain (r), and $M^{(r)}$ and $e^{(r)}$ are the local compliance and back-extrapolated term of grain (r)

$$\varepsilon = M^{(r)} \cdot \sigma + e^{(r)} \tag{6}$$

and $B^{(r)}$ and $b^{(r)}$ are the stress concentrations tensors of grain (r)

$$\overline{\sigma}^{(r)} = B^{(r)} \cdot \Sigma + b^{(r)} \tag{7}$$

where $\overline{\sigma}^{(r)}$ is the average stress of grain (r). Explicitly, the SC expressions of above tensors are given by[13]

$$B^{(r)} = \left(M^{(r)} + M^{*}\right)^{-1} \cdot \left(\widetilde{M} + M^{*}\right) \tag{8}$$

$$b^{(r)} = \left(M^{(r)} + M^{*}\right)^{-1} \cdot \left(\widetilde{e} - e^{(r)}\right) \tag{9}$$

where the interaction tensor M^{*} is given by

$$M^{*} = \left(I - S\right)^{-1} \cdot S \cdot \widetilde{M} \tag{10}$$

with S being the Eshelby tensor, a function of $\widetilde{M}$ and the grain-shape.

3 SECOND-ORDER MOMENTS OF THE STRESS FIELD

The average second-order moment of the stress over grain (r) is given by[12]

$$\left\langle \sigma \otimes \sigma \right\rangle^{(r)} = \frac{2}{c^{(r)}} \frac{\partial \widetilde{U}_T}{\partial M^{(r)}} \tag{11}$$

Using the explicit expression of $\widetilde{U}_T$ (Eq. 1), Eq. (11) becomes

$$\left\langle \sigma \otimes \sigma \right\rangle^{(r)} = \frac{1}{c^{(r)}} \frac{\partial \widetilde{M}}{\partial M^{(r)}} : (\Sigma \otimes \Sigma) + \frac{2}{c^{(r)}} \frac{\partial \widetilde{e}}{\partial M^{(r)}} \cdot \Sigma + \frac{1}{c^{(r)}} \frac{\partial \widetilde{g}}{\partial M^{(r)}} \tag{12}$$

The above derivatives will be obtained in the following sequence:

$$\frac{\partial B^{(s)}}{\partial M^{(r)}} \rightarrow \frac{\partial \widetilde{M}}{\partial M^{(r)}} \rightarrow \frac{\partial \widetilde{e}}{\partial M^{(r)}} \rightarrow \frac{\partial \widetilde{g}}{\partial M^{(r)}} \tag{13}$$

3.1 Calculation of $\partial B_{kj}^{(s)} / \partial M_{uv}^{(r)}$

From Eq. (8) we have

$$\frac{\partial B_{kj}^{(s)}}{\partial M_{uv}^{(r)}} = \frac{\partial}{\partial M_{uv}^{(r)}}\left[\left(M^{(s)}+M^{*}\right)^{-1}_{kl}\left(\tilde{M}+M^{*}\right)_{lj}\right] =$$

$$= -\left(M^{(s)}+M^{*}\right)^{-1}_{km}\left(\frac{\partial \tilde{M}_{mn}^{(s)}}{\partial M_{uv}^{(r)}}+\frac{\partial M_{mn}^{*}}{\partial M_{uv}^{(r)}}\right)\left(M^{(s)}+M^{*}\right)^{-1}_{nl}\left(\tilde{M}+M^{*}\right)_{lj}+ \qquad (14)$$

$$+\left(M^{(s)}+M^{*}\right)^{-1}_{km}\left(\frac{\partial \tilde{M}_{mj}}{\partial M_{uv}^{(r)}}+\frac{\partial M_{mj}^{*}}{\partial M_{uv}^{(r)}}\right)$$

Hence,

$$\frac{\partial B_{kj}^{(s)}}{\partial M_{uv}^{(r)}} = -\left(M^{(s)}+M^{*}\right)^{-1}_{km}\delta_{mu}\delta_{nv}\delta_{rs}B_{nj}^{(s)} + \left(M^{(s)}+M^{*}\right)^{-1}\cdot\left[\frac{\partial M^{*}}{\partial M_{uv}^{(r)}}\cdot\left(I-B^{(s)}\right)+\frac{\partial \tilde{M}}{\partial M_{uv}^{(r)}}\right] \qquad (15)$$

In the second term on the left, the indices (uv) (i.e.: the component of the local compliance with respect which the derivatives are calculated) appear only to indicate such derivative, while in the first term they are mixed-up with the other indices. For this reason, the first and second terms are written in explicit and implicit index notation, respectively.

Using the expression $\partial M^{*}/\partial M_{uv}^{(r)}$ derived in the Appendix (Eq. A3), Eq. (15) can be rewritten as

$$\frac{\partial B_{kj}^{(s)}}{\partial M_{uv}^{(r)}} = -\left(M^{(s)}+M^{*}\right)^{-1}_{ku}\delta_{rs}B_{vj}^{(s)} + \left(M^{(s)}+M^{*}\right)^{-1}\cdot\Phi^{(r)}\cdot\left(I-B^{(s)}\right)+$$

$$+\left(M^{(s)}+M^{*}\right)^{-1}\cdot\left[F\cdot\frac{\partial \tilde{M}}{\partial M_{uv}^{(r)}}\cdot\left(I-B^{(s)}\right)+\frac{\partial \tilde{M}}{\partial M_{uv}^{(r)}}\right] \qquad (16)$$

where $\Phi^{(r)}$ is a tensor that depends on the derivative of the Eshelby tensor $\partial S/\partial M_{uv}^{(r)}$ (see Appendix).

Working in explicit notation with the expression between brackets we obtain

$$F_{ik}\frac{\partial \tilde{M}_{kl}}{\partial M_{uv}^{(r)}}\left(I-B^{(s)}\right)_{lj}+\frac{\partial \tilde{M}_{ij}}{\partial M_{uv}^{(r)}} = \left[F_{ik}\left(I-B^{(s)}\right)_{lj}+\delta_{ik}\delta_{jl}\right]\frac{\partial \tilde{M}_{kl}}{\partial M_{uv}^{(r)}} = \alpha_{ijkl}^{(s)}\frac{\partial \tilde{M}_{kl}}{\partial M_{uv}^{(r)}} \qquad (17)$$

so, finally,

$$\frac{\partial B_{kj}^{(s)}}{\partial M_{uv}^{(r)}} = -\left(M^{(s)} + M^{*}\right)^{-1}_{ku} \delta_{rs} B_{vj}^{(s)} + \left(M^{(s)} + M^{*}\right)^{-1} \cdot \left[\Phi^{(r)} \cdot \left(I - B^{(s)}\right) + \alpha^{(s)} : \frac{\partial \tilde{M}}{\partial M_{uv}^{(r)}} \right] \quad (18)$$

3.2 Calculation of $\partial \tilde{M}_{ij} / \partial M_{uv}^{(r)}$

From Eq. (3) we have

$$\frac{\partial \tilde{M}_{ij}}{\partial M_{uv}^{(r)}} = \sum_s c^{(s)} \frac{\partial}{\partial M_{uv}^{(r)}} \left(M^{(s)} \cdot B^{(s)}\right) = \sum_s c^{(s)} \delta_{iu} \delta_{kv} \delta_{rs} B_{kj}^{(s)} + \sum_s c^{(s)} M_{ik}^{(s)} \frac{\partial B_{kj}^{(s)}}{\partial M_{uv}^{(r)}} \quad (19)$$

Using (18) and calling $\beta^{(s)} = M^{(s)} \cdot \left(M^{(s)} + M^{*}\right)^{-1}$ we get

$$\begin{aligned} \frac{\partial \tilde{M}_{ij}}{\partial M_{uv}^{(r)}} = {} & c^{(r)} \delta_{iu} B_{vj}^{(r)} - c^{(r)} \beta_{iu}^{(r)} B_{vj}^{(r)} + \sum_s c^{(s)} \beta^{(s)} \cdot \Phi^{(r)} \cdot \left(I - B^{(s)}\right) + \\ & + \left(\sum_s c^{(s)} \beta^{(s)} \cdot \alpha^{(s)} \right) : \frac{\partial \tilde{M}}{\partial M_{uv}^{(r)}} \end{aligned} \quad (20)$$

Calling $\lambda^{(r)} = \sum_s c^{(s)} \beta^{(s)} \cdot \Phi^{(r)} \cdot \left(I - B^{(s)}\right)$, defining $\pi_{ij}^{(r,uv)} = c^{(r)} \left(\delta_{iu} - \beta_{iu}^{(r)}\right) B_{vj}^{(r)} + \lambda_{ij}^{(r)}$ and $\Omega' = \sum_s c^{(s)} \beta^{(s)} \cdot \alpha^{(s)}$, Eq. (23) can be explicitly rewritten as

$$\frac{\partial \tilde{M}_{ij}}{\partial M_{uv}^{(r)}} = \pi_{ij}^{(r,uv)} + \Omega'_{ijkl} \frac{\partial \tilde{M}_{kl}}{\partial M_{uv}^{(r)}} \quad (21)$$

Finally, calling $\Omega_{ijkl} = \delta_{ik} \delta_{jl} - \Omega'_{ijkl}$ we have

$$\Omega_{ijkl} \frac{\partial \tilde{M}_{kl}}{\partial M_{uv}^{(r)}} = \pi_{ij}^{(r,uv)} \quad (22)$$

Equation (22) is a linear system of 25 equations with 25 unknowns (i.e. the components of $\partial \tilde{M}_{kl} / \partial M_{uv}^{(r)}$). This system can be solved for a given value of $\Phi^{(r)}$ that corresponds to a certain value of the Eshelby tensor derivative $\partial S / \partial M_{uv}^{(r)}$. This a priori unknown derivative can be calculated in terms of the also unknown $\partial \tilde{M} / \partial M_{uv}^{(r)}$, as shown in the Appendix. Therefore, the problem should be solved iteratively assuming an initial value of $\Phi^{(r)}$ (v.g. $\Phi^{(r)} = 0$),

getting $\partial\tilde{M}/\partial M_{uv}^{(r)}$ under this assumption, using the latter to get a new guess for $\Phi^{(r)}$, and so on. This iterative process should stop when the input and output values of $\Phi^{(r)}$ (and therefore those of $\partial\tilde{M}/\partial M_{uv}^{(r)}$) coincide within certain tolerance.

3.3 Calculation of $\partial\tilde{e}_j/\partial M_{uv}^{(r)}$

From Eq. (4) we have

$$\frac{\partial\tilde{e}_j}{\partial M_{uv}^{(r)}} = \sum_s c^{(s)} e_k^{(s)} \frac{\partial B_{kj}^{(s)}}{\partial M_{uv}^{(r)}} \tag{23}$$

With Eq. (18) and calling $\chi^{(s)} = \left(M^{(s)} + M^*\right)^{-1}$ we obtain

$$\frac{\partial\tilde{e}_j}{\partial M_{uv}^{(r)}} = -c^{(r)} e_k^{(r)} \chi_{ku}^{(r)} B_{vj}^{(r)} + \sum_s c^{(s)} e^{(s)} \cdot \chi^{(s)} \cdot \Phi^{(r)} \cdot \left(I - B^{(s)}\right) + \zeta : \frac{\partial\tilde{M}}{\partial M_{uv}^{(r)}} \tag{24}$$

where

$$\zeta_{ijk} = \sum_s c^{(s)} e_m^{(s)} \chi_{ml}^{(s)} \alpha_{lijk}^{(s)} \tag{25}$$

The value of $\partial\tilde{M}/\partial M_{uv}^{(r)}$ to be used in Eq. (24) comes from the procedure described in section 3-2.

3.4 Calculation of $\partial\tilde{g}/\partial M_{uv}^{(r)}$

From Eq. (5) we have

$$\frac{\partial\tilde{g}}{\partial M_{uv}^{(r)}} = \sum_s c^{(s)} e_i^{(s)} \frac{\partial b_i^{(s)}}{\partial M_{uv}^{(r)}} \tag{26}$$

Using Eq. (9), the derivative in the right term can be calculated as

$$\frac{\partial b_i^{(s)}}{\partial M_{uv}^{(r)}} = -\chi_{iu}^{(s)} \delta_{rs} \chi_{vl}^{(s)} \left(\tilde{e}_l - e_l^{(s)}\right) - \chi^{(s)} \cdot \frac{\partial M^*}{\partial M_{uv}^{(r)}} \cdot \chi^{(s)} \cdot \left(\tilde{e} - e^{(s)}\right) + \chi^{(s)} \cdot \frac{\partial\tilde{e}}{\partial M_{uv}^{(r)}} \tag{27}$$

Replacing Eq. (27) in Eq. (26) and using Eq. (A3)

$$\frac{\partial \tilde{g}}{\partial M_{uv}^{(r)}} = -c^{(r)} e_i^{(r)} \chi_{iu}^{(r)} \chi_{vl}^{(r)} \left(\tilde{e}_l - e_l^{(r)} \right)$$
$$- \sum_s c^{(s)} e^{(s)} \cdot \chi^{(s)} \cdot \left(\Phi^{(r)} + F \cdot \frac{\partial \tilde{M}}{\partial M_{uv}^{(r)}} \right) \cdot \chi^{(s)} \cdot \left(\tilde{e} - e^{(s)} \right) \qquad (28)$$
$$+ \sum_s c^{(s)} e^{(s)} \cdot \chi^{(s)} \cdot \frac{\partial \tilde{e}}{\partial M_{uv}^{(r)}}$$

The values of $\partial \tilde{M} / \partial M_{uv}^{(r)}$ and $\partial \tilde{e} / \partial M_{uv}^{(r)}$ to be used in Eq. (28) come from the procedure described in sections 3-2 and 3-3.

4 SECOND-ORDER MOMENTS OF THE STRAIN FIELD

Once the average second-order moments of the stress were obtained, the corresponding second-order moments of the strain (or strain-rate) can be calculated as follows:

$$M_{ik}^{(r)} M_{jl}^{(r)} \langle \sigma_k \sigma_l \rangle^{(r)} = \left\langle M_{ik}^{(r)} \sigma_k M_{jl}^{(r)} \sigma_l \right\rangle^{(r)} = \left\langle \left(\varepsilon_i - e_i^{(r)} \right) \left(\varepsilon_j - e_j^{(r)} \right) \right\rangle^{(r)} =$$
$$= \left\langle \varepsilon_i \varepsilon_j - \varepsilon_i e_j^{(r)} - e_i^{(r)} \varepsilon_j + e_i^{(r)} e_j^{(r)} \right\rangle^{(r)} = \left\langle \varepsilon_i \varepsilon_j \right\rangle^{(r)} - \langle \varepsilon_i \rangle^{(r)} e_j^{(r)} - e_i^{(r)} \langle \varepsilon_j \rangle^{(r)} + e_i^{(r)} e_j^{(r)} \qquad (29)$$

Hence, recalling that $\langle \varepsilon_i \rangle^{(r)} = \bar{\varepsilon}_i^{(r)}$

$$\left\langle \varepsilon_i \varepsilon_j \right\rangle^{(r)} = M_{ik}^{(r)} M_{jl}^{(r)} \langle \sigma_k \sigma_l \rangle^{(r)} + \bar{\varepsilon}_i^{(r)} e_j^{(r)} + e_i^{(r)} \bar{\varepsilon}_j^{(r)} - e_i^{(r)} e_j^{(r)} \qquad (30)$$

or, calling $M_{ik}^{(r)} M_{jl}^{(r)} = Z_{ijkl}^{(r)}$, in implicit notation we have

$$\langle \varepsilon \otimes \varepsilon \rangle^{(r)} = Z^{(r)} : \langle \sigma \otimes \sigma \rangle^{(r)} + \bar{\varepsilon}^{(r)} \otimes e^{(r)} + e^{(r)} \otimes \bar{\varepsilon}^{(r)} - e^{(r)} \otimes e^{(r)} \qquad (31)$$

5 NON-LINEAR SELF-CONSISTENT EXTENSIONS

Every non-linear extension of the SC formulation is based on a linearization of the actual non-linear local behavior. In the case of an aggregate of single crystal grains deforming by dislocation glide, the non-linear rate-sensitivity constitutive relation is approximated by:

$$\varepsilon = \gamma_o \sum_k \mu_{(k)}^{(r)} \left(\frac{\mu_{(k)}^{(r)} \cdot \sigma}{(\tau_o)_{(k)}} \right)^n \cong M^{(r)} \cdot \sigma + e^{(r)} \qquad (32)$$

In Eq. (32) $(\tau_o)_{(k)}$ and $\mu^{(r)}_{(k)}$ are the threshold stress and the Schmid tensor associated with slip system (k), γ_o is a normalization factor, and n is the rate-sensitivity exponent. If $M^{(r)}$ and $e^{(r)}$ are chosen to be certain functions of the average stress in grain (r), i.e. $\overline{\sigma}^{(r)}$, the corresponding non-linear SC extension is known as a first-order approximation. Otherwise, if both $\overline{\sigma}^{(r)}$ and $\langle \sigma \otimes \sigma \rangle^{(r)}$ are involved in the determination of $\overline{M}^{(r)}$ and $e^{(r)}$, the resulting SC approach becomes a second-order approximation.

5.1 First-order SC approximations

The three classical first-order approximations correspond to the following assumptions for $\overline{M}^{(r)}$ and $e^{(r)}$:

a) Secant[2]:

$$M^{(r)}_{sec} = \gamma_o \sum_k \frac{\mu^{(r)}_{(k)} \otimes \mu^{(r)}_{(k)}}{(\tau_o)_{(k)}} \left(\frac{\mu^{(r)}_{(k)} \cdot \overline{\sigma}^{(r)}}{(\tau_o)_{(k)}} \right)^{n-1} \tag{33a}$$

$$e^{(r)}_{sec} = 0 \tag{33b}$$

b) Affine[6, 13]:

$$M^{(r)}_{aff} = n\gamma_o \sum_k \frac{\mu^{(r)}_{(k)} \otimes \mu^{(r)}_{(k)}}{(\tau_o)_{(k)}} \left(\frac{\mu^{(r)}_{(k)} \cdot \overline{\sigma}^{(r)}}{(\tau_o)_{(k)}} \right)^{n-1} \tag{34a}$$

$$e^{(r)}_{aff} = \left(M^{(r)}_{sec} - M^{(r)}_{aff} \right) : \overline{\sigma}^{(r)} = (1-n)\, \overline{\varepsilon}^{(r)} \tag{34b}$$

c) Tangent[5]: in this case $M^{(r)}_{tg} = M^{(r)}_{aff}$ and $e^{(r)}_{tg} = e^{(r)}_{aff}$. However, instead of these expressions, use is made of the secant SC scheme (Eqs. 33) to get $\tilde{M}_{sec}$, in combination with the tangent-secant relation[2]: $\tilde{M}_{tg} = n\tilde{M}_{sec}$, so that the expression of the interaction tensor (see Eq. 10) is given by

$$M^* = (I-S)^{-1} \cdot S \cdot \tilde{M}_{tg} = n(I-S)^{-1} \cdot S \cdot \tilde{M}_{sec} \tag{35}$$

5.2 Second-order procedure

Once the average second-order moments of the stress field over each grain are obtained by means of the calculation of the derivatives appearing in Eq. (12), the implementation of the SO procedure follows the work of Liu and Ponte Castañeda[12]. The covariance tensor of stress fluctuations is given by

$$C_{\sigma}^{(r)} = \langle \sigma \otimes \sigma \rangle^{(r)} - \langle \sigma \rangle^{(r)} \otimes \langle \sigma \rangle^{(r)} \tag{36}$$

The average resolved shear stress on slip system (k) of grain (r) is given by

$$\bar{\tau}_{(k)}^{(r)} = \mu_{(k)}^{(r)} \cdot \langle \sigma \rangle^{(r)} \tag{37}$$

The corresponding average fluctuation of the resolved shear stress on slip system (k) of grain (r) is given by

$$\hat{\tau}_{(k)}^{(r)} = \bar{\tau}_{(k)}^{(r)} \pm \left(\mu_{(k)}^{(r)} \cdot C_{\sigma}^{(r)} \cdot \mu_{(k)}^{(r)} \right)^{1/2} \tag{38}$$

where the positive (negative) branch should be selected if $\bar{\tau}_{(k)}^{(r)}$ is positive (negative). The slip potential of slip system (k) in every grain is defined as

$$\phi_{(k)}(\tau) = \frac{(\tau_o)_{(k)}}{n+1} \left(\frac{|\tau|}{(\tau_o)_{(k)}} \right)^{n+1} \tag{39}$$

Two scalar magnitudes associated with each slip system (k) of each grain (r) are defined by

$$\alpha_{(k)}^{(r)} = \frac{\phi'^{(r)}_{(k)}\left(\hat{\tau}_{(k)}^{(r)}\right) - \phi'^{(r)}_{(k)}\left(\bar{\tau}_{(k)}^{(r)}\right)}{\hat{\tau}_{(k)}^{(r)} - \bar{\tau}_{(k)}^{(r)}} \tag{40}$$

$$e_{(k)}^{(r)} = \phi'^{(r)}_{(k)}\left(\bar{\tau}_{(k)}^{(r)}\right) - \alpha_{(k)}^{(r)} \bar{\tau}_{(k)}^{(r)} \tag{41}$$

The linearized local behavior associated with grain (r) is then given by

$$\varepsilon = M_{so}^{(r)} \cdot \sigma + e_{so}^{(r)} \tag{42}$$

where

$$M_{so}^{(r)} = \sum_{k} \alpha_{(k)}^{(r)} \left(\mu_{(k)}^{(r)} \otimes \mu_{(k)}^{(r)} \right) \tag{43}$$

$$e_{so}^{(r)} = \sum_{k} e_{(k)}^{(r)} \mu_{(k)}^{(r)} \tag{44}$$

The SO procedure consists in iterate over $M_{so}^{(r)}$ and $e_{so}^{(r)}$, defining improved estimations of a linear comparison polycrystal. Each of these polycrystals has associated different first- and second-order moments of the stress field in the grains. These statistical moments can be used to obtain new values of $\alpha_{(k)}^{(r)}$ and $e_{(k)}^{(r)}$, which in turn define a new linear comparison polycrystal, etc. This procedure converges when the input and output values of $\alpha_{(k)}^{(r)}$ and $e_{(k)}^{(r)}$ coincide within a certain tolerance.

6 RESULTS

6.1 Standard deviations of the stress and strain-rate fields predictions using first-order SC approximations. Case of hcp polycrytals with different contrasts

The average second-order moments over grain (r) (Eqs. 12 and 31) can be used to generate the average second-order moment of the equivalent stress and strain-rate in grain (r) as

$$\overline{\overline{\sigma}}_{eq}^{(r)} = \left(\frac{3}{2} I : \langle \sigma \otimes \sigma \rangle^{(r)} \right)^{1/2} \tag{45a}$$

$$\overline{\overline{\varepsilon}}_{eq}^{(r)} = \left(\frac{2}{3} I : \langle \varepsilon \otimes \varepsilon \rangle^{(r)} \right)^{1/2} \tag{45b}$$

The standard deviations of the equivalent magnitudes in grain (r) are defined as

$$SD^{(r)}(\sigma_{eq}) = \sqrt{\left(\overline{\overline{\sigma}}_{eq}^{(r)}\right)^2 - \left(\overline{\sigma}_{eq}^{(r)}\right)^2} \tag{46a}$$

$$SD^{(r)}(\varepsilon_{eq}) = \sqrt{\left(\overline{\overline{\varepsilon}}_{eq}^{(r)}\right)^2 - \left(\overline{\varepsilon}_{eq}^{(r)}\right)^2} \tag{46b}$$

Also, the standard deviations of the equivalent magnitudes over the whole polycrystal are defined as

$$SD(\sigma_{eq}) = \sqrt{\overline{\overline{\Sigma}}_{eq}^2 - \Sigma_{eq}^2} \tag{47a}$$

$$SD(\varepsilon_{eq}) = \sqrt{\overline{\overline{E}}_{eq}^2 - E_{eq}^2} \tag{47b}$$

where

$$\overline{\overline{\Sigma}}_{eq}^2 = \left\langle \left(\overline{\overline{\sigma}}_{eq}^{(r)}\right)^2 \right\rangle = \sum_r c^{(r)} \left(\overline{\overline{\sigma}}_{eq}^{(r)}\right)^2 \tag{48a}$$

$$\overline{\overline{E}}_{eq}^2 = \left\langle \left(\overline{\overline{\varepsilon}}_{eq}^{(r)} \right)^2 \right\rangle = \sum_r c^{(r)} \left(\overline{\overline{\varepsilon}}_{eq}^{(r)} \right)^2 \tag{48b}$$

It is worth noting that the overall SDs defined by Eqs. (47a,b) are a global scalar indicators that contain information about both intergranular and intragranular stress and strain-rate heterogeneity. For comparison purposes, let us define alternate SDs, that only reflects intergranular (but not intragranular) dispersion, i.e.:

$$SD'(\sigma_{eq}) = \sqrt{\left\langle \left(\overline{\sigma}_{eq}^{(r)} \right)^2 \right\rangle - \Sigma_{eq}^2} \tag{49a}$$

$$SD'(\varepsilon_{eq}) = \sqrt{\left\langle \left(\overline{\varepsilon}_{eq}^{(r)} \right)^2 \right\rangle - E_{eq}^2} \tag{49b}$$

In what follows we compare both types of SDs for an ice-type polycrystal with random texture, a rate-sensitivity exponent n=3, easy $(0001)\langle 11\bar{2}0\rangle$ basal slip ($\tau_{bas}^o = 1$), and hard $\{10\bar{1}0\}\langle 11\bar{2}0\rangle$ prismatic and $(11\bar{2}2)\langle 11\bar{2}\bar{3}\rangle$ pyramidal slip ($\tau_{pr}^o = \tau_{pyr}^o = M$), for different first-order approximations. Figure 1 shows the normalized SDs, i.e. $SD(\varepsilon_{eq})/E_{eq}$ and $SD(\sigma_{eq})/\Sigma_{eq}$ (*inter+intra* label), and $SD'(\varepsilon_{eq})/E_{eq}$ and $SD'(\sigma_{eq})/\Sigma_{eq}$ (*inter* label), versus the anisotropy parameter M. In the stress figure (Fig. 1b) we also present the results corresponding to a Taylor model (note that in this case, $SD(\sigma_{eq}) = SD'(\sigma_{eq})$ since there is no intragranular heterogeneity under Taylor assumption). When only intergranular heterogeneity is considered, the overall SD of the equivalent stress is highest for Taylor and decreases in the sequence secant-affine-tangent. Affine is closer to tangent at lower anisotropy and approaches secant at larger contrasts. Otherwise, when both intragranular and intergranular heterogeneity contributions are considered using the above calculation scheme for second-order moments, the SC approaches give in general higher dispersions than the Taylor model. As before, among the different SC linearization schemes, the secant formulation gives the highest dispersion, tangent the lowest, while affine lies in between, starting closer to tangent at low contrasts and approaching secant as the single crystal anisotropy increases.

In what concerns the strain-rate dispersions (Fig 1a), the overall intergranular SD is highest in the tangent and lowest in the secant case. Once again, the affine curve starts closer to tangent at lower anisotropy. Unlike the stress dispersions, in this case each model tends to saturate at different values, with the affine model closer to the secant than to the tangent saturation value. Same behavior is observed when both intergranular and intragranular dispersions are considered, but the SDs reach considerable higher levels than in the intergranular cases.

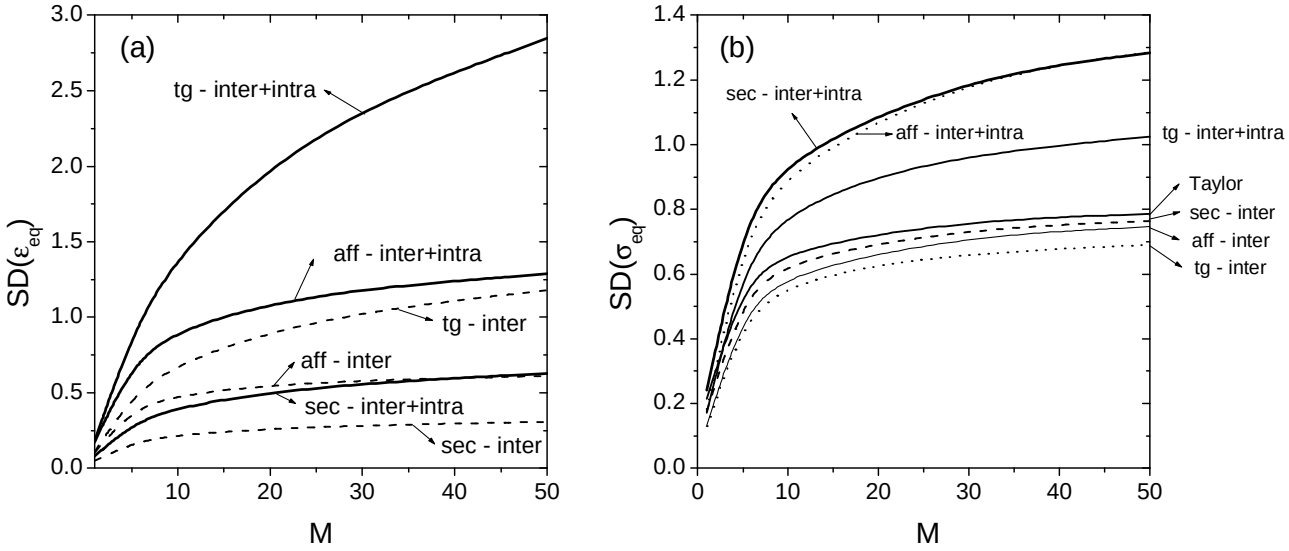

Figure 1: Overall intergranular (see Eqs. 49) and intergranular + intragranular (see Eqs. 47) standard deviations of the (a) strain-rate and (b) stress fields, for different first-order SC approximations in the case of an ice polycrystal with random texture, as functions of the anisotropy parameter M.

6.2 Effective behavior using first- and second-order SC approximations. Case of fcc polycrystals with different rate-sensitivities

Figure 2 shows a comparison between Taylor Factor (TF) vs. rate-sensitivity (1/n) curves, for a random fcc polycrystal under uniaxial tension. The TF was calculated as Σ_{eq} / τ_o, where τ_o is the threshold stress of the (111)<110> slip systems, and Σ_{eq} is the macroscopic equivalent stress corresponding to an unitary applied equivalent strain-rate $E_{eq} = 1$. The different curves correspond to the Taylor model, the different first-order SC approximations, and the second-order procedure. It can be observed that:

a) The TF curve predicted with Taylor approach is the highest, consistently with the upper bound status of this model.

b) All SC estimates coincide for n=1, i.e. the linear SC case.

c) For high and moderate rate-sensitivities, the SO procedure gives the lowest TF among the SC approaches. This is the reflection of an effective softer behavior at grain level that occurs when field fluctuations are considered for the determination of the linearized behavior of the grains.

d) In the rate-insensitive limit, while the secant and the tangent models tend respectively to the upper bound (Taylor) and the lower bound (i.e. TF=2.2 for $1/n \to 0$)[14], the affine and SO approximations remain between bounds.

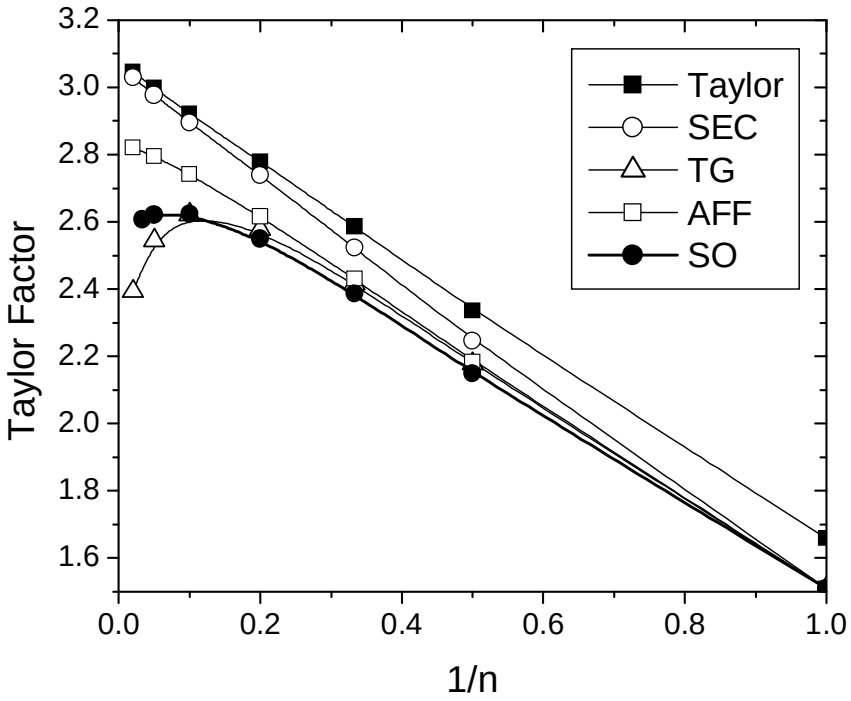

Figure 2: Taylor Factor vs. rate-sensitivity, for a random fcc polycrystal under unixial tension, as predicted with the Taylor model, several first-order SC approximations, and the second-order procedure.

7 CONCLUSIONS

A methodology for the calculation of second-order moments of the mechanical fields inside the grains of a polycrystal, within the framework of linear and non-linear SC models, has been given.

When both intergranular and intragranular field fluctuations are taken into account, the overall standard deviations of the stress and strain-rate distributions are appreciably higher than in the case of considering intergranular variations only.

Using the stress second-order moments inside the grains, the second-order SC procedure of Ponte Castañeda was implemented, and its estimates where compared with other SC approximations for the case of an fcc aggregate.

APPENDIX

A-1 Calculation of $\partial \mathrm{M}^{*} / \partial \mathrm{M}_{\mathrm{uv}}^{(\mathrm{r})}$

From Eq. (10) we have

$$\frac{\partial \mathrm{M}^{*}}{\partial \mathrm{M}_{uv}^{(r)}} = \frac{\partial}{\partial \mathrm{M}_{uv}^{(r)}}\left[(\mathrm{I}-\mathrm{S})^{-1}\cdot\mathrm{S}\cdot\tilde{\mathrm{M}}\right] = \\ = (\mathrm{I}-\mathrm{S})^{-1}\cdot\frac{\partial \mathrm{S}}{\partial \mathrm{M}_{uv}^{(r)}}\cdot\left[(\mathrm{I}-\mathrm{S})^{-1}\cdot\mathrm{S}\cdot\tilde{\mathrm{M}}+\tilde{\mathrm{M}}\right]+(\mathrm{I}-\mathrm{S})^{-1}\cdot\mathrm{S}\cdot\frac{\partial\tilde{\mathrm{M}}}{\partial \mathrm{M}_{uv}^{(r)}} \tag{A1}$$

where $\partial \mathrm{S}/\partial \mathrm{M}_{uv}^{(r)}$ can be calculated by means of the procedure explained below. Calling $\mathrm{F} = (\mathrm{I}-\mathrm{S})^{-1}\cdot\mathrm{S}$ and defining $\Phi^{(r)}$ as

$$\Phi^{(r)} = (\mathrm{I}-\mathrm{S})^{-1}\cdot\frac{\partial \mathrm{S}}{\partial \mathrm{M}_{uv}^{(r)}}\cdot\left[\mathrm{F}\cdot\tilde{\mathrm{M}}+\tilde{\mathrm{M}}\right] \tag{A2}$$

the interaction tensor derivative can be written as

$$\frac{\partial \mathrm{M}^{*}}{\partial \mathrm{M}_{uv}^{(r)}} = \Phi^{(r)} + \mathrm{F}\cdot\frac{\partial\tilde{\mathrm{M}}}{\partial \mathrm{M}_{uv}^{(r)}} \tag{A3}$$

A-2 Calculation of $\partial \mathrm{S}/\partial \mathrm{M}_{uv}^{(r)}$

The incompressible Eshelby tensor of an ellipsoidal inclusion of radii (a,b,c) embedded in an homogenous medium is given by

$$\mathrm{S} = \mathrm{T}\cdot\tilde{\mathrm{L}} \tag{A4}$$

where $\tilde{\mathrm{L}} = \tilde{\mathrm{M}}^{-1}$ is the stiffness of the medium (i.e. of the homogenized polycrystal) and, in tensorial notation

$$\mathrm{T}_{ijkl} = \frac{abc}{16\pi}\int_0^{2\pi}\int_0^{\pi}\frac{\lambda_{ijkl}(\alpha)}{[\rho(\alpha)]^3}\sin\theta\,d\theta\,d\varphi \tag{A5}$$

where α is an unitary vector of Fourier space; φ and θ are the spherical coordinates of α; $\rho(\alpha) = \left[(a\alpha_1)^2+(b\alpha_2)^2+(c\alpha_3)^2\right]^{1/2}$, and

$$\lambda_{ijkl} = \alpha_j\,\alpha_l\,A'^{-1}_{ik} + \alpha_i\,\alpha_l\,A'^{-1}_{jk} + \alpha_j\,\alpha_k\,A'^{-1}_{il} + \alpha_i\,\alpha_k\,A'^{-1}_{jl} \tag{A6}$$

with

$$A'_{ik} = \tilde{L}_{ijkl}\alpha_j\,\alpha_l \tag{A7}$$

Deriving (A4)[15]:

$$\frac{\partial \mathrm{S}}{\partial \mathrm{M}_{uv}^{(r)}} = \frac{\partial \mathrm{T}}{\partial \mathrm{M}_{uv}^{(r)}}\cdot\tilde{\mathrm{L}} + \mathrm{T}\cdot\frac{\partial\tilde{\mathrm{L}}}{\partial \mathrm{M}_{uv}^{(r)}} \tag{A8}$$

If $\partial\tilde{M}_{ij}/\partial M_{uv}^{(r)}$ is known, the second term in the left can be readily calculated recalling that

$$\frac{\partial\tilde{L}}{\partial M_{uv}^{(r)}} = -\tilde{L}\cdot\frac{\partial\tilde{M}}{\partial M_{uv}^{(r)}}\cdot\tilde{L} \tag{A9}$$

Using (A5), the derivative appearing in the first term of the left can be written as

$$\frac{\partial T_{ijkl}}{\partial M_{uv}^{(r)}} = \frac{abc}{16\pi}\int_0^{2\pi}\int_0^{\pi}\frac{\partial\lambda_{ijkl}}{\partial M_{uv}^{(r)}}\frac{\sin\theta\,d\theta\,d\varphi}{[\rho(\alpha)]^3} \tag{A10}$$

Using (A6), $\partial\lambda_{ijkl}/\partial M_{uv}^{(r)}$ is calculated as:

$$\frac{\partial\lambda_{ijkl}}{\partial M_{uv}^{(r)}} = \alpha_j\alpha_l\frac{\partial A'^{-1}_{ik}}{\partial M_{uv}^{(r)}} + \alpha_i\alpha_l\frac{\partial A'^{-1}_{jk}}{\partial M_{uv}^{(r)}} + \alpha_j\alpha_k\frac{\partial A'^{-1}_{il}}{\partial M_{uv}^{(r)}} + \alpha_i\alpha_k\frac{\partial A'^{-1}_{jl}}{\partial M_{uv}^{(r)}} \tag{A11}$$

Recalling (A7), $\partial A'^{-1}_{ik}/\partial M_{uv}^{(r)}$ can be obtained as:

$$\frac{\partial A'^{-1}_{ik}}{\partial M_{uv}^{(r)}} = -A'^{-1}_{ip}\left(\frac{\partial\tilde{L}_{pqrs}}{\partial M_{uv}^{(r)}}\alpha_q\alpha_s\right)A'^{-1}_{rk} \tag{A12}$$

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