CrossMark

A generalized-secant homogenization scheme for viscoplastic polycrystalline solids under imposed deformations

Une méthode d'homogénéisation sécante généralisée pour des matériaux polycristallins viscoplastiques en déformations imposées

Martín I. Idiart [a,b,*], Pierre-Guy Vincent [c,d]

[a] Departamento de Aeronáutica, Facultad de Ingeniería, Universidad Nacional de La Plata, Avda. 1 esq. 47, La Plata B1900TAG, Argentina
[b] Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), CCT La Plata, Calle 8 N° 1467, La Plata B1904CMC, Argentina
[c] Institut de radioprotection et de sûreté nucléaire (IRSN), BP 3, 13115 Saint-Paul-Lez-Durance cedex, France
[d] Laboratoire de micromécanique et d'intégrité des structures, IRSN–CNRS–UMII, BP 3, 13115 Saint-Paul-lez-Durance Cedex, France

ARTICLE INFO

ABSTRACT

Homogenization estimates for viscoplastic polycrystals are derived by applying the generalized-secant linearization scheme of Liu and Ponte Castañeda (2004) [1] to the constitutive description with strain rates as primary variables. The resulting estimates are thus particularly suitable for simulating mechanical processes where deformations are imposed and where the material softens. Their accuracy is preliminarily assessed in the context of a model material system. Good agreement with previous estimates is found.

© 2014 Académie des sciences. Published by Elsevier Masson SAS. All rights reserved.

RÉSUMÉ

Des estimations relatives à l'homogénéisation de polycristaux viscoplastiques sont obtenues en appliquant la méthode de linéarisation sécante généralisée de Liu et Ponte Castañeda (2004) [1] au cas d'une relation constitutive où les taux de déformation sont des variables primaires. Les estimations obtenues sont particulièrement adaptées pour simuler des chargements mécaniques où les déformations sont imposées et où le matériau s'adoucit. La précision de ces estimations est évaluée au préalable dans le cas d'un système matériau modèle. Un bon accord est obtenu avec des estimations antérieures.

© 2014 Académie des sciences. Published by Elsevier Masson SAS. All rights reserved.

1. Introduction

This work is concerned with homogenization techniques for correlating the macroscopic viscoplastic response of polycrystalline solids with the flow rules governing microscopic viscoplastic slip. We consider polycrystals consisting of a random

aggregate of perfectly bonded single crystals (i.e., grains) of a similar size, much smaller than the specimen size and the scale of variation of the applied loads, distributed in a statistically uniform and ergodic fashion. In the *current* configuration of the aggregate at a generic stage of deformation, the grain orientations are assumed to take on a set of N discrete values, characterized by rotation tensors $\mathbf{Q}^{(r)}$ ($r = 1, \ldots, N$). All grains with a given orientation $\mathbf{Q}^{(r)}$ occupy a possibly disconnected domain and are collectively referred to as 'phase' r. For definiteness, we focus on material systems made up of single crystals deforming along K slip systems according to microscopic flow rules of the form

$$\boldsymbol{D} = \frac{\partial u}{\partial \boldsymbol{\sigma}}(\mathbf{x}, \boldsymbol{\sigma}) \quad \text{with} \quad u(\mathbf{x}, \boldsymbol{\sigma}) = \sum_{r=1}^{N} \chi^{(r)}(\mathbf{x}) u^{(r)}(\boldsymbol{\sigma}), \quad u^{(r)}(\boldsymbol{\sigma}) = \sum_{k=1}^{K} \psi_{(k)}^{(r)}\big(\boldsymbol{\sigma} \cdot \boldsymbol{\mu}_{(k)}^{(r)}\big) \tag{1}$$

where $\boldsymbol{D}$ and $\boldsymbol{\sigma}$ are the Eulerian strain rate and Cauchy stress tensors, $\chi^{(r)}$ are the characteristic functions of each phase r, $\psi_{(k)}^{(r)}$ are convex viscoplastic slip potentials, and $\boldsymbol{\mu}_{(k)}^{(r)}$ are the Schmidt tensors indicating slip directions. The macroscopic homogenized response of the polycrystal is then given by (e.g., [1])

$$\overline{\boldsymbol{D}} = \frac{\partial \widetilde{u}}{\partial \overline{\boldsymbol{\sigma}}}(\overline{\boldsymbol{\sigma}}) \quad \text{with} \quad \widetilde{u}(\overline{\boldsymbol{\sigma}}) = \min_{\boldsymbol{\sigma} \in \mathcal{S}(\overline{\boldsymbol{\sigma}})} \langle u(\mathbf{x}, \boldsymbol{\sigma}) \rangle = \min_{\boldsymbol{\sigma} \in \mathcal{S}(\overline{\boldsymbol{\sigma}})} \sum_{r=1}^{N} c^{(r)} \langle u^{(r)}(\boldsymbol{\sigma}) \rangle^{(r)} \tag{2}$$

where $\overline{\boldsymbol{D}} = \langle \boldsymbol{D} \rangle$ and $\overline{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle$, $\langle \cdot \rangle$ and $\langle \cdot \rangle^{(r)}$ denote volume averages over the aggregate and over phase r, respectively, $c^{(r)}$ is the volume fraction of phase r, and $\mathcal{S}(\overline{\boldsymbol{\sigma}})$ is the set of statically admissible stress fields with average $\overline{\boldsymbol{\sigma}}$.

Amongst the various quasi-analytical techniques available to estimate the macroscopic potential $\widetilde{u}$ in terms of the microscopic properties, the so-called 'generalized-secant technique' proposed by Liu and Ponte Castañeda [1] seems to deliver the most accurate estimates to date — see, for instance, Refs. [2–4]. This technique is based on the concept of 'linear-comparison medium' whereby the variational problem $(2)_2$ is rewritten in terms of linearized microscopic slip potentials so that linear homogenization techniques, such as the well-known Self-Consistent technique [5], can be used to approximate the non-linear macroscopic potential. The resulting estimates are computationally inexpensive relative to full-field simulations, but they still require the numerical resolution of a large set of nonlinear algebraic equations. This fact can become an issue when simulating mechanical processes where deformations are imposed, which require inversion of the above constitutive description in order to express stresses in terms of strain rates; this can be particularly crucial in problems where the material exhibits softening.

The purpose of this work is to derive generalized-secant estimates for the inverted stress–strain-rate relation by applying the strategy of Liu and Ponte Castañeda [1] directly to the dual problem of (2). This problem was not tackled in Ref. [1] because the dual potential of $u^{(r)}$ does not exhibit the additive form $(1)_2$ on which the linearization strategy hinges. However, well-known results of convex analysis (e.g., [6]) do permit to write the inverted microscopic flow rule as

$$\boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{D}}(\mathbf{x}, \boldsymbol{D}) \quad \text{with} \quad w(\mathbf{x}, \boldsymbol{D}) = \sum_{r=1}^{N} \chi^{(r)}(\mathbf{x}) w^{(r)}(\boldsymbol{D}), \quad w^{(r)}(\boldsymbol{D}) = \min_{\gamma_{(k)}^{(r)} \in \Gamma^{(r)}(\boldsymbol{D})} \sum_{k=1}^{K} \phi_{(k)}^{(r)}\big(\gamma_{(k)}^{(r)}\big) \tag{3}$$

where

$$\phi_{(k)}^{(r)}(\gamma) = \sup_{\tau} \big[\tau \gamma - \psi_{(k)}^{(r)}(\tau) \big] \tag{4}$$

is the Legendre transform of the slip potentials $\psi_{(k)}^{(r)}$ and

$$\Gamma^{(r)}(\boldsymbol{D}) = \left\{ \gamma_{(k)}^{(r)} \ (k = 1, \ldots K) \text{ such that } \sum_{k=1}^{K} \gamma_{(k)}^{(r)} \boldsymbol{\mu}_{(k)}^{(r)} = \boldsymbol{D} \right\} \tag{5}$$

and to invert the macroscopic constitutive relation (2) to

$$\overline{\boldsymbol{\sigma}} = \frac{\partial \widetilde{w}}{\partial \overline{\boldsymbol{D}}}(\overline{\boldsymbol{D}}) \quad \text{with} \quad \widetilde{w}(\overline{\boldsymbol{D}}) = \min_{\boldsymbol{D} \in \mathcal{K}(\overline{\boldsymbol{D}})} \langle w(\mathbf{x}, \boldsymbol{D}) \rangle = \min_{\boldsymbol{D} \in \mathcal{K}(\overline{\boldsymbol{D}})} \sum_{r=1}^{N} c^{(r)} \langle w^{(r)}(\boldsymbol{D}) \rangle^{(r)} \tag{6}$$

where $\mathcal{K}(\overline{\boldsymbol{D}})$ is the set of kinematically admissible strain-rate fields with average $\overline{\boldsymbol{D}}$. Thus, the form $(3)_2$ for the dual potential $w^{(r)}$ exhibits an additive form analogous to that of $u^{(r)}$, except for an additional minimum operation. This fact is exploited next to derive generalized-secant estimates for the potential $\widetilde{w}$. The accuracy of the resulting estimates is then preliminarily assessed in the context of a model material system.

2. A strain-rate formulation of the generalized-secant scheme

2.1. An estimate for the effective potential

Following the strategy of Liu and Ponte Castañeda [1], we begin by expressing the slip potentials $\phi_{(k)}^{(r)}$ in the alternative form

$$\phi_{(k)}^{(r)}(\gamma) = \underset{\alpha_{(k)}^{(r)} \geq 0}{\mathrm{stat}} \left[\mathring{\phi}_{(k)}^{(r)}(\gamma; \alpha_{(k)}^{(r)}) + v_{(k)}^{(r)}(\alpha_{(k)}^{(r)}) \right] \tag{7}$$

where the functions $\mathring{\phi}_{(k)}^{(r)}$ denote comparison slip potentials given by

$$\mathring{\phi}_{(k)}^{(r)}(\gamma; \alpha_{(k)}^{(r)}) = \phi_{(k)}^{(r)}(\check{\gamma}_{(k)}^{(r)}) + \phi_{(k)}^{(r)'}(\check{\gamma}_{(k)}^{(r)})(\gamma - \check{\gamma}_{(k)}^{(r)}) + \frac{1}{2}\alpha_{(k)}^{(r)}(\gamma - \check{\gamma}_{(k)}^{(r)})^2 \tag{8}$$

and

$$v_{(k)}^{(r)}(\alpha_{(k)}^{(r)}) = \underset{\hat{\gamma}_{(k)}^{(r)}}{\mathrm{stat}} \left[\phi_{(k)}^{(r)}(\hat{\gamma}_{(k)}^{(r)}) - \mathring{\phi}_{(k)}^{(r)}(\hat{\gamma}_{(k)}^{(r)}; \alpha_{(k)}^{(r)}) \right] \tag{9}$$

In these expressions, $\alpha_{(k)}^{(r)}$ and $\check{\gamma}_{(k)}^{(r)}$ represent uniform-per-phase slip viscosities and reference slip rates, respectively, the stat denotes a stationary operation, and the prime denotes differentiation. Expression (7) is valid provided the correct stationary point is chosen in $v_{(k)}^{(r)}$. The reader is referred to [1] for details on the derivation of analogous expressions in terms of the stress potentials $\psi_{(k)}^{(r)}$.

Introducing the representation (7) for the slip potentials in expression (3) we obtain the alternative representation for the phase potentials

$$w^{(r)}(\boldsymbol{D}) = \underset{\alpha_{(k)}^{(r)} \geq 0}{\mathrm{stat}} \left[\mathring{w}^{(r)}(\boldsymbol{D}; \alpha_{(k)}^{(r)}) + \sum_{k=1}^{K} v_{(k)}^{(r)}(\alpha_{(k)}^{(r)}) \right] \tag{10}$$

where the functions $\mathring{w}^{(r)}$ are comparison phase potentials given by

$$\mathring{w}^{(r)}(\boldsymbol{D}; \alpha_{(k)}^{(r)}) = \min_{\gamma_{(k)}^{(r)} \in \Gamma^{(r)}(\boldsymbol{D})} \sum_{k=1}^{K} \mathring{\phi}_{(k)}^{(r)}(\gamma_{(k)}^{(r)}) \tag{11}$$

In deriving (10) we have commuted the stationary and the minimum operations based on the same arguments of Ref. [1]. Introducing expression (10) in (6) and commuting, once again, the stationary and minimum operations gives the *approximate* stationary estimate

$$\widetilde{w}(\overline{\boldsymbol{D}}) = \underset{\alpha_{(k)}^{(r)} \geq 0}{\mathrm{stat}} \left[\widetilde{\mathring{w}}(\overline{\boldsymbol{D}}; \alpha_{(k)}^{(r)}) + \sum_{r=1}^{N} \sum_{k=1}^{K} c^{(r)} v_{(k)}^{(r)}(\alpha_{(k)}^{(r)}) \right] \tag{12}$$

where $\widetilde{\mathring{w}}(\overline{\boldsymbol{D}}; \alpha_{(k)}^{(r)})$ is the effective potential of a comparison polycrystalline solid with the same microstructure as the original solid but with slip potentials $\mathring{\phi}_{(k)}^{(r)}$ as given by (8). Thus, this expression provides a nonlinear estimate given any linear homogenization estimate for the comparison potential $\widetilde{\mathring{w}}$.

2.2. The comparison polycrystal

The potential (8) can be written in the alternative form

$$\mathring{\phi}_{(k)}^{(r)}(\gamma; \alpha_{(k)}^{(r)}) = \frac{1}{2}\alpha_{(k)}^{(r)}\gamma^2 + e_{(k)}^{(r)}\gamma + f_{(k)}^{(r)} \tag{13}$$

where

$$e_{(k)}^{(r)} = \phi_{(k)}^{(r)'}(\check{\gamma}_{(k)}^{(r)}) - \alpha_{(k)}^{(r)}\check{\gamma}_{(k)}^{(r)} \quad \text{and} \quad f_{(k)}^{(r)} = \phi_{(k)}^{(r)}(\check{\gamma}_{(k)}^{(r)}) - \phi_{(k)}^{(r)'}(\check{\gamma}_{(k)}^{(r)})\check{\gamma}_{(k)}^{(r)} + \frac{1}{2}\alpha_{(k)}^{(r)}\check{\gamma}_{(k)}^{(r)2} \tag{14}$$

Performing the minimization in (11) we obtain

$$\mathring{w}^{(r)}(\boldsymbol{D}; \alpha_{(k)}^{(r)}) = \frac{1}{2}\boldsymbol{D} \cdot \mathbf{L}^{(r)}\boldsymbol{D} + \boldsymbol{\tau}^{(r)} \cdot \boldsymbol{D} + f^{(r)} \tag{15}$$

where

$$\mathbf{L}^{(r)} = \left[\sum_{k=1}^{K}(\alpha_{(k)}^{(r)})^{-1}\boldsymbol{\mu}_{(k)}^{(r)}\otimes\boldsymbol{\mu}_{(k)}^{(r)}\right]^{-1} \tag{16}$$

$$\boldsymbol{\tau}^{(r)} = \mathbf{L}^{(r)}\sum_{k=1}^{K}(\alpha_{(k)}^{(r)})^{-1}e_{(k)}^{(r)}\boldsymbol{\mu}_{(k)}^{(r)} \tag{17}$$

$$f^{(r)} = \frac{1}{2}\boldsymbol{\tau}^{(r)}\cdot(\mathbf{L}^{(r)})^{-1}\boldsymbol{\tau}^{(r)} + \sum_{k=1}^{K}\left[f_{(k)}^{(r)} - \frac{1}{2}(\alpha_{(k)}^{(r)})^{-1}(e_{(k)}^{(r)})^2\right] \tag{18}$$

Thus, the effective potential $\tilde{\tilde{w}}$ can be written as

$$\tilde{\tilde{w}}(\overline{\boldsymbol{D}};\alpha_{(k)}^{(r)}) = \tilde{\tilde{w}}(\overline{\boldsymbol{D}};\alpha_{(k)}^{(r)},e_{(k)}^{(r)},f_{(k)}^{(r)}) = \frac{1}{2}\overline{\boldsymbol{D}}\cdot\widetilde{\mathbf{L}}\overline{\boldsymbol{D}} + \widetilde{\boldsymbol{\tau}}\cdot\overline{\boldsymbol{D}} + \widetilde{f} \tag{19}$$

where $\widetilde{\mathbf{L}}$, $\widetilde{\boldsymbol{\tau}}$ and $\widetilde{f}$ are the effective properties of the linear comparison polycrystal. Their expressions in terms of the local properties $\mathbf{L}^{(r)}$, $\boldsymbol{\tau}^{(r)}$ and $f^{(r)}$ will depend on the linear homogenization scheme employed.

2.3. The stationarity conditions

The stationarity conditions in (9) and (12) lead to a system of nonlinear equations for the set of variables $\alpha_{(k)}^{(r)}$ and $\hat{\gamma}_{(k)}^{(r)}$ given by

$$\phi_{(k)}^{(r)'}(\hat{\gamma}_{(k)}^{(r)}) - \phi_{(k)}^{(r)'}(\check{\gamma}_{(k)}^{(r)}) = \alpha_{(k)}^{(r)}(\hat{\gamma}_{(k)}^{(r)} - \check{\gamma}_{(k)}^{(r)}) \tag{20}$$

$$(\hat{\gamma}_{(k)}^{(r)} - \check{\gamma}_{(k)}^{(r)})^2 = \frac{2}{c^{(r)}}\frac{\partial\tilde{\tilde{w}}}{\partial\alpha_{(k)}^{(r)}}(\overline{\boldsymbol{D}};\alpha_{(k)}^{(r)}) \equiv \langle(\gamma_{(k)}^{(r)} - \check{\gamma}_{(k)}^{(r)})^2\rangle^{(r)} \tag{21}$$

with $k = 1,\ldots,K$ and $r = 1,\ldots,N$. The first set of Eqs. (20) states that the optimal slip viscosities $\alpha_{(k)}^{(r)}$ are given by generalized secant linearizations of the nonlinear functions $\phi_{(k)}^{(r)'}$ passing through the points $\hat{\gamma}_{(k)}^{(r)}$ and $\check{\gamma}_{(k)}^{(r)}$, while the second set of equations states that the optimal $\hat{\gamma}_{(k)}^{(r)}$ are related to the intraphase fluctuations of the slip rates $\gamma_{(k)}^{(r)}$ about $\check{\gamma}_{(k)}^{(r)}$ in the linear comparison polycrystal. The last identity follows from well-known results for field statistics in heterogeneous media (e.g., [7]). We refer to [1] for further discussions on these type of conditions.

2.4. The reference slip rates

The estimate (12) is valid for any choice of reference strain rates $\check{\gamma}_{(k)}^{(r)}$. Thus far, no stationarity condition has been found for these parameters, and only physically motivated prescriptions are considered.

The simplest choice is

$$\check{\gamma}_{(k)}^{(r)} = 0 \tag{22}$$

In this case, the linearization (20) becomes a secant condition through the $\hat{\gamma}_{(k)}^{(r)}$, and the estimate (12) can be shown to reduce to the dual version of the secant estimate of deBotton and Ponte Castañeda [8]. These estimates are only exact to first order in the heterogeneity contrast.

Another possible choice is to identify the reference slip rates with the corresponding phase averages of the slip rates in the linear comparison polycrystal:

$$\check{\gamma}_{(k)}^{(r)} = \langle\gamma_{(k)}^{(r)}\rangle^{(r)} \equiv \overline{\gamma}_{(k)}^{(r)} \tag{23}$$

which can be computed from $\tilde{\tilde{w}}$ making use of the identity (e.g., [7])

$$\overline{\gamma}_{(k)}^{(r)} = \frac{1}{c^{(r)}}\frac{\partial\tilde{\tilde{w}}}{\partial e_{(k)}^{(r)}}(\overline{\boldsymbol{D}};\alpha_{(k)}^{(r)},e_{(k)}^{(r)},f_{(k)}^{(r)}) \tag{24}$$

This is analogous to the choice employed by Liu and Ponte Castañeda [1] in their stress formulation, and can be shown to deliver estimates that are exact to second order in the contrast. Despite the analogy, it can be shown that there is a duality gap between the resulting estimate (12) and its stress formulation, in general. However, the results provided below show that this gap is very small and can even vanish in some limiting cases. With the choice (24), expressions (20), (21) and
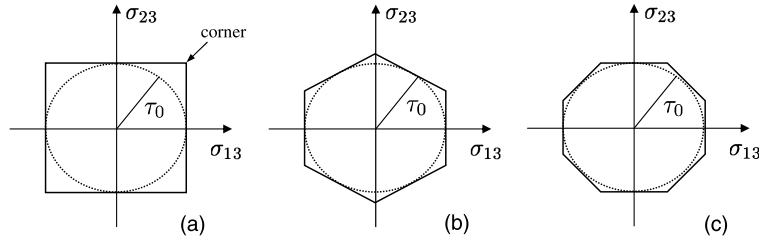
Fig. 1. Yield surfaces for square ($K = 2$), hexagonal ($K = 3$) and octagonal ($K = 4$) symmetries.

(24) constitute a system of $3N \times K$ nonlinear algebraic equations for the variables $\alpha_{(k)}^{(r)}$, $\hat{\gamma}_{(k)}^{(r)}$ and $\overline{\gamma}_{(k)}^{(r)}$, which must be solved numerically, in general.

Other prescriptions are certainly possible but will not be considered here for brevity.

2.5. Alternative form of the estimate

Making use of the stationarity conditions (20) and (21), it can be shown that the estimate (6) admits the alternative form

$$\widetilde{w}(\overline{\boldsymbol{D}}) = \sum_{r=1}^{N} \sum_{k=1}^{K} c^{(r)} \left[\phi_{(k)}^{(r)} \big(\hat{\gamma}_{(k)}^{(r)} \big) - \phi_{(k)}^{(r)\prime} \big(\check{\gamma}_{(k)}^{(r)} \big) \big(\hat{\gamma}_{(k)}^{(r)} - \overline{\gamma}_{(k)}^{(r)} \big) \right] \tag{25}$$

which proves more convenient for computational purposes.

3. Sample results for a model crystalline solid with second-phase inclusions

3.1. Problem setting and formulae

By way of example, we consider a special class of two-phase crystalline solids with 'particulate' microstructures, consisting of aligned cylindrical inclusions ($r = 2$) that are distributed *randomly* and *isotropically* in a viscoplastic *monocrystalline* matrix phase ($r = 1$). It is assumed that the cylindrical inclusions are aligned with the $\mathbf{e}_3$ direction, and that the crystalline matrix deforms along slip systems with Schmid tensors

$$\boldsymbol{\mu}_{(k)} = \frac{1}{2} (\mathbf{n}_{(k)} \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{n}_{(k)}) \quad \text{with} \quad \mathbf{n}_{(k)} = \cos\theta_{(k)} \mathbf{e}_1 + \sin\theta_{(k)} \mathbf{e}_2 \tag{26}$$

where $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ forms an orthonormal basis. The slip potentials are taken to be of the power-law form

$$\psi_{(k)}(\tau) = \frac{\dot{\gamma}_0 \tau_0}{1 + n} \left| \frac{\tau}{\tau_0} \right|^{1+n} \quad \Rightarrow \quad \phi_{(k)}(\gamma) = \frac{\dot{\gamma}_0 \tau_0}{1 + m} \left| \frac{\gamma}{\dot{\gamma}_0} \right|^{1+m} \tag{27}$$

where τ_0 and $\dot{\gamma}_0$ denote the flow stress and the reference strain rate of the slip system, n is a nonlinearity exponent, and $m = 1/n$ is the strain-rate sensitivity such that $0 \le m \le 1$. The limiting values $m = 1$ and $m = 0$ correspond to a linearly viscous and a rigid-perfectly plastic behavior, respectively. For simplicity, we assume that all slip systems have the same constitutive constants n, τ_0 and $\dot{\gamma}_0$.

The two-phase crystal is subjected to *anti-plane* loadings so that the relevant viscoplastic boundary value problem becomes a vectorial, two-dimensional problem, where the non-zero components of the stress and strain-rate vectors, namely, σ_{13}, σ_{23}, D_{13} and D_{23}, are functions of x_1 and x_2 only.

In order to assess the sensitivity of the predictions on material anisotropy, we consider three different matrix materials with sets of angles $\theta_{(k)}$ given by $\{0, \pi/2\}$, $\{0, \pm\pi/3\}$, and $\{0, \pm\pi/4, \pi/2\}$, which correspond to square ($K = 2$), hexagonal ($K = 3$), and octagonal ($K = 4$) symmetry, respectively. In the linear case, the anti-plane response of the matrix is actually isotropic for the three families of slip systems. In the nonlinear case, however, the response is anisotropic, such that in the ideally plastic limit it defines a polygonal yield surface in the σ_{13}–σ_{23} stress space, as shown in Fig. 1. Note that as the number of slip systems K increases, the potential approaches an isotropic yield surface with flow stress τ_0.

For brevity, we restrict attention to material systems with either voided or rigid inclusions, which correspond to the cases of extreme heterogeneity contrast and, as such, are particularly relevant for testing the capabilities of the new scheme. In these cases, the macroscopic potential $\widetilde{w}$ can be shown to be of the form

$$\widetilde{w}(\overline{\boldsymbol{D}}) = \frac{\widetilde{\tau}_0(\overline{\theta}) \dot{\gamma}_0}{1 + m} \left(\frac{\overline{D}_e}{\dot{\gamma}_0} \right)^{1+m} \tag{28}$$

where $\overline{D}_e = (\overline{D}_{13}^2 + \overline{D}_{23}^2)^{1/2}$ and $\overline{\theta} = \tan^{-1}(\overline{D}_{23}/\overline{D}_{13})$ are the macroscopic strain rate magnitude and direction, respectively. Thus, the macroscopic response can be completely characterized by the effective flow stress $\widetilde{\tau}_0(\overline{\theta})$ only. The generalized-secant estimate (25) for $\widetilde{w}$ with the prescription (23) leads to the estimate

$$\frac{\widetilde{\tau}_0}{\tau_0}(\overline{\theta}) = (1 - c) \sum_{k=1}^{K} \left[\left(\frac{\hat{\gamma}_{(k)}^{(1)}}{\overline{D}_e} \right)^{1+m} - (1+m) \left(\frac{\overline{\gamma}_{(k)}^{(1)}}{\overline{D}_e} \right)^m \left(\frac{\hat{\gamma}_{(k)}^{(1)}}{\overline{D}_e} - \frac{\overline{\gamma}_{(k)}^{(1)}}{\overline{D}_e} \right) \right] \tag{29}$$

for the effective flow stress of the material systems under consideration, where c denotes the volume fraction of inclusions. For the case of macroscopic loadings along the direction of a slip system (i.e., $\overline{\theta} = \theta_{(k)}$) and the effective potential of the linear comparison medium computed by means of the Hashin–Shtrikman estimates of Willis [5], the system of equations for the quantities $\hat{\gamma}_{(k)}^{(1)}/\overline{D}_e$ and $\overline{\gamma}_{(k)}^{(1)}/\overline{D}_e$ can be written as

$$\frac{\hat{\gamma}_{(k)}^{(1)}}{\overline{D}_e} = \frac{\overline{\gamma}_{(k)}^{(1)}}{\overline{D}_e} + \frac{\lambda_\|}{\alpha_{(k)}} \sqrt{\frac{c}{2} \frac{\sin^2 \theta_{(k)} + a \cos^2 \theta_{(k)}}{\sqrt{a}} A} \quad \text{and} \quad \frac{\overline{\gamma}_{(k)}^{(1)}}{\overline{D}_e} = [\lambda_\| B \cos \theta_{(k)}]^{1/m} \quad k = 1, \ldots, K \tag{30}$$

where

$$\lambda_\|^{-1} = \sum_{k=1}^{K} \frac{\cos^2 \theta_{(k)}}{\alpha_{(k)}}, \qquad \lambda_\perp^{-1} = \sum_{k=1}^{K} \frac{\sin^2 \theta_{(k)}}{\alpha_{(k)}}, \qquad a = \frac{\lambda_\|}{\lambda_\perp}, \qquad \eta = \sum_{k=1}^{K} \left[\frac{1}{\alpha_{(k)}} \left(\frac{\overline{\gamma}_{(k)}^{(1)}}{\overline{D}_e} \right)^m - \frac{\overline{\gamma}_{(k)}^{(1)}}{\overline{D}_e} \right] \cos \theta_{(k)} \tag{31}$$

$$\alpha_{(k)} = \frac{(\hat{\gamma}_{(k)}^{(1)}/\overline{D}_e)^m - (\overline{\gamma}_{(k)}^{(1)}/\overline{D}_e)^m}{\hat{\gamma}_{(k)}^{(1)}/\overline{D}_e - \overline{\gamma}_{(k)}^{(1)}/\overline{D}_e} \tag{32}$$

and the coefficients A and B depend on the inclusion type. For the case of *voided* crystals:

$$A = \left(\frac{1+\eta}{1+c\sqrt{a}} \right)^2 \quad \text{and} \quad B = \frac{1+\eta}{1+c\sqrt{a}} \tag{33}$$

while for the case of *rigidly reinforced* crystals:

$$A = \frac{a^{-1}}{(1-c)^2} \quad \text{and} \quad B = \frac{1}{(1-c)} + \eta \tag{34}$$

3.2. Results and discussion

Fig. 2 shows plots for the effective flow stress of voided and rigidly reinforced crystals loaded along the direction of a slip system, as a function of the strain-rate sensitivity m, for the choice $c = 0.25$. The new generalized-secant estimates (GSEC-γ) of the Hashin–Shtrikman type are compared with the elementary bounds of Taylor and Reuss, the corresponding secant estimates (SEC) of deBotton and Ponte Castañeda [8], and the stress-based generalized-secant estimates (GSEC-τ) of Liu and Ponte Castañeda [1]. Analytical expressions for various estimates applied to this model problem can be found in Refs. [9,10]. In addition, exact results are given for material systems with the infinite-rank, transversely isotropic, sequentially laminated microgeometries (LAM) of Idiart [11], with matrix behavior given by (26)–(27). It is recalled that the secant estimates provide rigorous upper bounds for all the other estimates considered. It is also recalled that the sequentially laminated microgeometries attain the linear Hashin–Shtrikman estimates, so that any difference between the LAM results and the linear-comparison estimates of the Hashin–Shtrikman type are solely due to the linearization procedure. We emphasize that the GSEC-τ and GSEC-γ are *different* estimates which can be independently used to estimate material behavior under arbitrary loading conditions.

The main observation in the context of this figure is that the new GSEC-γ estimates give very similar predictions to the dual GSEC-τ estimates for all cases considered; that is, the duality gap is small. Moreover, this duality gap vanishes not only in the linear case ($m = 1$) but also in the strongly nonlinear limit of ideal plasticity ($m = 0$). For intermediate values of m, the duality gap is virtually zero except for some range around $m = 0.1$ in the case of voided crystals. Within that range, the GSEC-γ are found to be less accurate than their GSEC-τ counterparts relative to the exact LAM results. Note that this range seems to widen with increasing number of slip systems.

However, in view of the fact that the material systems considered here exhibit extreme heterogeneity contrasts, it is expected that differences between the GSEC-γ and GSEC-τ estimates will be smaller in the context of fully dense polycrystals with realistic microstructures, even for relatively high crystal anisotropies. Moreover, it is expected that the additional inaccuracies incurred by the use of GSEC-γ estimates in *lieu* of GSEC-τ estimates, if any, will be entirely compensated by the concomitant computational simplifications for modeling mechanical processes under imposed deformations. Efforts to evaluate this compromise are currently under way and will be reported upon completion.
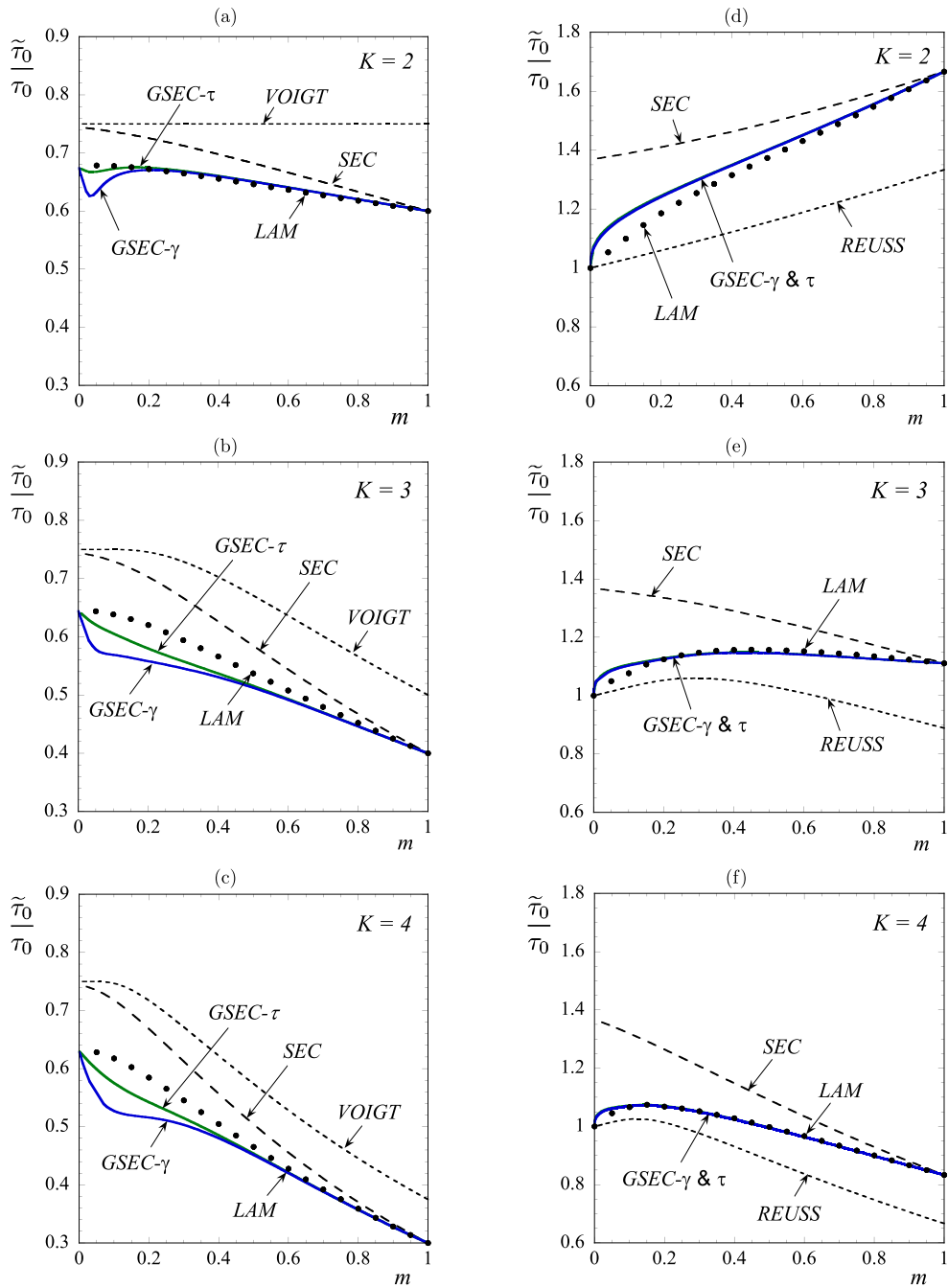
Fig. 2. (Color online.) Effective flow stress $\widetilde{\tau}_0$, normalized by the slip flow stress τ_0, for a two-phase monocrystal with K slip systems: (a–c) voided inclusion, (d–f) rigid inclusions. The volume fraction of inclusions is $c = 0.25$.

Acknowledgements

References

[1] Y. Liu, P. Ponte Castañeda, Second-order theory for the effective behavior and field fluctuations in viscoplastic polycrystals, J. Mech. Phys. Solids 52 (2004) 467–495.

[2] R.A. Lebensohn, M.I. Idiart, P. Ponte Castañeda, P.-G. Vincent, Dilatational viscoplasticity of polycrystalline solids with intergranular cavities, Philos. Mag. 91 (2011) 3038–3067.

[3] Y. Liu, P. Ponte Castañeda, Homogenization estimates for the average behavior and field fluctuations in cubic and hexagonal viscoplastic polycrystals, J. Mech. Phys. Solids 52 (2004) 1175–1211.

[4] Y. Liu, P. Gilormini, P. Ponte Castañeda, Variational self-consistent estimates for texture evolution in viscoplastic polycrystals, Acta Mater. 51 (2003) 5425–5437.

[5] J.R. Willis, Variational and related methods for the overall properties of composites, Adv. Appl. Mech. 21 (1981) 1–78.

[6] J. van Tiel, Convex Analysis, Wiley, New York, USA, 1984.

[7] M.I. Idiart, P. Ponte Castañeda, Field statistics in nonlinear composites. I. Theory, Proc. R. Soc. Lond. A 463 (2007) 183–202.

[8] G. deBotton, P. Ponte Castañeda, Variational estimates for the creep behavior of polycrystals, Proc. R. Soc. Lond. A 448 (1995) 121–142.

[9] M.I. Idiart, Macroscopic behavior and field statistics in viscoplastic composites, Ph.D. thesis, University of Pennsylvania, Philadelphia, PA, USA, 2006.

[10] M.I. Idiart, P. Ponte Castañeda, Variational linear comparison bounds for nonlinear composites with anisotropic phases. II. Crystalline materials, Proc. R. Soc. Lond. A 463 (2007) 925–943.

[11] M.I. Idiart, Modeling the macroscopic behavior of two-phase nonlinear composites by infinite-rank laminates, J. Mech. Phys. Solids 56 (2008) 2599–2617.