Second-order estimates of the self-consistent type for viscoplastic polycrystals

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The 'second-order' homogenization procedure of Ponte Castañeda is used to propose new estimates of the self-consistent type for the effective behaviour of viscoplastic polycrystals. This is accomplished by means of appropriately generated estimates of the self-consistent type for the relevant 'linear thermoelastic comparison composite', in the homogenization procedure. The resulting nonlinear self-consistent estimates are the only estimates of their type to be exact to second order in the heterogeneity contrast, which, for polycrystals, is determined by the grain anisotropy. In addition, they satisfy the recent bounds of Kohn & Little for two-dimensional power-law polycrystals, which are known to be significantly sharper than the Taylor bound at large grain anisotropy. These two features combined, suggest that the new self-consistent estimates, obtained from the second-order procedure, may be the most accurate to date. Direct comparison with other self-consistent estimates, including the classical incremental and secant estimates, for the special case of power-law creep, appear to corroborate this observation.

Keywords: rate-dependent plasticity; self-consistent estimates; heterogeneous materials; creep of polycrystals; second-order theory; nonlinear homogenization

1. Introduction

In spite of being a classical problem (Taylor 1938), the theoretical prediction of the effective response of plastic and viscoplastic polycrystals is still very much open. This is because the so-called 'classical' methods have been found to tend to overestimate the effective response, especially at large heterogeneity and nonlinearity (see, for example, Gilormini (1995) for the analogous problem of two-phase nonlinear composites). This paper is concerned with the application of a recently developed nonlinear homogenization method (Ponte Castañeda 1996), to estimate the effective flow stress of viscoplastic polycrystals. The method requires the computation of the effective response of a fictitious 'linear thermoelastic comparison polycrystal' as an intermediate step, which is accomplished by means of the self-consistent estimates of Laws (1973) and Willis (1981).

The resulting self-consistent estimates for the nonlinear viscoplastic polycrystals have the unique property of being exact to second order in the heterogeneity contrast. In other words, they agree to second order exactly in a suitable measure of the heterogeneity, which in the case of polycrystals is related to the grain anisotropy,

with the asymptotic results of Suquet & Ponte Castañeda (1993) for weakly heterogeneous systems. They are, in fact, the first estimates of the self-consistent type for nonlinear polycrystals to have this property, which is widely known to hold for the corresponding linear-elastic estimates. In addition, the new self-consistent estimates will be shown to satisfy a recently established bound (Kohn & Little 1999), for a certain class of model two-dimensional polycrystals, which is known to be significantly more restrictive than the corresponding Taylor and Hashin–Shtrikman bounds at large grain anisotropy (Dendievel *et al.* 1991; deBotton & Ponte Castañeda 1995). In fact, the Kohn–Little bound scales with the square root of the grain-anisotropy parameter, whereas the Taylor and Hashin–Shtrikman bounds scale linearly with this parameter. These two properties combined—that they are exact for small grain anisotropy and that they satisfy the Kohn–Little bound at large grain anisotropy—strongly suggest that these new self-consistent estimates may be the most accurate to date. That this may indeed be the case will be argued by direct comparison with the classical 'incremental' and 'secant' methods of Hill (1965; see also Hutchinson 1976) and Berveiller & Zaoui (1979), respectively, as well as with other more recent methods including the 'tangent' method of Molinari *et al.* (1987) and the related 'affine' method proposed by Zaoui & Masson (1998) and independently by P. Suquet (1996, personal communication). Comparisons will also be carried out with the variational self-consistent estimates of Ponte Castañeda & Nebozhyn (1997), which have already been found to satisfy both the Taylor and Kohn–Little bounds.

2. Effective behaviour of viscoplastic polycrystals

A *polycrystal* is an aggregate of a large number of perfectly bonded single-crystal grains with varying orientations. It is assumed to occupy a region in space, Ω, and can be thought of as an N-phase heterogeneous material, where each phase is defined as the subregion $\Omega^{(r)}$ $(r = 1, \ldots, N)$ occupied by all grains of a given orientation, as defined by a rotation tensor, $\boldsymbol{Q}^{(r)}$, relative to a reference crystal with known orientation. Each grain is assumed to undergo viscoplastic deformation on a set of K preferred crystallographic slip systems. These are defined by the second-order tensors

$$\boldsymbol{\mu}_{(k)}^{(r)} = \tfrac{1}{2}(\boldsymbol{n}_{(k)}^{(r)} \otimes \boldsymbol{m}_{(k)}^{(r)} + \boldsymbol{m}_{(k)}^{(r)} \otimes \boldsymbol{n}_{(k)}^{(r)}),$$

where the unit vectors $\boldsymbol{n}_{(k)}^{(r)}$ and $\boldsymbol{m}_{(k)}^{(r)}$ denote the normal to the slip plane and the slip direction in the kth $(k = 1, \ldots, K)$ system, respectively, for each grain orientation r $(r = 1, \ldots, N)$. The symbol $\otimes$ denotes the dyadic product. Note that

$$\boldsymbol{\mu}_{(k)}^{(r)} = \boldsymbol{Q}^{(r)\mathrm{T}} \boldsymbol{\mu}_{(k)} \boldsymbol{Q}^{(r)},$$

where the $\boldsymbol{\mu}_{(k)}$ define the slip systems of the reference crystal.

The resolved shear stress on the kth slip systems of grains with orientation r is defined by

$$\tau_{(k)}^{(r)} = \boldsymbol{\sigma} \cdot \boldsymbol{\mu}_{(k)}^{(r)}, \tag{2.1}$$

so that, neglecting elastic effects, the strain rate, $\boldsymbol{\varepsilon}$, and the stress, $\boldsymbol{\sigma}$, in these grains are related by

$$\boldsymbol{\varepsilon} = \frac{\partial u^{(r)}}{\partial \boldsymbol{\sigma}}, \qquad u^{(r)}(\boldsymbol{\sigma}) = \sum_{k=1}^{K} \phi_{(k)}(\tau_{(k)}^{(r)}), \tag{2.2}$$

where $u^{(r)}$ is the stress potential of the crystals with orientation r, defined in terms of the slip potentials $\phi_{(k)}$, typically assumed to be convex. In these relations, the dot denotes the inner product of two second-order tensors (e.g. $\boldsymbol{\sigma} \cdot \boldsymbol{\mu} = \sigma_{ij}\mu_{ij}$).

For reasons to be discussed in the following section, it is preferable to work with the dissipation potentials $w^{(r)}$, which are the Legendre transforms of the stress potentials $u^{(r)}$, such that

$$w^{(r)}(\boldsymbol{\varepsilon}) = (u^{(r)})^*(\boldsymbol{\varepsilon}) = \max_{\boldsymbol{\sigma}} \{\boldsymbol{\sigma} \cdot \boldsymbol{\varepsilon} - u^{(r)}(\boldsymbol{\sigma})\}. \tag{2.3}$$

Of course, $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ are related by

$$\boldsymbol{\sigma} = \frac{\partial w^{(r)}}{\partial \boldsymbol{\varepsilon}}, \tag{2.4}$$

which is the inverse of (2.2).

Given the dissipation potentials $w^{(r)}$ for the various grain orientations, the corresponding dissipation potential for the polycrystal may be written

$$w(\boldsymbol{x}, \boldsymbol{\varepsilon}) = \sum_{r=1}^{N} \chi^{(r)}(\boldsymbol{x}) w^{(r)}(\boldsymbol{\varepsilon}), \tag{2.5}$$

where the characteristic function $\chi^{(r)}$ is equal to one if the position vector $\boldsymbol{x}$ is inside a grain with orientation r (i.e. $\boldsymbol{x} \in \Omega^{(r)}$) and zero otherwise. The volume averages, $\langle\cdot\rangle$ and $\langle\cdot\rangle^{(r)}$, are defined over the polycrystal (Ω) and over grains with orientation r ($\Omega^{(r)}$), respectively, so that, for example, the scalars $c^{(r)} = \langle\chi^{(r)}\rangle$ serve to characterize the crystallographic texture of the polycrystal.

Then, assuming that the size of the typical grain is small relative to the size of the specimen under consideration, the *effective viscoplastic response* of the polycrystal may be written in the form

$$\bar{\boldsymbol{\sigma}} = \frac{\partial \tilde{W}}{\partial \bar{\boldsymbol{\varepsilon}}}, \tag{2.6}$$

where

$$\tilde{W}(\bar{\boldsymbol{\varepsilon}}) = \min_{\boldsymbol{\varepsilon} \in \mathcal{K}(\bar{\boldsymbol{\varepsilon}})} \langle w(\boldsymbol{x}, \boldsymbol{\varepsilon})\rangle = \min_{\boldsymbol{\varepsilon} \in \mathcal{K}(\bar{\boldsymbol{\varepsilon}})} \sum_{r=1}^{N} c^{(r)} \langle w^{(r)}(\boldsymbol{\varepsilon})\rangle^{(r)}, \tag{2.7}$$

is the *effective dissipation potential* for the polycrystal, $\bar{\boldsymbol{\sigma}} = \langle\boldsymbol{\sigma}\rangle$ and $\bar{\boldsymbol{\varepsilon}} = \langle\boldsymbol{\varepsilon}\rangle$ are the *average stress* and the *average strain rate* in the polycrystal, and $\mathcal{K}$ is the set of kinematically admissible strains:

$$\mathcal{K}(\bar{\boldsymbol{\varepsilon}}) = \{\boldsymbol{\varepsilon} \mid \text{there is } \boldsymbol{v} \text{ with } \boldsymbol{\varepsilon} = \tfrac{1}{2}[\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^{\mathrm{T}}] \text{ in } \Omega, \boldsymbol{v} = \bar{\boldsymbol{\varepsilon}}\boldsymbol{x} \text{ on } \partial\Omega\}. \tag{2.8}$$

3. Second-order estimates for viscoplastic polycrystals

As already mentioned in § 1, the second-order procedure was proposed by Ponte Castañeda (1996) to generate estimates for the effective behaviour of nonlinear composites that have the distinctive property of being *exact to second order* in the contrast. This is a particularly useful property for materials such as face-centred cubic polycrystals, which, because of the relatively low degree of anisotropy in the grains, exhibit fairly small levels of heterogeneity. However, as already demonstrated empirically by Ponte Castañeda (1996) for two-phase composites, the second-order procedure also seems to deliver accurate results at high contrast, for example, for rigidly

reinforced systems. In this section, an abbreviated derivation of the second-order procedure is given, together with an application to the computation of self-consistent estimates for the class of viscoplastic polycrystals described in § 2.

The basis for the second-order procedure is the first-order Taylor formula (with remainder) for the phase potentials $w^{(r)}$. Introducing reference strains $\bar{\boldsymbol{\varepsilon}}^{(r)}$, the Taylor formula for $w^{(r)}$ about $\bar{\boldsymbol{\varepsilon}}^{(r)}$ is given by

$$w^{(r)}(\boldsymbol{\varepsilon}) = w^{(r)}(\bar{\boldsymbol{\varepsilon}}^{(r)}) + \boldsymbol{\rho}^{(r)} \cdot (\boldsymbol{\varepsilon} - \bar{\boldsymbol{\varepsilon}}^{(r)}) + \tfrac{1}{2}(\boldsymbol{\varepsilon} - \bar{\boldsymbol{\varepsilon}}^{(r)}) \cdot \boldsymbol{L}^{(r)}(\boldsymbol{\varepsilon} - \bar{\boldsymbol{\varepsilon}}^{(r)}), \tag{3.1}$$

where $\boldsymbol{\rho}^{(r)}$ and $\boldsymbol{L}^{(r)}$ physically correspond to an internal stress and a tangent modulus tensor, respectively, with components

$$\rho_{ij}^{(r)} = \frac{\partial w^{(r)}}{\partial \varepsilon_{ij}}(\bar{\boldsymbol{\varepsilon}}^{(r)}) \quad \text{and} \quad \boldsymbol{L}_{ijkl}^{(r)} = \frac{\partial^2 w^{(r)}}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}(\boldsymbol{\gamma}^{(r)}), \tag{3.2}$$

respectively. Note that $\boldsymbol{L}^{(r)}$ depends on the strain

$$\boldsymbol{\gamma}^{(r)} = \lambda^{(r)} \bar{\boldsymbol{\varepsilon}}^{(r)} + (1 - \lambda^{(r)})\boldsymbol{\varepsilon},$$

where $\lambda^{(r)}$ depends on $\boldsymbol{\varepsilon}$ and is such that $0 < \lambda^{(r)} < 1$.

It then follows from equation (2.7)—by making the *approximation* that the reference strains, $\boldsymbol{\gamma}^{(r)} = \bar{\boldsymbol{\gamma}}^{(r)}$, are *constant* in each phase—that the effective potential, $\tilde{W}$, of the nonlinear composite may be estimated as

$$\tilde{W}(\bar{\boldsymbol{\varepsilon}}) \approx \sum_{r=1}^{N} c^{(r)} [w^{(r)}(\bar{\boldsymbol{\varepsilon}}^{(r)}) - \boldsymbol{\rho}^{(r)} \cdot \bar{\boldsymbol{\varepsilon}}^{(r)} + \tfrac{1}{2} \bar{\boldsymbol{\varepsilon}}^{(r)} \cdot \boldsymbol{L}^{(r)} \bar{\boldsymbol{\varepsilon}}^{(r)}] + \tilde{\Psi}, \tag{3.3}$$

where

$$\tilde{\Psi} = \min_{\boldsymbol{\varepsilon} \in \mathcal{K}(\boldsymbol{\varepsilon})} \langle \tfrac{1}{2} \boldsymbol{\varepsilon} \cdot \boldsymbol{L} \boldsymbol{\varepsilon} - \boldsymbol{l} \cdot \boldsymbol{\varepsilon} \rangle. \tag{3.4}$$

In this last relation, use has been made of the definitions:

$$\boldsymbol{l}^{(r)} = \boldsymbol{L}^{(r)} \bar{\boldsymbol{\varepsilon}}^{(r)} - \boldsymbol{\rho}^{(r)} \tag{3.5}$$

and

$$\boldsymbol{l}(\boldsymbol{x}) = \sum_{r=1}^{N} \chi^{(r)}(\boldsymbol{x}) \boldsymbol{l}^{(r)}, \qquad \boldsymbol{L}(\boldsymbol{x}) = \sum_{r=1}^{N} \chi^{(r)}(\boldsymbol{x}) \boldsymbol{L}^{(r)}. \tag{3.6}$$

Note that the variational problem $\tilde{\Psi}$, defined by (3.4), corresponds to a *thermoelastic polycrystal*, as made evident by the Euler–Lagrange equations:

$$(L_{ijkl} v_{k,l} - l_{ij})_{,j} = 0 \quad \text{in } \Omega, \qquad v_i = \bar{\varepsilon}_{ij} x_j \quad \text{on } \partial\Omega. \tag{3.7}$$

It follows that the approximation (3.3) for the effective potential, $\tilde{W}$, of the nonlinear polycrystal is easier to compute than the corresponding exact expression (2.7), because it requires the solution of a linear problem instead of a nonlinear one. Thus, given an estimate for $\tilde{\Psi}$, the expression (3.3) provides a corresponding estimate for $\tilde{W}$, for all choices of the $\bar{\boldsymbol{\varepsilon}}^{(r)}$ and $\bar{\boldsymbol{\gamma}}^{(r)}$.

The prescriptions consisting in setting

$$\bar{\boldsymbol{\varepsilon}}^{(r)} = \bar{\boldsymbol{\gamma}}^{(r)} = \langle \boldsymbol{\varepsilon} \rangle^{(r)}, \tag{3.8}$$

where $\boldsymbol{\varepsilon}$ is the strain in the thermoelastic comparison composite, were proposed by Ponte Castañeda (1996), based on the physical intuition that the strain, $\boldsymbol{\varepsilon}$, in

phase r would oscillate about its average, $\bar{\boldsymbol{\varepsilon}}^{(r)}$, in phase r, in such a way that large deviations would only be expected in regions of relatively small measure. A more rigorous justification for these prescriptions has been given by Ponte Castañeda & Willis (1999), who have shown that the resulting second-order estimates can be given a *stationary variational* interpretation.

The prescription (3.8) for the $\bar{\boldsymbol{\varepsilon}}^{(r)}$, also allows further simplification of the estimate (3.3) for $\tilde{W}$, as has been shown by Ponte Castañeda & Suquet (1998). In fact, the Hill condition for the thermoelastic comparison composite ensures that:

$$\langle \boldsymbol{\varepsilon} \cdot (\boldsymbol{L}\boldsymbol{\varepsilon} - \boldsymbol{l}) \rangle = \bar{\boldsymbol{\varepsilon}} \cdot \langle \boldsymbol{L}\boldsymbol{\varepsilon} - \boldsymbol{l} \rangle, \tag{3.9}$$

which, using the definition (3.5) for the polarizations $\boldsymbol{l}^{(r)}$, leads to

$$\tilde{\Psi} = \frac{1}{2} \sum_{r=1}^{N} c^{(r)} [\boldsymbol{\rho}^{(r)} \cdot (\bar{\boldsymbol{\varepsilon}} + \langle \boldsymbol{\varepsilon} \rangle^{(r)}) + (\langle \boldsymbol{\varepsilon} \rangle^{(r)} - \bar{\boldsymbol{\varepsilon}}^{(r)}) \cdot \boldsymbol{L}^{(r)} \bar{\boldsymbol{\varepsilon}} - \langle \boldsymbol{\varepsilon} \rangle^{(r)} \cdot \boldsymbol{L}^{(r)} \bar{\boldsymbol{\varepsilon}}^{(r)}]. \tag{3.10}$$

This result, combined with the prescription (3.8), can be used to rewrite the estimate (3.3) in the simpler form

$$\tilde{W}(\bar{\boldsymbol{\varepsilon}}) = \sum_{r=1}^{N} c^{(r)} \left\{ w^{(r)}(\bar{\boldsymbol{\varepsilon}}^{(r)}) + \frac{1}{2} \frac{\partial w^{(r)}}{\partial \boldsymbol{\varepsilon}} (\bar{\boldsymbol{\varepsilon}}^{(r)}) \cdot (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^{(r)}) \right\}, \tag{3.11}$$

where the $\bar{\boldsymbol{\varepsilon}}^{(r)}$ are determined by the prescriptions (3.8) and the approximate equality has been replaced by an exact equality for convenience.

It is also possible to work analogously with a Taylor expansion of the stress potentials, $u^{(r)}$, to generate a corresponding estimate for the effective stress potential, $\tilde{U}$. Unfortunately, the estimate for $\tilde{U}$ is not the Legendre dual of estimate (3.11) for $\tilde{W}$, and is therefore not equivalent to it. As suggested in Ponte Castañeda (1996), the expansion based on the dissipation potentials is preferred in plasticity, as a consequence of the fact that, for the physical nonlinearity present in plasticity and creep, the Taylor expansions on the dissipation potentials are expected to be more accurate than the corresponding expansions on the stress potentials. More details on this issue will be given in § 4.

Given the simplified form (3.11) for $\tilde{W}$, the implementation of the second-order procedure now only requires estimates for the phase averages, $\bar{\boldsymbol{\varepsilon}}^{(r)}$, of the strain field in the variational thermoelastic problem (3.4), or, equivalently, in the boundary-value problem (3.7). Since this problem is linear, the principle of superposition ensures that the phase averages, $\bar{\boldsymbol{\varepsilon}}^{(r)}$, can be given the form (Laws 1973):

$$\bar{\boldsymbol{\varepsilon}}^{(r)} = \boldsymbol{A}^{(r)} \bar{\boldsymbol{\varepsilon}} - \boldsymbol{a}^{(r)}, \tag{3.12}$$

where the $\boldsymbol{A}^{(r)}$ and $\boldsymbol{a}^{(r)}$ are the relevant fourth- and second-order localization tensors, respectively. Self-consistent estimates for these tensors have been given by Laws (1973) and Willis (1981). They can be written in the forms:

$$\boldsymbol{A}^{(r)} = [\boldsymbol{L}^{(r)} + \tilde{\boldsymbol{L}}^{\star}]^{-1} \tilde{\boldsymbol{P}}^{-1} \tag{3.13}$$

and

$$\boldsymbol{a}^{(r)} = [\boldsymbol{L}^{(r)} + \tilde{\boldsymbol{L}}^{\star}]^{-1} \left[\sum_{s=1}^{N} c^{(s)} (\boldsymbol{A}^{(s)})^{\mathrm{T}} \boldsymbol{l}^{(s)} - \boldsymbol{l}^{(r)} \right]. \tag{3.14}$$

In these relations, $\tilde{\boldsymbol{L}}^\star = \tilde{\boldsymbol{P}}^{-1} - \tilde{\boldsymbol{L}}$ is the constraint tensor defined by Hill (1965), where $\tilde{\boldsymbol{L}}$ is the self-consistent estimate for the effective modulus tensor which is obtained as the solution of the implicit equation

$$[\tilde{\boldsymbol{L}} + \tilde{\boldsymbol{L}}^\star]^{-1} = \sum_{s=1}^{N} c^{(s)} [\boldsymbol{L}^{(s)} + \tilde{\boldsymbol{L}}^\star]^{-1}, \tag{3.15}$$

also involving $\tilde{\boldsymbol{L}}^\star$. It is useful to recall that, while the derivation of Laws (1973) was based on the classical interpretation of the self-consistent method, in terms of the solution of the problem of an inclusion embedded in the effective medium, the more general derivation of Willis (1981) made use of the Hashin–Shtrikman variational principles allowing a more rigorous (i.e. variational) interpretation of the result in terms of two-point correlation functions. In the first case, the tensor $\tilde{\boldsymbol{P}}$ is associated with the solution of an ellipsoidal inclusion of given shape in an infinite matrix with modulus tensor $\tilde{\boldsymbol{L}}$. In the second, $\tilde{\boldsymbol{P}}$ depends on the shape of the two-point correlation functions (see Willis 1981).

The second-order estimates (3.11) hold for fairly general classes of viscoplastic polycrystals. In particular, they are able to account for different power-law exponents (or even more general flow rules) for different types of slip systems. In addition, elastic, hardening and texture evolution effects can, and should, be included for realistic modelling of metals (see Asaro & Needleman 1985). However, results will be presented here only for the *special case* of power-law creep, neglecting elastic, hardening and texture effects, since the objective in this short paper is to compare the second-order estimates with earlier estimates. More realistic applications will be given elsewhere.

4. Application to model power-law polycrystals

The results of § 3 will be used here to determine the effective behaviour of a special class of polycrystals consisting of columnar orthorhombic grains, such that the grains are cylindrical in shape, and their symmetry axes are all aligned with the x_3-axis. When such polycrystals are loaded in antiplane strain, only two slip systems can be activated. They are those defined by

$$\boldsymbol{\mu}_{(1)} = \tfrac{1}{2}(\boldsymbol{e}_1 \otimes \boldsymbol{e}_3 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_1) \quad \text{and} \quad \boldsymbol{\mu}_{(2)} = \tfrac{1}{2}(\boldsymbol{e}_2 \otimes \boldsymbol{e}_3 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_2), \tag{4.1}$$

and the problem becomes two-dimensional, where the stress, $\boldsymbol{\sigma}$, and strain rate, $\boldsymbol{\varepsilon}$, are characterized by two-dimensional vectors (with components σ_{13}, σ_{23} and ε_{13}, ε_{23}, respectively), and the modulus tensor, $\boldsymbol{L}$, by two-dimensional, symmetric, second-order tensors (with $2L_{1313}$ and $2L_{2323}$ for the diagonal entries and $2L_{1323}$ for the off-diagonal entry). In addition, the constitutive behaviour of the constituent grains will be assumed to be of the power-law type (e.g. Hutchinson 1976), so that the slip potentials in expression (2.2) will be taken to be of the form

$$\phi_{(k)}(\tau) = \frac{(\tau_0)_{(k)}}{n+1} \left(\frac{|\tau|}{(\tau_0)_{(k)}} \right)^{n+1}, \tag{4.2}$$

where $n \geqslant 1$ is the strain-rate sensitivity, and $(\tau_0)_{(1)}$ and $(\tau_0)_{(2)}$ denote the flow stresses associated with the two slip systems defined by (4.1). Note that the limit as n tends to ∞ is of special interest, as it corresponds to a rigid ideally plastic

polycrystal. A local dissipation potential may then be defined for the grains via relations (2.2), (2.3) and (4.2). Under antiplane strain conditions, it reduces to

$$w^{(r)}(\boldsymbol{\varepsilon}) = \frac{n}{n+1}[(\tau_0)_{(1)}|\varepsilon_{13}|^{1+(1/n)} + (\tau_0)_{(2)}|\varepsilon_{23}|^{1+(1/n)}]. \tag{4.3}$$

It follows, by assuming further that the statistical distribution of the grains in the transverse plane is isotropic both in space and orientation, that the polycrystal will exhibit isotropic properties in the plane. Therefore, under antiplane strain conditions, the effective behaviour of the polycrystal is determined by

$$\tilde{W}(\bar{\boldsymbol{\varepsilon}}) = \frac{n}{n+1}\tilde{\tau}_0(\bar{\gamma}_{\rm e})^{1+(1/n)}, \tag{4.4}$$

where $\bar{\gamma}_{\rm e} = [\bar{\varepsilon}_{13}^2 + \bar{\varepsilon}_{23}^2]^{1/2}$ and $\tilde{\tau}_0$ is the *effective flow stress* of the polycrystal.

The second-order estimates of the self-consistent type are obtained from expression (3.11), where the phase-average strains are obtained by solving equations (3.12)–(3.15) simultaneously for the $\bar{\boldsymbol{\varepsilon}}^{(r)}$. It is emphasized that the variables $\boldsymbol{L}^{(r)}$ and $\boldsymbol{l}^{(r)}$, as defined by (3.2) and (3.5), respectively, are dependent on $\bar{\boldsymbol{\varepsilon}}^{(r)}$, and therefore the above-mentioned set of equations are implicit on the $\bar{\boldsymbol{\varepsilon}}^{(r)}$ and are solved by iteration. Note that $\tilde{\boldsymbol{L}}$ is defined by relation (3.15), which is also implicit in $\tilde{\boldsymbol{L}}$ and must be solved by iteration. Noting that the two-point correlation functions for the distribution of the grain orientations within the polycrystal have been assumed to be isotropic in the plane (this is the so-called 'equiaxed grain' hypothesis), the relevant components of the tensor $\tilde{\boldsymbol{P}}$ are identical to those given in eqns (4.5) of Ponte Castañeda & Nebozhyn (1997).

Some sample second-order self-consistent (SC) predictions for the effective flow stress, $\tilde{\tau}_0$, are presented in figures 1 and 2 for various values of the nonlinearity exponent n, and the grain anisotropy parameter $M = (\tau_0)_{(2)}/(\tau_0)_{(1)}$. (An aggregate of 100 grain orientations was used to generate an isotropic texture in the transverse plane.) These predictions are compared against the Taylor and Sachs upper and lower bounds, the Hashin–Shtrikman (HS) upper bound of deBotton & Ponte Castañeda (1995) and the upper bound of Kohn & Little (1999). (Explicit expressions for the Taylor, Sachs and Kohn–Little bounds, as well as numerical results for the HS bounds, have been given by Ponte Castañeda & Nebozhyn (1997) for this case.) The new SC estimates are also compared against the classical 'incremental' SC estimates of Hill (1965) and Hutchinson (1976), the 'secant' SC estimate of Berveiller & Zaoui (1979), the 'tangent' (full anisotropic version) SC estimates of Molinari *et al.* (1987), the 'affine' SC estimate of Zaoui & Masson (1998) and P. Suquet (1996, personal communication), as well as the 'variational' SC estimates of Ponte Castañeda & Nebozhyn (1997).

In figure $1a, b$, results are shown for the various bounds and estimates for the effective flow stress $\tilde{\tau}_0$ as functions of the nonlinearity exponent, n, at fixed values of the grain anisotropy ($M = 1$ and 3, respectively). For $M = 1$, all the results—bounds and SC estimates—are in close agreement for n close to 1. The reason is that a two-dimensional linear material with square symmetry is known to be isotropic, and the polycrystal then becomes a homogeneous isotropic material with shear modulus proportional to $(\tau_0)_{(1)}$. For $M = 3$, all the SC estimates agree in the limit as n approaches 1, but they become increasingly different as n increases. The following additional observations can be made.

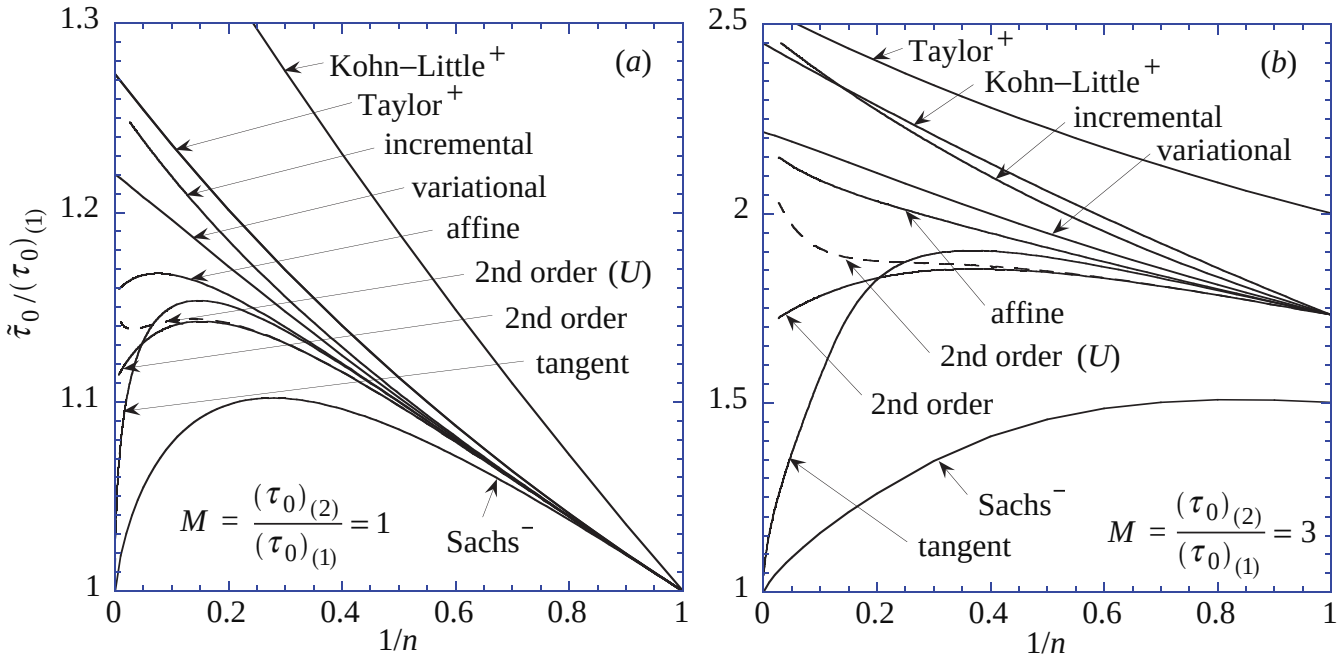

Figure 1. Comparison of the new second-order self-consistent estimates with various bounds and other self-consistent estimates for the effective flow stress $\tilde{\tau}_0$, as functions of n. Values of the grain anisotropy: (*a*) $M = (\tau_0)_{(2)}/(\tau_0)_{(1)} = 1$; (*b*) $M = (\tau_0)_{(2)}/(\tau_0)_{(1)} = 3$.

1. For low grain anisotropy ($M = 1$), the Taylor upper bound is sharper than the Kohn–Little bound. On the other hand, for the larger grain anisotropy ($M = 3$), the Kohn–Little bound improves on the Taylor bound for all values of n.

2. For $M = 3$, the 'incremental' SC estimate is seen to violate the Kohn–Little upper bound for values of $n \gtrsim 10$.

3. The rest of the SC estimates appear to satisfy the upper and lower bounds up to fairly large values of n. (Because of numerical error, in some cases it was not possible to generate results for n tending to ∞.) In general, the 'second-order' SC estimates are the least stiff, with the 'tangent', 'affine' and 'variational' following in order of increasing stiffness. However, the 'tangent' SC estimates become extremely soft, tending to the Sachs lower bound, in the limit as $n \to \infty$.

4. Two sets of results are shown here for the 'second-order' SC estimates: those obtained from the above-described dissipation potential formulation; and the corresponding estimates from the dual stress potential formulation (the latter are labelled U in figure 1 and appear as dashed lines). It is seen that, at least for these values of the grain anisotropy parameter, the two types of estimates are in very good agreement up to fairly large values of n. However, for sufficiently large n, the two sets of results begin to diverge with the stress potential estimates turning sharply toward the Taylor bound. Thus, in agreement with our earlier comments, the dissipation potential estimates appear to be more realistic.

In figure 2*a*, *b*, results are shown for the same bounds and estimates as in figure 1, but this time as functions of the grain anisotropy M, at fixed values of n (3 and 10). The following additional observations can be made.

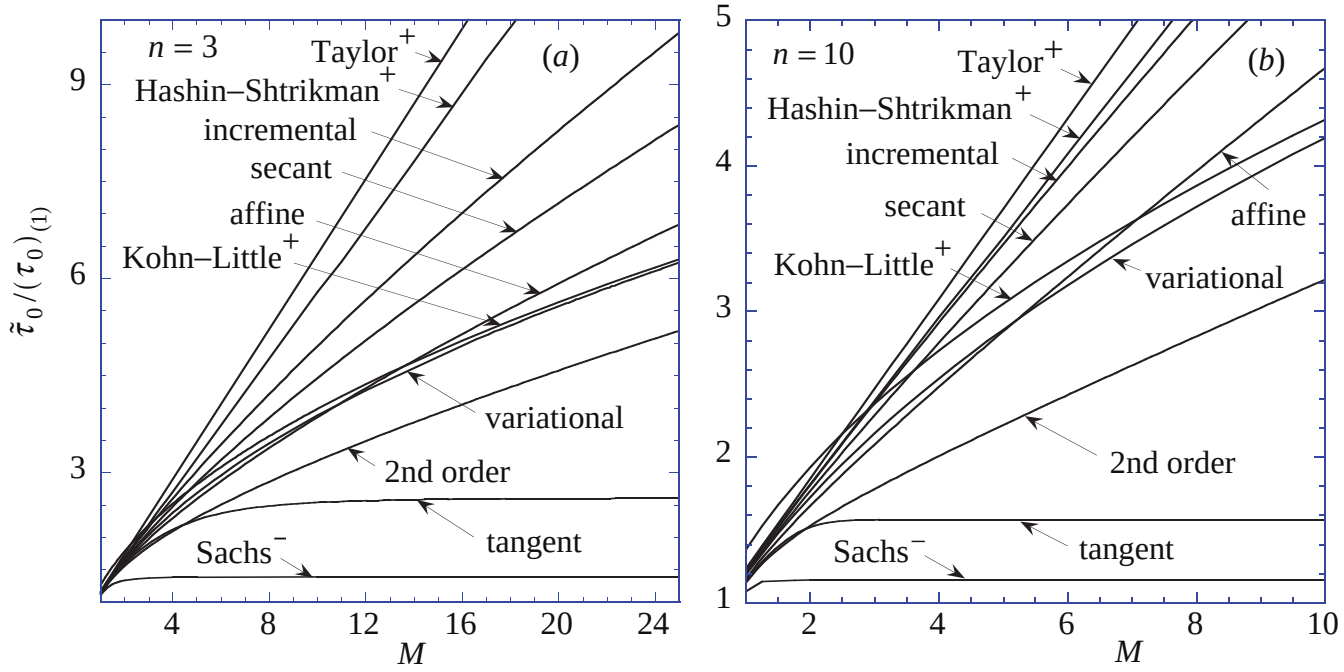

Figure 2. Comparison of the new second-order self-consistent estimates with various bounds and other self-consistent estimates for the effective flow stress, $\tilde{\tau}_0$, as functions of the grain anisotropy, $M = (\tau_0)_{(2)}/(\tau_0)_{(1)}$. (*a*) $n = 3$; (*b*) $n = 10$.

1. The new 'second-order' SC estimates should be the most accurate at low grain anisotropy because of their exact asymptotic status for small contrast. In this sense, it would appear that all the other SC estimates tend to *overestimate* the effective flow stress of the nonlinear polycrystals at low grain anisotropy.

2. Although the 'affine' SC estimates were found to satisfy all bounds in the previous set of figures, it is seen here that, even at a fairly low value of n, the 'affine' SC estimates appear to violate the Kohn–Little bound at sufficiently high grain anisotropy. For the larger value of n, the 'affine' SC estimates break down at even lower values of the grain anisotropy. (Note, however, that the 'affine' method of Zaoui & Masson (1998) can be implemented for elastic viscoplastic constitutive behaviour.) Similarly, the 'secant' SC estimates, which lie between the corresponding 'incremental' and 'affine' estimates, are seen to also violate the Kohn–Little bound. In conclusion, the 'variational', 'second-order' and 'tangent' SC estimates are the only that do not violate any bounds.

3. Because of their origin from a minimum principle (deBotton & Ponte Castañeda 1995), the 'variational' SC estimates should provide overestimates relative to the 'exact' SC estimates (i.e. those that would be obtained by means of the exact minimizing trial field in the context of the minimum principle). In this respect, the 'second-order' and 'tangent' SC estimates could be more accurate.

4. It is observed, however, that the 'tangent' SC estimates appear to satisfy a different scaling law than the 'second-order' and 'variational' SC estimates, which in turn appear to satisfy the same law as the Kohn–Little bound (i.e. square root in M). Thus, it is seen that the 'tangent' SC estimates reach a limiting state beyond which further increases in M lead to no corresponding increases

in the effective flow stress. While strictly unable to rule it out, this behaviour, especially for the low value of n ($n = 3$), would appear to be unrealistically soft.

5. Concluding remarks

In conclusion, the 'second-order' SC estimates—those obtained from the dissipation potential version (3.11) of the theory—would appear to be the most accurate of all, certainly when compared to the 'classical' SC estimates, and probably also when compared to other recently proposed SC estimates. This statement would be rigorously true at low grain anisotropy, but would still need to be proved more generally. In this connection, lower bounds that are sharper than Sachs, such as those that have been proposed by Talbot & Willis (1997) for two-phase nonlinear composites, would be extremely useful. Similarly, comparisons with direct numerical simulations could also be very insightful.

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References

Asaro, R. J. & Needleman, A. 1985 Texture development and strain hardening in rate-dependent polycrystals. *Acta Metall.* **33**, 923–953.

Berveiller, M. & Zaoui, A. 1979 An extension of the self-consistent scheme to plastically-flowing polycrystals. *J. Mech. Phys. Solids* **26**, 325–344.

deBotton, G. & Ponte Castañeda, P. 1995 Variational estimates for the creep behavior of polycrystals. *Proc. R. Soc. Lond.* A **448**, 121–142.

Dendievel, R., Bonnet, G. & Willis, J. R. 1991 Bounds for the creep behavior of polycrystalline materials. In *Inelastic deformation of composite materials* (ed. G. Dvorak), pp. 175–192. New York: Springer.

Gilormini, P. 1995 A shortcoming of the classical nonlinear extension of the self-consistent model. *C. R. Acad. Sci. Paris* IIb **320**, 115–122.

Hill, R. 1965 Continuum micro-mechanics of elastoplastic polycrystals. *J. Mech. Phys. Solids* **13**, 89–101.

Hutchinson, J. W. 1976 Bounds and self-consistent estimates for creep of polycrystalline materials. *Proc. R. Soc. Lond.* A **348**, 101–127.

Kohn, R. V. & Little, T. D. 1999 Some model problems of polycrystal plasticity with deficient basic crystals. *SIAM J. Appl. Math.* **59**, 172–197.

Laws, N. 1973 On the thermostatics of composite materials. *J. Mech. Phys. Solids* **21**, 9–17.

Molinari, A., Canova, G. R. & Ahzi, S. 1987 A self-consistent approach of the large deformation polycrystal viscoplasticity. *Acta Metall. Mater.* **35**, 2983–2994.

Ponte Castañeda, P. 1996 Exact second-order estimates for the effective mechanical properties of nonlinear composite materials. *J. Mech. Phys. Solids* **44**, 827–862.

Ponte Castañeda, P. & Nebozhyn, M. 1997 Variational estimates of the self-consistent type for some model nonlinear polycrystals. *Proc. R. Soc. Lond.* A **453**, 2715–2724.

Ponte Castañeda, P. & Suquet, P. 1998 Nonlinear composites. *Adv. Appl. Mech.* **34**, 171–302.

Ponte Castañeda, P. & Willis, J. R. 1999 Variational second-order estimates for nonlinear composites. *Proc. R. Soc. Lond.* A **455**. (In the press.)

Suquet, P. & Ponte Castañeda, P. 1993 Small-contrast perturbation expansions for the effective properties of nonlinear composites. *C. R. Acad. Sci. Paris* II **317**, 1515–1522.

Talbot, D. R. S. & Willis, J. R. 1997 Bounds of third order for the overall response of nonlinear composites. *J. Mech. Phys. Solids* **45**, 87–111.

Taylor, G. I. 1938 Plastic strains in metals. *J. Inst. Metals* **62**, 307–324.

Willis, J. R. 1981 Variational and related methods for the overall properties of composites. *Adv. Appl. Mech.* **21**, 1–78.

Zaoui, A. & Masson, R. 1998 Modeling stress-dependent transformation strains of heterogeneous materials. In *Transformation problems in composite and active materials (IUTAM Symp.)* (ed. Y. A. Bahei-El-Din & G. J. Dvorak), pp. 3–15. New York: Kluwer.