Variational estimates for the creep behaviour of polycrystals

BY G. deBotton¹ AND P. Ponte Castañeda²

¹Department of Mechanical Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel
²Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA 19104, U.S.A.

A variational procedure is developed for estimating the effective constitutive behaviour of polycrystalline materials undergoing high-temperature creep. The procedure is based on a new variational principle allowing the determination of the effective potential function of a given nonlinear polycrystal in terms of the corresponding potential for a linear comparison polycrystal with an identical geometric arrangements of its constituent single-crystal grains. As such, it constitutes an extension, to locally anisotropic behaviour, of the variational procedure developed by Ponte Castañeda (1991) for nonlinear heterogeneous media with locally isotropic behaviour. By way of an example, the procedure is applied to the determination of bounds of the Hashin–Shtrikman type for the effective potentials of statistically isotropic nonlinear polycrystals. The bounds are computed for the special class of untextured FCC polycrystals with isotropic pure power-law viscous behaviour, first considered by Hutchinson (1976), in the context of a calculation of the self-consistent type. The new bounds are found to be more restrictive than the corresponding classical Taylor–Bishop–Hill bounds, and also more restrictive, if only slightly so, than related bounds of the Hashin–Shtrikman type by Dendievel et al. (1991). The new procedure has the advantage over the self-consistent procedure of Hutchinson (1976) that it may be applied, without any essential complications, to aggregates of crystals with slip systems exhibiting different creep rules – with, for example, different power exponents – and to general loading conditions. However, the distinctive feature of the new variational procedure is that it may be used in conjunction with other types of known bounds and estimates for linear polycrystals to generate corresponding bounds and estimates for nonlinear polycrystals.

1. Introduction

The prediction of the effective constitutive behaviour of polycrystalline aggregates, directly from known information about the constitutive properties and geometric arrangement of their constituent single-crystal grains, has been the subject of numerous studies for quite some time. In the context of linear elasticity, Voigt (1889) and Reuss (1929) proposed estimates based on the assumptions of uniform strain and stress fields, respectively, within the polycrystals. Such estimates are known not to be exact because the associated stress and strain fields
violate equilibrium and compatibility, respectively; however, they were shown to be rigorous bounds for the actual effective behaviour of appropriate classes of polycrystals by Hill (1952), starting from the principles of minimum potential and minimum complementary energy, respectively. In parallel developments, Sachs (1928) and Taylor (1938) proposed uniform stress and uniform strain-rate estimates for the nonlinear stress-strain relations of polycrystalline aggregates of ductile, face-centred-cubic (fcc) single crystals. These types of estimates were rederived, and proved to be rigorous bounds for the effective yield strength of aggregates of rigid/perfectly plastic crystals by Bishop & Hill (1951a). In addition, Bishop & Hill (1951b) obtained explicit upper bounds for the yield strength of untextured fcc polycrystals; Hutchinson (1976) was the first to compute uniform strain-rate bounds for fcc polycrystals in power-law creep.

A different approach to the problem was proposed by Hershey (1954) and Kröner (1958), who independently advanced ‘self-consistent’ methods for estimating the effective behaviour of polycrystalline aggregates of linear-elastic single crystals. These methods may be alternatively derived by making use of the solution of Eshelby (1957) for the uniform stress and strain fields within an ellipsoidal inclusion embedded in an unbounded homogeneous medium, which is subjected to uniform stress on its ‘boundary’, as shown by Hill (1965). Extensions of these methods to polycrystalline aggregates of ductile single crystals were proposed by Kröner (1961) and Budiansky & Wu (1962). Computations based on these methods were carried out by Budiansky & Wu (1962) and Hutchinson (1964) for untextured fcc polycrystals. A different version of the self-consistent method for elastoplastic polycrystals was proposed by Hill (1965), essentially, by interpreting the nonlinear behaviour of the ductile crystals and polycrystal as incrementally linear, and applying the standard self-consistent procedures to the associated increments in the stress and strain-rate fields. In addition, Hill (1967) explored quite generally, but in qualitative terms, the implications of his self-consistent model for the structure of elastoplastic constitutive relations for polycrystals. A comparative study of the self-consistent Kröner–Budiansky–Wu (KBW) and Hill procedures was given by Hutchinson (1970), who found Hill’s method to be more realistic in accounting for the softer ductile interaction among the grains in the polycrystal, at the expense of significantly increased computational effort. In addition, Hutchinson (1976) extended the use of Hill’s method to power-law creep, and was able to ‘integrate’ the resulting incremental relations for the effective behaviour of polycrystals to obtain relatively simpler ‘total’ relations. Finally, Berveiller & Zaoui (1979) have been able to modify the KBW procedure to incorporate a softer interaction law for the grains in the self-consistent model of a polycrystal. For a review of many of the above mentioned developments for ductile polycrystals, emphasizing different aspects of single crystal behaviour, and including comparison with experimental results, the reader is referred to the article by Kocks (1970).

A third approach for characterizing the effective behaviour of linear-elastic polycrystals was proposed by Hashin & Shtrikman (1962a) in terms of new variational principles for the polarization stress and strain fields in the polycrystal relative to a homogeneous comparison material (see also Walpole 1966a). The idea is to prescribe bounds that are more restrictive than the Hill–Voigt–Reuss bounds, by making use of higher-order statistical information about the geometric arrangement of the grains within the polycrystal. Explicit upper and lower bounds
for the effective behaviour of statistically isotropic cubic polycrystals were given by Hashin & Shtrikman (1962b) (see also Hashin 1965 and Walpole 1966a, b). These bounds were indeed found to be more restrictive than the corresponding Hill–Voigt–Reuss bounds, and also to enclose the corresponding self-consistent estimate. An extension of the Hashin–Shtrikman (abbreviated from henceforth as ‘HS’) variational principles for more general geometric arrangements of the constituent phases was given by Willis (1977) in terms of two-point probability functions. Remarkably, however, it was not until fairly recently that appropriate generalizations of the HS variational principles for nonlinear media were suggested by Willis (1983) and developed further by Talbot & Willis (1985). An application of these variational principles to obtain upper bounds for the effective stress potentials of nonlinear polycrystals in the context of power-law creep was given by Dendievel et al. (1991). These bounds were found to be improvements on the corresponding uniform strain-rate bounds, and also to lie above the associated self-consistent estimates, as determined by Hutchinson (1976) for this class of polycrystals. One interesting feature, however, of these upper bounds is that they become virtually indistinguishable from the uniform-strain-rate bound of Bishop & Hill for sufficiently small ‘hardening’ (i.e. sufficiently close to rigid/perfectly plastic behaviour). This feature is apparently also exhibited, although to a lesser extent, by the self-consistent estimates of Hutchinson (1976).

In the present work, we make use of appropriate extensions of the variational principles of Ponte Castañeda (1991, 1992a), which were initially developed for nonlinear heterogeneous media with locally isotropic behaviour (but possibly anisotropic global behaviour). These variational principles serve to characterize the effective behaviour of nonlinear heterogeneous media in terms of the effective behaviour of certain classes of linear comparison heterogeneous media, and thus allow the direct translation of the large bodies of available information for the effective behaviour of linear systems directly to nonlinear systems. In particular, these variational principles may be used in conjunction with the HS bounds for linear systems to generate bounds of the HS type for nonlinear systems, but more generally, other types of linear estimates may also be used to generate corresponding types of nonlinear estimates.

The extension required in this investigation is one for nonlinear media with locally anisotropic behaviour, as appropriate for nonlinear polycrystals in the context of creep. After presenting the definition, in §2, of the effective behaviour of ‘generalized polycrystals’ (these are polycrystals with generally distinct single-crystal grains, and also generally distinct ‘hardening’ rules for the different slip systems within each type of crystal), a variational statement is developed, in §3, for the effective stress potentials of such generalized nonlinear polycrystals. The variational statement is expressed in terms of the effective potentials of appropriate classes of linear comparison polycrystals. In this connection, it is important to remark that, even if all the crystals in the nonlinear polycrystal are identical (except, of course, for their orientations), and all the hardening rules for the different slip systems in each crystal are also identical, in general, the corresponding ‘slip compliances’ in the linear comparison polycrystal will need to be chosen different for each crystal (i.e. each crystal in the linear comparison polycrystal is different), and also for each different slip system within each crystal. An application of this variational procedure to obtain bounds of the HS type for the effective stress potentials of the relevant class of nonlinear polycrystals is given

in §4. In addition, it is verified that the new variational procedure is capable of delivering the uniform strain-rate bounds. (In fact, a new and rather simple form is derived for these classical bounds.) We conclude, in §5, with an application of our proposed variational procedure to the computation of upper bounds of the HS type for FCC power-law polycrystals. These bounds are found to be more restrictive than the classical uniform strain-rate bounds, and also than the HS-type bounds of Dendievel et al. (1991), if only slightly so (for relatively large values of the creep exponent). Although we will not pursue this point here, we emphasize that one advantage of the proposed variational procedure is that it may be used in conjunction with other types of bounds and estimates for the linear comparison polycrystals to generate corresponding types of bounds and estimates for nonlinear polycrystals.

We note that alternative extensions of the variational procedure of Ponte Castañeda (1991) for composites with locally anisotropic behaviour have been suggested by Willis (1991) and Talbot and Willis (1992), the latter reference being more precisely a hybrid of the variational procedures of Talbot & Willis and Ponte Castañeda. However, as we shall see later, these extensions are more complicated than necessary because they consider classes of linear comparison polycrystals that are more general than necessary, at least for the nonlinear polycrystals considered in this paper. In addition, they are more difficult to implement numerically for reasons that will be discussed later. Yet a different type of extension was proposed by Bonnet et al. (1992), and bounds were computed, based on this extension, for the effective behaviour of the same class of power-law polycrystals considered by Hutchinson (1976) and Dendievel et al. (1991). However, these bounds were found to be weaker than the bounds originally proposed by Dendievel et al.; the reason presumably being that the class of linear polycrystals considered in this extension was not as broad as necessary. On the other hand, the extension proposed in this paper identifies the smallest possible class of linear comparison polycrystals that is capable, at least in principle, of delivering the exact constitutive behaviour of the nonlinear polycrystals (in a sense made explicit by expression (3.13) for the effective potential of a nonlinear polycrystal).

2. Characterization of the creep behaviour of single crystals and polycrystals

We consider a reference single crystal which is capable of undergoing creep on a set of $K$ preferred crystallographic slip systems. Each of the systems is characterized by a second-order tensor $\mu_{(k)}$ ($k = 1, \ldots, K$), such that

$$\mu_{(k)} = \frac{1}{2} (m_{(k)} \otimes n_{(k)} + n_{(k)} \otimes m_{(k)}),$$

(2.1)

where $n_{(k)}$ and $m_{(k)}$ denote respectively the unit vectors normal to the slip plane and along the slip direction of the $k$th system. Here, $\otimes$ denotes the dyadic product of two vectors.

In terms of $\mu_{(k)}$, the resolved shear stress on the $k$th slip system of the reference crystal is given by

$$\tau_{(k)} = \sigma \cdot \mu_{(k)},$$

(2.2)

where $\sigma$ is the stress field acting on the crystal, and where the dot denotes the inner product of two second-order tensors (i.e. $\sigma \cdot \mu = \sigma_{ij} \mu_{ij}$).

Following standard practice (see Hutchinson 1976), we assume that the shear strain-rate (engineering definition) in the $k$th slip system $\gamma_{(k)}$ depends only on the applied stress, through the resolved shear stress $\tau_{(k)}$ on that system, in such a way that

$$\gamma_{(k)} = \frac{d\phi_{(k)}}{d\tau_{(k)}}(\tau_{(k)}),$$

(2.3)

where $\phi_{(k)}$ is a convex function (Rice 1970; Mandel 1972), satisfying the condition $\phi_{(k)}(0) = 0$. In the above relation, we have implicitly assumed that the slip potential functions $\phi_{(k)}$ are differentiable; however, even when they are not differentiable, as would be the case for rigid/perfectly plastic crystals (e.g. $\phi_{(k)} = 0$, if $\tau_{(k)} \leq \tau_0$; and $\phi_{(k)} = \infty$, if $\tau_{(k)} > \tau_0$), it is still possible to relate $\gamma_{(k)}$ and $\tau_{(k)}$ via the subdifferential of convex analysis (see Van Tiel 1984), such that $\gamma_{(k)} \in \partial \phi_{(k)}(\tau_{(k)})$.

It follows from the definition of $\gamma_{(k)}$ that the overall strain-rate $\epsilon$ in the single crystal is given by the relation,

$$\epsilon = \sum_{k=1}^{K} \gamma_{(k)}\mu_{(k)},$$

(2.4)

or, alternatively, by

$$\epsilon = \frac{\partial u^{(c)}}{\partial \sigma}(\sigma),$$

(2.5)

where

$$u^{(c)}(\sigma) = \sum_{k=1}^{K} \phi_{(k)}(\tau_{(k)})$$

(2.6)

is the stress potential of the crystal. We note that a common choice for the slip potential functions $\phi_{(k)}$ is a pure-power law, as used by Hutchinson (1976) and Dendievel et al. (1991); however, in this work, we will consider general functions $\phi_{(k)}$ (satisfying the above convexity hypotheses). In particular, for rigid-perfectly plastic materials, relation (2.6) serves to characterize the yield strength domain of the single crystal, and (2.5), with the derivative interpreted as a subdifferential, implies that $\epsilon$ must lie in the appropriate cone of normals.

For our purposes, a polycrystal is an aggregate of a large number of identical single crystal grains, with generally distinct orientations. It is assumed that the size of the typical grain is much smaller than the size of the specimen of interest, and that the perfect grains are firmly bonded at their boundaries, so that, in particular, there are no cracks or holes within the polycrystal, and no sliding at the grain boundaries. We further assume that the polycrystals have no texture, so that the orientations of the single crystals within the polycrystal will be assumed to be random (i.e. no preferred orientations). In addition, we will assume that the geometric arrangement of the grains within the composite will be statistically uniform and isotropic, in a sense to be made more precise later on.

We consider next a representative specimen of the polycrystal occupying a domain $\Omega$, with unit volume and boundary $\partial \Omega$. The crystals within the polycrystal will be characterized by their orientation relative to the reference crystal, as given by rotation tensors $Q^{(r)}$ ($r = 1, \ldots, N$), in such a way that phase $r$ will be defined to be the region in $\Omega$ occupied by all crystals with orientations $Q^{(r)}$. Then,
letting
\[ u^{(r)}(\sigma) = u^{(o)}(Q^{(r)^T} \sigma Q^{(r)}) \] (2.7)
denote the stress potential of the \(r\)th phase, we may express the stress potential \(u\) of the polycrystal, depending on the position vector \(x\), via the relation,
\[ u(x; \sigma) = \sum_{r=1}^{N} \chi^{(r)}(x) u^{(r)}(\sigma), \] (2.8)
where \(\chi^{(r)}\) is the characteristic function of phase \(r\) (equal 1 when \(x\) is in phase \(r\), and 0 otherwise). With this definition, the volume fraction of the \(r\)th phase, or the proportion of crystals with orientation \(Q^{(r)}\), is given by
\[ c^{(r)} = \int_{\Omega} \chi^{(r)}(x) \, dx. \] (2.9)

We note that, since our polycrystals have no texture, \(c^{(r)} = c = N^{-1}\), but for later convenience we will continue to assume that the volume fractions of each phase are generally distinct. Also, by making use of relation (2.6) for \(u^{(o)}\), we remark, from (2.7), that \(u^{(r)}\) may be rewritten in the form,
\[ u^{(r)}(\sigma) = \sum_{k=1}^{K} \phi^{(k)}(\tau_{(k)}^{(r)}), \] (2.10)
where
\[ \tau_{(k)}^{(r)} = \sigma \cdot \mu^{(r)}(k). \] (2.11)

with \(\mu^{(r)}(k) = Q^{(r)^T} \mu(k) Q^{(r)}\).

Rigorous mathematical definitions for the effective behaviour of heterogeneous solids were introduced by Hill (1963) in the context of linear elasticity. Analogous definitions may be given for the nonlinear creep of polycrystals (see Rice 1970; Mandel 1972; Hutchinson 1976). Thus, when a polycrystal is subjected to the uniform traction boundary condition,
\[ \sigma n = \bar{\sigma} n, \quad x \in \partial \Omega, \] (2.12)
where \(n\) is the outward unit normal to \(\partial \Omega\) and \(\bar{\sigma}\) is a constant symmetric tensor, it is possible to show that the mean value (over \(\Omega\)) of the stress field is precisely \(\bar{\sigma}\). It then follows that the effective behaviour of the polycrystal may be characterized by means of
\[ \bar{\epsilon} = \frac{\partial U}{\partial \bar{\sigma}}(\bar{\sigma}) \] (2.13)
[or \(\bar{\epsilon} \in \partial U(\bar{\sigma})\)], where \(\bar{\epsilon}\) is the mean value of the strain-rate field and \(\bar{U}\) denotes the effective stress potential of the polycrystal. In turn, \(\bar{U}\) may be determined from the principle of minimum complementary energy (in its rate form), stating that
\[ \bar{U}(\bar{\sigma}) = \sigma \min_{(x) \in S} \left\{ \int_{\Omega} u(x; \sigma) \, dx \right\}, \] (2.14)
where
\[ S = \{ \sigma \mid \nabla \cdot \sigma = 0 \text{ in } \Omega, \text{ and } \sigma n = \bar{\sigma} n \text{ on } \partial \Omega \} \] (2.15)
is the appropriate set of statically admissible stress fields. (Note that $S$ depends on $\sigma$.) We observe that the solution of the variational problem (2.14) is in general extremely difficult, in particular, because of the nonlinear constitutive behaviour of the single crystals. As we have mentioned in §1, relatively few estimates are available for the effective behaviour of nonlinear polycrystals, whereas significantly more information is available for linear polycrystals. For this reason, in the next section, we introduce an alternative variational representation for $\tilde{U}$, which may be used to estimate the effective behaviour of the nonlinear polycrystals in terms of the effective behaviour of linear polycrystals.

Finally, for later reference, we note that there exists a dual characterization of the effective behaviour of the polycrystal, in terms of the local strain-rate potential function $\omega = u^*$, where $u^*$ denotes the Legendre–Fenchel transform of $u$, defined by

$$u^*(x; \varepsilon) = \sup_{\sigma} \{ \sigma \cdot \varepsilon - u(x; \sigma) \}. \quad (2.16)$$

The alternative representation is given by

$$\tilde{\sigma} = \frac{\partial \tilde{W}}{\partial \varepsilon}(\varepsilon), \quad (2.17)$$

in terms of the effective strain-rate potential $\tilde{W}$, obtained from the principle of minimum potential energy via

$$\tilde{W}(\varepsilon) = \min_{\varepsilon(\sigma) \in K} \left\{ \int_{\Omega} \omega(x; \varepsilon) \, dx \right\}, \quad (2.18)$$

where $K = \{ \varepsilon \mid \exists \text{ a velocity field } v \text{ such that} \}

$$\varepsilon = \frac{1}{2} [\nabla v + (\nabla v)^T] \text{ in } \Omega, \text{ and } v = \varepsilon x \text{ on } \partial\Omega \} \quad (2.19)$$

is the appropriate set of kinematically admissible strain-rates. With the above hypotheses for the polycrystal, it can be shown that $\tilde{W} = \tilde{U}^*$ and also that $\tilde{U} = \tilde{W}^*$, so that, in fact, the two representations (2.13) with (2.14) and (2.17) with (2.18) for the effective behaviour of the polycrystal are exactly dual. We emphasize that the dual formulation (2.18) usually offers no advantage over the original formulation (2.14) because the strain-rate potentials $\omega$ appearing in (2.18) are not easily determined for the nonlinear polycrystals of interest here.

3. New variational representation for the creep behaviour of polycrystalline aggregates

The variational statement developed in this section is a direct extension of the variational principles introduced by Ponte Castañeda (1991, 1992a), for nonlinear heterogeneous materials with locally isotropic behaviour, to classes of nonlinear heterogeneous materials with a special type of locally anisotropic behaviour, broad enough to include the nonlinear polycrystalline aggregates discussed in the previous section. Thus, in this section, we obtain an exact variational representation for the effective stress potential of $N$-phase heterogeneous materials with
potential functions as given by (2.8) and (2.10), except that the slip potential functions \( \phi_{(k)} \) will not be assumed to be the same for each phase, and therefore will be replaced by phase-dependent functions \( \phi_{(k)}^{(r)} \). The specialization of the relevant results for the polycrystals of the previous section (with identical grains) will be given later; however, for simplicity, we will also refer to the more general class of heterogeneous materials of this section as polycrystals.

Following the development of Ponte Castañeda (1992a, b), we introduce variables

\[
\nu = |\tau|^2 \quad \text{or} \quad \nu_{(k)}^{(r)} = |\tau_{(k)}^{(r)}|^2 ,
\]

(3.1)

and assume that the generalized slip potential functions \( \phi_{(k)}^{(r)} \) are such that there exist corresponding functions \( g_{(k)}^{(r)} \) satisfying the relation,

\[
g_{(k)}^{(r)}(\nu) = \phi_{(k)}^{(r)}(\tau).
\]

(3.2)

The functions \( g_{(k)}^{(r)} \) clearly satisfy the condition \( g_{(k)}^{(r)}(0) = 0 \), but are not necessarily convex. For reasons that will become evident in the following development, we further assume that the functions \( \phi_{(k)}^{(r)} \) are such that the associated functions \( g_{(k)}^{(r)} \) are convex (note that convexity of the \( \phi_{(k)}^{(r)} \) is thus ensured). We then say that the functions \( \phi_{(k)}^{(r)} \) are strongly convex. For example, the power-law functions,

\[
\phi_{(k)}^{(r)}(\tau) = \frac{\gamma_0 (\tau_{(k)}^{(r)})}{(n + 1)} \left[ \frac{\tau}{(\tau_{(k)}^{(r)})} \right]^{n+1},
\]

(3.3)

with creep exponent \( n \geq 1 \), and reference stresses and strain \( (\tau_{(k)}^{(r)}) \) and \( \gamma_0 \), respectively, are strongly convex.

Next, defining the convex polar function (or Legendre–Fenchel transform) of \( g_{(k)}^{(r)} \) via

\[
(g_{(k)}^{(r)})^*(\alpha) = \sup_{\nu \geq 0} \left\{ \alpha \nu - g_{(k)}^{(r)}(\nu) \right\},
\]

(3.4)

we observe that (see Ponte Castañeda 1992b)

\[
g_{(k)}^{(r)}(\nu) = \sup_{\alpha \geq 0} \left\{ \alpha \nu - (g_{(k)}^{(r)})^*(\alpha) \right\},
\]

(3.5)

which, on account of (3.1) and (3.2), may be rewritten as

\[
\phi_{(k)}^{(r)}(\tau) = \sup_{\alpha \geq 0} \left\{ \alpha |\tau|^2 - V_{(k)}^{(r)}(\alpha) \right\},
\]

(3.6)

where

\[
V_{(k)}^{(r)}(\alpha) = \sup_{\tau} \left\{ \alpha |\tau|^2 - \phi_{(k)}^{(r)}(\tau) \right\}.
\]

(3.7)

It then follows from (2.10) that

\[
u^{(r)}(\sigma) = \sup_{\alpha_{(k)}^{(r)}, \geq 0} \left\{ \sum_{k=1}^{K} \alpha_{(k)}^{(r)} |\tau_{(k)}^{(r)}|^2 - \sum_{k=1}^{K} V_{(k)}^{(r)}(\alpha_{(k)}^{(r)}) \right\},
\]

(3.8)

and therefore, from (2.8), also that

\[ u(x; \sigma) = \sup_{\substack{\alpha^{(r)}(x) \geq 0 \\ \alpha^{(r)}(x) \geq 0 \\ a_i = 1, \ldots, N \atop l=1, \ldots, K}} \left\{ \sum_{r=1}^{N} \sum_{k=1}^{K} \chi^{(r)}(x) \alpha^{(r)}(x) \right\} - \sum_{r=1}^{N} \sum_{k=1}^{K} \chi^{(r)}(x) V^{(r)}(x) \alpha^{(r)}(x) \right\} \quad (3.9) \]

We emphasize that the equalities (=) in (3.5), (3.6), (3.8) and (3.9) would need to be replaced by inequalities (\(\geq\)) if the functions \(\phi^{(r)}(k)\) were not assumed to be strongly convex.

In view of relations (3.8) and (3.9), it is expedient to introduce a ‘linear comparison polycrystal’ with potential function,

\[ u_0(x; \sigma) = \sum_{r=1}^{N} \chi^{(r)}(x) u^{(r)}(\sigma), \quad (3.10) \]

such that the quadratic potential of phase \(r\), in the linear comparison polycrystal, is given by

\[ u^{(r)}(\sigma) = \sum_{k=1}^{K} \alpha^{(r)}(\sigma) \gamma^{(r)}(\sigma)^2 \quad (3.11) \]

By comparison with (2.8) and (3.10), respectively, we observe that the linear comparison polycrystal has the same distribution of phases as the original nonlinear polycrystal. In addition, the grains belonging to a given phase \(r\) of the linear comparison polycrystal have exactly the same slip systems as the corresponding grains of the nonlinear polycrystal. However, we emphasize that, even when all the grains of the nonlinear polycrystal are identical (except, of course, for their orientations), the corresponding grains of the linear comparison polycrystal need not be identical. This is because the ‘slip system compliances’ \(\alpha^{(r)}(k)\) of the linear comparison polycrystal depend not only on the corresponding slip potentials \(\phi^{(r)}(k)\), but also on the actual state of stress within the grains, which in general will vary from grain to grain.

The above observations motivate the substitution of relation (3.9), making use of (3.10) and (3.11), into expression (2.14) for the effective potential of the nonlinear polycrystal. This leads to the following expression for \(\hat{U}\), namely,

\[ \hat{U}(\sigma) = \min_{\sigma(x) \in S} \left\{ \sup_{\alpha^{(r)}(x) \geq 0 \atop a_i = 1, \ldots, N \atop l=1, \ldots, K} \left[ \int_S u_0(x; \sigma) \, dx - \int_S \sum_{r=1}^{N} \sum_{k=1}^{K} \chi^{(r)}(x) V^{(r)}(x) \alpha^{(r)}(x) \, dx \right] \right\}. \quad (3.12) \]

Finally, by an argument completely analogous to that used by Ponte Castañeda (1992a) for locally isotropic composites (essentially the observation that the functional inside the square brackets is convex in \(\sigma\) and concave in the variables \(\alpha^{(r)}\), so that the minimum and supremum operations may be interchanged according to the saddle point theorem), we arrive at the following variational statement for

the effective stress potential of the nonlinear polycrystal,

$$
\tilde{U}(\sigma) = \sup_{\alpha_{(s)}^{(r)}(x) \geq 0 \atop s=1,\ldots,N \atop t=1,\ldots,K} \left\{ \tilde{U}_0(\sigma) - \int_{\Omega} \sum_{r=1}^{N} \sum_{k=1}^{K} \chi^{(r)}(x)V^{(r)}_{(s)}(\alpha^{(r)}_{(s)}(x)) \mathrm{d}x \right\},
$$

(3.13)

where

$$
\tilde{U}_0(\sigma) = \min_{\sigma(\alpha) \in S} \int_{\Omega} u_0(x; \sigma) \mathrm{d}x
$$

(3.14)

denotes the effective stress potential of a class of linear comparison polycrystals, defined by the local stress potentials (3.10) and (3.11). We emphasize that the $N$ sets of optimization variables $\alpha_{(s)}^{(r)} (k = 1, \ldots, K)$ are actually sets of non-negative functions of $x$, each set of functions being defined over its corresponding phase ($s = 1, \ldots, N$). Because of this variability of the slip compliances $\alpha_{(s)}^{(r)}$ – not only from grain to grain – but also within each grain, we note that the effective potential of the associated class of linear comparison polycrystals would be extremely difficult to compute in general. For these reasons, it is extremely difficult to make direct use of the above variational statement in the computation of $\tilde{U}$ for a specific nonlinear polycrystal. However, as it was found by Ponte Castañeda (1992a) for the corresponding locally isotropic composites, the above variational statement lends itself to a useful approximation.

Such an approximation for the effective potential $\tilde{U}$ in (3.13) is obtained by restricting the class of optimization functions $\alpha_{(s)}^{(r)}(x)$ to the strictly smaller class of piecewise uniform functions (a different constant for each phase and slip system). This approximation leads to a finite-dimensional optimization problem over $N \times K$ constant variables $\alpha_{(k)}^{(r)}$, which bounds the effective potential of the nonlinear polycrystal from below, that is

$$
\tilde{U}(\sigma) \geq \sup_{\alpha_{(s)}^{(r)} \geq 0 \atop s=1,\ldots,N \atop t=1,\ldots,K} \left\{ \tilde{U}_0(\sigma) - \sum_{r=1}^{N} \sum_{k=1}^{K} \epsilon^{(r)} V^{(r)}_{(k)}(\alpha^{(r)}_{(s)}(x)) \right\},
$$

(3.15)

where $\tilde{U}_0$ now stands for the effective potential of a linear polycrystal with precisely the same microstructural distribution of phases as the nonlinear polycrystal (since the distribution of the homogeneous phases is exactly the same). In summary, the above approximation suggests that we may take advantage of the wealth of results available for linearly viscous polycrystals (mathematically analogous to linear elastic polycrystals) to obtain, via (3.15), corresponding results for nonlinear polycrystals.

In passing, we note that the stress potentials $u_0^{(r)}$ of the phases of the linear comparison polycrystal, as characterized by (3.11), may be expressed alternatively in terms of fourth-order (viscous) compliance tensors $M_0^{(r)}$, such that (see (3.11))

$$
\begin{align*}
u_0^{(r)}(\sigma) & = \frac{1}{2} \sigma \cdot (M_0^{(r)} \sigma), \\
M_0^{(r)} & = 2 \sum_{k=1}^{K} \alpha_{(k)}^{(r)} \mu_{(k)}^{(r)} \otimes \mu_{(k)}^{(r)}.
\end{align*}
$$

(3.16)

(3.17)
Thus, the linear comparison polycrystal may be characterized as a heterogeneous material with compliance tensor $M_{ij}^{(r)}$ in phase $r$. This observation partly justifies the labelling of the optimization variables $\alpha_{(k)}^{(r)}$ as slip system compliances.

We conclude this section by recalling that an expression for a lower bound for the effective potential of heterogeneous materials with anisotropic phases was obtained by Willis (1991), extending previous results of Ponte Castañeda (1991). In this expression, which is also given in terms of an optimization problem over the properties of a linear heterogeneous comparison material, $21N$ optimization variables are required since the phases in the linear comparison are completely arbitrary. On the other hand, expression (3.15) for the lower bound is given in terms of $N \times K$ optimization variables, and thus, for example, when dealing with aggregates of rcc crystals with $K = 12$ and large number of phases, the prescription given here is more efficient. Another advantage in favour of (3.15) becomes evident when making the common choice of power-law behaviour for the slip potential functions $\phi_{(k)}^{(r)}$ (see (3.3)). This is because the functions $V_{(k)}^{(r)}$, as defined by (3.7), can be determined explicitly in this case, whereas the corresponding functions in the prescription of Willis (1991) are determined instead in terms of $N$ sets of non-trivial six-dimensional optimization problems (which, in general, would require numerical computation).

4. Application of the variational procedure to the computation of bounds

In this section, we apply the variational procedure developed in the previous section to obtain bounds for the effective potential of classes of nonlinear polycrystals from bounds for corresponding classes of linear polycrystals. We first recall the classical bounds of Taylor (1938) and Bishop & Hill (1951) for the class of nonlinear polycrystals with overall isotropic properties (no texture), as extended by Hutchinson (1976) to nonlinear creep. These bounds may be obtained directly from the classical minimum energy principles, and constitute direct extensions of the Voigt–Reuss bounds for linear elastic polycrystals, first proved by Hill (1952). We then show that the classical nonlinear bounds may also be obtained from the corresponding linear bounds via the new variational procedure. (In passing, a new, simple form is derived for the classical Taylor–Bishop–Hill bound.) This serves to demonstrate that the new variational procedure can deliver at least the same amount of information as the classical variational principles. However, the new variational procedure has the capability of delivering other types of bounds and estimates that are not directly available by the classical methods. Thus, we obtain a new lower bound for the stress potential of the class of untextured nonlinear polycrystals with a statistically isotropic geometric arrangement of the phases, as characterized by the two-point probability functions of the microstructure of the polycrystals. The starting point is provided by the Hashin–Shtrikman (HS) lower bounds for linear composites with prescribed two-point correlation functions of Willis (1977). We recall from the Introduction that a nonlinear bound of this type has been obtained earlier by Dendievel et al. (1991), but using instead the variational procedure of Talbot & Willis (1985). Additional bounds of this type were also obtained by Bonnet et al. (1991), but these bounds were found to be weaker than those of Dendievel et al.

(a) The classical bounds

It is well known that an upper bound $\bar{U}^{(R)}$ may be obtained for the effective stress potential $\bar{U}$ of the class of polycrystals with $N$ phases in prescribed volume fractions $c^{(r)}$ (and no other assumptions about the microstructural distribution of the phases), directly from the minimum complementary-energy representation (2.14), by selecting a constant trial field $\sigma(x) = \bar{\sigma}$. The result is

$$\bar{U}^{(R)}(\bar{\sigma}) = \sum_{r=1}^{N} c^{(r)} u^{(r)}(\bar{\sigma}). \quad (4.1)$$

We note that, in practice, the volume average implied by (4.1) is replaced by an orientation average over all possible orientations of the reference crystal. The result may again be expressed in the form (4.1), where the ‘volume fractions’ $c^{(r)}$ now represent weight factors associated with the textures (preferred orientations) of the polycrystal. As discussed in §2, however, in this paper, we are only concerned with isotropic polycrystals (i.e., with no texture), and so the $c^{(r)}$ may be selected equal to $N^{-1}$. We also note that the above bound, when specialized to linear polycrystals, states the fact that the effective compliance of the polycrystal is bounded above by the arithmetic average of the compliance.

Similarly, an upper bound $\bar{W}^{(V)}$ may be obtained for the effective strain-rate potential $\bar{W}$ of the class of polycrystals with $N$ phases in prescribed volume fractions $c^{(r)}$ by choosing the uniform trial strain-rate field $\epsilon(x) = \bar{\epsilon}$ in (2.18), to obtain

$$\bar{W}^{(V)}(\bar{\epsilon}) = \sum_{r=1}^{N} c^{(r)} w^{(r)}(\bar{\epsilon}), \quad (4.2)$$

where $w^{(r)}$ denotes the strain-rate potential of phase $r$. This result may be rewritten as a lower bound for effective stress potential $\bar{U} = \bar{W}^{*}$ of the composite, in terms of the phase stress potentials $u^{(r)}$. The result is

$$\bar{W}^{(V)}(\bar{\sigma}) = \left( \sum_{r=1}^{N} c^{(r)} (u^{(r)})^* \right)^*(\bar{\sigma}). \quad (4.3)$$

As was the case for the Reuss upper bound for $\bar{U}$, the average operations in (4.2) and (4.3) are interpreted as orientation averages in practice. In the linear context, the above result states that effective compliance of the polycrystal is bounded by the harmonic average of the compliance of the constituent grains.

In the following discussion, we present an alternative derivation of the above uniform-strain-rate bound. The purpose will be not only to demonstrate that the new variational representation (3.15) may be used to obtain the classical lower bound for $\bar{U}$, but also to obtain an alternative form for this lower bound, which will be used in the next section.

To be able to generate a lower bound for $\bar{U}$ from (3.15) for the class of nonlinear polycrystals with $N$ phases in prescribed volume fractions $c^{(r)}$, we require a bound for the effective potential $\bar{U}_0$ of the corresponding class of linear polycrystals (with the same microstructures). Such a lower bound is given by

$$\bar{U}_0^{(V)}(\bar{\sigma}) = \frac{1}{2} \bar{\sigma} \cdot (\bar{M}_0^{(V)} \bar{\sigma}), \quad (4.4)$$

where, as mentioned above,

$$\bar{\mathbf{M}}_0^{(V)} = \left[ \sum_{r=1}^{N} c^{(r)} (\mathbf{M}_0^{(r)})^{-1} \right]^{-1},$$

and where we denote by $\mathbf{M}_0^{(r)}$ the fourth-order compliance tensor associated with $u_0^{(r)}$, as given by (3.16) and (3.17). This is, of course, the same result that would be obtained by specializing (4.3) to the linear case. In fact, directly from that result, specialized to the linear case, we obtain

$$\bar{U}_0^{(V)}(\bar{\sigma}) = \sup_{\bar{\varepsilon}} \left\{ \bar{\varepsilon} \cdot \bar{\sigma} - \left[ \sum_{r=1}^{N} c^{(r)} \sup_{\sigma^{(r)}} \left[ \bar{\varepsilon} \cdot \sigma^{(r)} - u_0^{(r)}(\sigma^{(r)}) \right] \right] \right\},$$

which, in turn, may be rewritten as

$$\bar{U}_0^{(V)}(\bar{\sigma}) = \sup_{\bar{\varepsilon}} \inf_{\sigma^{(1)}, \ldots, \sigma^{(N)}} \left\{ \bar{\varepsilon} \cdot \left[ \bar{\sigma} - \sum_{r=1}^{N} c^{(r)} \sigma^{(r)} \right] + \sum_{r=1}^{N} c^{(r)} u_0^{(r)}(\sigma^{(r)}) \right\}.$$  \hfill (4.7)

It then follows, by interchanging the order of the supremum and the infima (allowed by the saddle point theorem since the expression inside the curly brackets is concave in $\bar{\varepsilon}$ and convex in the $\sigma^{(r)}$), that

$$\bar{U}_0^{(V)}(\bar{\sigma}) = \inf_{\sigma^{(1)}, \ldots, \sigma^{(N)}} \left\{ \sum_{r=1}^{N} c^{(r)} u_0^{(r)}(\sigma^{(r)}) \right\},$$

Thus, we have replaced the harmonic-type average associated with (4.5) by an arithmetic-type average, at the expense of introducing an $N$-dimensional optimization problem, with a simple linear constraint in the optimization variables $\sigma^{(r)}$. The advantages of this type of transformation, first used by deBotton & Ponte Castañeda (1992) in connection with the development of nonlinear bounds for locally isotropic composites, are discussed in that reference.

Given expression (4.8) for the lower bound for the effective potential $\bar{U}_0$ of the pertinent class of linear comparison polycrystals, we may now make use of representation (3.15) to obtain a corresponding lower bound for the effective potential $\bar{U}$ of the class of nonlinear polycrystals with identical microstructures.

Thus, we may write

$$\bar{U}(\bar{\sigma}) \geq \sup_{\alpha^{(r)}(i) \in 0 \atop s=1, \ldots, N \atop i=1, \ldots, K} \left\{ \inf_{\sigma^{(1)}, \ldots, \sigma^{(N)}} \left[ \sum_{r=1}^{N} c^{(r)} \left( u_0^{(r)}(\sigma^{(r)}) - \sum_{k=1}^{K} V^{(r)}_{(k)} (\alpha^{(r)}(i)) \right) \right] \right\},$$

which in turn may be rewritten, again by virtue of the saddle point theorem (since the expression inside the curly brackets is concave in the variables $\alpha^{(r)}(i)$ and $\alpha^{(r)}(j)$),
convex in the $\sigma^{(r)}$, as

$$
\bar{U}(\bar{\sigma}) \geq \inf_{\sigma^{(1)}, \ldots, \sigma^{(N)}} \left\{ \sum_{r=1}^{N} c^{(r)} u^{(r)}(\sigma^{(r)}) \right\},
$$

(4.10)

where we have additionally made use of relations (3.8) and (3.11).

However, by following, in reverse order, the procedure that led from (4.3) to (4.8), for the linear polycrystals, we observe that the lower bound given by (4.10), for the nonlinear polycrystal, is precisely the nonlinear uniform strain-rate bound $\bar{U}^{(V)}$ of (4.3). Thus, we have shown that the classical nonlinear lower bound for $\bar{U}$ may be obtained, via the new variational procedure, by means of the corresponding classical linear bound for $\bar{U}_0$. It is important to note that the derivation required the use of the full set of optimization variables $\alpha^{(r)}_{\alpha}$ in the context of the variational statement (3.15) (i.e. the slip compliances within each grain and for each slip system are generally distinct). If, instead, it is assumed $a$ priori that the slip compliances are the same, even if it is only for the same slip system in different grains, or for different slip systems in the same grain, the above demonstration would fail, and a bound that is strictly weaker than the Taylor bound would result. Similarly, it may be shown that the classical nonlinear upper bound may also be obtained from the corresponding linear bound. In this case, we need to make use of the exact version of the variational principle (3.13), instead of the approximate version (3.15).

Finally, we remark that the expression (4.10) for the classical lower bound of the nonlinear polycrystals is significantly simpler than the equivalent expression (4.3); this is because (4.10) involves a $6N$-dimensional optimization problem, with a simple linear constraint, instead of the $6(N+1)$-dimensional optimization problem implied by (4.3). In fact, the linear constraint may be easily embedded in the optimization problem (4.10) to further reduce its order by one (to $6(N-1)$).

(b) Hashin–Shtrikman lower bound

Our goal in this section is to obtain a lower bound for the effective stress potential of the class of untextured nonlinear polycrystals, with statistically isotropic geometric arrangement of the constituent phases. More specifically, we assume that all crystal orientations are equally likely, and that the two-point probability functions, characterizing the geometric arrangement of its phases in the polycrystal, are isotropic. We emphasize that overall isotropy does not necessarily imply a statistically isotropic arrangement of the phases within the polycrystal; see Schulgasser (1977) for an example of an anisotropic polycrystal, in the context of linear conductivity, lacking statistical isotropy (for the geometric arrangement of the phases). Further, it is well known in the linear context (see Willis 1981) that the specification of the two-point correlation functions in the variational principles of Hashin & Shtrikman (1962a, b) leads to bounds that are tighter than the corresponding classical bounds, which in turn do not utilize such higher-order statistical information. Thus, we will make use of the variational representation (3.15), together with a lower bound for the class of linear heterogeneous materials with a random distribution (and isotropic two-point correlation functions) of $N$ distinct phases with compliance tensors $\mathbf{M}_0^{(r)}$ as given by relation (3.17), to

generate the corresponding nonlinear bounds. The lower bound for the effective potential of such a class of linear comparison polycrystals may be written as (see Walpole 1969; Willis 1981)

\[ \hat{U}_0^{(\text{HS})}(\tilde{\sigma}) = \frac{1}{2} \tilde{\sigma} \cdot (\tilde{M}_0^{(\text{HS})} \tilde{\sigma}), \]  

(4.11)

where

\[ \tilde{M}_0^{(\text{HS})} = \left[ \sum_{r=1}^{N} c^{(r)} \left[ M_0^{(r)} + M_0^* \right]^{-1} \right]^{-1} - M_0^*, \]  

(4.12)

and where

\[ M_0^* = Q_0^{-1} - M_0. \]  

(4.13)

In this last relation, \( M_0 \) is an isotropic tensor, with shear and bulk moduli \( \mu_0 \) and \( \kappa_0 \), respectively, satisfying the restrictions

\[ \frac{1}{2} \tilde{\sigma} \cdot (M_0 \tilde{\sigma}) \leq u_0^{(s)}(\tilde{\sigma}) \quad (s = 1, \ldots, N), \]  

(4.14)

for all symmetric tensors \( \tilde{\sigma} \). In addition, the tensor \( Q_0 \) is also isotropic (because of the hypothesis of statistical isotropy for the geometric arrangement of the phases; see Willis 1981) and may be expressed, taking advantage of the notation of Hill (1965), in the form

\[ Q_0 = \begin{pmatrix} \frac{12 \kappa_0 \mu_0}{3 \kappa_0 + 4 \mu_0} & \frac{2 \mu_0 (9 \kappa_0 + 8 \mu_0)}{5 (3 \kappa_0 + 4 \mu_0)} \end{pmatrix}. \]  

(4.15)

Before proceeding with the nonlinear polycrystals, it is useful to notice that the nonlinear polycrystals, and hence the linear comparison polycrystals, are incompressible. Because of this, we may take \( M_0 \) to be an isotropic, incompressible (i.e. \( \kappa_0 = \infty \)) tensor with shear modulus \( \mu_0 \) satisfying the inequalities

\[ \frac{1}{6 \mu_0} \sigma_e^2 \leq u_0^{(s)}(\tilde{\sigma}) \quad (s = 1, \ldots, N), \]  

(4.16)

for all symmetric tensors \( \tilde{\sigma} \), where \( \sigma_e = \sqrt{\frac{2}{3}} s \cdot s \) is the equivalent tensile stress and \( s \) the stress deviator tensor associated with \( \tilde{\sigma} \) (i.e. \( s = \tilde{\sigma} - \sigma_m I \), where \( \sigma_m \) denotes the hydrostatic stress and \( I \) the identity tensor). It follows that \( M_0^* \) may be simplified to take the form

\[ M_0^* = \begin{pmatrix} 1 & 1 \\ 4 \mu_0 & 3 \mu_0 \end{pmatrix}. \]  

(4.17)

Expression (4.11), together with (4.12) and (4.17), serves to characterize the bound for the effective potentials of the class of linear comparison polycrystals to be used in conjunction with (3.15) and (3.7) to determine the corresponding bound for the nonlinear polycrystals. We note that condition (4.16) must be enforced to ensure that the resulting expression is indeed a bound; the best bound is obtained by choosing \( \mu_0 \) according to

\[ \frac{1}{\mu_0} = 6 \min_{s=1,\ldots,N} \left\{ \inf_{\tilde{\sigma}} \left[ \sum_{k=1}^{K} \alpha^{(s)}_k \left( \tilde{\sigma} \cdot \mu^{(s)}_k \right)^2 \right] \right\}. \]  

(4.18)

We further note (see also Dendievel et al. 1991) that the resulting nonlinear

lower bound also holds for textured polycrystals, if the phase volume fractions \( c^{(s)} \) are chosen such that certain crystal orientations are more likely than others. In addition, we note that an anisotropic lower bound could be obtained for the polycrystals, even when all crystal orientations are equally likely, if the two-point probability functions, further characterizing the geometric arrangement of the phases within the polycrystal, were chosen to be anisotropic (Willis (1977), for example, gives general linear bounds for composites with ‘ellipsoidal’ two-point probability functions).

(c) Comments regarding possible simplifications of the Hashin–Shtrikman lower bound

In this section, we mention briefly some possible simplifications, that were tried in the course of this work, of the result discussed in the previous section for the HS lower bound. The first such possibility is concerned with the determination of \( \mu_0 \) from expression (4.18); it follows trivially from this expression that

\[
\frac{1}{\mu_0} \geq 6 \min_{s=1, \ldots, N} \left\{ \left\{ \alpha^{(s)}_{(l)} \right\} \inf_{\sigma_k} \sum_{k=1}^{K} (\sigma \cdot \mu_{(k)})^2 \right\}.
\]

The use of the right-hand side of this inequality in place of expression (4.18) for \( \mu_0 \) simplifies the computation of the HS bound, at the expense of weakening it. However, it was found that, while this approximation was rather innocuous for small values of the creep exponent \( n \), it led to significantly weaker results for large values of \( n \). Because of this, we did not make use of this approximation in the results presented in the next section for power-law FCC polycrystals.

Another possibility for simplifying the computation of the HS bound is to reduce the number of optimization variables \( \alpha^{(r)}_{(k)} \) in expression (3.15); this, of course, preserves the inequality, but it makes it less sharp. In general, the more restrictions we add, the weaker the associated bounds become. Since in this work we are mostly concerned with polycrystals with identical grains and ‘isotropic hardening’, we may let all the slip system compliances in expression (3.15) be identical in each grain and for all the slip systems (i.e. \( \alpha^{(r)}_{(k)} = \alpha \) for all \( r = 1, \ldots, N \) and \( k = 1, \ldots, K \)). Under this restriction, the following lower bound for the effective potential of polycrystals is obtained, namely,

\[
\tilde{U}(\sigma) \geq \sup_{\alpha \geq 0} \left\{ \tilde{U}_0(\sigma) - KV(\alpha) \right\},
\]

where \( \tilde{U}_0 \) may be chosen to correspond to a HS bound for the effective potential of a linear comparison polycrystal with identical grains and isotropic hardening.

(By contrast, in the previous section we required HS bounds for the class of linear comparison polycrystals with generally distinct grains and different slip compliances for each grain, even if all the grains and slip compliances for the nonlinear polycrystal are identical.) However, again in the context of the power-law polycrystals discussed in the next section, this approximation leads to bounds that become progressively weaker (relative to the ‘exact’ bound of the previous section) with increasing nonlinearity. We remark that such weaker bounds are closely related to the so-denoted ‘Ponte Castañeda bounds’ of Bonnet et al. (1991). The present discussion makes it clear that the relative weakness of such bounds arises from the fact that the class of slip compliances considered by these authors is
not large enough to capture the significantly locally anisotropic behaviour of the nonlinear polycrystal.

5. Application to power-law creeping FCC polycrystals

Here we apply the results of the previous section to obtain bounds for the effective creep behaviour of the class of untextured, statistically isotropic FCC polycrystals, with ‘isotropic hardening’ of the power-law type. Thus, we deal with polycrystalline aggregates made up of randomly oriented, and distributed FCC crystals, each of which may undergo creep on a set of twelve crystallographic slip systems. The slip systems of the reference FCC single crystal are determined by four slip planes of the \( \{1,1,1\} \) type and three slip directions (per plane) of the \( (1,1,0) \) type, which in turn serve to determine, via relation (2.1), the 12 possible values of the tensor \( \mu_{(k)} \).

Because of the assumption of ‘isotropic hardening’ for the constituent crystals, the reference stresses associated with the slip potentials of the identical single crystal grains, as given by relations (3.3), are taken to be equal (i.e. \( \tau_0 = \tau_0 \)). Of course, the creep exponent \( n \) is also the same for all the slip systems and all the grains in the polycrystal. This means that the effective potential of the polycrystal \( \hat{U} \) must be a homogeneous function of degree \( n + 1 \) in the average stress \( \bar{s} \). In addition, since the polycrystal is isotropic and incompressible, \( \hat{U} \) must depend on \( \bar{s} \) only through the two invariants of the stress deviator \( \hat{s} \), namely, \( \hat{\sigma}_e = \sqrt{\left( \frac{3}{2} \hat{s} \cdot \hat{s} \right)} \) and \( \hat{\sigma}_d = \frac{3}{2} \left[ \frac{1}{3} \text{det}(\hat{s}) \right]^{1/3} \). (Note that, in particular, \( \hat{U} \) is independent of the hydrostatic stress \( \hat{\sigma}_m = \frac{1}{3} \text{tr} \hat{\sigma} \).) It follows that the effective potential of the polycrystal may be written in the form

\[
\hat{U}(\bar{s}) = \frac{\gamma_0 \bar{\tau}_0}{(n + 1)} \left( \frac{\hat{\sigma}_e}{\bar{\tau}_0} \right)^{n+1}, \tag{5.1}
\]

where the effective reference stress for the polycrystal, denoted \( \bar{\tau}_0 \), is a function of the dimensionless ratio \( \bar{\rho} = \hat{\sigma}_d / \hat{\sigma}_e \) only. It can be shown (see Dendievel et al. (1991)) that \( \bar{\rho} \) must lie in the interval \([0, 1]\), with the endpoints 0 and 1 corresponding to the stress states of pure shear and uniaxial tension, respectively. In conclusion, we may now characterize the lower/upper bounds for \( \hat{U} \), discussed in the previous section, in terms of upper/lower bounds for the effective reference stress \( \bar{\tau}_0 \), as a function of the ratio \( \bar{\rho} \).

Figure 1a, b presents results for various bounds and estimates, in terms of the normalized reference stress \( \bar{\tau}_0 / \tau_0 \), plotted as a function of \( 1/n \), for uniaxial tension (\( \bar{\rho} = 1 \)) and simple shear (\( \bar{\rho} = 0 \)), respectively. The dashed top and bottom curves correspond to the Taylor and Reuss bounds, respectively, as computed from expressions (4.1) and (4.10) of § 4 a. These curves were obtained by considering 648 different orientations for the constituent grains. We note that progressively larger numbers of orientations were necessary to ensure the accuracy of the results for increasing values of the creep exponent. For comparison with our results, we include in figure 1a, b the results for the Taylor bound for perfectly plastic polycrystals of Bishop & Hill (1951b) (dark triangles), the results for the Taylor bound for power-law hardening polycrystals of Hutchinson (1976) (clear triangles) and the results for the Reuss bound of Dendievel et al. (1991) (inverted...
clear triangles). Thus, we observe that our results for the classical bounds are in good agreement with those of other authors.

The continuous lines in figure 1 correspond to the new HS upper bound for $\bar{\tau}_0$, computed using the procedure indicated in § 4 b. These results were obtained using up to 648 different orientations for the single crystal grains, and they agree with the linear HS upper bound given by Hutchinson (1976), in the limit as $n \to 1$. We observe that this upper bound lies between the classical bounds of Taylor and Reuss, but is much closer to the Taylor bound. In fact, we find that the HS upper bound becomes very close to the Taylor bound in the limit as $n \to \infty$ (i.e. in the rigid/perfectly plastic limit). For comparison, we also include in figure 1 some selected results for the HS bound of Dendievel et al. (1991) (actually taken from Bonnet et al. 1991) (squares), as well as the self-consistent estimates of Hutchinson (1976) (circles).

By comparison to the results of Dendievel et al., we observe that our results for the HS bound are in good agreement with theirs for relatively small values of the creep exponent. However, figure 1 of Dendievel et al. (1991) shows that, in tension, their results for the HS bound become virtually indistinguishable from the Taylor-bound results for values of $n$ greater than about 4, whereas we observe from figure 1a (of the present work) that our results for the HS bound are clearly distinguishable from the Taylor-bound results for values of $n$ up to 10. This shows that our HS bound is actually stronger, if only slightly so, than the corresponding bound of Dendievel et al. One possible explanation for this is, of course, the fact that the two bounds are obtained by different methods; however, it is known that the two methods give the same bounds of the HS type, at least for locally isotropic composites with power-law viscous behaviour. A more likely reason for the different predictions is related to a certain approximation introduced by Dendievel et al. to facilitate the computation of their HS bound. This

Variational estimates for creep behaviour

Figure 2. Results for the new HS upper bound for the effective reference stress $\tau_0$ of isotropic FCC polycrystals plotted as functions of $\bar{\rho} = \sigma_\infty/\sigma_0$, for four different values of the creep exponent $n$ (1, 2, 5 and 8).

approximation consists in the replacement of the lower convex envelope of the sum of some functions by the sum of their respective envelopes, which in general would lead to a weaker result. However, we emphasize that the differences between the two bounds are relatively small, so that the approximation introduced by Dendievel et al. appears to be rather sharp. Regarding the self-consistent estimates of Hutchinson (1976) for $\tau_0$ (given only for tensile loading), we note that they are fairly close to our HS bounds, but more importantly, they do not appear to violate these bounds for the whole range of $n$.

Finally, figure 2 shows results for our HS upper bounds, in the form of plots of the effective reference stress $\tau_0$ for the isotropic FCC polycrystals as functions of $\bar{\rho}$, for four different values of the creep exponent $n$. We observe that for low values of the creep exponent the curves exhibit low sensitivity to the magnitude of $\bar{\rho}$ (of course, in the limit as $n \to 1$, the HS bounds must become independent of $\bar{\rho}$). On the other hand, the dependence of the bounds for $\tau_0$ on $\bar{\rho}$ becomes more noticeable for larger values of the creep exponent; however, even for $n = 8$ the variation of the HS upper bound is less than 5%.

6. Concluding remarks

The main contribution of this paper is the development of an extension of the variational procedure of Ponte Castañeda (1991, 1992a), for nonlinear heterogeneous media with locally isotropic behaviour, to nonlinear media with locally anisotropic behaviour. The result is expressed as a finite-dimensional optimization problem over $N \times K$ variables, which correspond to the 'slip compliances' of a linear comparison polycrystal with $N$ different crystals and $K$ distinct slip systems (for each crystal). The procedure was applied to the class of FCC polycrystals with identical power-law creep rules for each slip system. Under the assumption that the polycrystals exhibit no texture (i.e. no preferred orientations), the classical Taylor–Bishop–Hill bounds of Hutchinson (1976) for power-law polycrystals were reproduced. In addition, bounds of the Hashin–Shtrikman type for the nonlinear polycrystals were computed under the additional assumption of.

statistical isotropy (i.e. isotropic two-point correlation functions). These Hashin–Shtrikman bounds were found to be tighter than other bounds of this type, previously determined by Dendievel et al. (1991), using an alternative procedure based on the work of Talbot & Willis (1985). However, the difference between the two sets of bounds was small and only noticeable for relatively large values of the creep exponent. Finally, it was found that the self-consistent estimates of Hutchinson (1976) for power-law polycrystals not only appear to satisfy the Hashin–Shtrikman bounds, but also that they are rather close to these bounds. However, it is important to note that the self-consistent procedure of Hutchinson for creep of polycrystals, in its (simpler) ‘total’ formulation, relies critically on the assumptions of pure power-law behaviour for the constituent grains, whereas the present procedure may be applied equally well to polycrystals with more complex behaviour for the constituent grains. In particular, this would be useful in the analysis of polycrystalline aggregates of single crystals exhibiting different types of slip systems (i.e. slip systems with essentially different creep rules, with different powers, for example). In addition, the new procedure may be used for general loading conditions, including simple shear, and may also account for texture in an approximate way (see also Dendievel et al. 1991).

We conclude by remarking the curious result (see also Hutchinson 1976; Dendievel et al. 1991) that both the Hashin–Shtrikman bounds and self-consistent estimates become virtually indistinguishable from the Taylor estimate in the limit as the creep exponent becomes large (corresponding to rigid/perfectly plastic behaviour), at least for FCC polycrystals with identical hardening for all slip systems. Indeed, it is known that the Taylor estimate for the effective yield stress of rigid/perfectly plastic FCC polycrystals (in uniaxial tension, approximately three times the yield stress of the typical slip system) is a rigorous upper bound for untextured polycrystals. On the other hand, Bishop & Hill (1951b) also provided a rigorous lower bound for this class of FCC polycrystals (in uniaxial tension, two times the yield stress of the typical system). Therefore, it would seem reasonable to expect that the incorporation of additional morphological information into a bound or estimate for the effective yield strength of such a class of polycrystals would lead to results that lie somewhere in between the two classical bounds. The fact that, at least for FCC polycrystals, neither the Hashin–Shtrikman upper bound developed here (or that of Dendievel et al.), which includes additional two-point statistical information, nor for the self-consistent estimate of Hutchinson, which also includes additional morphological information, appear to improve on the Taylor bound is unexpected. It remains to verify whether this result is specific to aggregates of fairly ductile single crystals, such as FCC crystals, or whether similar results would be obtained for other less ductile types of polycrystals, such as ionic polycrystals. Calculations for this type of polycrystals are currently in progress. In addition, it also remains to consider the application of the present variational procedure to other types of bounds and estimates for polycrystalline materials, incorporating alternative types of information about the microstructural distribution of the grains in the polycrystal.

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G. deBotton and P. Ponte Castañeda


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