Bounds and estimates for the overall plastic behaviour of composites with strain gradient effects

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The macroscopic plastic response is estimated for a composite with each phase satisfying a strain gradient constitutive description. In a $J_2$ deformation theory of strain gradient plasticity, the strain energy function is assumed to depend on both the von Mises strain invariant $\varepsilon_e$ and on a curvature invariant $\chi_e$. For a general coupling between $\varepsilon_e$ and $\chi_e$, a nonlinear variational principle is formulated generalizing that of Ponte Castañeda (1992 J. Mech. Phys. Solids 40, 1757). The minimum principle is used to derive bounds and estimates for the overall plastic response of statistically homogeneous and isotropic strain gradient composites. An essential ingredient of the strategy is the use of previous results of the authors (1994 J. Mech. Phys. Solids 42, 1851) for a linear comparison composite. For a particular coupling between $\varepsilon_e$ and $\chi_e$, suggested earlier by Fleck & Hutchinson (1993), the Hashin–Shtrikman upper bounds and lower estimates are calculated for a power-law hardening solid (including the rigid–perfectly plastic limit). The results demonstrate a size effect.

1. Introduction

The size effect observed in plasticity is usually modelled by including gradients of strain in the constitutive law (Aifantis 1984; Muhlhaus & Aifantis 1991; Zbib & Aifantis 1992; Fleck & Hutchinson 1993; Fleck et al. 1994). This has the effect of introducing a material length scale $l$ into the constitutive relations.

If such theories are used to derive a macroscopic plastic response of a microscopically heterogeneous composite, it should be expected that the response will depend on the competition between two length scales: the ‘intrinsic’ length scale $l$ and the scale of the microstructure $a$. The overall properties of the composite are functions of $l/a$, which reflects the size effect. The purpose of this paper is to study the macroscopic plastic response of composites whose phases satisfy a $J_2$ deformation theory of strain gradient plasticity. In this theory, it is assumed that the strain energy density depends on both the von Mises strain invariant $\varepsilon_e$ and on a curvature invariant $\chi_e$. A physical interpretation of this constitutive law has been given by Fleck et al. (1994).

Much progress has been made on the bounding and estimating of macroscopic properties of composites: this work has focused on conventional constitutive laws.

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which do not account for gradient effects. Most of these bounding techniques are based on new variational methods laid down by Hashin & Shtrikman (1962, 1963) for linear problems, and developed further by Willis (1983), Talbot & Willis (1985), Ponte Castañeda (1991, 1992), Willis (1991) and Talbot & Willis (1994a, b) to include nonlinear effects. These methods have been developed further to address specifically problems of determining the effective plastic behaviour of heterogeneous materials (Ponte Castañeda & De Botton 1992; Suquet 1993; Olson 1994). These homogenization methods are based on constitutive descriptions which contain no length scale and give, therefore, predictions which are independent of the scale of the microstructure.

In our recent paper (Smyshlyaev & Fleck 1994) we have suggested an extension of the Hashin–Shtrikman procedure to include strain gradient effects for linear composites. In the present paper we employ these results to derive upper bounds and (lower) estimates for the overall plastic response of statistically homogeneous and isotropic strain gradient composites. Our construction is based on a nonlinear variational principle (§3) generalizing that of Ponte Castañeda (1992) for $J_2$ strain gradient solids. Upon solving a one-dimensional optimization problem by numerical means, we obtain upper bounds for the effective parameters of the composite with power-law hardening. In the limit of a rigid–perfectly plastic solid, an explicit upper bound is achieved for the yield strength of the composite.

Estimates for the effective parameters are also derived by making use of the linear Hashin–Shtrikman lower bounds for the comparison solid. The results of the study demonstrate a size effect for the plastic response of two-phase composites. These results agree with those obtained by Ponte Castañeda (1992), Ponte Castañeda & De Botton (1992) and Suquet (1993) in the limiting case of a conventional solid where strain gradient effects vanish.

2. Formulation

(a) Basic equations

We consider a heterogeneous nonlinear ‘strain gradient’ solid occupying a volume $V$ with boundary $S$. In a deformation theory of strain gradient plasticity, the strain energy density $\psi$ at each point $x$ of $V$ is assumed to depend upon both the strain tensor $\varepsilon$ and the curvature tensor $\chi$. The tensors $\varepsilon$ and $\chi$ are derived kinematically from the displacement field $u$ and the rotation field $\Theta$ via

$$
\varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}), \quad \chi_{ij} = \theta_{i,j},
$$

where $\theta$ in turn is derived from the displacement as $\theta_i = \frac{1}{2} \varepsilon_{ijk} u_{k,j}$, i.e. $\Theta = \frac{1}{2} \text{curl}(u)$. Simple manipulations give

$$
\chi_{ij} = \varepsilon_{ikl} \varepsilon_{jl,k},
$$

which means that both the strain and certain combinations of the strain gradient are involved in the constitutive description. Note that the rotation $\theta$ is the material rotation: we are concerned with the so-called reduced couple stress theory.

A strain gradient analogue of $J_2$ theory for isotropic and incompressible solids assumes that $\psi$ depends only on the von Mises strain invariant

$$
\varepsilon_e = \sqrt{\frac{2}{3} \varepsilon_{ij} \varepsilon_{ij}}
$$

and curvature invariants. Since the curvature tensor $\chi$ is unsymmetric, it has, in

fact, two independent $J_2$ invariants

$$\chi^e = \sqrt{\frac{2}{3} \chi^{s}_i \chi^{s}_j} \quad \text{and} \quad \chi^a = \sqrt{\frac{2}{3} \chi^{a}_i \chi^{a}_j},$$

according to decomposition of $\chi$ into the symmetric part $\chi^{s}$ and the antisymmetric part $\chi^{a}$

$$\chi^{s}_{ij} = \frac{1}{2} (\chi_{ij} + \chi_{ji}), \quad \chi^{a}_{ij} = \frac{1}{2} (\chi_{ij} - \chi_{ji}).$$

In order to deal with a single length scale within the constitutive law, we assume that there is no dependence of $w$ on the antisymmetric component $\chi^{a}$, so that

$$w = w(x; \varepsilon_e, \chi^{s}_e).$$

(2.1)

A dependence of $w$ upon both $\chi^{s}$ and $\chi^{a}$ can be developed without serious difficulties, but at the expense of unnecessary complication. In the remainder of the paper (2.1) is enforced; the superscript ‘s’ is omitted and the symmetric curvature is introduced as

$$\chi_{ij} = \frac{1}{2} (\theta_{i,j} + \theta_{j,i}) = \frac{1}{2} (e_{i,k} \varepsilon_{j,k} + e_{j,k} \varepsilon_{i,k}).$$

It is further supposed that the function $w$ is smooth and convex in $\varepsilon_e$ and $\chi_e$, for each $x \in V$. The deviatoric stress $s$ and couple stress $m$ are defined as work conjugates of $\varepsilon$ and $\chi$ respectively:

$$s_{ij} = \frac{\partial w}{\partial \varepsilon_{ij}} = \frac{2}{3} \frac{\partial w}{\partial \varepsilon_e} \cdot \varepsilon_{ij}, \quad m_{ij} = \frac{\partial w}{\partial \chi_{ij}} = \frac{2}{3} \frac{\partial w}{\partial \chi_e} \cdot \chi_{ij}.$$

(2.2)

We shall make extensive use of a power-law description along the lines of that given by Fleck & Hutchinson (1993), so that

$$w(\varepsilon_e, \chi_e) = \frac{n}{n+1} \Sigma_0 \varepsilon_0 \left( \frac{\mathcal{E}(\varepsilon_e, \chi_e)}{\varepsilon_0} \right)^{(n+1)/n},$$

(2.3)

where $\chi_e \equiv \chi^{s}_e$ and

$$\mathcal{E} = (\varepsilon_e^2 + l^2 \chi_e^2)^{1/2}.$$  

(2.4)

The scalar strain measure $\mathcal{E}$ is a natural measure of total dislocation density, as discussed by Fleck et al. (1994). In (2.4), $l$ is an ‘intrinsic’ material length scale interpreted as a free slip distance between statistically stored dislocations; $n$ is the hardening index and ranges from unity to infinity. In particular, for the linear case, $n = 1$ and (2.3) assumes the form

$$w_L(\varepsilon_e, \chi_e) = \frac{3}{2} \mu \mathcal{E}^2 = \frac{3}{2} \mu \varepsilon_e^2 + \frac{3}{2} \mu l^2 \chi_e^2$$

(2.5)

and

$$s_{ij} = 2 \mu \varepsilon_{ij}, \quad m_{ij} = 2 \mu l^2 \chi_{ij}.$$  

(2.6)

Note that assumption (2.1) implies that $m$ is symmetric.

It is also natural to introduce a kinematic assumption of continuity of the displacement $u$ and the rotation $\theta$ throughout $V$ including interfaces. This is equivalent to the statement that the phases are perfectly bonded. We call such displacement fields ‘kinematically admissible’.

Now consider the energy functional

$$W(u) = \int_V w(x; \varepsilon_e(u), \chi_e(u)) \, dx$$

within the class of kinematically admissible displacement fields, which satisfy prescribed boundary conditions. Stationarity of this functional recovers the equations of couple stress theory (see, for example, Fleck & Hutchinson 1993; Smyshlyaev & Fleck 1994). The equation of equilibrium reads

\[ \sigma_{ij,j} + \tau_{ji,j} = 0. \]

Here the symmetric part \( \sigma \) of the stress tensor is related to its deviatoric part \( s \) via

\[ \sigma_{ij} = s_{ij} + \delta_{ij}\sigma_h, \]

and \( \sigma_h(x) \) is the hydrostatic stress. The antisymmetric part \( \tau \) of the stress tensor is defined by

\[ \tau_{ji} = -\frac{1}{2} \epsilon_{kji} m_{pk,p}. \] (2.7)

Note that, in couple stress theory, (2.7) is a restatement of moment equilibrium.

Attention is focused on the response of a composite material occupying the volume \( V \), subjected to ‘uniform strain’ boundary conditions

\[ u_i = \varepsilon_{ij}^0 x_j, \quad \theta_i \equiv 0 \] (2.8)

over the boundary \( S \). The composite is regarded as a microscopically heterogeneous but macroscopically homogeneous body, with a microstructural dimension \( a \) that is small compared to the size of the volume. Therefore, \( \varepsilon^0 \) in (2.8) plays the part of a ‘macroscopic’ strain: it is the uniform strain which a homogeneous material would experience under displacement conditions (2.8). We emphasize here that under boundary conditions (2.8), the macroscopic strain is constant and therefore the macroscopic curvature is zero. The microscopic (local) curvature and couple stress, however, do not vanish.

Our objective is to deduce effective properties of the composite via an estimation of the strain energy \( \tilde{W} \) of the composite, where

\[ \tilde{W} = \int_V w(x; \varepsilon_e(x), \chi_e(x)) \, dx. \] (2.9)

This is performed using variational principles for the strain energy (2.9). We give here a brief account of available results.

(b) Minimum energy principle and the Voigt bound

A minimum principle may be stated for \( \tilde{W} \) (see, for example, Fleck & Hutchinson 1993) provided the strain energy density is strictly convex with respect to \( (\varepsilon, \chi) \) at each point \( x \in V \). This nonlinear minimum principle generalizes that given by Koiter (1964) for linear solids. It states that the ‘true’ energy \( \tilde{W} \) minimizes the functional \( W(u) \) within the class of kinematically admissible fields \( u \) satisfying the boundary conditions (2.8):

\[ \tilde{W} \leq W(u). \] (2.10)

The Voigt upper bound follows by substituting \( u^0(x) \) (see (2.8)) into the right-hand side of (2.10):

\[ \tilde{W} \leq W_V, \]

where

\[ W_V = \int_V w(x; \varepsilon^0_e, 0) \, dx. \]
For the case of an \( N \)-phase composite with the energy densities \( w_1, w_2, \ldots, w_N \) and volume fractions \( c_1, c_2, \ldots, c_N \), we have

\[
W_V = |V| \sum_{j=1}^{N} c_j w_j(x; \varepsilon_0^e, 0).
\]  

(2.11)

Consider now a two-phase power-law composite with each phase described by the energy density function (2.3), (2.4) with common hardening index \( n \) (\( 1 < n < \infty \)) and common normalizing parameter \( \varepsilon_0 \). The properties of the phases are characterized by the ‘strength’ parameters \( \Sigma_0^{(j)} \) and the length scale parameters \( l_j; j = 1, 2 \). It is also expected that the composite itself shows a power-law behaviour (2.3), (2.4) with the effective parameters \( \Sigma^*, l^* \). In particular, under the ‘uniform strain’ boundary conditions (2.8), the macroscopic strain energy \( \tilde{W} \) assumes the form

\[
\tilde{W} = |V| \frac{1}{1 + m} \Sigma^* \varepsilon_0 \left( \frac{\varepsilon_0^e}{\varepsilon_0} \right)^{1+m},
\]

where \( m \equiv 1/n \) is in the range \( 0 < m < 1 \). Then the Voigt bound (2.11) reads

\[
\Sigma^* \leq c_1 \Sigma_0^{(1)} + c_2 \Sigma_0^{(2)}.
\]

(2.13)

(c) Minimum complementary energy principle and the Reuss bound

The complementary minimum principle has also been introduced by Fleck & Hutchinson (1993). Define at each point \( x \) a stress potential \( \phi(x; \sigma, m) \) as a dual to \( w(\varepsilon, \chi) \):

\[
\phi(x; \sigma, m) = \max_{\varepsilon, \chi} \{ \sigma_{ij} \varepsilon_{ij} + m_{ij} \chi_{ij} - w(x; \varepsilon, \chi) \}. 
\]

(2.14)

Note that \( \phi \) is finite as long as \( w \) is strictly convex. Elementary considerations show that the potential \( \phi \) is a function of

\[
\sigma_e = \sqrt{\frac{3}{2} s_{ij} s_{ij}} \quad \text{and} \quad m_e = \sqrt{\frac{3}{2} m_{ij} m_{ij}},
\]

where \( \sigma_e \) is the von Mises effective stress and \( m_e \) is the analogous effective couple stress.

Consider a composite of volume \( V \) with boundary conditions

\[
n_i \sigma_{ij} + n_i \tau_{ij} = n_i \sigma_{ij}^0, \quad n_i m_{ij} = 0,
\]

(2.15)

e.i. with prescribed ‘uniform stress’ tractions on \( S \). Define the complementary energy by

\[
\Phi(\sigma, m) \equiv \int_V \phi(\sigma, m) \, dx.
\]

(2.16)

The complementary minimum principle states that, for all statically admissible fields compatible with (2.15), the ‘true’ complementary energy \( \tilde{\Phi} \) minimizes the functional (2.16):

\[
\tilde{\Phi} \leq \Phi(\sigma, m).
\]

(2.17)

The Reuss bound for \( \tilde{\Phi} \) now follows by substituting \( \sigma(x) = \sigma^0, m \equiv 0 \) into the right-hand side:

\[
\tilde{\Phi} \leq \Phi_R,
\]

where

\[
\Phi_R \equiv \int_V \phi(x; \sigma_e^0, 0) \, dx.
\]

For an $N$-phase composite
\[ \Phi_R = |V| \Sigma_j \phi_j(x; \sigma_e^0, 0), \] (2.18)
where the $\phi_j$ are defined from $w_j$ via (2.14).

For the power-law case (2.3), the stress potential for each phase reads
\[ \phi(\sigma, m) = \frac{1}{n+1} \Sigma_0 \Sigma^* \left( \frac{\Sigma}{\Sigma_0} \right)^{n+1}, \]
where
\[ \Sigma = (\sigma_e^2 + l^{-2} m_e^2)^{1/2} \]
is a scalar stress measure. Assuming that the effective strength parameter $\Sigma^*$ for the composite is determined via
\[ \tilde{\Phi} = |V| \frac{1}{n+1} \Sigma_0 \Sigma^* \left( \frac{\sigma_e^0}{\Sigma^*} \right)^{n+1}, \]
we arrive at the Reuss lower bound for an isotropic power-law composite
\[ \Sigma^* \geq \Sigma_R, \]
where
\[ \Sigma_R \equiv \left( \frac{c_1}{\Sigma_0^{(1)}} + \frac{c_2}{\Sigma_0^{(2)}} \right)^{-1/n}. \] (2.19)
In the rigid/perfectly plastic limit ($n \to \infty$), (2.19) transforms to
\[ \Sigma_R = \min\{\Sigma_0^{(1)}, \Sigma_0^{(2)}\}. \] (2.20)

It is worth emphasizing that the elementary bounds (2.11) and (2.18) do not capture the size effect, i.e. they are insensitive to the scale of the microstructure. Smyshlyaev & Fleck (1994) have demonstrated that, in the linear case, an extension of the Hashin–Shtrikman technique does capture the size effect, as summarized in the next section.

(d) Linear Hashin–Shtrikman bounds

Smyshlyaev & Fleck (1994) have established a Hashin–Shtrikman-type variational principle for strain gradient composites and applied it to derive Hashin–Shtrikman bounds for linear statistically homogeneous and isotropic incompressible two-phase composites. We reproduce here the bounds.

In the linear case, the strain energy function assumes the form (2.5) and the constitutive relations are given by (2.6). The effective shear modulus $\mu^*$ of an isotropic composite is defined as
\[ \tilde{W}_L \equiv \mu^* |V| \varepsilon_{ij}^0 \varepsilon_{ij}^0, \] (2.21)
where $\tilde{W}_L$ is the true stored energy of the linear composite under the boundary conditions (2.8), i.e. under the uniform macroscopic strain $\varepsilon^0$.

Explicit expressions for upper and lower bounds were given by Smyshlyaev & Fleck (1994) in terms of the moduli of the phases $(\mu_1, l_1)$ and $(\mu_2, l_2)$, volume fractions $c_1$ and $c_2$, and a correlation coefficient
\[ h(|z|) = (\Psi_{11}(z) - c_1^2)/(c_1 c_2). \]
Here $\Psi_{11}(\boldsymbol{z})$ is a two-point correlation function describing a probability of finding both the point $\boldsymbol{x}$ and the point $\boldsymbol{x} + \boldsymbol{z}$ in phase one. By definition, $h(0) = 1$; isotropy ensures that $h$ depends only on the length of the vector $\boldsymbol{z}$.

The lower Hashin–Shtrikman bound $\mu_{\text{HS}}^-$ and the upper Hashin–Shtrikman bound $\mu_{\text{HS}}^+$ for the effective shear modulus $\mu^*$ read

$$\mu_{\text{HS}}^- = \mu_1 \left\{ 1 + \frac{c_2}{(\mu_1/(\mu_2 - \mu_1)) + c_1 \psi^+} \right\}, \quad (2.22)$$

$$\mu_{\text{HS}}^+ = \mu_2 \left\{ 1 + \frac{c_1}{(\mu_2/(\mu_1 - \mu_2)) + c_2 \psi^-} \right\}. \quad (2.23)$$

It has been assumed here that $\mu_1 \geq \mu_2$ without loss of generality. The parameters $\psi^+$ and $\psi^-$ are defined by

$$\psi^+ = \psi(l^+), \quad \psi^- = \psi(l^-), \quad (2.24)$$

where

$$l^+ = \max \left\{ l_1, \frac{\sqrt{\mu_2}}{\mu_1} l_2 \right\}, \quad l^- = \min \left\{ l_2, \frac{\sqrt{\mu_1}}{\mu_2} l_1 \right\} \quad (2.25)$$

and the function $\psi(l)$ is related to the correlation coefficient $h$ by

$$\psi(l) = \frac{8}{5} \int_0^{+\infty} e^{-2t} h(lt) t \, dt. \quad (2.26)$$

In the limit $l \to 0$, $\psi(l) \to \psi(0) = \frac{2}{5}$ and (2.22), (2.23) transform into the conventional Hashin–Shtrikman (1963) bounds.

It is worth emphasizing that the Hashin–Shtrikman variational principle developed by Smyshlyaev & Fleck (1994, §3) does not necessarily assume that the phases are linear. This should lead to a direct derivation of nonlinear bounds following the pattern of Willis (1983, 1991), and Talbot & Willis (1985). We prefer here, however, to develop a strain gradient version of an elegant nonlinear variational principle suggested by Ponte Castañeda (1992).

### 3. A nonlinear variational principle

The underlying idea behind the analysis of Ponte Castañeda (1991, 1992) is that a nonlinear solid behaves like an *instantaneously linear* one with the same secant modulus. Indeed, comparison of (2.2) and (2.6) demonstrates that

$$\tilde{\mu}(\boldsymbol{x}) = \frac{1}{3} \frac{\partial w(\varepsilon_0, \chi_0)}{\partial \varepsilon_0} \cdot \frac{1}{\varepsilon_0} \quad (3.1)$$

plays the part of the instantaneous shear modulus; similarly, the instantaneous length scale is determined from

$$\tilde{\mu}(\boldsymbol{x}) l^2(\boldsymbol{x}) = \frac{1}{3} \frac{\partial w(\varepsilon_0, \chi_0)}{\partial \chi_0} \cdot \frac{1}{\chi_0}. \quad (3.2)$$

This simple observation means that a nonlinear solid under prescribed boundary conditions experiences the same response as a *linear inhomogeneous* couple stress solid with variable parameters $\tilde{\mu}(\boldsymbol{x})$ and $l(\boldsymbol{x})$ determined from (3.1) and (3.2).
other words, if we know \( \tilde{\mu}(x) \) and \( \tilde{l}(x) \) and could also solve the linear problem, we would also know the solution to the nonlinear problem.

Suppose \( \tilde{\mu}(x) \) and \( \tilde{l}(x) \) are known. The strain energy \( \tilde{W} \) for the nonlinear solid under boundary conditions (2.8) is related to the strain energy \( \tilde{W}_L \) for the linear solid with spatially varying properties \( (\tilde{\mu}(x), \tilde{l}(x)) \) and the same boundary conditions by

\[
\tilde{W} = \tilde{W}_L + \int_V \tilde{U}(x; \tilde{\mu}(x), \tilde{l}(x), \tilde{\varepsilon}_e, \tilde{\chi}_e) \, dx. \tag{3.3}
\]

Here the correction term \( \tilde{U} \) is defined via (2.5) as

\[
\tilde{U}(x; \tilde{\mu}, \tilde{l}, \tilde{\varepsilon}_e, \tilde{\chi}_e) = w(x; \tilde{\varepsilon}_e(x), \tilde{\chi}_e(x)) - \frac{3}{2} \tilde{\mu}(x) \tilde{\varepsilon}_e^2(x) - \frac{3}{2} \tilde{\mu}(x) \tilde{l}^2(x) \tilde{\chi}_e^2(x). \tag{3.4}
\]

(Here and elsewhere, the tilde symbol denotes the true value of any quantity.)

We follow Ponte Castañeda (1992) by assuming that \( w(x; \varepsilon_e, \chi_e) \) grows slower than quadratically with respect to \( \varepsilon_e, \chi_e \), and, moreover, is concave with respect to the new variables \( p = \varepsilon_e^2, q = \chi_e^2 \). This is usually the case for plasticity with hardening, e.g. for the power law (2.3) of Fleck & Hutchinson (1993). Further, introduce the function \( U(x; \tilde{\mu}, \tilde{l}) \) defined by

\[
U(x; \tilde{\mu}, \tilde{l}) \equiv \max_{\varepsilon_e, \chi_e} \left\{ w(x; \varepsilon_e, \chi_e) - \frac{3}{2} \tilde{\mu} \varepsilon_e^2 - \frac{3}{2} \tilde{\mu} \tilde{l}^2 \chi_e^2 \right\}. \tag{3.4}
\]

Equality of \( \tilde{U} \) and \( U \) is ensured by the definitions (3.1) and (3.2) of \( \tilde{\mu}(x) \) and \( \tilde{l}(x) \), which provide the extremum conditions for the right-hand side of (3.4).

Combination of (3.3) and (3.4) gives

\[
\tilde{W} = \tilde{W}_L(\tilde{\mu}(x), \tilde{l}(x)) + \int_V U(x; \tilde{\mu}(x), \tilde{l}(x)) \, dx \tag{3.5}
\]

with \( \tilde{\mu}(x), \tilde{l}(x) \) given by (3.1), (3.2).

We shall now argue that the left-hand side of (3.5) is less than or equal to the right-hand side for arbitrary \( \mu(x) \) and \( l(x) \) within the volume \( V \).

We start by considering an arbitrary \( \mu(x) \) and \( l(x) \), and an arbitrary kinematically admissible displacement field \( u(x) \), which satisfies the boundary conditions (2.8). Then by the definition (3.4) of \( U \) we have

\[
U(x; \mu(x), l(x)) \geq w(x, \varepsilon_e(u), \chi_e(u)) - w_L(\mu(x), l(x), u),
\]

where the strain energy density for the linear solid \( w_L \) is defined via (2.5). Integration of the above inequality over \( V \) gives

\[
\int_V w(x, u) \, dx \leq \int_V w_L(\mu(x), l(x); u) \, dx + \int_V U(x; \mu(x), l(x)). \tag{3.6}
\]

Next, take the minimum value of both sides of (3.6) over all possible kinematically admissible \( u(x) \) which satisfy the boundary conditions. The minimum value of \( \int_V w \, dx \) is \( \tilde{W} \) by (2.10), and the minimum value of \( \int_V w_L \, dx \) is \( \tilde{W}_L \) by the same argument. As a result,

\[
\tilde{W} \leq \tilde{W}_L(\mu(x), l(x)) + \int_V U(x, \mu(x), l(x)) \, dx \tag{3.7}
\]

† The variational procedure which follows is easily generalized to energy functions without the concavity restriction with the \( (\leq) \) inequality instead of the equality in the final result (3.8).
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for arbitrary \( \mu(x) \) and \( l(x) \).

By combining (3.5) and (3.7), we arrive finally at

\[
\hat{W} = \min_{\mu(x), l(x)} \left\{ \hat{W}_L(\mu(x), l(x)) + \int_V U(x, \mu(x), l(x)) \, dx \right\},
\]

(3.8)

and the minimum is attained for the true fields \( \hat{\mu}(x) \) and \( \hat{l}(x) \), as defined by (3.1) and (3.2).

The variational statement (3.8) is a strain gradient version of that introduced by Ponte Castañeda (1992) for conventional solids. It is regarded as a starting point for the derivation of upper bounds for the strain energy \( \hat{W} \) by a suitable choice of linear parameters \( \mu(x) \) and \( l(x) \), subject to the availability of appropriate ‘linear’ bounds for \( \hat{W}_L \). The quality of the bounds depends upon the amount of available information on the microstructure. Basically, the more information that is available, the tighter are the bounds which can be derived, at the expense, however, of more elaborate computations. We focus in the sequel on the derivation of ‘nonlinear’ bounds of Hashin–Shtrikman type for statistically homogeneous and isotropic incompressible two-phase composites with prescribed volume fractions and a two-point correlation function. To this end, we can employ in (3.8) the ‘linear’ results of Smyshlyaev & Fleck (1994), as summarized in §2c.

Similar methods can be developed for bounding of the nonlinear complementary energy \( \Phi \), starting from the complementary minimum principle (2.17); this is not pursued here.

4. Bounds and estimates for power-law plasticity

Consider a statistically homogeneous and isotropic composite with two nonlinear phases specified by the energy densities \( w_1 \) and \( w_2 \). If the only available statistical information is volume fractions and a two-point correlation function, a natural option is to choose the trial parameters \( \mu(x) \) and \( l(x) \) to be piecewise constant within each phase:

\[
\mu(x) = \hat{\mu}_1 f_1(x) + \hat{\mu}_2 f_2(x), \quad l(x) = \hat{l}_1 f_1(x) + \hat{l}_2 f_2(x).
\]

Here \( f_1(x) \) and \( f_2(x) \) are characteristic functions of phases one and two, respectively: \( f_1(x) = 1 \) if \( x \) belongs to phase one; \( f_1(x) = 0 \) otherwise; and \( f_2(x) = 1 - f_1(x) \).

The variational statement (3.8) gives

\[
\hat{W} \leq \hat{W}_L(\hat{\mu}_1, \hat{l}_1; \hat{\mu}_2, \hat{l}_2) + c_1 V |U_1(\hat{\mu}_1, \hat{l}_1) + c_2 V |U_2(\hat{\mu}_2, \hat{l}_2)
\]

(4.1)

for any \( \hat{\mu}_j, \hat{l}_j; j = 1, 2 \). In (4.1), \( \hat{W}_L \) is the strain energy stored in a linear two-phase ‘comparison’ composite with the same geometrical arrangement of phases and with the properties \( \hat{\mu}_1, \hat{l}_1 \) and \( \hat{\mu}_2, \hat{l}_2 \) of phases one and two, respectively. The duals \( U_1 \) and \( U_2 \) emerge from definition (3.4) with \( w \) replaced by \( w_1 \) and \( w_2 \).

(a) Nonlinear Hashin–Shtrikman bounds

Both \( \hat{W} \) and \( \hat{W}_L \) in inequality (4.1) depend on the microstructure. Upon assuming statistical homogeneity and by taking the representative volume \( V \) to be much larger than the scale of the microstructure, the inequality in (4.1) is preserved upon taking a statistical average. Further, the energy \( \hat{W}_L \) of the linear composite can be bounded by (2.21) and (2.22), which makes use of the results of Smyshlyaev & Fleck (1994):

\[
\hat{W} \leq \hat{W}^{\pm}_{HS}(\hat{\mu}_1, \hat{l}_1; \hat{\mu}_2, \hat{l}_2) + c_1 V |U_1(\hat{\mu}_1, \hat{l}_1) + c_2 V |U_2(\hat{\mu}_2, \hat{l}_2).
\]

(4.2)

Here
\[ \hat{W}^+_{\text{HS}} \equiv \mu^+_{\text{HS}} |V| \varepsilon^0_{ij} \varepsilon^0_{ij}, \]
and \( \mu^+_{\text{HS}} \) is given explicitly by (2.22), (2.24)–(2.26) with \( \mu_1 = \hat{\mu}_1, \mu_2 = \hat{\mu}_2, \ell_1 = \hat{\ell}_1 \)
and \( l_2 = \hat{l}_2 \), provided \( \hat{\mu}_1 \leq \hat{\mu}_2 \). If \( \hat{\mu}_1 \geq \hat{\mu}_2 \), there is a straightforward interchange of the indices.

Inequality (4.2) represents a family of upper bounds for a nonlinear strain energy function \( \hat{W} \), for arbitrary linear parameters \( \hat{\mu}_1, \hat{l}_1, \hat{\mu}_2 \) and \( \hat{l}_2 \). Its further optimization with respect to these parameters requires explicit analysis of the dual potentials \( U_1 \)
and \( U_2 \). For the case of power-law strain gradient plasticity (2.3), (2.4), the duals \( U_1 \)
and \( U_2 \) are calculated explicitly as follows. The dual potentials introduced by (3.4) specialize for power-law hardening (2.3) to
\[
U_j(\mu_j, \ell_j) = \max_{\varepsilon_0, \lambda \geq 0} \left\{ \frac{1}{m+1} \sum_0 (\varepsilon_0^2 + \ell_j \lambda)^{1+m/2} - \frac{3}{2} \mu_j \varepsilon_0^2 - \frac{3}{2} \mu_j \ell_j \lambda \right\}, \quad j = 1, 2.
\]

Straightforward analytical procedure gives
\[
U_j(\hat{\mu}_j, \hat{\ell}_j) = \begin{cases} 
U_0(\mu_j, \Sigma_0^{(j)}), & \text{if } \hat{\ell}_j \geq \ell_j, \\
U_0 \left( \frac{\hat{\mu}_j}{\ell_j}, \frac{\hat{\ell}_j}{\ell_j}, \Sigma_0^{(j)} \right), & \text{if } \hat{\ell}_j \leq \ell_j,
\end{cases}
\]
(4.3)
where
\[
U_0(\mu, \Sigma) \equiv \frac{3}{2} \cdot \frac{1 - m}{1 + m} \left( \frac{1}{3 \Sigma_0} \right)^{2/(1-m)} \frac{\Sigma^{2/(1-m)}}{\mu^{1/(1+m)}} \mu^{1/(1-m)}.
\]

The objective is to minimize the right-hand side of (4.2) by a suitable choice of parameters \( \hat{\mu}_1, \hat{l}_1, \hat{\mu}_2, \hat{l}_2 \), with \( U_j, j = 1, 2 \) explicitly given by (4.3). Fixed values are assumed for \( \Sigma_0^{(j)}, \ell_j; j = 1, 2 \) and \( m = 1/n \) is taken in the range \( 0 < m < 1 \). The power-law self-similarity and a particular form of coupling via the scalar strain measure (2.4) permit us to reduce this four-dimensional optimization problem to that with one variable (see the Appendix). The resulting upper bound for \( \Sigma^* \) reads
\[
\Sigma^* \leq \Sigma^+_{\text{HS}},
\]
where
\[
\Sigma^+_{\text{HS}} \equiv \min \{ \Sigma^{(1)}, \Sigma^{(2)} \},
\]
(4.4)
and†
\[
\Sigma^{(1)} \equiv \min_{0 \leq \gamma \leq 1} \left\{ 1 - \frac{c_2}{1/(1-\gamma) - \psi^{(1)}_1(\gamma)c_1} \right\}^{(1+m)/2} \times \left\{ c_1 \Sigma_1^{2/(1-m)} + c_2 \frac{\Sigma_2^{2/(1-m)}}{\gamma^{(1+m)/(1-m)}} \right\}^{(1-m)/2},
\]
\[
\Sigma^{(2)} \equiv \min_{0 \leq \gamma \leq 1} \left\{ 1 - \frac{c_1}{1/(1-\gamma) - \psi^{(1)}_2(\gamma)c_2} \right\}^{(1+m)/2},
\]

† We write henceforth \( \Sigma_1 \) and \( \Sigma_2 \) instead of \( \Sigma_0^{(1)} \) and \( \Sigma_0^{(2)} \) to simplify the notation.

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\[ \times \left( c_2 \Sigma_2^{2/(1-m)} + c_1 \frac{\Sigma_1^{2/(1-m)}}{\gamma^{(1+m)/(1-m)}} \right)^{(1-m)/2}. \] (4.5)

The functions \( \psi_1^+ (\gamma) \) and \( \psi_2^+ (\gamma) \) are defined by

\[ \psi_1^+ (\gamma) = \psi (\gamma_1^+), \quad \psi_2^+ (\gamma) = \psi (\gamma_2^+), \] (4.6)

with

\[ \gamma_1^+ = \max \{ l_1, \sqrt[3]{l_2} \}, \quad \gamma_2^+ = \max \{ l_2, \sqrt[3]{l_1} \}, \] (4.7)

and the function \( \psi (\cdot) \) defined by (2.26).

The value of \( \Sigma_{HS}^+ \) can be easily computed numerically from (4.4), (4.5), (4.7) and (2.26) for chosen parameters of the phases and the correlation function \( h \). They can be however simplified further in the limit \( n \to \infty \) (\( m \to 0 \)) which corresponds to a rigid–perfectly plastic composite.

(i) **Bounds for rigid–perfectly plastic limit**

When the hardening index \( n \) tends to infinity, expression (2.3) for the strain energy function transforms to

\[ w = \Sigma_0 \mathcal{E} \] (4.8)

and the parameter \( \Sigma_0 \) plays the part of the yield strength of a rigid–perfectly plastic strain gradient body. A straightforward formulation for the strain energy (4.8) suffers from the drawback that the function \( w (\mathcal{E}, \chi) \) is not strictly convex. We avoid related discussion, regarding (4.8) as a limiting case of (2.3). Then the expressions (4.5) for the Hashin–Shtrikman upper bound reduce to

\[ \Sigma^{(1)} = \min_{0 \leq \gamma \leq 1} \left\{ 1 - \frac{c_2}{1/(1-\gamma) - \psi_1^+ (\gamma)c_1} \right\}^{1/2} \left\{ c_1 \Sigma_1^2 + c_2 \frac{\Sigma_2^2}{\gamma} \right\}^{1/2}, \] (4.9)

\[ \Sigma^{(2)} = \min_{0 \leq \gamma \leq 1} \left\{ 1 - \frac{c_1}{1/(1-\gamma) - \psi_2^+ (\gamma)c_2} \right\}^{1/2} \left\{ c_2 \Sigma_2^2 + c_1 \frac{\Sigma_1^2}{\gamma} \right\}^{1/2}, \] (4.10)

Consider a ‘well-ordered’ composite where \( l_1 \geq l_2 \) for the case \( \Sigma_1 \geq \Sigma_2 \). Then, \( \psi_1^+ (\gamma) = \psi (l_1) \equiv \psi^+ \) from the definitions (4.6) and (4.7), which is a constant independent of \( \gamma \). Consequently, the minimization in (4.9) and (4.10) can be done explicitly by differentiation with respect to \( \gamma \). Then relation (4.4) provides, via routine analytical manipulations, the following explicit bound for \( \Sigma_{HS}^+ \):

\[ \frac{\Sigma_{HS}^+}{\Sigma_2} = \frac{c_2}{1 - c_1 \psi^+} + c_1 \sqrt{\frac{1 - \psi^+}{1 - c_1 \psi^+} - \frac{\Sigma_1^2}{\Sigma_2^2} - \frac{c_2 \psi^+ (1 - \psi^+)}{(1 - c_1 \psi^+)^2}}. \] (4.11)

In the conventional limit (\( l \to 0 \), \( \psi^+ \to \frac{2}{3} \)) and (4.11) reproduces the results of Ponte Castañeda & De Botton (1992, formula (15)) and Suquet (1993, formula (3.16)) for the effective yield stress of a rigid–perfectly plastic composite.

(b) **Hashin–Shtrikman (lower) estimates**

A similar prescription to obtain Hashin–Shtrikman lower bounds for power-law composites (2.3) is not available.† Instead, estimates can be derived based on the

† Talbot & Willis (1994a, b) have recently suggested a new extension of the Hashin–Shtrikman methodology using a nonlinear ‘comparison medium’, which permits derivation of both upper and lower bounds. Possibility of an extension of their method to strain gradient composites is not discussed here.

linear Hashin–Shtrikman lower bounds in a way suggested by Ponte Castañeda & De Botton (1992) for conventional composites. Their idea is to substitute into (4.1) the lower bound (2.21), (2.23) for $\bar{W}_L$, and then to minimize the right-hand side with respect to $(\hat{\mu}_1, \hat{\mu}_2, \hat{l}_1, \hat{l}_2)$. The expectation is that the opposite tendencies of overestimation provided by inequality (4.2) and of underestimation provided by the bounds (2.21), (2.23) tend to cancel each other. Performing finite element calculations for a particular packing of spheres, Suquet (1993) found that in some cases the estimate is indeed in relatively good agreement with the results of direct calculations.

Manipulations similar to those employed for the derivation of the upper bounds (see the Appendix) give the following expressions for the estimates:

$$\Sigma^* = \min\{\Sigma^{(1)}_e, \Sigma^{(2)}_e\}, \quad (4.12)$$

$$\Sigma^{(1)}_e \equiv \min_{0 < \gamma < 1} \left\{ 1 + \frac{c_1}{\gamma/(1-\gamma) + \psi^-_1(\gamma)c_2} \right\}^{(1+m)/2} 
\times \left\{ c_2 \Sigma_2^{2/(1-m)} + c_1 \Sigma_1^{2/(1-m)} \gamma^{(1+m)/(1-m)} \right\}^{(1-m)/2},$$

$$\Sigma^{(2)}_e \equiv \min_{0 < \gamma < 1} \left\{ 1 + \frac{c_2}{\gamma/(1-\gamma) + \psi^-_2(\gamma)c_1} \right\}^{(1+m)/2} 
\times \left\{ c_1 \Sigma_1^{2/(1-m)} + c_2 \Sigma_2^{2/(1-m)} \gamma^{(1+m)/(1-m)} \right\}^{(1-m)/2}, \quad (4.13)$$

$$\psi^-_1 = \psi(l_1^-), \quad \psi^-_2 = \psi(l_2^-), \quad l_1^- \equiv \min\{l_1, \gamma^{-1/2}l_1\}, \quad l_2^- \equiv \min\{l_1, \gamma^{-1/2}l_2\}.$$ 

This permits a simple numerical calculation of the estimates.

Also, for the rigid–plastic limit $n \to \infty (m \to 0)$, the explicit expressions for estimates of the effective yield strength are available provided the phases are well-ordered ($\Sigma_1 \geq \Sigma_2, l_1 \geq l_2$):

$$\frac{\Sigma^*_e}{\Sigma_2} = \begin{cases} 
\frac{c_1}{1 - c_2 \psi^-} \left( \frac{\Sigma_1}{\Sigma_2} \right) + c_2 \sqrt{1 - \psi^-} \frac{1 - \psi^-}{1 - c_2 \psi^-} - \frac{c_1 \psi^- (1 - \psi^-)}{(1 - c_2 \psi^-)^2} \left( \frac{\Sigma_1}{\Sigma_2} \right)^2, \\
\quad \text{if } \psi^- \sqrt{1 + \frac{1 - \psi^-}{\psi^-}c_1} < \Sigma_2 \Sigma_1 < 1, \\
\sqrt{1 + c_1 \left( \frac{1}{\psi^-} - 1 \right)}, \quad \text{if } \frac{\Sigma_2}{\Sigma_1} \leq \psi^- \sqrt{1 + \frac{1 - \psi^-}{\psi^-}c_1}, \end{cases} \quad (4.14)$$

where

$$\psi^- \equiv \psi(l_2).$$

In the conventional limit $l \to 0$, $\psi^- \to 2/\psi$ and (4.14) conforms to ‘conventional’ estimates of Ponte Castañeda & De Botton (1992, formula (16)).

5. Numerical results

The correlation function has been taken as

$$h(|z|) = e^{-|z|/a},$$

where $a$ is a correlation length parameter which specifies the scale of the microstructure. Both the Hashin–Shtrikman upper bounds and the lower estimates have been
computed. They lie between the elementary Voigt and Reuss bounds, calculated via (2.13), (2.19) and (2.20).

Some representative results are given in figures 1–3 for the Hashin–Shtrikman upper bounds and lower estimates of the macroscopic strength $\Sigma$ of a two-phase composite; Voigt and Reuss bounds are included for completeness. Figure 1 shows the effect upon the effective strength $\Sigma$ of the scale of the microstructure $a$ in relation to the material length scale $l$; results are given for $c_1 = 0.3$, $\Sigma_1/\Sigma_2 = 5$, $l_1 = l_2 = l$ and $n$ in the range $1 \leq n \leq \infty$. It is clear from figure 1 that the Hashin–Shtrikman upper bound and lower estimate approach the upper bound with increasing $l/a$.

The effect of concentration $c_1$ upon the macroscopic strength is given in figure 2 for $l_1 = l_2 = l = a$ and for the conventional limit $l_1 = l_2 = l = 0$. We note that the Voigt and Reuss bounds are independent of length scale $l/a$, and that the Hashin–Shtrikman upper bound lies close to the Voigt bound for both $l_1 = l_2 = l = a$ and $l_1 = l_2 = l = 0$: the size effect is relatively small.

Figure 3 displays the bounds and estimates as a function of hardening index $n$, for $l_1 = l_2 = l = a$ and $l_1 = l_2 = l = 0$. The Hashin–Shtrikman upper bound increases with increasing $n$ and Hashin–Shtrikman lower estimate decreases with increasing $n$. The degree of strengthening due to the size effect is fairly insensitive to the value of $n$.

We conclude from the numerical results that the Hashin–Shtrikman upper bound strength increases by up to 10%, as $l/a$ is increased from zero to unity, for all $n$ and $c_1$ considered. By comparison, the Hashin–Shtrikman lower estimate of strength increases by up to 20% as $l/a$ is increased from zero to unity.

6. Concluding remarks

We have shown that the macroscopic plastic response of a two-phase strain gradient composite depends upon the ratio of the intrinsic length scale $l$ and the scale
Figure 2. Effect of concentration \( c_1 \) upon the macroscopic strength \( \Sigma \). Results are shown for both \( l/a = 0 \) and \( l/a = 1 \), with \( l_1 = l_2 = l \) and \( \Sigma_1/\Sigma_2 = 5 \).

Figure 3. Bounds and estimates for the macroscopic strength \( \Sigma \) as a function of the hardening index \( n \), for \( \Sigma_1 = 5\Sigma_2 \), \( l_1 = l_2 = l \) and \( c_1 = 0.3 \).

of the microstructure \( a \). The ‘accuracy’ of the bounds depends on the amount of available information on the microstructure. The more information is available, the tighter the bounds can be derived in principle, at the expense, however, of more elaborate computations. We have chosen here a simple option leading to constant trial parameters \( \mu(\mathbf{x}) \) and \( l(\mathbf{x}) \) for the nonlinear variational principle, as well as to constant trial polarizations in the linear case (Smyshlyaev & Fleck 1994), provided
minimal statistical information is available. Tighter bounds could be derived using non-constant polarizations and/or non-constant parameters $\mu(x), l(x)$, provided more statistical or morphological information on the microstructure is available. This would require additional computational effort.

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Appendix A. Optimization

We seek to minimize the right-hand side of (4.2) by a suitable choice of the parameters $(\hat{\mu}_1, \hat{\mu}_2, \hat{l}_1, \hat{l}_2)$ for $U_1$ and $U_2$ given by (4.3).

We argue first that the best choice is to take $\hat{l}_1 = l_1, \hat{l}_2 = l_2$. This reflects the fact that the instantaneous length scale $l(x)$ determined from (3.1) and (3.2) equals the material length scale $l$ if the strain energy function $w$ depends on $\varepsilon$ and $\chi_0$ via the scalar strain measure $\varepsilon$. This is easily verified by substituting $w = w(\varepsilon, \chi_0)$ into (3.1), (3.2) and performing differentiations. This observation permits us to suppose that $l_1 = l, l_2 = l$ does provide the best choice. A straightforward proof of this fact has also been obtained by a direct analysis of the explicit formulae (4.2), (2.22)–(2.25) and (4.3). As a result the four-dimensional optimization problem reduces to that with two variables $\hat{\mu}_1$ and $\hat{\mu}_2$.

Assuming that $\hat{\mu}_1 \geq \hat{\mu}_2$, the right-hand side of (4.2) specializes via (2.22)–(2.25) and (4.3) to

$$\frac{3}{2} \left( \varepsilon^2_0 \right)^2 \hat{\mu}_1 \left\{ 1 - \frac{c_2}{(1/(1 - \gamma)) - \psi^*_1(\gamma)c_1} \right\} + \frac{3}{2} \frac{1 - m}{1 + m} \left( \frac{1}{3\varepsilon^m_0} \right)^{2/(1-m)} \times \frac{1}{\hat{\mu}((1+m)/(1-m))} \left\{ \frac{c_1 \Sigma^2_1}{1 - \gamma^2(1+m)/(1-m)} + \frac{c_2 \Sigma^2_2}{\gamma^2(1+m)/(1-m)} \right\},$$

(A1)

where $\gamma \equiv \hat{\mu}_2/\hat{\mu}_1, 0 \leq \gamma \leq 1$ and $\psi^*_1(\gamma)$ is given by (4.6)–(4.7).

Minimization of (A1) with respect to $\hat{\mu}_1 \geq 0$, and regarding $\gamma$ as an independent constant parameter, leads to a bound $\Sigma^{(1)}$ for the effective strength parameter $\Sigma^*$ in (2.12). This minimization process is stated in (4.9).

Similarly, the bound $\Sigma^{(2)}$ in (4.10) is derived from the alternative assumption $\hat{\mu}_2 \geq \hat{\mu}_1$. Finally, the Hashin–Shtriknam bound (4.4) is taken as the minimum of $\Sigma^{(1)}$ and $\Sigma^{(2)}$.

Derivation of the formulae (4.12)–(4.14) for the lower estimates follows the same formal pattern, as based on explicit formulae for the linear lower bound (2.23).

References


† This employs in effect the power-law self-similarity as discussed by Suquet (1993).


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