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THE ROLE OF STRAIN GRADIENTS IN THE GRAIN SIZE EFFECT FOR POLYCRYSTALS

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ABSTRACT

The role of grain size on the overall behaviour of polycrystals is investigated by using a strain gradient constitutive law for each slip system for a reference single crystal. Variational principles of Hashin–Shtrikman type are formulated for the case where the strain energy density is a convex function of both strain and strain gradient. The variational principles are specialized to polycrystals with a general multi-slip strain gradient constitutive law. An extension of the Hashin–Shtrikman bounding methodology to general strain gradient composites is discussed in detail and then applied to derive bounds for arbitrary linear strain gradient composites or polycrystals. This is achieved by an extensive study of kernel operators related to the Green's function for a general "strain-gradient" linear isotropic incompressible comparison medium. As a simple illustrative example, upper and lower bounds are computed for linear face-centred cubic polycrystals: a size effect is noted whereby smaller grains are stiffer than large grains. The relation between the assumed form of the constitutive law for each slip system and the overall response is explored.

1. INTRODUCTION

It is well established that the macroscopic properties of polycrystals depend on the grain size. The well-known Hall–Petch effect (Hall, 1951; Petch 1953) states that the strength of polycrystalline metals increases with decreasing grain size. It is thought that the grain size effect is due to the presence of spatial gradients of strain in each single grain. These gradients are associated with the plastic inhomogeneity of slip and are expected to be particularly significant near grain boundaries.

A qualitative physical interpretation of such constitutive behaviour as resulting from a combination of "statistically stored" and "geometrically necessary" dislocations has been proposed by Ashby (1970), and developed further by Fleck *et al.* (1994). Their arguments suggest that a single crystal's behaviour is controlled by a strain gradient constitutive law. The geometrically necessary dislocations (and strain gradient effects associated with them) introduce a length scale l into the constitutive law and account for a size effect in the macroscopic response of a polycrystal.

In this paper we focus on the *quantitative* aspects of the *homogenization problem* for polycrystals with constituent single crystals described by a strain gradient law. Upon selecting the crystal's constitutive law the question arises as to what is the

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resulting macroscopic behaviour of the polycrystal. The homogenization procedure is expected to reflect a competition between two length scales: the intrinsic length scale l introduced into crystal's constitutive law by the gradient effects, and the scale of the grain size a. The overall properties of the polycrystal are functions of l/a, which reflects the grain size effect.

The prediction of the effective properties of polycrystals from the constitutive properties of the component crystals has been a focus of investigations for a long time: this work, however, has focussed on *conventional* constitutive laws which do not include a length scale and do not account for the size effect. One established approach is based on variational methods laid down by Hashin and Shtrikman (1962a,b) is the context of elasticity, and seeks to bound the total energy of the polycrystal subjected to a macroscopic deformation. Hutchinson (1976) has obtained elementary bounds and self-consistent estimates for the creep of polycrystals; each individual crystal is treated as a multislip system (of Schmid type) with a power law characterizing each slip. The model of Hutchinson was extensively studied by applying more advanced nonlinear versions of the Hashin–Shtrikman method by Willis and co-workers (e.g. Dendievel *et al.*, 1991), and by deBotton and Ponte Castañeda (1995). These more sophisticated approaches resulted in the attainment of improved bounds for the overall behaviour of the polycrystal.

In the paper by Smyshlyaev and Fleck (1994) we have proposed an extension of the Hashin–Shtrikman procedure to account for strain gradient effects, and applied it to two-phased composites with a linear couple stress constitutive law for each phase. This approach was developed further (Smyshlyaev and Fleck, 1995) to address the overall *nonlinear* behaviour of two-phase composites with a J_2 isotropic strain gradient constitutive law for the phases. Here we develop the above ideas and apply them to polycrystals.

We begin with a general discussion of "strain-gradient" deformation theories (linear or nonlinear), and state the minimum principles. This framework is then specialized to *crystals* which are assumed to deform by slip on a discrete number of slip systems. The strain gradient crystal plasticity framework of Fleck and Hutchinson (1996) is summarized, and a property of "instantaneous linearity" of such crystals is then discussed. The instantaneous linearity motivates an extensive study of *linear* strain gradient polycrystals which is the focus of the rest of the paper. We discuss in detail an extension of the Hashin–Shtrikman methodology as interpreted by Willis (1977, 1981, 1983, 1986, 1991) to general (not necessarily linear) strain-gradient composites. This requires an extensive study of kernel operators related to a general "strain-gradient" Green's function, and of a "canonic" representation for an incompressible, linear, isotropic strain-gradient constitutive law. Bounds are then derived for arbitrary linear polycrystals. As a simple illustrative example, upper and lower bounds are computed for a linear face-centred cubic strain-gradient polycrystal: a grain size effect is noted.

Results are given for the macroscopic shear modulus μ^* of the face-centred cubic polycrystals as a function of the shear modulus for each slip system μ and the grain size a. It is found that μ^* varies roughly as $a^{-1/2}$ in qualitative support of the Hall–Petch grain-size effect. We emphasise that the Hall–Petch effect relates to the dependence of yield strength of polycrystal upon grain size, and so the results presented here for the

dependence of the macroscopic shear modulus upon grain size are meant only for a qualitative comparison. Further, the analysis of the linear case is the first step in the estimation of the grain size for non-linear polycrystals: in order to use the nonlinear variational principle of Ponte Castañeda (1991, 1992) the effective properties of the linear solid are required.

2. REVIEW OF "GRADIENT THEORIES"

2.1. *The Toupin–Mindlin higher-order deformation theory*

Toupin (1962) and Mindlin (1964, 1965) have developed a theory of linear elasticity whereby the strain energy density w depends upon both the symmetric strain tensor $\varepsilon_{ij} \equiv \frac{1}{2}(u_{i,j}+u_{j,i})$ and the second gradient of displacement $\eta_{ijk} \equiv u_{k,ij}$. Their theory admits a straightforward generalization to nonlinear and inhomogeneous behaviour as follows.

The strain energy function w is assumed to be a convex function with respect to its arguments $(\boldsymbol{\varepsilon}, \boldsymbol{\eta})$ for each point $\mathbf{x}$ of a solid of volume V. The total energy W stored in the solid is determined by the displacement field $\mathbf{u}(\mathbf{x})$ within V

$$W(\mathbf{u}) \equiv \int_V w(\boldsymbol{\varepsilon}(\mathbf{u}), \boldsymbol{\eta}(\mathbf{u}); \mathbf{x})\, \mathrm{d}\mathbf{x}$$

with $\boldsymbol{\varepsilon}$ and $\boldsymbol{\eta}$ derived from $\mathbf{u}$, as given above.

The energy increment of the solid due to an arbitrary variation of the displacement $\mathbf{u}$ is

$$\delta W = \int_V (\sigma_{jk}\delta\varepsilon_{jk} + \tau_{ijk}\delta\eta_{ijk})\, \mathrm{d}\mathbf{x}. \tag{2.1}$$

Here the "conventional" stress $\boldsymbol{\sigma}$ is defined as the work conjugate to $\boldsymbol{\varepsilon}$ and, in analogous fashion, the "higher stress" $\boldsymbol{\tau}$ is defined as the work conjugate to $\boldsymbol{\eta}$

$$\sigma_{ij} \equiv \frac{\partial w}{\partial \varepsilon_{ij}}; \quad \tau_{ijk} \equiv \frac{\partial w}{\partial \eta_{ijk}}. \tag{2.2}$$

Use of the divergence theorem transforms (2.1) into

$$\delta W = -\int_V [(\sigma_{jk,j} - \tau_{ijk,ij})\delta u_k]\, \mathrm{d}\mathbf{x} + \int_S [(\sigma_{jk} - \tau_{ijk,i})n_j \delta u_k + \tau_{ijk} n_i \delta u_{k,j}]\, \mathrm{d}S, \tag{2.3}$$

where S is the surface bounding the volume V. Stationarity of the energy integral with respect to variations of displacement field provides the equilibrium relation

$$\sigma_{jk,j} - \tau_{ijk,ij} = 0. \tag{2.4}$$

To identify the required boundary conditions we note that $\delta u_{k,j}$ is not independent of δu_k on the surface S because, if δu_k is known on S, so is the surface gradient of δu_k. Therefore, six independent displacement boundary conditions are required for correct

formulation of the problem, e.g. prescribed values for u_i, $i = 1, 2, 3$ and their normal derivatives.

In order to identify independent *traction* boundary conditions we resolve the gradient $\delta u_{k,j}$ into a surface gradient $D_j \delta u_k$ and a normal gradient $n_j D\delta u_k$,

$$\delta u_{k,j} = D_j \delta u_k + n_j D\delta u_k, \tag{2.5}$$

where

$$D_j \equiv (\delta_{jp} - n_j n_p)\partial_p, \quad D \equiv n_p \partial_p \tag{2.6}$$

and ∂_p denotes the partial derivative with respect to x_p. Now substitute (2.4), (2.5), (2.6) into (2.3) and make use of the surface divergence theorem (see, e.g. Mindlin, 1965) to obtain the following final form of the principle of virtual work

$$\delta W = \int_S [t_k \delta u_k] \, \mathrm{d}S + \int_S [R_k \cdot (D\delta u_k)] \, \mathrm{d}S, \tag{2.7}$$

where the *surface traction* t_k on the surface S is

$$t_k = n_i(\sigma_{ik} - \tau_{ijk,j}) + n_i n_j \tau_{ijk}(D_p n_p) - D_j(n_i \tau_{ijk}) \tag{2.8}$$

and the *double stress traction* R_k on S is

$$R_k = n_i n_j \tau_{ijk}. \tag{2.9}$$

To summarize, the displacement field $\mathbf{u}(\mathbf{x})$ must satisfy three equilibrium equations given by relation (2.4) and either six traction boundary conditions given by (2.8) and (2.9), or six displacement boundary conditions

$$u_i(\mathbf{x}) = u_i^0(\mathbf{x}), \quad Du_i(\mathbf{x}) = v_i^0(\mathbf{x}), \quad i = 1, 2, 3, \tag{2.10}$$

(or a mixture of them).

A corollary of the above principle of virtual work is the stationarity principle

$$\int_V (\sigma_{ij}\varepsilon_{ij} + \tau_{ijk}\eta_{ijk}) = 0 \tag{2.11}$$

for any $(\boldsymbol{\varepsilon}, \boldsymbol{\eta})$ derived kinematically from a displacement field $\mathbf{u}(\mathbf{x})$ and for any $(\boldsymbol{\sigma}, \boldsymbol{\tau})$ satisfying the equilibrium condition (2.4) and zero traction conditions $t_k = R_k = 0$.

Note that in general the equilibrium relation (2.4) is understood in a "weak" sense which implies that tractions and higher-order tractions are continuous across interfaces if there are any. This makes the above framework applicable to composites.

2.2. *Minimum principle*

A minimum principle can be stated for W provided the strain energy density w is strictly convex in $(\boldsymbol{\varepsilon}, \boldsymbol{\eta})$. It states that the "true" energy $\tilde{W}$ of the solid minimizes the functional $W(\mathbf{u})$ within the class of kinematically admissible fields $\mathbf{u}$ satisfying the boundary conditions (2.10)

$$\tilde{W} \leqslant W(\mathbf{u}). \tag{2.12}$$

Derivation of this principle follows along standard lines (see, e.g. Fleck and Hutchinson, 1993). Let $\mathbf{u}^*$ be the "true" displacement field satisfying both the equilibrium conditions (2.4) and the boundary conditions (2.10). Consider an arbitrary displacement field $\mathbf{u}(\mathbf{x}) = \mathbf{u}^*(\mathbf{x}) + \Delta\mathbf{u}(\mathbf{x})$ satisfying the same boundary conditions. Denote similarly the strain and strain gradient field derived from $\mathbf{u}$

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \boldsymbol{\varepsilon}^*(\mathbf{x}) + \Delta\boldsymbol{\varepsilon}(\mathbf{x}), \quad \boldsymbol{\eta}(\mathbf{x}) = \boldsymbol{\eta}^*(\mathbf{x}) + \Delta\boldsymbol{\eta}(\mathbf{x}).$$

Convexity implies

$$w(\boldsymbol{\varepsilon}^* + \Delta\boldsymbol{\varepsilon}, \boldsymbol{\eta}^* + \Delta\boldsymbol{\eta}\,; \mathbf{x}) \geqslant w(\boldsymbol{\varepsilon}^*, \boldsymbol{\eta}^*\,; \mathbf{x}) + \frac{\partial w}{\partial \varepsilon_{ij}}(\boldsymbol{\varepsilon}^*, \boldsymbol{\eta}\,; \mathbf{x})\Delta\varepsilon_{ij} + \frac{\partial w}{\partial \eta_{ijk}}(\boldsymbol{\varepsilon}^*, \boldsymbol{\eta}^*; \mathbf{x})\Delta\eta_{ijk}$$

for any $(\Delta\boldsymbol{\varepsilon}, \Delta\boldsymbol{\eta})$. Upon integration over the volume V this inequality results in

$$W(\mathbf{u}^* + \Delta\mathbf{u}) \equiv \int_V w(\boldsymbol{\varepsilon}^* + \Delta\boldsymbol{\varepsilon}, \boldsymbol{\eta}^* + \Delta\boldsymbol{\eta}\,; \mathbf{x})\,\mathrm{d}\mathbf{x} \geqslant W(\mathbf{u}^*) + \int_V [\sigma^*_{ij}\Delta\varepsilon_{ij} + \tau^*_{ijk}\Delta\eta_{ijk}]\,\mathrm{d}\mathbf{x}, \tag{2.13}$$

where σ^*_{ij} and τ^*_{ijk} are the "true" stress and higher stress, respectively. Use of the virtual work principle (2.7) for $\boldsymbol{\delta}\mathbf{u} \equiv \Delta\mathbf{u}$, coupled with zero displacement boundary conditions for the virtual field $\boldsymbol{\delta}\mathbf{u}$ results in vanishing of the integral on the right hand side of (2.13). This immediately gives the inequality (2.12) for $\tilde{W} \equiv W(\mathbf{u}^*)$ and arbitrary $\mathbf{u} = \mathbf{u}^* + \Delta\mathbf{u}$.

2.3. *Complementary minimum principle*

The complementary energy density (stress potential) ϕ can be introduced as a dual to w

$$\phi(\boldsymbol{\sigma}, \boldsymbol{\tau}\,; \mathbf{x}) = \sup_{(\boldsymbol{\varepsilon}, \boldsymbol{\eta})} \{\boldsymbol{\varepsilon}\cdot\boldsymbol{\sigma} + \boldsymbol{\eta}\cdot\boldsymbol{\tau} - w(\boldsymbol{\varepsilon}, \boldsymbol{\eta}\,; \mathbf{x})\}. \tag{2.14}$$

Here and henceforth the dot sign means the scalar product of the tensors involved, i.e. $\boldsymbol{\varepsilon}\cdot\boldsymbol{\sigma} \equiv \varepsilon_{ij}\sigma_{ij}$, $\boldsymbol{\eta}\cdot\boldsymbol{\tau} \equiv \eta_{ijk}\tau_{ijk}$. If the function w is smooth and strictly convex then for a fixed $\boldsymbol{\sigma} = \boldsymbol{\sigma}^*$ and $\boldsymbol{\tau} = \boldsymbol{\tau}^*$ the supremum is attained at $\boldsymbol{\varepsilon}^*$ and $\boldsymbol{\eta}^*$ such that

$$\sigma^*_{ij} = \frac{\partial w}{\partial \varepsilon_{ij}}(\boldsymbol{\varepsilon}^*, \boldsymbol{\eta}^*\,; \mathbf{x}), \quad \tau^*_{ijk} = \frac{\partial w}{\partial \eta_{ijk}}(\boldsymbol{\varepsilon}^*, \boldsymbol{\eta}^*\,; \mathbf{x}).$$

Thus, for a given stress $(\boldsymbol{\sigma}^*, \boldsymbol{\tau}^*)$ the corresponding strain $(\boldsymbol{\varepsilon}^*, \boldsymbol{\eta}^*)$ delivers the supremum of (2.14), and

$$\phi(\boldsymbol{\sigma}^*, \boldsymbol{\tau}^*\,; \mathbf{x}) = \boldsymbol{\varepsilon}^*\cdot\boldsymbol{\sigma}^* + \boldsymbol{\eta}^*\cdot\boldsymbol{\tau}^* - w(\boldsymbol{\varepsilon}^*, \boldsymbol{\eta}^*\,; \mathbf{x}). \tag{2.15}$$

The complementary function ϕ as defined by (2.14) is a convex function of its arguments $(\boldsymbol{\sigma}, \boldsymbol{\tau})$. Therefore (2.15) implies that, in turn, the strain energy function w is the dual of ϕ

$$w(\boldsymbol{\varepsilon}^*, \boldsymbol{\eta}^*\,; \mathbf{x}) = \sup_{(\boldsymbol{\sigma}, \boldsymbol{\tau})} \{\boldsymbol{\varepsilon}^*\cdot\boldsymbol{\sigma} + \boldsymbol{\eta}^*\cdot\boldsymbol{\tau} - \phi(\boldsymbol{\sigma}, \boldsymbol{\tau}\,; \mathbf{x})\}$$

with the supremum attained at $\boldsymbol{\sigma} = \boldsymbol{\sigma}^*$, $\boldsymbol{\tau} = \boldsymbol{\tau}^*$, and therefore

$$\varepsilon^*_{ij} = \frac{\partial \phi}{\partial \sigma_{ij}}(\boldsymbol{\sigma}^*, \boldsymbol{\tau}^*; \mathbf{x}), \quad \eta^*_{ijk} = \frac{\partial \phi}{\partial \tau_{ijk}}(\boldsymbol{\sigma}^*, \boldsymbol{\tau}^*; \mathbf{x}). \tag{2.16}$$

To formulate the complementary minimum principle define the complementary energy of the solid of volume V by

$$\tilde{\Phi} = \int_V \phi(\boldsymbol{\sigma}^*, \boldsymbol{\tau}^*; \mathbf{x})\, \mathrm{d}\mathbf{x}.$$

The minimum principle states that for all stress fields $(\boldsymbol{\sigma}(\mathbf{x}), \boldsymbol{\eta}(\mathbf{x}))$ in V which are

(i) statically admissible, i.e. satisfy the equilibrium equation (2.4), and
(ii) satisfy prescribed traction boundary conditions (2.8), (2.9) on the boundary S,

the true complementary energy $\tilde{\Phi}$ minimizes the functional

$$\Phi(\boldsymbol{\sigma}, \boldsymbol{\tau}) \equiv \int_V \phi(\boldsymbol{\sigma}(\mathbf{x}), \boldsymbol{\tau}(\mathbf{x}); \mathbf{x})\, \mathrm{d}\mathbf{x}. \tag{2.17}$$

This may be re-written as

$$\tilde{\Phi} \equiv \Phi(\boldsymbol{\sigma}^*, \boldsymbol{\tau}^*) \leqslant \Phi(\boldsymbol{\sigma}, \boldsymbol{\tau}). \tag{2.18}$$

To sketch the derivation of (2.18) take an arbitrary stress field $\boldsymbol{\sigma} = \boldsymbol{\sigma}^* + \Delta\boldsymbol{\sigma}$, $\boldsymbol{\tau} = \boldsymbol{\tau}^* + \Delta\boldsymbol{\tau}$ which satisfies conditions (i) and (ii). Employing convexity of ϕ and (2.16) gives

$$\Phi(\boldsymbol{\sigma}^* + \Delta\boldsymbol{\sigma}) \geqslant \int_V \phi(\boldsymbol{\sigma}^*, \boldsymbol{\tau}^*; \mathbf{x})\, \mathrm{d}\mathbf{x} + \int_V [\Delta\sigma_{ij}\varepsilon^*_{ij} + \Delta\tau_{ijk}\eta^*_{ijk}]\, \mathrm{d}\mathbf{x}.$$

According to (2.11) the last integral vanishes since $(\Delta\boldsymbol{\sigma}, \Delta\boldsymbol{\tau})$ is an equilibrium stress field with vanishing tractions on the boundary and $(\boldsymbol{\varepsilon}^*, \boldsymbol{\eta}^*)$ is derived from a displacement field $\mathbf{u}^*$. Thus,

$$\Phi(\boldsymbol{\sigma}^* + \Delta\boldsymbol{\sigma}) \geqslant \int_V \phi(\boldsymbol{\sigma}^*, \boldsymbol{\tau}^*; \mathbf{x})\, \mathrm{d}\mathbf{x} \equiv \tilde{\Phi}$$

and the complementary energy principle has been proved.

3. SUMMARY OF STRAIN GRADIENT MODEL FOR CRYSTALS

We summarize in Sections 3.1 and 3.2 below the crystal plasticity formulation of Fleck and Hutchinson (1996). The instantaneous secant modulus is then defined in Section 3.3: this motivates a study of linear polycrystals in the remainder of the paper.

3.1. *Crystal kinematics*

The general framework of the previous section is now specialized to crystals. The crystal is assumed to deform by slip on a discrete number of slip systems. A particular slip system, α, is characterized by a slip plane with normal $\mathbf{m}^\alpha$ and the direction of slip $\mathbf{s}^\alpha$ in the slip plane. By neglecting elastic stretching of the crystal lattice and assuming deformations to be small, the displacement gradient can be expressed as

$$u_{i,j} = \gamma_{ij} + \phi_{ij}.$$

Here, the slip tensor γ_{ik} is associated with an amount of slip $\gamma^{(\alpha)}$ on each of the slip systems, i.e.

$$\gamma_{ik} = \sum_\alpha \gamma^{(\alpha)} s_i^{(\alpha)} m_j^{(\alpha)} \tag{3.1}$$

(summation is taken over all slip systems), and ϕ_{ij} is the antisymmetric *lattice rotation tensor*. Obviously, such deformation is incompressible, i.e. $u_{i,i} \equiv 0$.

The objective is to develop a higher order constitutive law which involves both the slips $\gamma^{(\alpha)}$ and the slip gradients.† To this end we express both the strain tensor $\boldsymbol{\varepsilon}$ and the strain-gradient tensor $\boldsymbol{\eta}$ in terms of $\gamma^{(\alpha)}$ and $\gamma_{,k}^{(\alpha)}$. The strain tensor may be written in the form

$$\varepsilon_{ij} \equiv \tfrac{1}{2}(u_{i,j} + u_{j,i}) = \sum_\alpha \gamma^{(\alpha)} \mu_{ij}^{(\alpha)}, \quad \text{where} \quad \mu_{ij}^{(\alpha)} \equiv \tfrac{1}{2}(s_i^{(\alpha)} m_j^{(\alpha)} + m_i^{(\alpha)} s_j^{(\alpha)}), \tag{3.2}$$

and the strain-gradient tensor may be written as

$$\eta_{jki} \equiv u_{i,jk} = \gamma_{ij,k} + \phi_{ij,k}.$$

Kinematic compatibility dictates that the gradients of rotation are pre-determined to accomodate the gradients of the slip (see Fleck and Hutchinson, 1996)

$$\phi_{ij,k} = \gamma_{ki,j} - \gamma_{kj,i} - \tfrac{1}{2} e_{ijk} e_{spq} \gamma_{sp,q}.$$

This results in the following kinematic connection between the strain-gradient tensor η_{ijk} and the "slip-gradient" tensor $\gamma_{jk,i}$

$$\eta_{jki} = \gamma_{ij,k} + \gamma_{ki,j} - \gamma_{kj,i} - \tfrac{1}{2} e_{ijk} e_{spq} \gamma_{sp,q}. \tag{3.3}$$

Note that by definition tensor η_{jki} is symmetric in its first two indices, and is also *incompressible*, i.e. $\eta_{jkk} = \eta_{kjk} = 0$ for $j = 1, 2, 3$. Assuming small deformations (3.1) implies‡

$$\gamma_{ij,k} = \sum_\alpha \gamma_{,k}^{(\alpha)} s_i^{(\alpha)} m_j^{(\alpha)}. \tag{3.4}$$

Substitution of (3.4) into (3.3) results in

† Fleck *et al.* (1994) give the underlying physical motivation in their discussion of dislocation hardening by "statistically stored" and "geometrically necessary" dislocations.

‡ The terms containing $s_{i,k}^{(\alpha)}$ and $m_{j,k}^{(\alpha)}$ are negligible. Indeed, if e.g. $\mathbf{s}^0$ is the undeformed slip direction, then for the "rotated" $\mathbf{s}$, $s_i \sim s_i^0 + \phi_{ij} s_j^0$. Therefore $s_{i,k} \sim \phi_{ij,k} s_j^0$ which is negligible provided $\gamma^{(\alpha)}$ are small (see (3.3)).

$$\eta_{ijk} = \sum_{\alpha} \gamma^{(\alpha)}_{,p} \psi^{(\alpha)}_{pijk} \tag{3.5}$$

where the resolution tensor $\boldsymbol{\psi}^{(\alpha)}$ is given by

$$\psi^{(\alpha)}_{pijk} = \delta_{pi} s^{(\alpha)}_k m^{(\alpha)}_j + \delta_{pj} s^{(\alpha)}_i m^{(\alpha)}_k - \delta_{pk} s^{(\alpha)}_i m^{(\alpha)}_j + \tfrac{1}{2} t^{(\alpha)}_p e_{ijk} \quad \text{(no sum on } \alpha\text{)}, \tag{3.6}$$

upon introducing the "transverse" unit vector $\mathbf{t}^{(\alpha)} \equiv \mathbf{s}^{(\alpha)} \times \mathbf{m}^{(\alpha)}$. Note that $(\mathbf{s}^{(\alpha)}, \mathbf{m}^{(\alpha)}, \mathbf{t}^{(\alpha)})$ forms a right-handed triad with $\mathbf{t}^{(\alpha)}$ in the slip plane and orthogonal to the slip direction $\mathbf{s}^{(\alpha)}$.

It is convenient to express the slip gradient $\gamma^{(\alpha)}_{,i}$ in terms of the slip gradient $\gamma^{(\alpha)}_{,S}$ along the slip direction $\mathbf{s}^{(\alpha)}$, the slip gradient $\gamma^{(\alpha)}_{,M}$ along the normal $\mathbf{m}^{(\alpha)}$ to the slip plane, and the slip gradient $\gamma^{(\alpha)}_{,T}$ along the transverse direction $\mathbf{t}^{(\alpha)}$

$$\gamma^{(\alpha)}_{,S} \equiv \gamma^{(\alpha)}_{,p} s^{(\alpha)}_p; \quad \gamma^{(\alpha)}_{,M} \equiv \gamma^{(\alpha)}_{,p} m^{(\alpha)}_p; \quad \gamma^{(\alpha)}_{,T} \equiv \gamma^{(\alpha)}_{,p} t^{(\alpha)}_p.$$

Since $(\mathbf{s}^{(\alpha)}, \mathbf{m}^{(\alpha)}, \mathbf{t}^{(\alpha)})$ form an orthonormal basis, (3.5) transforms to

$$\eta_{ijk} = \sum_{\alpha} \{\gamma^{(\alpha)}_{,S} \psi^{(\alpha)S}_{ijk} + \gamma^{(\alpha)}_{,M} \psi^{(\alpha)M}_{ijk} + \gamma^{(\alpha)}_{,T} \psi^{(\alpha)T}_{ijk}\}, \tag{3.7}$$

where the notation

$$\begin{aligned} \psi^{(\alpha)S}_{ijk} &\equiv s^{(\alpha)}_i s^{(\alpha)}_j m^{(\alpha)}_k, \\ \psi^{(\alpha)M}_{ijk} &\equiv m^{(\alpha)}_i m^{(\alpha)}_j s^{(\alpha)}_k, \\ \psi^{(\alpha)T}_{ijk} &\equiv [t^{(\alpha)}_i m^{(\alpha)}_j s^{(\alpha)}_k + s^{(\alpha)}_i t^{(\alpha)}_j m^{(\alpha)}_k - s^{(\alpha)}_i m^{(\alpha)}_j t^{(\alpha)}_k + \tfrac{1}{2} e_{ijk}] \end{aligned} \tag{3.8}$$

has been introduced. Relation (3.7) gives the strain-gradient tensor $\boldsymbol{\eta}$ in terms of slip gradients for each slip system.

Following the argument of Fleck *et al.* (1994), the slip $\gamma^{(\alpha)}$ on each slip system gives rise to a density of "statistically stored dislocations". The slip gradient $\gamma^{(\alpha)}_{,S}$ is associated with the storage of a density $\gamma^{(\alpha)}_{,S}/b$ of "geometrically necessary" edge dislocations along the $\mathbf{t}^{(\alpha)}$ direction, with Burgers vector $\mathbf{b}$ aligned with $\mathbf{s}^{(\alpha)}$. Similarly, the slip gradient $\gamma^{(\alpha)}_{,T}$ is associated with the storage of a density $\gamma^{(\alpha)}_{,T}/b$ of "geometrically necessary" screw dislocations along the $\mathbf{s}^{(\alpha)}$ direction with Burgers vector $\mathbf{b}$ also aligned with $\mathbf{s}^{(\alpha)}$. A slip gradient $\gamma^{(\alpha)}_{,M}$ along the normal $\mathbf{m}^{(\alpha)}$ to the slip plane does not result in the storage of "geometrically necessary" dislocations.

3.2. *Resolved stresses; crystal constitutive laws*

To specialize the principle of virtual work to the crystal multislip deformation, substitute the kinematic relations (3.2) and (3.5) into (2.1). The energy increment due to crystallographic slip $\gamma^{(\alpha)}$ is written in the form

$$\delta W = \int_V \sum_{\alpha} [\tau^{(\alpha)} \delta\gamma^{(\alpha)} + Q^{(\alpha)}_p \delta\gamma^{(\alpha)}_{,p}] \, \mathrm{d}\mathbf{x}. \tag{3.9}$$

Here, the work conjugate to $\gamma^{(\alpha)}$ is the Schmid resolved stress

$$\tau^{(\alpha)} \equiv \sigma_{ij}\mu_{ij}^{(\alpha)}, \tag{3.10}$$

and, similarly, the work conjugate to the slip gradient $\gamma_{,p}^{(\alpha)}$ is

$$Q_p^{(\alpha)} \equiv \tau_{ijk}\psi_{pijk}^{(\alpha)},$$

which can be called the *vector of higher order Schmid stress*, $\mathbf{Q}^{(\alpha)}$. Recall that the hydrostatic part of $\boldsymbol{\sigma}$ does not contribute to the Schmid stress $\tau^{(\alpha)}$. In similar fashion, the hydrostatic part of $\boldsymbol{\tau}$ does not contribute to the higher order Schmid stress $\mathbf{Q}^{(\alpha)}$. The hydrostatic part $\boldsymbol{\tau}^{\mathrm{h}}$ of $\boldsymbol{\tau}$ can be written in the form†

$$\tau_{ijk}^{\mathrm{h}} = \tfrac{1}{4}(\delta_{ik}\tau_{jpp} + \delta_{jk}\tau_{ipp}). \tag{3.11}$$

Note that $\boldsymbol{\tau}^{\mathrm{h}}$ does not work through any incompressible strain gradient tensor $\boldsymbol{\eta}$ since $\tau_{ijk}^{\mathrm{h}}\eta_{ijk} = 0$.

Specializing (3.9) to the basic triad $(\mathbf{s}^{(\alpha)}, \mathbf{m}^{(\alpha)}, \mathbf{t}^{(\alpha)})$ gives

$$\delta W = \int_V \sum_\alpha [\tau^{(\alpha)}\delta\gamma^{(\alpha)} + Q_S^{(\alpha)}\delta\gamma_{,S}^{(\alpha)} + Q_M^{(\alpha)}\delta\gamma_{,M}^{(\alpha)} + Q_T^{(\alpha)}\delta\gamma_{,T}^{(\alpha)}]\,\mathrm{d}\mathbf{x}.$$

Explicit formulae for the resolved higher stress components $Q_S^{(\alpha)}$, $Q_M^{(\alpha)}$ and $Q_T^{(\alpha)}$ derived from (3.7) and (3.8) are

$$\begin{aligned} Q_S^{(\alpha)} &= \tau_{ijk}\psi_{ijk}^{(\alpha)S}, \\ Q_M^{(\alpha)} &= \tau_{ijk}\psi_{ijk}^{(\alpha)M}, \\ Q_T^{(\alpha)} &= \tau_{ijk}\psi_{ijk}^{(\alpha)T}. \end{aligned} \tag{3.12}$$

A fundamental assumption of Schmid's model for a deformation theory version of crystal plasticity states that the amount of slip $\gamma^{(\alpha)}$ on the slip system α depends on stress $\boldsymbol{\sigma}$ only through the resolved stress $\tau^{(\alpha)}$. A "gradient" extension of this law is to require that both the slip $\gamma^{(\alpha)}$ and the slip gradients $\gamma_{,S}^{(\alpha)}$, $\gamma_{,M}^{(\alpha)}$ and $\gamma_{,T}^{(\alpha)}$ depend only on the resolved stress $\tau^{(\alpha)}$ and the resolved higher stress $\mathbf{Q}^{(\alpha)} \equiv (Q_S^{(\alpha)}, Q_M^{(\alpha)}, Q_T^{(\alpha)})$. This assumption is supported micromechanically by the notion of statistically stored and geometrically necessary dislocations (see, e.g. Ashby, 1970; Fleck *et al.*, 1994) which suggests that the amount of strain hardening of the slip system is governed by the accumulated slip and the accumulated slip gradient on each slip system. Note that the component $\gamma_{,M}^{(\alpha)}$ of the slip gradient does not result in the storage of geometrically necessary dislocations as has been discussed by Fleck *et al.* (1994): the work conjugates $Q_M^{(\alpha)}$ are included for mathematical completeness. "Physically" $Q_M^{(\alpha)}$ should vanish which imposes constraints on the higher order stress $\boldsymbol{\tau}$: $\tau_{ijk}\psi_{ijk}^{(\alpha)M} = 0$, for all α.

The stress potential $\phi(\boldsymbol{\sigma}, \boldsymbol{\tau})$, as introduced in Section 2.2, is of the form

$$\phi(\boldsymbol{\sigma}, \boldsymbol{\tau}) = \sum_\alpha \phi^{(\alpha)}(\boldsymbol{\sigma}, \boldsymbol{\tau}), \tag{3.13}$$

where the contribution of the slip system α *is taken to depend only on the resolved stresses associated with this slip system*

$$\phi^{(\alpha)} = \phi^{(\alpha)}(\tau^{(\alpha)}, \mathbf{Q}^{(\alpha)}) \equiv \phi^{(\alpha)}(\tau^{(\alpha)}; Q_S^{(\alpha)}, Q_M^{(\alpha)}, Q_T^{(\alpha)}). \tag{3.14}$$

† Obviously, the component $\boldsymbol{\tau}^{\mathrm{d}} \equiv \boldsymbol{\tau} - \boldsymbol{\tau}^{\mathrm{h}}$ is "deviatoric" in the sense that $\tau_{ijj}^{\mathrm{d}} = \tau_{jij}^{\mathrm{d}} = 0$.

Here and elsewhere we assume no sum on α unless otherwise stated. Relation (3.14) is equivalent to an independent hardening assumption. The strain $\boldsymbol{\varepsilon}$ and the strain gradient $\boldsymbol{\eta}$ are determined by the stress potential (3.13), (3.14) via (2.16), (3.10) and (3.12) as

$$\varepsilon_{ij} \equiv \frac{\partial \phi}{\partial \sigma_{ij}} = \sum_{\alpha} \frac{\partial \phi^{(\alpha)}}{\partial \tau^{(\alpha)}} \mu_{ij}^{(\alpha)},$$

$$\eta_{ijk} \equiv \frac{\partial \phi}{\partial \tau_{ijk}} = \sum_{\alpha} \left[\frac{\partial \phi^{(\alpha)}}{\partial Q_S^{(\alpha)}} \psi_{ijk}^{(\alpha)S} + \frac{\partial \phi^{(\alpha)}}{\partial Q_M^{(\alpha)}} \psi_{ijk}^{(\alpha)M} + \frac{\partial \phi^{(\alpha)}}{\partial Q_T^{(\alpha)}} \psi_{ijk}^{(\alpha)T} \right]. \tag{3.15}$$

Comparison of (3.15) with (3.2) and (3.7) implies

$$\gamma^{(\alpha)} = \frac{\partial \phi^{(\alpha)}}{\partial \tau^{(\alpha)}}, \quad \gamma_{,S}^{(\alpha)} = \frac{\partial \phi^{(\alpha)}}{\partial Q_S^{(\alpha)}}, \quad \gamma_{,M}^{(\alpha)} = \frac{\partial \phi^{(\alpha)}}{\partial Q_M^{(\alpha)}}, \quad \gamma_{,T}^{(\alpha)} = \frac{\partial \phi^{(\alpha)}}{\partial Q_T^{(\alpha)}}. \tag{3.16}$$

Thus, we may interpret $\phi^{(\alpha)}$ as "single slip potentials".

Note that the $\phi^{(\alpha)}$ must be convex functions of their arguments $(\tau^{(\alpha)}, \mathbf{Q}^{(\alpha)})$ to ensure convexity of the "total" potential $\phi(\boldsymbol{\sigma}, \boldsymbol{\tau})$. Apart from this we impose no restrictions on $\phi^{(\alpha)}$. Their exact form describes micromechanically the combined effect of densities of statistically stored and geometrically necessary dislocations on the material's hardening, and must be found experimentally or through explicit modelling of dislocation–dislocation interactions.

3.3. *Linear constitutive laws and the "instantaneous linearity" of nonlinear Schmid's crystals*

Linear constitutive relations form an important particular case of (3.13) as will be clarified later in this section. To describe such a linear behaviour an assumption is made that the slips $\gamma^{(\alpha)}$ and the slip gradients $\gamma_{,S}^{(\alpha)}$, $\gamma_{,M}^{(\alpha)}$ and $\gamma_{,T}^{(\alpha)}$ are linearly related to their work conjugates $\tau^{(\alpha)}$, $Q_S^{(\alpha)}$, $Q_M^{(\alpha)}$ and $Q_T^{(\alpha)}$ via

$$\gamma^{(\alpha)} = \frac{1}{\mu_\alpha} \tau^{(\alpha)},$$

$$\gamma_{,S}^{(\alpha)} = \frac{1}{\mu_\alpha l_S^{(\alpha)2}} Q_S^{(\alpha)},$$

$$\gamma_{,M}^{(\alpha)} = \frac{1}{\mu_\alpha l_M^{(\alpha)2}} Q_M^{(\alpha)},$$

$$\gamma_{,T}^{(\alpha)} = \frac{1}{\mu_\alpha l_T^{(\alpha)2}} Q_T^{(\alpha)}. \tag{3.17}$$

Here μ_α plays the role of the shear modulus of the slip system α; the three lengthscales $l_S^{(\alpha)}$, $l_M^{(\alpha)}$ and $l_T^{(\alpha)}$ are introduced for dimensional consistency and adopt the role of material lengthscales in the constitutive description.

The total stress potential corresponding to (3.17) is

$$\phi(\boldsymbol{\sigma},\boldsymbol{\tau}) = \sum_{\alpha}\frac{1}{2\mu_\alpha}[(\tau^{(\alpha)})^2 + (l_S^{(\alpha)^{-1}}Q_S^{(\alpha)})^2 + (l_M^{(\alpha)^{-1}}Q_M^{(\alpha)})^2 + (l_T^{(\alpha)^{-1}}Q_T^{(\alpha)})^2]. \tag{3.18}$$

The slip shear moduli μ_α and the length scales $l_S^{(\alpha)}$, $l_M^{(\alpha)}$, $l_T^{(\alpha)}$ may vary from one slip system to the next, and, for "inhomogeneous" linear crystals, from one material point to the next.

The stress potential (3.18) for the linear crystal can be presented symbolically as a quadratic form

$$\phi(\boldsymbol{\sigma},\boldsymbol{\tau}) = \tfrac{1}{2}\sigma_{ij}M_{ijpq}\sigma_{pq} + \tfrac{1}{2}\tau_{ijk}\mathscr{M}_{ijkpqr}\tau_{pqr}, \tag{3.19}$$

where

$$M_{ijpq} \equiv \sum_{\alpha}\frac{1}{\mu_\alpha}\mu_{ij}^{(\alpha)}\mu_{pq}^{(\alpha)} \tag{3.20}$$

is the conventional compliance tensor, and

$$\mathscr{M}_{ijkpqr} \equiv \sum_{\alpha}\left[\frac{1}{\mu_\alpha(l_S^{(\alpha)})^2}\psi_{ijk}^{(\alpha)S}\psi_{pqr}^{(\alpha)S} + \frac{1}{\mu_\alpha(l_M^{(\alpha)})^2}\psi_{ijk}^{(\alpha)M}\psi_{pqr}^{(\alpha)M} + \frac{1}{\mu_\alpha(l_T^{(\alpha)})^2}\psi_{ijk}^{(\alpha)T}\psi_{pqr}^{(\alpha)T}\right] \tag{3.21}$$

is a higher-order compliance tensor. It follows directly from (3.19) that

$$\varepsilon_{ij} = M_{ijpq}\sigma_{pq}, \quad \eta_{ijk} = \mathscr{M}_{ijkpqr}\tau_{pqr}.$$

We note in passing that both $\mathbf{M}$ and $\mathscr{M}$ are symmetric, i.e. $M_{ijpq} = M_{pqij}$ and $\mathscr{M}_{ijkpqr} = \mathscr{M}_{pqrijk}$, which will be assumed henceforth whenever tensors of such type are introduced.

The linear constitutive law (3.18) plays a critical role in the study of the overall behaviour of polycrystals with *nonlinear* constitutive laws (3.13), (3.14) due to the property of **instantaneous linearity** of a general Schmid crystal. Comparison of (3.16) with (3.17) demonstrates that

$$\tilde{\mu}_\alpha(\mathbf{x}) = \tau^{(\alpha)}\left[\frac{\partial\phi^{(\alpha)}}{\partial\tau^{(\alpha)}}(\tau^{(\alpha)},\mathbf{Q}^{(\alpha)})\right]^{-1}$$

plays the part of the "instantaneous" shear modulus of the slip system; similarly, the instantaneous length scales $\tilde{l}_S^{(\alpha)}$, $\tilde{l}_M^{(\alpha)}$ and $\tilde{l}_T^{(\alpha)}$ are determined from

$$\begin{aligned}
\tilde{\mu}_\alpha(\mathbf{x})\tilde{l}_S^{(\alpha)2} &= Q_S^{(\alpha)}\left[\frac{\partial\phi^{(\alpha)}}{\partial Q_S^{(\alpha)}}(\tau^{(\alpha)},\mathbf{Q}^{(\alpha)})\right]^{-1},\\
\tilde{\mu}_\alpha(\mathbf{x})\tilde{l}_M^{(\alpha)2} &= Q_M^{(\alpha)}\left[\frac{\partial\phi^{(\alpha)}}{\partial Q_M^{(\alpha)}}(\tau^{(\alpha)},\mathbf{Q}^{(\alpha)})\right]^{-1},\\
\tilde{\mu}_\alpha(\mathbf{x})\tilde{l}_T^{(\alpha)2} &= Q_T^{(\alpha)}\left[\frac{\partial\phi^{(\alpha)}}{\partial Q_T^{(\alpha)}}(\tau^{(\alpha)},\mathbf{Q}^{(\alpha)})\right]^{-1}.
\end{aligned} \tag{3.22}$$

This simple observation means that a nonlinear crystal under prescribed loading experiences the same response as a linear inhomogeneous crystal with variable parameters $\tilde{\mu}_\alpha(\mathbf{x})$, $\tilde{l}_S^{(\alpha)}(\mathbf{x})$, $\tilde{l}_M^{(\alpha)}(\mathbf{x})$ and $\tilde{l}_T^{(\alpha)}(\mathbf{x})$. In other words, if we knew these parameters and could also solve the linear problem, we would know also the solution to the nonlinear problem. Of course, these parameters themselves depend on the solution via $\tau^{(\alpha)}$ and $\mathbf{Q}^{(\alpha)}$ as a consequence of nonlinearity.

This important property makes the strategy of Ponte Castañeda (1991, 1992), deBotton & Ponte Castañeda (1995) applicable to study the effective properties of *nonlinear* strain-gradient polycrystals in terms of the effective properties of related *linear* polycrystals. This is worth a separate discussion which is beyond the purposes of the present paper. This also motivates an extensive study of the effective properties of linear strain-gradient polycrystals in the rest of this paper.

Now take as an example the case where the slip potentials $\phi^{(\alpha)}$ are functions of a scalar "resolved stress measure" $s^{(\alpha)}$, where

$$s^{(\alpha)} \equiv [(\tau^{(\alpha)})^2 + (l_S^{(\alpha)^{-1}} Q_S^{(\alpha)})^2 + (l_M^{(\alpha)^{-1}} Q_M^{(\alpha)})^2 + (l_T^{(\alpha)^{-1}} Q_T^{(\alpha)})^2]^{1/2}.$$

The measure $s^{(\alpha)}$ can be interpreted as the dual to one possible strain measure

$$e^{(\alpha)} \equiv [(\gamma^{(\alpha)})^2 + (l_S^{(\alpha)} \gamma_{,S}^{(\alpha)})^2 + (l_M^{(\alpha)} \gamma_{,M}^{(\alpha)})^2 + (l_T^{(\alpha)} \gamma_{,T}^{(\alpha)})^2]^{1/2}$$

associated with the total density $\rho^{(\alpha)}$ of dislocations accumulated due to slip on the system α. Recall that physically $\gamma_{,M}^{(\alpha)}$ should not contribute to the total dislocation density which can be achieved by taking the limit $l_M^{(\alpha)} \to 0$.

For such coupling $\phi(\boldsymbol{\sigma}, \boldsymbol{\tau})$ assumes the form

$$\phi = \sum_\alpha \phi^{(\alpha)}(s^{(\alpha)})$$

and (3.22) implies that the instantaneous linear parameters are

$$\tilde{\mu}_\alpha = s^{(\alpha)}[(\sigma^{(\alpha)})'(s^{(\alpha)})]^{-1}$$

and

$$\tilde{l}_S^{(\alpha)} = l_S^{(\alpha)}, \quad \tilde{l}_M^{(\alpha)} = l_M^{(\alpha)}, \quad \tilde{l}_T^{(\alpha)} = l_T^{(\alpha)}.$$

4. OVERALL PROPERTIES OF POLYCRYSTALS WITH STRAIN-GRADIENT EFFECTS

4.1. *Homogenization problem*

A polycrystal is regarded as a collection of single crystals specified by a constitutive law (3.13), (3.14) with a large number N of distinct orientations. The orientations of the crystals are characterized by rotation tensors $\boldsymbol{\Omega}^{(r)}$, $(r = 1, 2, \ldots, N)$. Therefore, the stress potential of a rotated crystal $\phi^{(r)}$ relates to the "reference" stress potential via

$$\phi^{(r)}(\boldsymbol{\sigma}, \boldsymbol{\tau}) = \phi(\boldsymbol{\sigma}^{(r)}, \boldsymbol{\tau}^{(r)}),$$

where $\boldsymbol{\sigma}^{(r)}$ and $\boldsymbol{\tau}^{(r)}$ are the stress and the higher stress in the rotated frame

$$\sigma_{ij}^{(r)} = \Omega_{pi}\Omega_{qj}\sigma_{pq}, \quad \tau_{ijk}^{(r)} = \Omega_{pi}\Omega_{qj}\Omega_{rk}\tau_{pqr}.$$

The total stress potential is

$$\phi(\boldsymbol{\sigma}, \boldsymbol{\tau}) = \sum_{r=1}^{N} f^{(r)}(\mathbf{x})\phi^{(r)}(\boldsymbol{\sigma}, \boldsymbol{\tau}), \tag{4.1}$$

where $f^{(r)}(\mathbf{x})$, $r = 1, 2, \ldots, N$ are characteristic functions for the crystals orientations; $f^{(r)}(\mathbf{x}) = 1$ if $\mathbf{x}$ belongs to a crystal with orientation r; $f^{(r)} = 0$ otherwise.

Assume the polycrystal occupies a volume V and is subjected to uniform stress boundary conditions†

$$t_k = \bar{\sigma}_{ik}n_i, \quad R_k = 0. \tag{4.2}$$

over the boundary S.

The size of the polycrystal $V^{1/3}$ is supposed to be much large then the "typical" grain size a (the scale of the microstructure). The polycrystal is regarded as a *macroscopically homogeneous* body and, therefore, $\bar{\boldsymbol{\sigma}}$ in (4.2) plays the part of a uniform macroscopic stress: it is the uniform stress which a homogeneous material would experience under the traction conditions (4.2). We emphasize here that under these boundary conditions the macroscopic stress and strain are constant and therefore the macroscopic strain gradient and higher order stresses vanish. The *macroscopic* (local) gradients, however, do not vanish which affects indirectly the overall macroscopic behaviour of the solid and gives rise to the grain size effect.

The objective is to estimate the total complementary energy of the polycrystal as a function of $\bar{\boldsymbol{\sigma}}$

$$\tilde{\Phi}(\bar{\boldsymbol{\sigma}}) = \frac{1}{|V|}\int_V \phi(\boldsymbol{\sigma}, \boldsymbol{\tau})\, \mathrm{d}\mathbf{x} \tag{4.3}$$

which can be regarded as an "effective" stress potential of the polycrystal.‡ If the polycrystal displays no texture, i.e. if all crystals' orientations are equally likely, then $\tilde{\Phi}(\bar{\boldsymbol{\sigma}})$ is isotropic.

The influence of the scale of the microstructure a on the overall behaviour of the polycrystal described by $\tilde{\Phi}(\bar{\boldsymbol{\sigma}})$, i.e. the grain size effect, is anticipated to be a result of a competition between the internal crystal lengthscales $l_S^{(\alpha)}$, $l_M^{(\alpha)}$ and $l_T^{(\alpha)}$ and a.

Although the main motivation of this study is to develop homogenization methods for *nonlinear* polycrystals to model the so-called Hall–Petch effect (the grain size effect in plasticity) we concentrate in the remainder of this paper on the overall behaviour of *linear* polycrystals. This step is critical due to the "instantaneous linearity" of polycrystals with gradient effects as discussed above. This opens an avenue for

† Recall that the higher order constitutive law (3.13) for (4.1) implies that the displacements, displacement gradients, tractions (2.8) and double tractions (2.9) are continuous at grain boundaries.

‡ We avoid here discussion of the dependence of $\tilde{\Phi}$ on the macroscopic higher stress $\bar{\tau}$ which is zero due to the boundary conditions (4.2). More accurately, $\tilde{\Phi}(\bar{\sigma})$ as introduced by (4.3) could be regarded as the value of $\tilde{\Phi}(\bar{\sigma}, \bar{\tau})$ at $\bar{\tau} = 0$.

implementation of the linear results to nonlinear homogenization problems following the general strategy of Ponte Castañeda (1991, 1992) which has been adopted recently to conventional polycrystals (deBotton and Ponte Castañeda, 1995). This strategy has already been adopted by Smyshlyaev and Fleck (1995) for nonlinear two-phase composites with strain gradient effects included. In the following section a Hashin–Shtrikman variational principle is formulated in a form which does not necessarily assume that the phases (or the reference crystal) are linear. We then specialize to the linear case. Willis and co-workers (Dendievel *et al.*, 1991) have used a nonlinear variational principle of this type to derive bounds for nonlinear polycrystals. In principle, this avenue is also open for nonlinear polycrystals with strain gradient effects.

4.2. *Hashin–Shtrikman variational principle*

It is convenient to regard a polycrystal with a large number N of possible orientations as a particular example of an N-phase composite. Each phase r, $r = 1, 2, \ldots, N$ is described by a stress potential $\phi^{(r)}(\boldsymbol{\sigma}, \boldsymbol{\tau})$ specified in the linear case by compliance moduli $\mathbf{M}^{(r)}$ and $\mathscr{M}^{(r)}$ given by (3.19). The whole aggregate is subjected to the traction boundary conditions (4.2). The objective is to bound the total complementary energy $\tilde{\Phi}$ of the polycrystal.

We follow here a general strategy laid down by Hashin and Shtrikman (1962 a,b) and developed further by Willis (1977, 1981, 1983) and Talbot and Willis (1985) both for linear and nonlinear "conventional" composites. First, a comparison medium with stress potential $\phi_0(\boldsymbol{\sigma}, \boldsymbol{\tau})$ is introduced.

To derive a family of lower bounds a function $V(\boldsymbol{\zeta}, \boldsymbol{\kappa})$ can be defined as the dual to $\phi(\boldsymbol{\sigma}, \boldsymbol{\theta}) - \phi_0(\boldsymbol{\sigma}, \boldsymbol{\tau})$,

$$V(\boldsymbol{\zeta}, \boldsymbol{\kappa}) = \sup_{\boldsymbol{\sigma}, \boldsymbol{\tau}} \{\boldsymbol{\sigma} \cdot \boldsymbol{\zeta} + \boldsymbol{\tau} \cdot \boldsymbol{\kappa} - \phi(\boldsymbol{\sigma}, \boldsymbol{\tau}) + \phi_0(\boldsymbol{\sigma}, \boldsymbol{\tau})\} \tag{4.4}$$

for arbitrary "stress polarizations" ζ_{ij} and "higher order stress polarizations" κ_{ijk}. It follows immediately from the definition (4.4) that

$$\phi(\boldsymbol{\sigma}, \boldsymbol{\tau}) \geqslant \boldsymbol{\sigma} \cdot \boldsymbol{\zeta} + \boldsymbol{\tau} \cdot \boldsymbol{\kappa} + \phi_0(\boldsymbol{\sigma}, \boldsymbol{\tau}) - V(\boldsymbol{\zeta}, \boldsymbol{\kappa}) \tag{4.5}$$

for any values of $\boldsymbol{\sigma}$, $\boldsymbol{\tau}$, $\boldsymbol{\zeta}$ and $\boldsymbol{\kappa}$. Therefore, for the complementary energy functional defined by (2.17),

$$\Phi(\boldsymbol{\sigma}, \boldsymbol{\tau}) \geqslant \int_V [\boldsymbol{\sigma} \cdot \boldsymbol{\zeta} + \boldsymbol{\tau} \cdot \boldsymbol{\kappa} + \phi(\boldsymbol{\sigma}, \boldsymbol{\tau}) - V(\boldsymbol{\zeta}, \boldsymbol{\kappa})] \, \mathrm{d}\mathbf{x}.$$

Taking the infimum of both sides of the inequality within the class of statically admissible $(\boldsymbol{\sigma}(\mathbf{x}), \boldsymbol{\tau}(\mathbf{x}))$ compatible with the boundary conditions (4.2), and employing the complementary energy principle (2.18) results in

$$\tilde{\Phi}(\bar{\boldsymbol{\sigma}}) \geqslant \inf_{(\boldsymbol{\sigma}(\mathbf{x}), \boldsymbol{\tau}(\mathbf{x}))} \int_V [\boldsymbol{\sigma} \cdot \boldsymbol{\zeta} + \boldsymbol{\tau} \cdot \boldsymbol{\kappa} + \phi_0(\boldsymbol{\sigma}, \boldsymbol{\tau}) - V(\boldsymbol{\zeta}, \boldsymbol{\kappa})] \, \mathrm{d}\mathbf{x}. \tag{4.6}$$

The inequality (4.6) displays a family of bounds for the complementary energy $\tilde{\Phi}(\bar{\boldsymbol{\sigma}})$, for arbitrary polarization fields $(\boldsymbol{\zeta}(\mathbf{x}), \boldsymbol{\kappa}(\mathbf{x}))$.

If the comparison medium is chosen to be linear, i.e.

$$\phi_0(\boldsymbol{\sigma}, \boldsymbol{\tau}) = \tfrac{1}{2}\boldsymbol{\sigma} \cdot \mathbf{M}_0 \boldsymbol{\sigma} + \tfrac{1}{2}\boldsymbol{\tau} \cdot \mathscr{M}_0 \boldsymbol{\tau} \tag{4.7}$$

then the infimum of (4.6) may be expressed in terms of linear operators $\boldsymbol{\Delta}^{ij}$, $i = 1, 2$; $j = 1, 2$ which are related to the Green's function for the comparison medium (Appendix A). The result is

$$\tilde{\Phi}(\bar{\boldsymbol{\sigma}}) \geqslant \tfrac{1}{2}\bar{\boldsymbol{\sigma}} \cdot \mathbf{M}_0 \bar{\boldsymbol{\sigma}} |V| + \int_V [\bar{\boldsymbol{\sigma}} \cdot \boldsymbol{\zeta} - \tfrac{1}{2}\boldsymbol{\zeta} \cdot \boldsymbol{\Delta}^{11} \boldsymbol{\zeta} - \tfrac{1}{2}\boldsymbol{\zeta} \cdot \boldsymbol{\Delta}^{12} \boldsymbol{\kappa} - \tfrac{1}{2}\boldsymbol{\kappa} \cdot \boldsymbol{\Delta}^{21} \boldsymbol{\zeta} - \tfrac{1}{2}\boldsymbol{\kappa} \cdot \boldsymbol{\Delta}^{22} \boldsymbol{\kappa} - V(\boldsymbol{\zeta}, \boldsymbol{\kappa}; \mathbf{x})] \, d\mathbf{x}, \tag{4.8}$$

where the operators $\boldsymbol{\Delta}^{ij}$ are given in the Appendix A.

The lower bounds (4.8) generalize those developed by Hashin and Shtrikman (1962a,b), Willis (1983) and Talbot and Willis (1985) to include gradient effects. The inequality in (4.8) holds for any fields $\boldsymbol{\zeta}(\mathbf{x})$ and $\boldsymbol{\kappa}(\mathbf{x})$. Note that the dual potential $V(\boldsymbol{\zeta}, \boldsymbol{\kappa})$ specialized to a N-phase composite (4.1) is of similar form

$$V(\boldsymbol{\zeta}, \boldsymbol{\kappa}; \mathbf{x}) = \sum_{r=1}^{N} V^{(r)}(\boldsymbol{\zeta}, \boldsymbol{\kappa}) f^{(r)}(\mathbf{x}) \tag{4.9}$$

with $V^{(r)}$ related to $\phi^{(r)}$ as in (4.4).

For a linear composite $\phi^{(r)}$ having the form (3.19) the function $V^{(r)}(\boldsymbol{\zeta}, \boldsymbol{\kappa})$ is easily found explicitly from the definition (4.4)

$$V^{(r)}(\boldsymbol{\zeta}, \boldsymbol{\kappa}) = \tfrac{1}{2}\boldsymbol{\zeta} \cdot (\mathbf{M}^{(r)} - \mathbf{M}_0)^{-1} \boldsymbol{\zeta} + \tfrac{1}{2}\boldsymbol{\kappa} \cdot (\mathscr{M}^{(r)} - \mathscr{M}_0)^{-1} \boldsymbol{\kappa} \tag{4.10}$$

provided

$$\mathbf{M}^{(r)} > \mathbf{M}_0 \quad \text{and} \quad \mathscr{M}^{(r)} > \mathscr{M}_0. \tag{4.11}$$

The inequalities in (4.11) are interpreted in the sense of positive definiteness, i.e. $\boldsymbol{\sigma} \cdot (\mathbf{M}^{(r)} - \mathbf{M}^0)\boldsymbol{\sigma} > 0$ and $\boldsymbol{\tau} \cdot (\mathscr{M}^{(r)} - \mathscr{M}^0)\boldsymbol{\tau} > 0$ for any nonvanishing $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$. When (4.11) is violated $V^{(r)}(\boldsymbol{\zeta}, \boldsymbol{\kappa}) = +\infty$ which makes the lower bound in (4.8) trivial.

Note in conclusion that for $(\phi(\boldsymbol{\sigma}, \boldsymbol{\tau}) - \phi_0(\boldsymbol{\sigma}, \boldsymbol{\tau}))$ strictly convex, (such as for linear composites with a comparison medium satisfying (4.11)) the relation (4.8) holds equality if

$$\zeta_{ij}(\mathbf{x}) = \varepsilon_{ij}(\mathbf{x}) - \frac{\partial \phi_0}{\partial \sigma_{ij}}(\boldsymbol{\sigma}(\mathbf{x}), \boldsymbol{\tau}(\mathbf{x})),$$

$$\kappa_{ijk}(\mathbf{x}) = \eta_{ijk}(\mathbf{x}) - \frac{\partial \phi_0}{\partial \tau_{ijk}}(\boldsymbol{\sigma}(\mathbf{x}), \boldsymbol{\tau}(\mathbf{x})),$$

by evaluation of the supremum of (4.4). By choosing ϕ_0 to have the form of (4.7) the above relations specialize to

$$\boldsymbol{\zeta} = \boldsymbol{\varepsilon} - \mathbf{M}_0 \boldsymbol{\sigma}, \quad \boldsymbol{\kappa} = \boldsymbol{\eta} - \mathscr{M}_0 \boldsymbol{\tau}, \tag{4.12}$$

which establishes the connection with the standard definition of polarization.

4.3. *Hashin–Shtrikman lower bounds*

If the "true" polarizations (4.12) were known, their substitution into the right hand side of (4.8) would provide the exact value of the complementary energy $\tilde{\Phi}(\bar{\boldsymbol{\sigma}})$. However, the polarizations depend on all the details of the microstructure which are unknown precisely, though some partial statistical information may be available. By substituting relatively simple "trial" polarizations into the variational principle (4.8), employing available statistical information and performing an optimization, bounds for $\tilde{\Phi}$ are sought instead. These bounds are expected to reflect dispersion in the parameters of the overall behaviour due to remaining uncertainty in the details of the microstructure.

We specialize to linear composites, and choose the trial polarizations to be constant within each phase

$$\boldsymbol{\zeta}(\mathbf{x}) = \sum_{r=1}^{N} \boldsymbol{\zeta}_r f^{(r)}(\mathbf{x}), \quad \boldsymbol{\kappa}(\mathbf{x}) = \sum_{r=1}^{N} \boldsymbol{\kappa}_r f^{(r)}(\mathbf{x}). \tag{4.13}$$

Let $c_r \equiv |V|^{-1} \int_V f^{(r)}(\mathbf{x})\, d\mathbf{x}$ be the volume fraction of each phase, $r = 1, 2, \ldots, N$. Consequently

$$\bar{\boldsymbol{\zeta}} \equiv \sum c_r \boldsymbol{\zeta}_r, \quad \bar{\boldsymbol{\kappa}} \equiv \sum c_r \boldsymbol{\kappa}_r$$

are the mean values of the polarization field (4.13). The "true" higher-order polarization $\boldsymbol{\kappa}(\mathbf{x})$ satisfying (4.12) has zero mean value because no macroscopic higher stress and strain gradient are generated by the boundary conditions (4.2) in a statistically uniform composite. Likewise, upon making the approximation (4.13) one can expect that the mean value $\bar{\boldsymbol{\kappa}}$ should be zero, which is enforced henceforth.

To proceed, we substitute (4.9) and (4.10) into (4.8). The terms containing the operators $\boldsymbol{\Delta}^{ij}$ are simplified considerably by assuming that the constituent phases are arranged in a statistically uniform and isotropic fashion. Note first that (4.8) can be replaced by

$$\begin{aligned}\tilde{\Phi}(\bar{\boldsymbol{\sigma}}) \geqslant \tfrac{1}{2}\bar{\boldsymbol{\sigma}} \cdot \mathbf{M}_0 \bar{\boldsymbol{\sigma}} |V| + \int_V [&\bar{\boldsymbol{\sigma}} \cdot \boldsymbol{\zeta} - \tfrac{1}{2}(\boldsymbol{\zeta} - \bar{\boldsymbol{\zeta}}) \cdot \boldsymbol{\Delta}^{11}(\boldsymbol{\zeta} - \bar{\boldsymbol{\zeta}}) \\ &- \tfrac{1}{2}(\boldsymbol{\zeta} - \bar{\boldsymbol{\zeta}}) \cdot \boldsymbol{\Delta}^{12}(\boldsymbol{\kappa} - \bar{\boldsymbol{\kappa}}) - \tfrac{1}{2}(\boldsymbol{\kappa} - \bar{\boldsymbol{\kappa}}) \cdot \boldsymbol{\Delta}^{21}(\boldsymbol{\zeta} - \bar{\boldsymbol{\zeta}}) - \tfrac{1}{2}(\boldsymbol{\kappa} - \bar{\boldsymbol{\kappa}}) \cdot \boldsymbol{\Delta}^{22}(\boldsymbol{\kappa} - \bar{\boldsymbol{\kappa}}) - \\ &\tfrac{1}{2}\boldsymbol{\zeta} \cdot (\mathbf{M} - \mathbf{M}_0)^{-1} \boldsymbol{\zeta} - \tfrac{1}{2}\boldsymbol{\kappa} \cdot (\mathscr{M} - \mathscr{M}_0)^{-1} \boldsymbol{\kappa}],\end{aligned} \tag{4.14}$$

where $\boldsymbol{\zeta}$ is replaced by $(\boldsymbol{\zeta} - \bar{\boldsymbol{\zeta}})$ due to the properties of the operators $\boldsymbol{\Delta}^{ij}$ (see Appendix A):

$$\int_V (\boldsymbol{\zeta} \boldsymbol{\Delta}^{11} \bar{\boldsymbol{\zeta}} + \boldsymbol{\kappa} \boldsymbol{\Delta}^{21} \bar{\boldsymbol{\zeta}}) = \int_V \bar{\boldsymbol{\zeta}} (\boldsymbol{\Delta}^{11} \boldsymbol{\zeta} + \boldsymbol{\Delta}^{12} \boldsymbol{\kappa}) = 0. \tag{4.15}$$

Recall that $\bar{\boldsymbol{\kappa}}$ is taken to be zero and $(\boldsymbol{\kappa} - \bar{\boldsymbol{\kappa}})$ has been introduced in (4.14) instead of $\boldsymbol{\kappa}$ for convenience. Making use of (4.13), the bounds (4.14) are transformed into

$$\frac{1}{|V|}\tilde{\Phi}(\bar{\boldsymbol{\sigma}}) \geqslant \tfrac{1}{2}\bar{\boldsymbol{\sigma}}\cdot\mathbf{M}_0\bar{\boldsymbol{\sigma}} - \bar{\boldsymbol{\sigma}}\bar{\boldsymbol{\zeta}} - \tfrac{1}{2}\sum_{r=1}^{N}\sum_{s=1}^{N}\{\boldsymbol{\zeta}_r\cdot\mathbf{B}_{11}^{(rs)}\boldsymbol{\zeta}_s + \boldsymbol{\zeta}_r\cdot\mathbf{B}_{12}^{(rs)}\boldsymbol{\kappa}_s + \boldsymbol{\kappa}_r\cdot\mathbf{B}_{21}^{(rs)}\boldsymbol{\zeta}_s$$

$$+\boldsymbol{\kappa}_r\cdot\mathbf{B}_{22}^{(rs)}\boldsymbol{\kappa}_s\} - \tfrac{1}{2}\sum_{r=1}^{N} c_r\{\boldsymbol{\zeta}_r\cdot(\mathbf{M}^{(r)}-\mathbf{M}_0)^{-1}\boldsymbol{\zeta}_r + \boldsymbol{\kappa}_r\cdot(\mathscr{M}^{(r)}-\mathscr{M}_0)^{-1}\boldsymbol{\kappa}_r\}, \quad (4.16)$$

where

$$\mathbf{B}_{ij}^{(rs)} \equiv \frac{1}{|V|}\int_V d\mathbf{x}' \int_V d\mathbf{x}\boldsymbol{\Delta}^{ij}(\mathbf{x}',\mathbf{x})(f^{(r)}(\mathbf{x}')-c_r)(f^{(s)}(\mathbf{x})-c_s)\,d\mathbf{x}, \quad i,j=1,2. \quad (4.17)$$

The polycrystal's size is much larger than the scale of the microstructure specified by the characteristic functions $f^{(r)}$ and, due to statistical uniformity $[f^{(r)}(\mathbf{x}')-c_r]$ in (4.17) rapidly oscillate about zero throughout the volume V. Following Willis (e.g. 1981) this permits us to implement an ensemble averaging in (4.17), and to replace $\boldsymbol{\Delta}^{ij}(\mathbf{x}',\mathbf{x})$ by its infinite-body form $\boldsymbol{\Delta}^{ij,\infty}(\mathbf{x}'-\mathbf{x})$ which is translationary invariant. As a result,

$$\mathbf{B}_{ij}^{(rs)} \cong \int d\mathbf{z}\boldsymbol{\Delta}^{ij,\infty}(\mathbf{z})[\psi_{rs}(\mathbf{z})-c_rc_s] \quad (4.18)$$

with the integration performed over the infinite body. Here the (two-point) correlation function ψ_{rs} is defined as an expectation value (local average) of $f^{(r)}(\mathbf{x})f^{(s)}(\mathbf{x}+\mathbf{z})$ for any point $\mathbf{x}$ within the composite. Due to the statistical uniformity it may be alternatively introduced as a volume average

$$\psi_{rs}(\mathbf{z}) = \frac{1}{|V|}\int_V f^{(r)}(\mathbf{x})f^{(s)}(\mathbf{x}+\mathbf{z})\,d\mathbf{x}.$$

The right hand side of (4.16) represents an algebraic quadratic form with respect to $\boldsymbol{\zeta}_1,\ldots,\boldsymbol{\zeta}_N, \boldsymbol{\kappa}_1,\ldots,\boldsymbol{\kappa}_N$. It is maximized by making its value stationary. For composites with isotropic microstructure ψ_{rs} depend only on the modulus of $\mathbf{z}$. Then, $\mathbf{B}_{12}^{(rs)} = \mathbf{B}_{21}^{(rs)} = 0$ from (4.18) since $\boldsymbol{\Delta}^{12,\infty}$ and $\boldsymbol{\Delta}^{21,\infty}$ are odd functions of $\mathbf{x}$ (Appendix A). Consequently, the optimization problems uncouple for $\boldsymbol{\zeta}_r$, $r=1,2,\ldots,N$ and for $\boldsymbol{\kappa}_r$, $r=1,2,\ldots,N$. The parameters $\boldsymbol{\kappa}_r$ appear only as a pure quadratic form without linear terms involved. Their optimal choice is trivial: $\boldsymbol{\kappa}_r = 0$, $r=1,\ldots,N$.

To optimize (4.16) with respect to $\{\boldsymbol{\zeta}_r\}$ the correlation functions ψ_{rs} must first be specialized to the "cell" structure of the polycrystal. The polycrystal is regarded as consisting of many single grains with each grain adopting one of N orientations with probabilities c_r, $r=1,2,\ldots,N$. Assume that the orientation of *different* grains is totally uncorrelated, and introduce a "single grain" correlation function $h(\mathbf{z})$, as the probability that both $\mathbf{x}$ and $\mathbf{x}+\mathbf{z}$ belong to the same grain. Then it follows immediately that

$$\psi_{rs}(\mathbf{z}) = c_r\delta_{rs}h(\mathbf{z}) + c_rc_s(1-h(\mathbf{z}))$$

(see, e.g. Talbot and Willis, 1982), and therefore

$$\mathbf{B}^{rs}_{(11)} = (c_r\delta_{rs} - c_r c_s)\mathbf{Q},$$

where

$$\mathbf{Q} \equiv \int \boldsymbol{\Delta}^{11,\infty}(\mathbf{x}) h(\mathbf{x})\, d\mathbf{x}. \tag{4.19}$$

The remaining optimization with respect to $\{\zeta_r\}$ is straightforward. Algebraically, it is equivalent to that in the conventional case (see, e.g. Willis, 1981) and the resulting optimal value for the right hand side of (4.16) is

$$\tilde{\Phi}(\bar{\boldsymbol{\sigma}}) \geqslant \tfrac{1}{2}\bar{\boldsymbol{\sigma}} \cdot \mathbf{M}^{-}_{\mathrm{HS}}\bar{\boldsymbol{\sigma}}, \tag{4.20}$$

where

$$\mathbf{M}^{-}_{\mathrm{HS}} \equiv \left(\sum_{r=1}^{N} c_r [\mathbf{M}^{(r)} + \hat{\mathbf{M}}]^{-1} \right)^{-1} - \hat{\mathbf{M}}, \tag{4.21}$$

and

$$\hat{\mathbf{M}} \equiv \mathbf{Q}^{-1} - \mathbf{M}_0. \tag{4.22}$$

Note that the expression for the lower bound (4.21) formally coincides with that in the conventional case (compare, e.g. to Willis, 1981; deBotton and Ponte Castañeda, 1995). The only but essential difference is in the tensor $\mathbf{Q}$ which is derived from the *strain gradient* Green's function corresponding to $(\mathbf{M}_0, \mathscr{M}_0)$ (see Appendix A), in contrast to the "conventional" tensor $\mathbf{Q}$ related to the Eshelby tensor and derived from a conventional Green's function (Willis, 1981).

We remind the reader that (4.20) and (4.21) represent a lower bound for any chosen comparison medium with compliance moduli $(\mathbf{M}_0, \mathscr{M}_0)$ such that the restrictions (4.11) hold for all orientations $r = 1, 2, \ldots, N$.

4.4. *Hashin–Shtrikman upper bounds*

The upper bounds for the effective compliance are derived following the same strategy with some obvious changes. To this end the dual function $V_+(\boldsymbol{\zeta}, \boldsymbol{\kappa})$ is introduced as

$$V_+(\boldsymbol{\zeta}, \boldsymbol{\kappa}) = \inf_{\boldsymbol{\sigma},\boldsymbol{\tau}} \{\boldsymbol{\sigma}\cdot\boldsymbol{\zeta} + \boldsymbol{\tau}\cdot\boldsymbol{\kappa} - \phi(\boldsymbol{\sigma},\boldsymbol{\tau}) + \phi_0(\boldsymbol{\sigma},\boldsymbol{\tau})\}$$

(compare with (4.4)). If both ϕ and ϕ_0 are potentials for the linear media, V is still determined by (4.10) in each phase r provided, however,

$$\mathbf{M}^{(r)} < \mathbf{M}_0 \quad \text{and} \quad \mathscr{M}^{(r)} < \mathscr{M}_0 \tag{4.23}$$

for all r. If (4.23) is violated then $V_+ = -\infty$. Following the same prescription as for the lower bounds with obvious alterations we end up with the upper bounds for $\tilde{\Phi}$ analogous to (4.21)

$$\tilde{\Phi}(\bar{\boldsymbol{\sigma}}) \leqslant \tfrac{1}{2}\bar{\boldsymbol{\sigma}} \cdot \mathbf{M}^{+}_{\mathrm{HS}}\bar{\boldsymbol{\sigma}},$$

where

$$\mathbf{M}^{+}_{\mathrm{HS}} \equiv \left(\sum_{r=1}^{N} c_r[\mathbf{M}^{(r)} + \hat{\mathbf{M}}]^{-1}\right) - \hat{\mathbf{M}} \tag{4.24}$$

with $\hat{\mathbf{M}}$ related to the tensor $\mathbf{Q}$ as in (4.22). We emphasize that, although the right hand sides of (4.21) and (4.24) formally coincide, the bounds hold subject to *opposite restrictions* (4.11) and (4.23) for the comparison medium $(\mathbf{M}_0, \mathscr{M}_0)$.

5. EXAMPLE: ISOTROPIC F.C.C. LINEAR POLYCRYSTAL

5.1. *Bounds for the effective shear modulus*

The general formulae (4.21) and (4.24) for the lower and upper bounds are now specialized to linear isotropic polycrystals. Note first that the bounds (4.21) and (4.24) hold also in the continuum limit when the number of orientations N tends to infinity. In this case the orientations r are identified with the rotation tensor $\boldsymbol{\Omega}$, $\mathbf{M}^{(r)}$ is replaced by $\mathbf{M}(\boldsymbol{\Omega})$, and the summation over r is replaced by an integration averaging over $\boldsymbol{\Omega}$, where $\boldsymbol{\Omega}$ are all possible rotation matrices. Assuming there is no texture, i.e. all orientations are equally likely, the continuous analogues of (4.21) and (4.24) are

$$\mathbf{M}^{\pm}_{\mathrm{HS}} = \langle[\mathbf{M}(\boldsymbol{\Omega}) + \hat{\mathbf{M}}]^{-1}\rangle^{-1} - \hat{\mathbf{M}}, \tag{5.1}$$

where $\langle \cdot \rangle$ is the average over all orientations $\boldsymbol{\Omega}$ of the crystal. For the linear polycrystal a "rotated" compliance tensor $\mathbf{M}(\boldsymbol{\Omega})$ is related to a reference tensor $\mathbf{M}^{\mathrm{R}}$ via

$$\mathbf{M}_{ijpq}(\boldsymbol{\Omega}) = \Omega_{ik}\Omega_{jl}\Omega_{pr}\Omega_{qs}M^{\mathrm{R}}_{klrs}. \tag{5.2}$$

The bounds hold for $\hat{\mathbf{M}}$ derived from any $\mathbf{M}^0$ and $\mathscr{M}^0$ such that

$$\mathbf{M}^0 \leqslant \mathbf{M}(\boldsymbol{\Omega}), \quad \mathscr{M}^0 \leqslant \mathscr{M}(\boldsymbol{\Omega}) \tag{5.3}$$

for all $\boldsymbol{\Omega}$ for the lower bound, and,

$$\mathbf{M}^0 \geqslant \mathbf{M}(\boldsymbol{\Omega}), \quad \mathscr{M}^0 \geqslant \mathscr{M}(\boldsymbol{\Omega}) \tag{5.4}$$

for the upper bound. The tensor $\mathscr{M}(\boldsymbol{\Omega})$ is determined similarly from the reference tensor $\mathscr{M}^{\mathrm{R}}$

$$\mathscr{M}_{ijkpqr}(\boldsymbol{\Omega}) = \Omega_{il}\Omega_{jm}\Omega_{kn}\Omega_{ps}\Omega_{qt}\Omega_{ru}\mathscr{M}^{\mathrm{R}}_{lmnstu}.$$

Because of rotation symmetry the optimal $(\mathbf{M}^0, \mathscr{M}^0)$ satisfying (5.3) or (5.4) are isotropic. This implies that the tensor $\mathbf{Q}$ related to the infinite body Green's function $\mathbf{G}^0$ of this medium via (4.19) and (B.15) is also isotropic. Isotropy also follows (for untextured polycrystals) for the tensors $\mathbf{M}^{-}_{\mathrm{HS}}$ and $\mathbf{M}^{+}_{\mathrm{HS}}$ defined by (5.1) and (4.22), and for the effective compliance modulus $\mathbf{M}^*$ defined via

$$\tilde{\Phi}(\bar{\boldsymbol{\sigma}}) = \tfrac{1}{2}\bar{\boldsymbol{\sigma}} \cdot \mathbf{M}^*\bar{\boldsymbol{\sigma}}|V|.$$

For *incompressible* polycrystals associated with the multislip deformation discussed in Section 3 the isotropic tensor $\mathbf{M}^*$ is fully specified by the shear modulus μ^*

$$\tfrac{1}{2}\bar{\boldsymbol{\sigma}}\cdot\mathbf{M}^*\bar{\boldsymbol{\sigma}} = \frac{1}{4\mu^*}\bar{\boldsymbol{\sigma}}\cdot\bar{\boldsymbol{\sigma}}$$

provided $\bar{\boldsymbol{\sigma}}$ is "deviatoric", i.e. $\bar{\sigma}_{kk} = 0$. It follows that

$$\mu^* = \tfrac{5}{2}(M^*_{ijij})^{-1} = \frac{1}{4M^*_{1212}}.$$

Similarly, the tensors $\mathbf{M}^+_{\mathrm{HS}}$ and $\mathbf{M}^-_{\mathrm{HS}}$ are specified by the shear moduli μ^-_{HS} and μ^+_{HS}, respectively

$$\mu^-_{\mathrm{HS}} = [4(M^+_{\mathrm{HS}})_{1212}]^{-1}, \quad \mu^+_{\mathrm{HS}} = [4(M^-_{\mathrm{HS}})_{1212}]^{-1}.$$

Note that μ^-_{HS} provides a lower bound for the effective shear modulus μ^* in contrast to $\mathbf{M}^+_{\mathrm{HS}}$ associated with it, which provides the upper bound for the total compliance tensor; the same comment applies to μ^+_{HS} and $\mathbf{M}^-_{\mathrm{HS}}$.

As shown in Appendix B the shear part $\mu_Q \equiv Q_{1212}$ of the tensor $\mathbf{Q}$ is related to the shear modulus $\mu_0 \equiv (4M^0_{1212})^{-1}$ identifying $\mathbf{M}^0$, and to the lengthscales l_1, l_2 and l_3 identifying $\mathscr{M}_0$ via

$$\mu_Q = \mu_0(1-\psi(l_0)), \tag{5.5}$$

where

$$l_0 \equiv 2(\tfrac{4}{15}l_1^2+\tfrac{1}{3}l_2^2+\tfrac{2}{5}l_3^2)^{1/2}.$$

The function $\psi(l)$ is related to the grain-size correlation function h via (B.19).

Specialize now to a face-centred cubic (f.c.c.) linear polycrystal. The reference single crystal has twelve slip systems defined by four slip planes of the $\{1,1,1\}$ type and by three slip directions for each plane of the $\{1,1,0\}$ type. This defines the basic triads $(\mathbf{s}^{(\alpha)}, \mathbf{m}^{(\alpha)}, \mathbf{t}^{(\alpha)})$ for each $\alpha = 1, 2, \ldots, 12$ and determines the reference compliances $\mathbf{M}$ and $\mathscr{M}$ via (3.20), (3.21) once the parameters μ_α, $l_S^{(\alpha)}$, $l_M^{(\alpha)}$ and $l_T^{(\alpha)}$ have been specified. The crystal is expected to display cubic symmetry which implies that the above single slip parameters are actually independent of α (i.e. $\mu_\alpha = \mu$; $l_S^{(\alpha)} = l_S$, etc).

It is well known that a cubic compliance tensor $\mathbf{M}$ which is also incompressible is fully characterized by two quantities $v' \equiv (M_{1111}-M_{1122})/2$ and $v'' \equiv M_{1212}$, see, e.g. Walpole (1981). The parameters v' and v'' are explicitly found from (3.20):

$$v' = \frac{1}{\mu}, \quad v'' = \frac{1}{3\mu}.$$

To find expressions for μ^-_{HS} and μ^+_{HS} from (5.1), well known rules of algebraic manipulations with cubic tensors $\mathbf{M} = (2v', 2v'')$ have been employed (see, e.g. Walpole, 1981): if $\mathbf{M}_1 = (2v_1', 2v_1'')$ and $\mathbf{M}_2 = (2v_2', 2v_2'')$ then $(\mathbf{M}_1+\mathbf{M}_2) = (2v_1'+2v_2'', 2v_1''+2v_2'')$, $\mathbf{M}_1\mathbf{M}_2 = (4v_1'v_2', 4v_1''v_2'')$ and $\mathbf{M}_1^{-1} = ((2v_1')^{-1}, (2v_1'')^{-1})$. For isotropic tensors $v' = v''$; a simple relation for the shear modulus v^{I} associated with the "isotropic average" $\langle M\rangle = (2v^{\mathrm{I}}, 2v^{\mathrm{I}})$ of the cubic tensor $\mathbf{M}$ is

$$v^{\mathrm{I}} = \tfrac{1}{10}M_{ijij} = \frac{2v' + 3v''}{5}.$$

This follows from

$$v^{\mathrm{I}} \equiv \tfrac{1}{10}\langle \mathbf{M} \rangle_{ijij} = \tfrac{1}{10}\langle M_{ijij} \rangle$$

and the fact that the invariant M_{ijij} is itself rotation invariant and therefore needs no rotational averaging.

One immediate implication of cubic symmetry is that for the optimal choice of the comparison medium

$$\frac{1}{4\mu_0} = \min\{v', v''\} = \frac{1}{3\mu} \tag{5.6}$$

for the restrictions (4.11) corresponding to the lower bound, and

$$\frac{1}{4\mu_0} = \max\{v', v''\} = \frac{1}{\mu} \tag{5.7}$$

for the upper bound conforming to (4.23).

Expressions for μ^{-}_{HS} and μ^{+}_{HS} follow now from (5.1) and (5.5) by implementing together all the above properties. The result is

$$\mu^{-}_{\mathrm{HS}} \leqslant \mu^{*} \leqslant \mu^{+}_{\mathrm{HS}},$$

$$\mu^{+}_{\mathrm{HS}} = \frac{\mu}{4}\left(3 - \frac{4}{5 - 2\psi^{+}}\right), \tag{5.8}$$

$$\mu^{-}_{\mathrm{HS}} = \frac{\mu}{4}\left(1 + \frac{6}{5 + 4\psi^{-}}\right), \tag{5.9}$$

where

$$\psi^{+} \equiv \psi(l^{+}) = \frac{8}{5}\int_0^{+\infty} \mathrm{e}^{-2t} h(l^{+}t)t\,\mathrm{d}t,$$

$$\psi^{-} \equiv \psi(l^{-}) = \frac{8}{5}\int_0^{+\infty} \mathrm{e}^{-2t} h(l^{+}t)t\,\mathrm{d}t. \tag{5.10}$$

Note that the grain size effect for μ^{*} is expressed in the above relations via the grain size correlation function $h(|\mathbf{z}|)$.

The lengthscales l^{+} and l^{-} are found from optimal choice of the Toupin–Mindlin isotropic strain gradient comparison medium (see Appendix B) to satisfy the second restrictions of (4.11) and (4.23), respectively.

5.2. *Numerical implementation and results*

The formulae (5.8)–(5.10) have been employed for calculation of bound for the effective shear modulus of an f.c.c. strain-gradient composite for various combinations

of the single slip lengthscales l_S, l_M and l_T. As a simple illustrative example the grain size correlation function was taken as

$$h(|\mathbf{z}|) = \mathrm{e}^{-|\mathbf{z}|/a}, \tag{5.11}$$

where a is a correlation length parameter which can be interpreted loosely as a "typical" grain size. In this case the integrals in (5.10) are easily found

$$\psi(l^{\pm}) = \tfrac{8}{5}\left(\frac{l^{\pm}}{a}+2\right)^{-2}.$$

Observe that in the limit $l \ll a\psi^{\pm} = 2/5$, and (5.8) and (5.9) conform to the "conventional" Hashin–Shtrikman (1962b) values

$$\mu^{-}_{\mathrm{HS}} = \tfrac{21}{44}\mu, \quad \mu^{+}_{\mathrm{HS}} = \tfrac{43}{84}\mu.$$

The optimal value l^{+} is found by minimizing the value of

$$l_0(l_1, l_2, l_3) \equiv 2(\tfrac{4}{15}l_1^2 + \tfrac{1}{3}l_2^2 + \tfrac{2}{5}l_3^2)^{1/2}, \tag{5.12}$$

as defined in (B.13), over all possible lengthscales (l_1, l_2, l_3). The minimization of l_0 is constrained by values for (l_1, l_2, l_3) such that the second of inequalities (4.11) holds

$$\boldsymbol{\tau}\cdot\mathscr{M}_0\boldsymbol{\tau} \leqslant \boldsymbol{\tau}\cdot\mathscr{M}\boldsymbol{\tau} \tag{5.13}$$

for any incompressible $\boldsymbol{\tau}$. The isotropic incompressible tensor $\mathscr{M}_0$ is associated with (l_1, l_2, l_3) via

$$\boldsymbol{\tau}\cdot\mathscr{M}_0\boldsymbol{\tau} \equiv \frac{1}{\mu_0 l_1^2}\boldsymbol{\tau}^{(1)}\cdot\boldsymbol{\tau}^{(1)} + \frac{1}{\mu_0 l_2^2}\boldsymbol{\tau}^{(2)}\cdot\boldsymbol{\tau}^{(2)} + \frac{1}{\mu_0 l_3^2}\boldsymbol{\tau}^{(3)}\cdot\boldsymbol{\tau}^{(3)}, \tag{5.14}$$

where $\boldsymbol{\tau} = \boldsymbol{\tau}^{(1)}+\boldsymbol{\tau}^{(2)}+\boldsymbol{\tau}^{(3)}$ is the decomposition of the incompressible tensor τ_{ijk} into three orthogonal invariant subspaces (Appendix B). Recall that μ_0 is the shear modulus and its optimal choice is given by (5.6).

Similarly, l^{+} is sought to maximize $l_0(l_1, l_2, l_3)$ subject to the opposite restriction

$$\boldsymbol{\tau}\cdot\mathscr{M}_0\boldsymbol{\tau} \geqslant \boldsymbol{\tau}\cdot\mathscr{M}\boldsymbol{\tau} \tag{5.15}$$

for any incompressible $\boldsymbol{\tau}$. The shear modulus μ_0 is now given by (5.7).

For given single crystal lengthscales l_S, l_M and l_T the optimal values l^{+} and l^{-} have been computed numerically using NAG minimization routines.† The numerical strategy was to minimize (or maximize) the right hand side of (5.12) with respect to such l_1, l_2 and l_3 that the constraint (5.13) (or (5.15)) is met.

The physically important case is $l_M^{(\alpha)} \to 0$ which reflects the absence of the dislocation storage due to the slip gradient in the normal direction $\mathbf{m}^{(\alpha)}$, see Fleck *et al.* (1994). In this case the second term in the right hand side of (3.21) results in infinitely large contributions unless

$$\boldsymbol{\tau}\cdot\boldsymbol{\psi}^{(\alpha)M} = 0, \quad \alpha = 1, 2, \ldots, 12. \tag{5.16}$$

In the limit (5.16) imposes a family of constraints for the higher order stress tensor $\boldsymbol{\tau}$.

† The NAG Fortran Library Manual, Mark 14. The Numerical Algorithms Group Limited, 1990.

Then, the upper bound for the effective shear modulus is found by performing the above optimization strategy subject to these additional constraints. The lower bound, however, degenerates into the conventional Hashin–Shtrikman value $\mu_{\overline{HS}}/\mu = 21/44$ uniformly with respect to l_S and l_T. This follows from the observation that if (5.15) holds and l_T in (3.21) tends to zero, then necessarily $l_1 \to 0$, $l_2 \to 0$ and $l_3 \to 0$ and therefore $l^- \to 0$ from (5.12).

Figure 1 shows results of sample calculations of the upper and lower bounds for various values of l_S, l_M and l_T. The solid curves correspond to $l_S = l_T = l_M = l$. The results of calculations demonstrate strengthening of the polycrystal with diminishing grain size a. For the polycrystals with coarse grains ($a \gg 1$) our results reproduce the Hashin–Shtrikman (1962b) bounds for "conventional" polycrystals. In the opposite limit of large l/a both the upper and the lower(!) bounds approach the Voigt uniform strain upper bound $\mu_V^+ = 0.55$ (the upper margin of the figure). This is consistent with the expectation that the displacement field of the polycrystal tends to the uniform strain pattern (which contains no gradients), when the strain gradient terms dominate in the energy functional. For both the *upper* and *lower* bounds the optimal values of l_1, l_2 and l_3 have been numerically found to be

$$l_1/l = 1.4142, \quad l_2/l = 0.7072 \quad \text{and} \quad l_3/l = 0.8660,$$

with the "effective" lengthscale $l^{\pm} \equiv l_0(l_1, l_2, l_3) = 2l$.

The dashed curves correspond to the case when $l_S = l_T = l$, but $l_M \to 0$. The (constrained) optimization for the upper bound gave the following values of the optimal comparison lengthscales

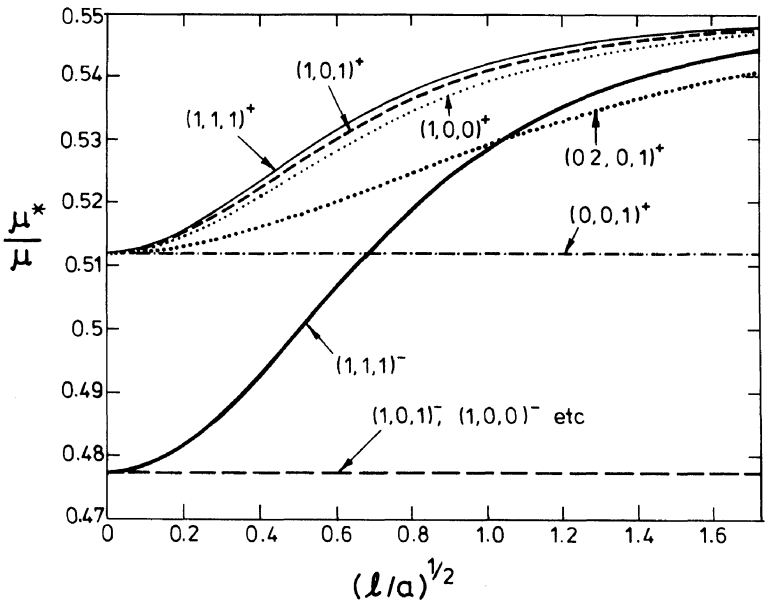

Fig. 1. Effect of the grain size a upon the Hashin–Strikman upper and lower bounds for a linear f.c.c. polycrystal for various lengthscales l_S, l_M and l_T, scaled against a "normalizing" lengthscale l. The notation $(l_S/l, l_M/l, l_T/l)^+$ is used for the upper bound, and $(l_S/l, l_M/l, l_T/l)^-$ for the lower bound. The grain size correlation function is taken as in (5.11).

$$l_1/l = 1.4142, \quad l_2/l = 0.5345 \quad \text{and} \quad l_3/l = 0.5774,$$

and the "effective" lengthscale $l^+/l = 1.7457$. The lower bound is a horizontal line $\mu_{\mathrm{HS}}^- = \frac{21}{44}\mu = 0.4773\mu$ as $l^- \to 0$ when $l_M \to 0$. It is well above the "elementary" Reuss bound $\mu_{\mathrm{R}}^- = 0.4167\mu$ (not displayed).

The dotted curve displays the upper bound for the case $l_S = l$, $l_M \to 0$ and $l_T \to 0$. Physically, this corresponds to accumulation of geometrically necessary *edge* dislocations only, and, mathematically, results in constraints

$$\boldsymbol{\tau} \cdot \boldsymbol{\psi}^{(\alpha)T} = 0, \quad \alpha = 1, 2, \ldots, 12 \tag{5.17}$$

in addition to (5.16). Direct analysis shows that these constraints make $\boldsymbol{\tau}$ fully symmetric, i.e. $\boldsymbol{\tau} = \boldsymbol{\tau}^{(1)}$, and so $\boldsymbol{\tau}^{(2)} = \boldsymbol{\tau}^{(3)} = 0$. Therefore, to satisfy (5.13) l_2 and l_3 can be chosen arbitrarily. The remaining lengthscale l_1 is found numerically to satisfy $l_1 \geqslant \sqrt{2}$ to ensure (5.13). Therefore, the choice of l_1, l_2 and l_3 to deliver the minimum to (5.12) is $l_1 = 1.4142l$, $l_2 \to 0$, $l_3 \to 0$ which results in $l^+/l = 1.4606$. The lower bound coincides with the horizontal dotted line at the "conventional" Hashin–Shtrikman value $\mu_{\mathrm{HS}}^-/\mu = 21/44$, and displays no scale effect.

Finally consider the limiting case $l_T = l$, $l_M \to 0$ and $l_S \to 0$. This corresponds to a hardening contribution by geometrically necessary screw dislocations only. In this case the constraints $\boldsymbol{\tau} \cdot \boldsymbol{\psi}^{(\alpha)S} = 0$, $\alpha = 1, 2, \ldots, 12$ in combination with (5.16) cover the full 15-dimensional linear space of incompressible higher-order stresses $\boldsymbol{\tau}$. The resulting optimization procedure degenerates and $l^+ = 0$ which corresponds to $l_1 \to 0$, $l_2 \to 0$, $l_3 \to 0$. This results in the uniform upper bound displayed by the dash–dotted horizontal line.

The bold–dotted curve displays the upper bound for an "intermediate" case $l_S = 0.2l$, $l_T = l$, $l_M \to 0$. The optimal lengthscales were found to be $l_1/l = 0.3746$, $l_2/l = 0.3299$, $l_3/l = 0.1732$, and, as a result, $l^+/l = 0.5855$.

Comparison of results of calculations demonstrates that for f.c.c. polycrystals the lengthscale l_S (edge dislocations) have a major impact on the scale effect for the upper bound, whereas variations of the other lengthscale l_T (screw dislocations) have a less pronouncing effect.

Note that the Fig. 1 is in qualitative agreement with the Hall–Petch relations: $\mu^* \sim \mu_0^* + c(l/a)^{1/2}$ for some constant c. One can see that the behaviour is indeed close to linear for, approximately, $0.2 < (l/a)^{1/2} < 1$. We emphasise that the Hall–Petch effect relates to the dependence of yield strength of polycrystal upon grain size, and so the results presented here for the dependence of the macroscopic shear modulus upon grain size are meant only for a qualitative comparison. Further, the analysis of the linear case is the first step in the estimation of the grain size effect for non-linear polycrystals: in order to use the non-linear variational principle of Ponte Castañeda (1991, 1992) the effective properties of the linear solid are required.

6. CONCLUDING DISCUSSION

We regard this paper as a first step towards quantitative modelling of the scale effect in the plastic behaviour of polycrystals (the Hall–Petch effect). For this purpose,

a study of the linear polycrystals is the first and critical step. The instantaneous linearity of a nonlinear crystal permits us to implement ideas of Ponte Castañeda (1991, 1992) and deBotton and Ponte Castañeda (1995) to nonlinear polycrystals with strain-gradient effects. As an alternative, the Hashin–Shtrikman variational principle formulated in Section 4 in a more general "nonlinear" form permits us to pursue the strategy of Willis and co-workers (Willis, 1983, 1991; Dendievel *et al.*, 1991) to derive bounds for *nonlinear* polycrystals with strain-gradient effects directly. The avenues for implementation of these homogenization techniques are open as soon as the appropriate coupling between the slip and the slip gradients for the reference single crystal has been selected. This has to be done experimentally, or through explicit modelling dislocation–dislocation interactions.

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APPENDIX A

We start by seeking the infimum of the right hand side of (4.6) and (4.7) with respect to the class of statically admissible $(\boldsymbol{\sigma}(\mathbf{x}), \boldsymbol{\tau}(\mathbf{x}))$ compatible with (4.2). We follow here the strategy of Willis (e.g. 1981). To this end consider the variation of

$$I(\boldsymbol{\sigma}, \boldsymbol{\tau}) = \int_V [\boldsymbol{\sigma} \cdot \boldsymbol{\zeta} + \boldsymbol{\tau} \cdot \boldsymbol{\kappa} + \tfrac{1}{2}\boldsymbol{\sigma} \cdot \mathbf{M}_0 \boldsymbol{\sigma} + \tfrac{1}{2}\boldsymbol{\tau} \cdot \mathscr{M}_0 \boldsymbol{\tau}] \, \mathrm{d}\mathbf{x},$$

which is

$$\delta I(\boldsymbol{\sigma}, \boldsymbol{\tau}) = \int_V [(\mathbf{M}_0 \boldsymbol{\sigma} + \boldsymbol{\zeta}) \cdot \delta\boldsymbol{\sigma} + (\mathscr{M}_0 \boldsymbol{\tau} + \boldsymbol{\kappa}) \cdot \delta\boldsymbol{\tau}] \, \mathrm{d}\mathbf{x}$$

by using the symmetry of $\mathbf{M}_0$ and $\mathscr{M}_0$. Both $\mathbf{M}_0$ and $\mathscr{M}_0$ are assumed to be positive definite, i.e. $\boldsymbol{\sigma} \cdot \mathbf{M}_0 \boldsymbol{\sigma} > 0$, $\boldsymbol{\tau} \cdot \mathscr{M}_0 \boldsymbol{\tau} > 0$ for any nonvanishing $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$. Therefore, a stationary value of I is also a minimum. To ensure that $\delta I = 0$ it is sufficient to find a displacement field $\mathbf{u}(\mathbf{x})$ such that

$$\begin{aligned} \mathbf{M}_0 \boldsymbol{\sigma} + \boldsymbol{\zeta} &= \boldsymbol{\varepsilon} \\ \mathscr{M}_0 \boldsymbol{\tau} + \boldsymbol{\kappa} &= \boldsymbol{\eta}, \end{aligned} \tag{A.1}$$

where $\boldsymbol{\varepsilon}$ and $\boldsymbol{\eta}$ are the strain and the strain gradient kinematically derived from $\mathbf{u}$. This follows from the stationary principle (2.11).

Relations (A.1) can be re-expressed as

$$\begin{aligned} \boldsymbol{\sigma} &= \mathbf{L}_0 \boldsymbol{\varepsilon} - \mathbf{L}_0 \boldsymbol{\zeta}, \\ \boldsymbol{\tau} &= \mathscr{L}_0 \boldsymbol{\eta} - \mathscr{L}_0 \boldsymbol{\kappa}, \end{aligned} \tag{A.2}$$

where $\mathbf{L}_0 \equiv \mathbf{M}_0^{-1}$ and $\mathscr{L} \equiv \mathscr{M}_0^{-1}$ are the "stiffness" tensors. By substituting (A.2) into the equilibrium relation (2.4) we achieve the governing partial differential equation for $\mathbf{u}(\mathbf{x})$, given by

$$L^0_{kjpq}u_{p,jq}(\mathbf{x}) - \mathscr{L}^0_{ijkpqr}u_{r,pqij}(\mathbf{x}) + f_k(\mathbf{x}) = 0. \tag{A.3}$$

Here

$$f_k \equiv -L^0_{kjpq}\zeta_{pq,j}(\mathbf{x}) + \mathscr{L}^0_{ijkpqr}\kappa_{pqr,ij} \tag{A.4}$$

may be interpreted as a body force which would cause the same displacement field within V if the composite solid were replaced by the homogeneous linear comparison medium with parameters $\mathbf{M}_0$ and $\mathscr{M}_0$.

We seek the solution of the displacement equation of equilibrium (A.3) such that $(\boldsymbol{\sigma}, \boldsymbol{\tau})$ satisfies the boundary conditions (4.2). The total displacement field $\mathbf{u}(\mathbf{x})$ is obtained as the sum of the solutions to two problems:

(i) the solution $\tilde{\mathbf{u}}(\mathbf{x})$ of (A.2) due to the body force f_k given by (A.3) but with vanishing tractions on the boundary S, and
(ii) the solution $\bar{\mathbf{u}}(\mathbf{x})$ of (A.2) due to the surface tractions (4.2) but with vanishing body force f_k.

To obtain the solution $\tilde{\mathbf{u}}(\mathbf{x})$ of (A.2) introduce the Green's function $G_{ik}(\mathbf{x}, \mathbf{x}')$ in V,

$$L^0_{kjpq}G_{lp,jq}(\mathbf{x}) - \mathscr{L}^0_{ijkpqr}G_{lr,pqij}(\mathbf{x}) + \delta_{lk}\delta(\mathbf{x}-\mathbf{x}') = 0,$$

with "traction free" boundary conditions on S

$$t_k = 0, \quad R_k = 0,$$

where t_k and R_k are defined by (2.8) and (2.9). Then by comparison of the above governing equations for $G_{ik}(\mathbf{x}, \mathbf{x}')$ with (A.1) we obtain

$$\tilde{u}_k = \int_V G_{kl}(\mathbf{x}, \mathbf{x}')f_l(\mathbf{x}')\,d\mathbf{x}'.$$

The total displacement field is

$$u_k = \bar{u}_k(\mathbf{x}) + \int_V G_{kl}(\mathbf{x}, \mathbf{x}')f_l(\mathbf{x}')\,d\mathbf{x}', \tag{A.5}$$

where $\bar{\boldsymbol{\varepsilon}} \equiv \mathbf{M}_0\bar{\boldsymbol{\sigma}}$ and $\bar{\mathbf{u}}(\mathbf{x})$ is the related linear displacement field.

It follows from (A.2), (A.5) and (A.4) that

$$\boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}} - \boldsymbol{\Delta}^{11}\boldsymbol{\zeta} - \boldsymbol{\Delta}^{12}\boldsymbol{\kappa},$$

$$\boldsymbol{\tau} = -\boldsymbol{\Delta}^{21}\boldsymbol{\zeta} - \boldsymbol{\Delta}^{22}\boldsymbol{\kappa},$$

where the operators $\boldsymbol{\Delta}^{ij}$ can be given explicitly in terms of the Green's function, for example

$$(\boldsymbol{\Delta}^{11}\boldsymbol{\zeta})_{ij} = (\mathbf{L}_0\boldsymbol{\zeta})_{ij} - L^0_{ijpq}\int_V \frac{\partial^2 G_{pr}}{\partial x_q \partial x'_s}(\mathbf{x}, \mathbf{x}')L^0_{rskl}\zeta_{kl}(\mathbf{x}')\,d\mathbf{x}'. \tag{A.6}$$

The relations (4.15) follow from the stationarity principle (2.11) applied to

$$\tilde{\boldsymbol{\sigma}} = -\boldsymbol{\Delta}^{11}\boldsymbol{\zeta} - \boldsymbol{\Delta}^{12}\boldsymbol{\kappa}, \quad \tilde{\boldsymbol{\tau}} = -\boldsymbol{\Delta}^{21}\boldsymbol{\zeta} - \boldsymbol{\Delta}^{22}\boldsymbol{\kappa}$$

and $\boldsymbol{\varepsilon} = \bar{\boldsymbol{\zeta}}$, $\boldsymbol{\eta} \equiv 0$, and the reciprocity property of the operators $\boldsymbol{\Delta}^{ij}$:

$$\int_V \boldsymbol{\zeta}_1 \cdot \boldsymbol{\Delta}^{11}\boldsymbol{\zeta}_2 = \int_V \boldsymbol{\zeta}_2 \cdot \boldsymbol{\Delta}^{11}\boldsymbol{\zeta}_1, \quad \int_V \boldsymbol{\zeta} \cdot \boldsymbol{\Delta}^{12}\boldsymbol{\kappa} = \int_V \boldsymbol{\kappa} \cdot \boldsymbol{\Delta}^{21}\boldsymbol{\zeta}$$

for arbitrary ζ, κ, ζ_1, ζ_2. The latter can be checked directly by expressing $\mathbf{\Delta}^{ij}$ in terms of G, and using the symmetry properties of $\mathbf{L}^0$ and $\mathscr{L}^0$.

To prove that $\mathbf{B}_{12}^{(rs)}$ and $\mathbf{B}_{21}^{(rs)}$ defined by (4.17) vanish for isotropic $\psi_{rs}(\mathbf{z})$ observe that $\mathbf{G}^\infty(-\mathbf{z}) = \mathbf{G}^\infty(\mathbf{z})$ for the infinite body Green's function and, therefore,

$$\mathbf{\Delta}^{12,\infty}(-\mathbf{z}) = -\mathbf{\Delta}^{12,\infty}(\mathbf{z}), \quad \mathbf{\Delta}^{21,\infty}(-\mathbf{z}) = -\mathbf{\Delta}^{21,\infty}(\mathbf{z})$$

since they are determined by third order derivatives of $\mathbf{G}^\infty$.

APPENDIX B: LINEAR ISOTROPIC STRAIN GRADIENT MEDIUM

The "gradient" part of the strain energy of a linear isotropic solid due to an arbitrary strain gradient $\boldsymbol{\eta}$ can be written as

$$\tfrac{1}{2}\boldsymbol{\eta}\cdot\mathscr{L}^0\boldsymbol{\eta} = a_1\eta_{ijk}\eta_{ijk} + a_2\eta_{ijk}\eta_{jki} + a_3\eta_{jji}\eta_{kki} + a_4\eta_{iik}\eta_{kjj} + a_5\eta_{kii}\eta_{kjj} \tag{B.1}$$

(see, e.g. Mindlin, 1964, 1965). Recall that $\eta_{ijk} \equiv u_{k,ij}$ is the tensor of the second-order gradient of displacement and is symmetric in its first two indices. In (B.1) the coefficients $(a_1, a_2, \ldots, a_5)$ are arbitrary real numbers which should satisfy certain restrictions to ensure positive definiteness of $\mathscr{L}$.

Since the linear operators introduced via (3.21) are incompressible, it is sufficient for our purposes to consider a general form for the isotropic incompressible comparison medium. If the displacement field $\mathbf{u}$ is incompressible then $\eta_{kjj} = 0$ for $k = 1, 2, 3$, and to enforce this one can consider the limit $a_4 \to \infty$, $a_5 \to \infty$. As a result the last two terms in (B.1) vanish and

$$\tfrac{1}{2}\boldsymbol{\eta}\cdot\mathscr{L}^0\boldsymbol{\eta} = a_1\eta_{ijk}\eta_{ijk} + a_2\eta_{ijk}\eta_{jki} + a_3\eta_{jji}\eta_{kki}, \tag{B.2}$$

where the tensor $\boldsymbol{\eta}$ is constrained: $\eta_{kjj} = 0$ for $k = 1, 2, 3$.

The representation (B.2) indicates that the family of isotropic incompressible operators is three-dimensional, i.e. any such operator $\mathscr{L}^0$ can be decomposed into a linear combination of "canonic" isotropic incompressible operators $\mathscr{L}^{(1)}$, $\mathscr{L}^{(2)}$ and $\mathscr{L}^{(3)}$

$$\mathscr{L}^0 = b_1\mathscr{L}^{(1)} + b_2\mathscr{L}^{(2)} + b_3\mathscr{L}^{(3)}.$$

The canonic operators $\mathscr{L}^{(j)}$ are sought to be projectors† to mutually orthogonal subspaces of the 15-dimensional linear space of incompressible tensors $\boldsymbol{\eta}$. To this end, we develop here some ideas of Mindlin (1964, 1965) by decomposing first the strain gradient tensor $\boldsymbol{\eta}$ into the symmetric part and the rotation gradient part.

The symmetric part of η_{ijk} is

$$\eta^s_{ijk} \equiv \tfrac{1}{3}(\eta_{ijk} + \eta_{jki} + \eta_{kij}) = \tfrac{1}{3}(u_{k,ij} + u_{i,jk} + u_{j,ki}), \tag{B.3}$$

i.e. $\boldsymbol{\eta}^s$ is symmetric with respect to any permutation of the indices. An arbitrary strain gradient tensor $\boldsymbol{\eta}$ therefore can be decomposed into its symmetric and "antisymmetric" parts

$$\boldsymbol{\eta} = \boldsymbol{\eta}^s + \boldsymbol{\eta}^a. \tag{B.4}$$

The antisymmetric part is specified by the curvature tensor $\boldsymbol{\chi}$ (see, e.g. Mindlin, 1964). Indeed,

$$\begin{aligned}\eta^a_{ijk} &= \tfrac{1}{3}(u_{k,i} - u_{i,k})_{,j} + \tfrac{1}{3}(u_{k,j} - u_{j,k})_{,i} \\ &= \tfrac{2}{3}e_{ikp}\chi_{pj} + \tfrac{2}{3}e_{jkq}\chi_{qi},\end{aligned} \tag{B.5}$$

where

† This is analogous to decomposition of an isotropic operator into its bulk and shear parts in "conventional" elasticity theory.

$$\chi_{ij} \equiv \theta_{i,j} = \tfrac{1}{2} e_{iqr} u_{r,jq} = \tfrac{1}{2} e_{iqr} \eta_{jqr}$$

is the curvature tensor and $\theta_i \equiv \frac{1}{2} e_{ikl} u_{l,k}$ is the rotation vector. Note that for any $\boldsymbol{\eta}$ (B.4) is an orthogonal decomposition, i.e. $\eta^s_{ijk} \eta^a_{ijk} = 0$.

Further decomposition of $\boldsymbol{\eta}^a$ is done splitting the curvature tensor $\boldsymbol{\chi}$ into its symmetric and antisymmetric parts

$$\chi_{ij} = \chi^s_{ij} + \chi^a_{ij}; \quad \chi^s_{ij} \equiv \tfrac{1}{2}(\chi_{ij} + \chi_{ji}), \quad \chi^a_{ij} \equiv \tfrac{1}{2}(\chi_{ij} - \chi_{ji}) \tag{B.6}$$

and by substituting (B.6) into (B.5). As a result the tensor $\boldsymbol{\eta}^a$ splits into two parts $\boldsymbol{\eta}^{as}$ and $\boldsymbol{\eta}^{aa}$ as follows

$$\boldsymbol{\eta}^a = \boldsymbol{\eta}^{as} + \boldsymbol{\eta}^{aa}, \tag{B.7}$$

$$\begin{aligned}
\eta^{as}_{ijk} &\equiv \tfrac{2}{3} e_{ikp} \chi^s_{pj} + \tfrac{2}{3} e_{jkp} \chi^s_{pi} \\
&= \tfrac{1}{6}(e_{ikp} e_{jlm} \eta_{lpm} + e_{jkp} e_{ilm} \eta_{lpm} + 2\eta_{ijk} - \eta_{jki} - \eta_{kij}); \\
\eta^{aa}_{ijk} &\equiv \tfrac{2}{3} e_{ikp} \chi^a_{pj} + \tfrac{2}{3} e_{jkp} \chi^a_{pi} \\
&= \tfrac{1}{6}(-e_{ikp} e_{jlm} \eta_{lpm} - e_{jkp} e_{ilm} \eta_{lpm} + 2\eta_{ijk} - \eta_{jki} - \eta_{kij}).
\end{aligned}$$

To summarize, we decompose an arbitrary $\boldsymbol{\eta}$ into the three components

$$\boldsymbol{\eta} = \boldsymbol{\eta}^s + \boldsymbol{\eta}^{as} + \boldsymbol{\eta}^{aa}.$$

These components are mutually orthogonal. For example, for any $\boldsymbol{\eta}$ and $\tilde{\boldsymbol{\eta}}$

$$\boldsymbol{\eta}^s \cdot \tilde{\boldsymbol{\eta}}^{as} = \tfrac{2}{3} \eta^s_{ijk} e_{ikp} \tilde{\chi}^s_{pj} + \tfrac{2}{3} \eta^s_{ijk} e_{jkp} \tilde{\chi}^s_{pi}$$

is zero because, e.g. η^s_{ijk} is symmetric in (ik) but e_{ikp} is antisymmetric. Similarly, $\boldsymbol{\eta}^s \cdot \tilde{\boldsymbol{\eta}}^{aa} = 0$. Finally,

$$\begin{aligned}
\boldsymbol{\eta}^{as} \cdot \tilde{\boldsymbol{\eta}}^{aa} &= \tfrac{4}{9}(e_{ikp} \chi^s_{pj} + e_{jkq} \chi^s_{qi})(e_{ikr} \chi^a_{rj} + e_{jks} \chi^a_{si}) \\
&= \tfrac{4}{9}(6\chi^s_{pj} \chi^a_{pj} - 2\chi^s_{ii} \chi^a_{jj}) = 0.
\end{aligned}$$

Specialize now to the incompressible case, i.e. to such $\boldsymbol{\eta}$ that $\eta_{kjj} = 0$, $k = 1, 2, 3$. Observe first that η^s_{ijk} as defined by (B.3) does not fall algebraically into the class of incompressible tensors, i.e. η^s_{kjj} may not be zero even though $\eta_{kjj} = 0$. To maintain incompressibility we subtract from $\boldsymbol{\eta}^s$ its "hydrostatic symmetric" part and introduce

$$\eta^{(1)}_{ijk} = \eta^s_{ijk} - \tfrac{1}{5}(\delta_{ij} \eta^s_{kpp} + \delta_{jk} \eta^s_{ipp} + \delta_{ki} \eta^s_{jpp}),$$

which is both symmetric and "incompressible".

Introduce next the tensor $\boldsymbol{\eta}^{(2)} \equiv \boldsymbol{\eta}^{as}$ as defined by (B.7). It is incompressible and needs no modification as above. Indeed,

$$\eta^{as}_{kjj} = \tfrac{2}{3} e_{kjp} \chi^s_{pj} + \tfrac{2}{3} e_{jjq} \chi^s_{qk} = 0.$$

Finally, let

$$\eta^{(3)}_{ijk} \equiv \eta_{ijk} - \eta^{(1)}_{ijk} - \eta^{(2)}_{ijk} = \eta^{aa}_{ijk} + \tfrac{1}{5}(\delta_{ij} \eta^s_{kpp} + \delta_{jk} \eta^s_{ipp} + \delta_{ki} \eta^s_{jpp}),$$

which is incompressible by construction.

The resulting new decomposition

$$\boldsymbol{\eta} = \boldsymbol{\eta}^{(1)} + \boldsymbol{\eta}^{(2)} + \boldsymbol{\eta}^{(3)}$$

maintains incompressibility and is still orthogonal. The latter may be checked directly, e.g.

$$\boldsymbol{\eta}^{(1)} \cdot \tilde{\boldsymbol{\eta}}^{(3)} = \boldsymbol{\eta}^{(1)} \cdot \tilde{\boldsymbol{\eta}}^{aa} + \tfrac{1}{5}\eta^{(1)}_{ijk}(\delta_{ij}\tilde{\eta}^{s}_{kpp} + \delta_{jk}\tilde{\eta}^{s}_{ipp} + \delta_{ki}\tilde{\eta}^{s}_{jpp}) = 0$$

due to incompressibility of $\boldsymbol{\eta}^{(1)}$, i.e. $\eta^{(1)}_{iik} = \eta^{(1)}_{iki} = \eta^{(1)}_{kii} = 0$, $k = 1, 2, 3$.

The above considerations imply that three isotropic operators $\mathscr{L}^{(1)}$, $\mathscr{L}^{(2)}$ and $\mathscr{L}^{(3)}$ can be introduced such that for any $\boldsymbol{\eta}$

$$\boldsymbol{\eta}^{(1)} \equiv \mathscr{L}^{(1)}\boldsymbol{\eta}, \quad \boldsymbol{\eta}^{(2)} \equiv \mathscr{L}^{(2)}\boldsymbol{\eta}, \quad \boldsymbol{\eta}^{(3)} \equiv \mathscr{L}^{(3)}\boldsymbol{\eta}.$$

The operators $\mathscr{L}^{(j)}$, $j = 1, 2, 3$ are in fact projectors to mutually orthogonal subspaces of the linear space of the isotropic incompressible tensors $\boldsymbol{\eta}$. From dimensional considerations an arbitrary isotropic incompressible operator $\mathscr{L}^0$ of form (B.2) must be of the form

$$\mathscr{L}^0 = b_1\mathscr{L}^{(1)} + b_2\mathscr{L}^{(2)} + b_3\mathscr{L}^{(3)},$$

where (b_1, b_2, b_3) are linearly related to (a_1, a_2, a_3). The corresponding energy functional is

$$\tfrac{1}{2}\boldsymbol{\eta} \cdot \mathscr{L}^0\boldsymbol{\eta} = \tfrac{1}{2}b_1\boldsymbol{\eta}^{(1)} \cdot \boldsymbol{\eta}^{(1)} + \tfrac{1}{2}b_2\boldsymbol{\eta}^{(2)} \cdot \boldsymbol{\eta}^{(2)} + \tfrac{1}{2}b_3\boldsymbol{\eta}^{(3)} \cdot \boldsymbol{\eta}^{(3)} \tag{B.8}$$

since

$$\boldsymbol{\eta} \cdot \mathscr{L}^{(1)}\boldsymbol{\eta} = \boldsymbol{\eta} \cdot \boldsymbol{\eta}^{(1)} = (\boldsymbol{\eta}^{(1)} + \boldsymbol{\eta}^{(2)} + \boldsymbol{\eta}^{(3)}) \cdot \boldsymbol{\eta}^{(1)} = \boldsymbol{\eta}^{(1)} \cdot \boldsymbol{\eta}^{(1)}$$

for example.

The resulting "canonical" representation (B.8) gives a general form of the strain-gradient energy functional. It provides a particularly simple condition of positive definiteness of $\mathscr{L}^0$: this holds if and only if $b_1 > 0$, $b_2 > 0$ and $b_3 > 0$. One can write $b_j = \mu_0 l_j^2$, $j = 1, 2, 3$ where $\mu_0 = (4M^0_{1212})^{-1}$ is the "conventional" shear modulus, and $l_j > 0$ have dimensions of length. Another advantage of the canonic form (B.8) is that the operator $\mathscr{L}^0$ can be easily inverted since it acts as a simple multiplication by b_j in corresponding subspace: if $\mathscr{M}^0 = (\mathscr{L}^0)^{-1}$ then

$$\mathscr{M}^0\boldsymbol{\tau} = \frac{1}{\mu_0 l_1^2}\boldsymbol{\tau}^{(1)} + \frac{1}{\mu_0 l_2^2}\boldsymbol{\tau}^{(2)} + \frac{1}{\mu_0 l_3^2}\boldsymbol{\tau}^{(3)}.$$

Here, similarly to $\boldsymbol{\eta}$, $\boldsymbol{\tau}^{(j)}$ denote projections of $\boldsymbol{\tau}$ on the jth subspace ($j = 1, 2$, or 3): $\boldsymbol{\tau}^{(j)} = \mathscr{L}^{(j)}\boldsymbol{\tau}$ with all the above algebraic representations applied by simple replacement of η by τ. In particular, the energy may be re-written as

$$\tfrac{1}{2}\boldsymbol{\eta} \cdot \mathscr{L}^0\boldsymbol{\eta} = \tfrac{1}{2}\boldsymbol{\tau} \cdot \mathscr{M}^0\boldsymbol{\tau} = \frac{1}{2\mu_0 l_1^2}\boldsymbol{\tau}^{(1)} \cdot \boldsymbol{\tau}^{(1)} + \frac{1}{2\mu_0 l_2^2}\boldsymbol{\tau}^{(2)} \cdot \boldsymbol{\tau}^{(2)} + \frac{1}{2\mu_0 l_3^2}\boldsymbol{\tau}^{(3)} \cdot \boldsymbol{\tau}^{(3)}.$$

Note that

$$\boldsymbol{\tau} = b_1\boldsymbol{\eta}^{(1)} + b_2\boldsymbol{\eta}^{(2)} + b_3\boldsymbol{\eta}^{(3)} \tag{B.9}$$

defines the deviatoric part of the higher-order stress analogously to $\boldsymbol{\sigma} = 2\mu_0\boldsymbol{\varepsilon}$ identifying the deviatoric part of the conventional stress.

Consider now the Green's function corresponding to a linear incompressible comparison medium with tensors $(\mathbf{M}^0, \mathscr{M}^0)$ characterized by the parameters μ_0, l_1, l_2 and l_3 as discussed above. Note first that due to incompressibility the deviatoric parts $\boldsymbol{\sigma} = \mathbf{L}^0\boldsymbol{\varepsilon}$ and $\boldsymbol{\tau} = \mathscr{L}^0\boldsymbol{\eta}$ satisfy the equilibrium equation (2.4) in a corrected form

$$\sigma_{jk,j} - \tau_{ijk,ij} + H_{,k} = 0 \tag{B.10}$$

with some scalar field $H(\mathbf{x})$ accounting for the hydrostatic components of the stresses. To obtain the equilibrium equation in displacement form substitute $\sigma_{jk} = 2\mu_0\varepsilon_{jk} = \mu_0(u_{j,k} + u_{k,j})$ and (B.9) into (B.10) using the explicit formulae for $\boldsymbol{\eta}^{(1)}$, $\boldsymbol{\eta}^{(2)}$, $\boldsymbol{\eta}^{(3)}$ and employing the incompressibility of displacement, i.e. $u_{i,i} = 0$, $u_{i,ji} = 0$. As a result,

$$\mu_0\Delta u_k - \mu_0(\tfrac{4}{15}l_1^2 + \tfrac{1}{3}l_2^2 + \tfrac{2}{5}l_3^2)\Delta^2 u_k + H_{,k} = 0, \tag{B.11}$$

where Δ is the Laplacian operator. The infinite body Green's functions G_{ik}^{∞} satisfies (B.11) with a point load

$$\mu_0 \Delta G_{ik}^{\infty} - \tfrac{1}{4}\mu_0 l_0^2 \Delta^2 G_{ik}^{\infty} + \tilde{H}_{i,k} + \delta_{ik}\delta(\mathbf{x}) = 0, \tag{B.12}$$

where

$$l_0 \equiv 2(\tfrac{4}{15}l_1^2 + \tfrac{1}{3}l_2^2 + \tfrac{2}{5}l_3^2)^{1/2}. \tag{B.13}$$

The equation (B.12) formally coincides with that emerging in a reduced couple stress theory (Smyshlyaev and Fleck, 1994; Appendices A and B), and its solution is given by

$$G_{ij}(\mathbf{x}) = \frac{1}{8\pi\mu_0 l_0}\int_{|\xi|=1}(\delta_{ij} - \xi_i\xi_j)\exp\left\{-\frac{2|\boldsymbol{\xi}\cdot\mathbf{x}|}{l_0}\right\}\mathrm{d}S(\boldsymbol{\xi}). \tag{B.14}$$

To obtain the shear part μ_Q of tensor $\mathbf{Q}$ defined by (4.19) note first that in the case of the infinite body (A.6) defines $\boldsymbol{\Delta}^{11,\infty}$ as a translationary invariant operator with kernel

$$\Delta_{ijkl}^{11,\infty} = L_{ijkl}^{0}\delta(\mathbf{x}) + L_{ijpq}^{0}G_{pr,qs}^{\infty}(\mathbf{x})L_{rskl}. \tag{B.15}$$

Relation (4.19) then reads

$$\mathbf{Q} = \mathbf{L}^0 - \mathbf{L}^0\mathbf{S}^{\infty}\mathbf{L}^0, \tag{B.16}$$

where

$$S_{ijkl}^{\infty} \equiv -\int G_{il,kj}(\mathbf{x})_{|(ij),(kl)}h(|\mathbf{x}|)\,\mathrm{d}\mathbf{x} \tag{B.17}$$

and (ij) denotes symmetrization with respect to the relevant indices.

As all the tensors involved are isotropic, (B.16) leads to the following expression for $\mu_Q \equiv Q_{1212}$

$$\mu_Q = \mu_0 - 4\mu_0^2\mu_S, \tag{B.18}$$

where $\mu_S \equiv S_{1212}^{\infty}$ is the shear part of the tensor $\mathbf{S}^{\infty}$. The shear modulus μ_S is found from (B.17) and (B.14) to be (see Smyshlyaev and Fleck, 1994, Appendix B)

$$\mu_S = \frac{1}{4\mu_0}\psi(l_0),$$

where

$$\psi(l) \equiv \frac{8}{5}\int_0^{+\infty} \mathrm{e}^{-2t}h(lt)t\,\mathrm{d}t. \tag{B.19}$$

Thus, μ_Q assumes the form

$$\mu_Q = \mu_0(1 - \psi(l_0)). \tag{B.20}$$