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The role of interfaces in enhancing the yield strength of composites and polycrystals

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Abstract

A deformation-theory version of strain-gradient plasticity is employed to assess the influence of microstructural scale on the yield strength of composites and polycrystals. The framework is that recently employed by Fleck and Willis (J. Mech. Phys. Solids 52 (2004) 1855–1888), but it is enhanced by the introduction of an interfacial ‘‘energy’’ that penalises the build-up of plastic strain at interfaces. The most notable features of the new interfacial potential are: (a) internal surfaces are treated as surfaces of discontinuity and (b) the scale-dependent enhancement of the overall yield strength is no longer limited by the ‘‘Taylor’’ or ‘‘Voigt’’ upper bound. The variational structure associated with the theory is developed in generality and its implications are demonstrated through consideration of simple one-dimensional examples. Results are presented for a single-phase medium containing interfaces distributed either periodically or randomly.

Keywords: Strain-gradient plasticity; Variational principles; Hall–Petch effect

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1. Introduction

The first theory of plasticity which incorporated effects of gradients of plastic strain was that introduced by Aifantis (1984, 1987), who recognised that gradient terms could resolve small-scale deformation features such as the width and spacing of shear bands. Subsequent contributions on problems of this type include those of Zbib and Aifantis (1988) and Leroy and Molinari (1993). More recently, theories of strain-gradient plasticity have gained prominence through increasing interest in scale effects in small specimens and devices. Several theories have been proposed, including those of Fleck and Hutchinson (1993), Fleck et al. (1994) and Fleck and Hutchinson (2001) and the so-called "mechanism-based strain-gradient theory" of Gao et al. (1999). These theories are intended to make allowance, at least qualitatively, for the influence on hardening of the long-range stresses produced by "geometrically necessary" as opposed to "forest" dislocations. Rather precise theory has also been developed in the context of single-crystal plasticity (Gurtin, 2000, 2002). All such theories have associated with them a characteristic (internal) length, and the influence of the gradient term becomes apparent as soon as some dimension of the specimen is reduced to a small multiple of this characteristic length. The basic question of how to choose between the competing theories remains incompletely resolved. Qualitatively, any will show the right trend, but differences of detail, obtained by fixing parameters relative to one experimental setup and then predicting outcomes for different experiments, can provide evidence in favour of one theory relative to another, but will not definitively identify one theory as "correct". Another approach is to compare predictions made by use of a strain-gradient theory with corresponding predictions obtained from a simulation which employs discrete dislocations. A drawback here is that the discrete dislocation simulation inevitably employs an idealised version of the underlying physics. Examples of work of this type include Cleveringa et al. (1997), Shu et al. (2001), Bittencourt et al. (2003).

Strain-gradient theory has one additional feature which has so far not yielded to precise physical interpretation. This is that introduction of a gradient term requires the introduction of an additional boundary condition and a corresponding additional jump condition across any surface of discontinuity. The mathematical structure shows what quantity needs to be specified but provision of the actual value can only follow from a clear recognition of the physics that the strain-gradient theory is supposed to represent. Exactly what boundary or interface conditions can be imposed depends on the precise strain-gradient theory that is adopted. For instance, a single-crystal model such as that of Gurtin (2002), in which the plastic distortion is defined in terms of slips on slip planes, contains sufficient detail to allow the tracking of the motion of the (geometrically necessary) dislocations. Implications for boundaries and interfaces, associated with this model, have recently been developed by Gurtin and Needleman (2005). Retention of this degree of detail is, however, likely to be difficult in the context of applications.

Previous studies (Smyshlyaev and Fleck, 1995, 1996; Fleck and Willis, 2004) have employed strain-gradient plasticity to predict the influence of scale on the yield strength of a composite. In these works, methods for calculating the effective response of nonlinear composites (Talbot and Willis, 1985; Ponte Castañeda, 1991; Ponte Castañeda and Suquet, 1998) were adapted and extended to find the effective macroscopic response of a composite whose constituents conformed to deformation-theory versions of strain-gradient plasticity. The earlier work of Smyshlyaev and Fleck (1995, 1996) was based on strain-gradient theory of the type proposed by Fleck and Hutchinson (1993), while that of Fleck and Willis (2004) used a modified version of the ‘‘reformulated’’ theory of Fleck and Hutchinson (2001). In all of this work, the effective yield strength was predicted to increase as the scale of the microstructure decreased, but it could not increase above the level given by the elementary ‘‘Taylor’’ or ‘‘Voigt’’ upper bound. The reason for this was that a mathematical assumption, ‘‘natural’’ for the structure of the equations, of continuity of plastic strain and higher-order traction across interfaces, was made. This conclusion can be altered, however, by injection of some additional physics, corresponding to the fact that an interface usually presents an obstruction to the motion of a dislocation, and hence to plastic flow. This mechanism can be accounted for by augmenting the variational principle of Fleck and Willis (2004) with an interfacial ‘‘energy’’ term which penalises the build-up (accumulation) of plastic strain on internal surfaces and hence depends on the plastic strain there. It should be noted that the assumption of continuity of plastic strain across interfaces is retained.

The introduction of such an energy penalty is fully compatible with the structure of this strain-gradient theory. It would have no effect in the absence of the strain-gradient term in the constitutive relation. In the context of strain-gradient theory, however, it induces a relation between the jump in higher-order traction (hence also plastic strain gradient) and the interfacial plastic strain. This has a qualitative relationship with the admission of dislocation pileups near boundaries leading to the classical Hall–Petch mechanism for grain-refinement strengthening; dislocation pileups correspond to local gradients in plastic strain.

Some elementary illustrations of the effects of admitting jump conditions across interfaces have been developed by Aifantis and Willis (2005). They formulated a system of ordinary differential equations, applied to one-dimensional (1-D) problems, and solved them in simple cases in which the differential equations were linear. In the present study the associated variational structure, slightly generalising that employed by Fleck and Willis (2004), is developed and exploited.

The flexibility of strain-gradient theories in allowing the introduction of jump conditions across interfaces has been independently recognised by Gudmundson (2004). His remarks on this aspect are, however, more ‘‘generic’’ than ‘‘specific’’ and admit the possibility of jumps in both plastic strain and higher-order traction, through a generalised interfacial ‘‘penalty’’ that is a function of the plastic strains $(\varepsilon^{p,1}, \varepsilon^{p,2})$ on either side of the interface. This, however, is so general that it has the potential to uncouple completely the solutions for the stresses and strains in each constituent phase, and hence some care in the choice of the functions of $\varepsilon^{p,1}$ and $\varepsilon^{p,2}$ will be required. The present work, in contrast, offers explicit models and develops their implications for the influence of scale on the effective response of a composite.

2. Gradient plasticity with an interfacial penalty

2.1. Deformation theory version of classical plasticity

The mathematical structure that is employed throughout this work is first placed in context by displaying the corresponding formulation for the deformation theory version of "classical" plasticity, with no allowance for strain-gradients. Throughout the whole of Section 2, the presentation is kept as simple as possible by assuming that displacements are prescribed on the boundary $\partial\Omega$ of the body, which occupies the domain Ω.

In the deformation theory framework of classical plasticity an energy-like functional for the domain Ω under consideration can be defined as

$$\Psi(\varepsilon_{ij}, \varepsilon^{\mathrm{p}}_{ij}) \equiv \int_{\Omega} U(\varepsilon_{ij}, \varepsilon^{\mathrm{p}}_{ij})\,\mathrm{d}x, \tag{2.1}$$

where

$$U(\varepsilon_{ij}, \varepsilon^{\mathrm{p}}_{ij}) \equiv \tfrac{1}{2}(\varepsilon_{ij} - \varepsilon^{\mathrm{p}}_{ij})L_{ijkl}(\varepsilon_{kl} - \varepsilon^{\mathrm{p}}_{kl}) + V(\varepsilon^{\mathrm{p}}_{ij}). \tag{2.2}$$

The quantities $\varepsilon_{ij}, \varepsilon^{\mathrm{p}}_{ij}$ denote the total strain and plastic strain, respectively; L_{ijkl} is the elastic stiffness tensor and the first term of the right-hand side of Eq. (2.2) is the elastic strain energy. The second term, $V(\varepsilon^{\mathrm{p}}_{ij})$, is a "dissipation function", dual to the "plastic potential". In the present context of deformation theory, the distinction between dissipated and recoverable energy is blurred. In the sequel, it is convenient to refer to V simply as a "potential". The displacement is taken to be continuous across interfaces. The problem posed is to find the fields $(\varepsilon_{ij}, \varepsilon^{\mathrm{p}}_{ij})$ that minimise Eq. (2.1), where the total strain tensor ε_{ij} is related to the displacement vector u_i by the usual relationship

$$\varepsilon_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}). \tag{2.3}$$

For convenience, the following variables conjugate to the elastic and plastic strain are introduced

$$\begin{aligned}\sigma_{ij} &= \frac{\partial U}{\partial \varepsilon_{ij}} = L_{ijkl}(\varepsilon_{kl} - \varepsilon^{\mathrm{p}}_{kl}),\\ s_{ij} &= \frac{\partial U}{\partial \varepsilon^{\mathrm{p}}_{ij}} = -L_{ijkl}(\varepsilon_{kl} - \varepsilon^{\mathrm{p}}_{kl}) + \frac{\partial V}{\partial \varepsilon^{\mathrm{p}}_{ij}} = -\sigma_{ij} + \frac{\partial V}{\partial \varepsilon^{\mathrm{p}}_{ij}}.\end{aligned} \tag{2.4}$$

The quantity σ_{ij} is the usual Cauchy stress tensor and s_{ij} may be viewed as a type of back stress. Setting the first variation of Eq. (2.1) equal to zero, $\delta\Psi = 0$, gives the principle of virtual work:

$$\int_{\Omega} \{\sigma_{ij}\delta\varepsilon_{ij} + s_{ij}\delta\varepsilon^{\mathrm{p}}_{ij}\}\,\mathrm{d}x = 0 \Rightarrow \int_{\Omega} \{-\sigma_{ij,j}\delta u_i + s_{ij}\delta\varepsilon^{\mathrm{p}}_{ij}\}\,\mathrm{d}x = 0 \tag{2.5}$$

which must hold true for all admissible variations $\delta u_i, \delta\varepsilon^{\mathrm{p}}_{ij}$. As a result, the following field equations are obtained:

$$\left.\begin{aligned} \sigma_{ij,j} &= 0, \\ s_{ij} = 0 \Rightarrow \sigma_{ij} &= \frac{\partial V}{\partial \varepsilon^{\mathrm{p}}_{ij}} \end{aligned}\right\} \quad \text{in } \Omega \tag{2.6}$$

which are to be solved together with the given boundary condition

$$u_i = u_i^0 \quad \text{on } \partial\Omega. \tag{2.7}$$

The second equation of Eq. (2.6) shows that the potential V provides a stress–plastic strain relation, from which plastic strain can be eliminated to yield, in conjunction with Eq. $(2.4)_1$, the conventional stress–total strain relation of deformation theory. The use of plastic strain as an intermediate (or internal) variable will, however, be essential for the developments to follow. It is perhaps worth noting that no requirement of continuity is made for the plastic strain. Imposition of such a requirement would compromise the existence of a plastic strain field which would minimise Ψ. It would be necessary instead to seek the infimum, which would be approached by use of sequences of continuous plastic strain fields whose limit would be the possibly discontinuous plastic strain obtained from the solution of Eqs. (2.6) and (2.7).

2.2. *Variational formulation for the strain-gradient theory*

The gradient formulation to be presented is a direct generalisation of that employed by Fleck and Willis (2004) which, as in the previous section, takes as its primary independent kinematic variables the total displacement u_i and the plastic strain $\varepsilon^{\mathrm{p}}_{ij}$. In admitting the influence of gradients of plastic strain in the constitutive equation the effects of "geometrically necessary" dislocations are qualitatively accounted for but there is no relation which matches the precise correspondence $\alpha_{ij} = \varepsilon_{jkl}\beta^{\mathrm{p}}_{il,k}$ between the (geometrically necessary) dislocation density tensor α_{ij} and the plastic distortion tensor β^{p}_{ij}. The development of more general theory, allowing for plastic distortion or some other "internal variables", is desirable but it seems appropriate first to consider the influence of the new interfacial feature in relation to a model whose implications have already been investigated.

The gradient deformation theory under consideration is defined by reference to a functional Ψ given by

$$\Psi(\varepsilon_{ij}, \varepsilon^{\mathrm{p}}_{ij}) \equiv \int_\Omega U(\varepsilon_{ij}, \varepsilon^{\mathrm{p}}_{ij}, \varepsilon^{\mathrm{p}}_{ij,k})\,\mathrm{d}x + \int_\Gamma \phi(\varepsilon^{\mathrm{p}}_{ij})\,\mathrm{d}\Gamma, \tag{2.8}$$

where Ω is the domain occupied by the composite material. Its external surface is denoted $\partial\Omega$, while internal interfaces between different constituents are denoted collectively by Γ. The total strain ε_{ij} is related to the displacement u_i by Eq. (2.3), and it is assumed that both the displacement and plastic strain are continuous throughout the whole domain under consideration (including across Γ). The potential $U(\varepsilon_{ij}, \varepsilon^{\rm p}_{ij}, \varepsilon^{\rm p}_{ij,k})$ is defined as in Fleck and Willis (2004), i.e.

$$U(\varepsilon_{ij}, \varepsilon^{\rm p}_{ij}, \varepsilon^{\rm p}_{ij,k}) = \tfrac{1}{2}(\varepsilon_{ij} - \varepsilon^{\rm p}_{ij})L_{ijkl}(\varepsilon_{kl} - \varepsilon^{\rm p}_{kl}) + V(\varepsilon^{\rm p}_{ij}, \varepsilon^{\rm p}_{ij,k}). \tag{2.9}$$

It should be noted that the elastic moduli L_{ijkl} and the gradient potential $V(\varepsilon^{\rm p}_{ij}, \varepsilon^{\rm p}_{ij,k})$ vary with position x, depending on the material constituent present at x. The new feature of the present formulation is the introduction of the potential $\phi(\varepsilon^{\rm p}_{ij})$, defined over the interfaces Γ. If the composite is subjected to given displacements $u_i = u^0_i$ at its surface $\partial\Omega$, the fields within the composite are taken to be those that minimise the functional $\Psi(\varepsilon_{ij}, \varepsilon^{\rm p}_{ij})$ over total strain fields ε_{ij} that satisfy Eq. (2.3) for some continuous displacement u_i that takes values u^0_i on $\partial\Omega$, and over continuous plastic strain fields $\varepsilon^{\rm p}_{ij}$. No other restrictions of a "physical" nature are imposed, but a more careful mathematical specification requires at least that the integrals in Eq. (2.8) should exist. The problem then posed is to find the fields ε_{ij} (or u_i), $\varepsilon^{\rm p}_{ij}$ that yield the infimum value

$$\Xi = \inf_{\varepsilon_{ij}, \varepsilon^{\rm p}_{ij}} \Psi(\varepsilon_{ij}, \varepsilon^{\rm p}_{ij}). \tag{2.10}$$

The Euler–Lagrange equations associated with the infimum problem (2.10) are best expressed by introducing the conjugate variables

$$\begin{aligned}
\sigma_{ij} &= \frac{\partial U}{\partial \varepsilon_{ij}} = L_{ijkl}(\varepsilon_{kl} - \varepsilon^{\rm p}_{kl}),\\
s_{ij} &= \frac{\partial U}{\partial \varepsilon^{\rm p}_{ij}} = -L_{ijkl}(\varepsilon_{kl} - \varepsilon^{\rm p}_{kl}) + \frac{\partial V}{\partial \varepsilon^{\rm p}_{ij}},\\
\tau_{ijk} &= \frac{\partial U}{\partial \varepsilon^{\rm p}_{ij,k}} = \frac{\partial V}{\partial \varepsilon^{\rm p}_{ij,k}}.
\end{aligned} \tag{2.11}$$

It should be noted that the two first conjugate variable relations are the same as those used in the classical case, but use of the gradient of $\varepsilon^{\rm p}_{ij}$ as an additional independent variable resulted in the definition $(2.11)_3$ of the higher-order stress τ_{ijk}. The requirement that the functional Ψ is minimised implies the principle of virtual work, that the first variation of Eq. (2.8) has to be zero for all allowed variations $\delta\varepsilon_{ij}$ and $\delta\varepsilon^{\rm p}_{ij}$; hence

$$\int_\Omega (\sigma_{ij}\delta\varepsilon_{ij} + s_{ij}\delta\varepsilon^{\rm p}_{ij} + \tau_{ijk}\delta\varepsilon^{\rm p}_{ij,k})\,{\rm d}x + \int_\Gamma \phi'(\varepsilon^{\rm p}_{ij})\delta\varepsilon^{\rm p}_{ij}\,{\rm d}\Gamma = 0. \tag{2.12}$$

Integration by parts and allowing for admissible discontinuities across interfaces gives

$$\begin{aligned}
&\int_\Omega \{-\sigma_{ij,j}\delta u_i + (s_{ij} - \tau_{ijk,k})\delta\varepsilon^{\rm p}_{ij}\}\,{\rm d}x + \int_{\partial\Omega} \{\sigma_{ij}n_j\delta u_i + \tau_{ijk}n_k\delta\varepsilon^{\rm p}_{ij}\}\,{\rm d}S\\
&\quad + \int_\Gamma \{-[\sigma_{ij}n_j]\delta u_i + (\phi'(\varepsilon^{\rm p}_{ij}) - [\tau_{ijk}n_k])\delta\varepsilon^{\rm p}_{ij}\}\,{\rm d}\Gamma = 0
\end{aligned} \tag{2.13}$$

for all allowed variations δu_i and $\delta\varepsilon^{\rm p}_{ij}$. This implies the field equations

$$\left.\begin{aligned}\sigma_{ij,j}&=0,\\ s_{ij}-\tau_{ijk,k}&=0\end{aligned}\right\}\quad \text{in } \Omega\backslash\Gamma, \tag{2.14}$$

the "natural" boundary condition

$$\tau_{ijk}n_k=0\quad \text{on } \partial\Omega \tag{2.15}$$

and the interface conditions

$$\left.\begin{aligned}[][\sigma_{ij}n_j]&=0,\\ [\tau_{ijk}n_k]&=\phi'(\varepsilon^{\rm p}_{ij})\end{aligned}\right\}\quad \text{across } \Gamma. \tag{2.16}$$

Here and in the sequel, $\phi'(\varepsilon^{\rm p}_{ij})$ is written for $\partial\phi/\partial\varepsilon^{\rm p}_{ij}$. It can be seen that a jump condition is induced by the interfacial energy term, which is solely due to the admission of the gradient of $\varepsilon^{\rm p}_{ij}$ in the total energy functional. In Eqs. (2.13) and (2.16) and equations to follow, $[f]$ denotes the jump f_1-f_2 across a point of Γ, where the normal n_i points in the direction from "side 2" to "side 1". There is no condition for $\sigma_{ij}n_j$ on the external boundary $\partial\Omega$ because displacement is prescribed there; with similar reasoning it can be seen that if $\varepsilon^{\rm p}_{ij}$ were prescribed on $\partial\Omega$, the boundary condition (2.15) would not be present. Imposing other boundary conditions on $\partial\Omega$ would require the addition of surface integrals (over $\partial\Omega$) to the basic infimum problem (2.10) (see Fleck and Willis, 2004; Aifantis and Willis, 2005). Finally, it should be noted that setting $\phi=0$ results in the original Fleck–Willis formulation; the second condition in Eq. (2.16) reduces then to the requirement of continuity of higher-order tractions.

3. Effective response

If the medium under consideration has very fine microstructure relative to the (macroscopic) length scale of the domain Ω, and if the boundary data $u_i=u^0_i$ vary smoothly relative to the scale of Ω, problem (2.10) can be replaced asymptotically by the homogenised problem

$$\Xi=\inf_{\bar\varepsilon_{ij},\bar\varepsilon^{\rm p}_{ij}}\int_\Omega U^{\rm eff}(\bar\varepsilon_{ij},\bar\varepsilon^{\rm p}_{ij})\,{\rm d}x, \tag{3.1}$$

where $U^{\rm eff}$ is a "local average" defined over a "representative volume element" D:

$$U^{\rm eff}(\bar\varepsilon_{ij},\bar\varepsilon^{\rm p}_{ij})\equiv\inf_{\varepsilon_{ij},\varepsilon^{\rm p}_{ij}}\left\{\frac{1}{|D|}\left[\int_D U(\varepsilon_{ij},\varepsilon^{\rm p}_{ij},\varepsilon^{\rm p}_{ij,k})\,{\rm d}x+\int_{\Gamma_D}\phi(\varepsilon^{\rm p}_{ij})\,{\rm d}\Gamma\right]\right\}, \tag{3.2}$$

where Γ_D represents the interfaces within D, $|D|$ denotes the volume of D and the infimum is taken over fields which satisfy the relations

$$\begin{aligned}
&\varepsilon_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}) \quad \text{for some displacement } u_i, \\
&\langle \varepsilon_{ij} \rangle \equiv \frac{1}{|D|}\int_D \varepsilon_{ij}\,\mathrm{d}x = \bar{\varepsilon}_{ij}, \\
&\langle \varepsilon^{\mathrm{p}}_{ij} \rangle \equiv \frac{1}{|D|}\int_D \varepsilon^{\mathrm{p}}_{ij}\,\mathrm{d}x = \bar{\varepsilon}^{\mathrm{p}}_{ij}.
\end{aligned} \tag{3.3}$$

The infimum for problem (3.2) is attained when an equation like (2.13) is satisfied, except that now u_i is not prescribed on ∂D and the allowed total and plastic strains have to be compatible with $(3.3)_{2,3}$. Such considerations result in the following field equations:

$$\left.\begin{aligned} \sigma_{ij,j} &= 0, \\ s_{ij} - \tau_{ijk,k} &= s^*_{ij} \end{aligned}\right\} \quad \text{in } D \backslash \Gamma_D, \tag{3.4}$$

$$\left.\begin{aligned} (\sigma_{ij} - \bar{\sigma}_{ij})n_j &= 0, \\ \tau_{ijk}n_k &= 0 \end{aligned}\right\} \quad \text{on } \partial D, \tag{3.5}$$

$$\left.\begin{aligned} [\sigma_{ij}n_j] &= 0, \\ [\tau_{ijk}n_k] &= \phi'(\varepsilon^{\mathrm{p}}_{ij}) \end{aligned}\right\} \quad \text{across } \Gamma_D. \tag{3.6}$$

Here, $\bar{\sigma}_{ij}, s^*_{ij}$ are constants, unknown a priori, that play the role of Lagrange multipliers corresponding to the constraints $(3.3)_2$ and $(3.3)_3$, respectively. It follows from the first of each of the pairs of Eqs. (3.4)–(3.6) that $\bar{\sigma}_{ij}$ is the mean value of σ_{ij} over D. An elementary calculation, based on considering the variation of $U^{\mathrm{eff}}(\bar{\varepsilon}_{ij}, \bar{\varepsilon}^{\mathrm{p}}_{ij})$ with respect to small changes in $\bar{\varepsilon}_{ij}$ and $\bar{\varepsilon}^{\mathrm{p}}_{ij}$, delivers the "effective constitutive relations"

$$\bar{\sigma}_{ij} = \frac{\partial U^{\mathrm{eff}}}{\partial \bar{\varepsilon}_{ij}}, \quad s^*_{ij} = \frac{\partial U^{\mathrm{eff}}}{\partial \bar{\varepsilon}^{\mathrm{p}}_{ij}}. \tag{3.7}$$

The second of these relations is new, in view of the presence of the surface potential $\phi(\varepsilon^{\mathrm{p}}_{ij})$. As in Section 2.1, the infimum with respect to $\bar{\varepsilon}^{\mathrm{p}}_{ij}$ for (3.1) is achieved by taking $s^*_{ij} = 0$.

4. Bounds

Henceforth, following Fleck and Willis (2004), the simplifying assumption is made that the tensor of elastic moduli L is the same for every constituent, and hence also describes the elastic response of the composite. In this case, it is natural to express the "effective" potential U^{eff} in the form

$$U^{\text{eff}}(\bar{\varepsilon}_{ij}, \bar{\varepsilon}^{\text{p}}_{ij}) = \tfrac{1}{2}(\bar{\varepsilon}_{ij} - \bar{\varepsilon}^{\text{p}}_{ij})L_{ijkl}(\bar{\varepsilon}_{kl} - \bar{\varepsilon}^{\text{p}}_{kl}) + V^{\text{eff}}(\bar{\varepsilon}^{\text{p}}_{ij}) \tag{4.1}$$

which provides the kind of classical deformation-theory effective response for the composite that was discussed in Section 2.1. Relation (4.1) defines the potential $V^{\text{eff}}(\bar{\varepsilon}^{\text{p}}_{ij})$; hence it is necessary to prove that V^{eff} is independent of $\bar{\varepsilon}_{ij}$. First, performing a minimisation over ε_{ij}, with $\varepsilon^{\text{p}}_{ij}$ fixed, requires the following calculation:

$$\inf_{\varepsilon_{ij}} \frac{1}{|D|}\int_D \frac{1}{2}(\varepsilon_{ij} - \varepsilon^{\text{p}}_{ij})L_{ijkl}(\varepsilon_{kl} - \varepsilon^{\text{p}}_{kl})\,\mathrm{d}x = \inf_{\varepsilon^1_{ij}} \frac{1}{|D|}\int_D \frac{1}{2}(\bar{\varepsilon}_{ij} + \varepsilon^1_{ij} - \varepsilon^{\text{p}}_{ij})L_{ijkl} \times(\bar{\varepsilon}_{kl} + \varepsilon^1_{kl} - \varepsilon^{\text{p}}_{kl})\,\mathrm{d}x, \tag{4.2}$$

where ε^1_{ij} is any strain field with mean value zero over D. Expansion of this expression, exploiting the fact that ε^1_{ij} has mean value zero, now gives

$$\frac{1}{2}(\bar{\varepsilon}_{ij} - \bar{\varepsilon}^{\text{p}}_{ij})L_{ijkl}(\bar{\varepsilon}_{kl} - \bar{\varepsilon}^{\text{p}}_{kl}) + \inf_{\varepsilon^1_{ij}} \frac{1}{|D|}\int_D \frac{1}{2}(\varepsilon^1_{ij} + \bar{\varepsilon}^{\text{p}}_{ij} - \varepsilon^{\text{p}}_{ij})L_{ijkl}(\varepsilon^1_{kl} + \bar{\varepsilon}^{\text{p}}_{kl} - \varepsilon^{\text{p}}_{kl})\,\mathrm{d}x. \tag{4.3}$$

Thus,

$$V^{\text{eff}}(\bar{\varepsilon}^{\text{p}}_{ij}) = \inf_{\varepsilon^1_{ij},\varepsilon^{\text{p}}_{ij}}\left\{\frac{1}{|D|}\left[\int_D\left(\frac{1}{2}(\varepsilon^1_{ij} + \bar{\varepsilon}^{\text{p}}_{ij} - \varepsilon^{\text{p}}_{ij})L_{ijkl}(\varepsilon^1_{kl} + \bar{\varepsilon}^{\text{p}}_{kl} - \varepsilon^{\text{p}}_{kl}) + V(\varepsilon^{\text{p}}_{ij}, \varepsilon^{\text{p}}_{ij,k})\right)\mathrm{d}x + \int_{\Gamma_D}\phi(\varepsilon^{\text{p}}_{ij})\,\mathrm{d}\Gamma\right]\right\}. \tag{4.4}$$

The infimum over ε^1_{ij} makes a contribution to V^{eff}, which depends on $\bar{\varepsilon}^{\text{p}}_{ij}$ but not on $\bar{\varepsilon}_{ij}$. A more explicit form for this term is given in Fleck and Willis (2004, Eq. (3.6)).

4.1. Elementary upper and lower bounds

Definition (3.2) of U^{eff} permits the immediate derivation of an upper bound by substituting into the right side any admissible fields ε_{ij}, $\varepsilon^{\text{p}}_{ij}$. Choosing these to be $\bar{\varepsilon}_{ij}$, $\bar{\varepsilon}^{\text{p}}_{ij}$, respectively, delivers the upper bound

$$U^{\text{eff}}(\bar{\varepsilon}_{ij}, \bar{\varepsilon}^{\text{p}}_{ij}) \leqslant \frac{1}{|D|}\left\{\int_D U(\bar{\varepsilon}_{ij}, \bar{\varepsilon}^{\text{p}}_{ij}, 0)\,\mathrm{d}x + \int_{\Gamma_D}\phi(\bar{\varepsilon}^{\text{p}}_{ij})\,\mathrm{d}\Gamma\right\} \tag{4.5}$$

which is analogous to the Voigt upper bound of classical elasticity. In the case that the elastic constant tensor L is constant over D, this bound, together with definition (4.4), gives the corresponding bound for V^{eff},

$$V^{\text{eff}}(\bar{\varepsilon}^{\text{p}}_{ij}) \leqslant V_V(\bar{\varepsilon}^{\text{p}}_{ij}) \equiv \frac{1}{|D|}\left\{\int_D V(\bar{\varepsilon}^{\text{p}}_{ij}, 0)\,\mathrm{d}x + \int_{\Gamma_D}\phi(\bar{\varepsilon}^{\text{p}}_{ij})\,\mathrm{d}\Gamma\right\}. \tag{4.6}$$

In the absence of the interface potential ϕ, this bound is insensitive to the scale of the microstructure and so sets a scale-independent upper limit for the effective plastic response, as found by Smyshlyaev and Fleck (1995, 1996) and Fleck and Willis (2004). The presence of the interfacial potential removes this restriction; the bound increases linearly with the ratio of surface area to volume.

An elementary lower bound, of Reuss type, can also be derived, by making use of the Fenchel inequality

$$U^*(\sigma_{ij}, s_{ij}, \tau_{ijk}) \geqslant \sigma_{ij}\varepsilon_{ij} + s_{ij}\varepsilon^{\mathrm{p}}_{ij} + \tau_{ijk}\varepsilon^{\mathrm{p}}_{ij,k} - U(\varepsilon_{ij}, \varepsilon^{\mathrm{p}}_{ij}, \varepsilon^{\mathrm{p}}_{ij,k}) \tag{4.7}$$

in conjunction with definition (3.2). In the case of constant L, and taking $\sigma_{ij} = \overline{\sigma}_{ij}$, $s_{ij} = \overline{s}_{ij}$, constants, and $\tau_{ijk} = 0$, this gives

$$\begin{aligned} U^{\mathrm{eff}}(\overline{\varepsilon}_{ij}, \overline{\varepsilon}^{\mathrm{p}}_{ij}) \geqslant \inf_{\varepsilon^{\mathrm{p}}_{ij}} \Bigg\{ & \overline{\sigma}_{ij}\overline{\varepsilon}_{ij} + \overline{s}_{ij}\overline{\varepsilon}^{\mathrm{p}}_{ij} - \frac{1}{2}\overline{\sigma}_{ij}(L^{-1})_{ijkl}\overline{\sigma}_{kl} \\ & - \frac{1}{|D|}\left[\int_D V^*(\overline{\sigma}_{ij} + \overline{s}_{ij}, 0)\,\mathrm{d}x - \int_{\Gamma_D} \phi(\varepsilon^{\mathrm{p}})\,\mathrm{d}\Gamma \right] \Bigg\} \end{aligned} \tag{4.8}$$

for any $\overline{\sigma}_{ij}$ and $\overline{s}_{ij}$, where V^* is the convex dual of V. Assuming that $\phi(\varepsilon^{\mathrm{p}}_{ij}) \geqslant \phi(0) = 0$, it follows, by minimising the surface integral (over which the mean-value constraint has no influence) and optimising over $\overline{\sigma}_{ij}$, $\overline{s}_{ij}$, that

$$V^{\mathrm{eff}}(\overline{\varepsilon}^{\mathrm{p}}_{ij}) \geqslant V_{\mathrm{R}}(\overline{\varepsilon}^{\mathrm{p}}_{ij}), \tag{4.9}$$

where

$$V_{\mathrm{R}}(\overline{\varepsilon}^{\mathrm{p}}_{ij}) \equiv \sup_{\overline{s}_{ij}} \left\{ \overline{s}_{ij}\overline{\varepsilon}^{\mathrm{p}}_{ij} - \frac{1}{|D|}\int_D V^*(\overline{s}_{ij}, 0)\,\mathrm{d}x \right\}. \tag{4.10}$$

This lower bound is scale-independent. It was derived by Fleck and Willis (2004) under the assumption that $\phi = 0$.

4.2. *Refined upper bound*

It may be possible to find the effective potential exactly, or else find good approximations, if the response of the composite is linear, so that V and ϕ are quadratic functions of their arguments. Such a composite has no direct physical relevance but it permits the development of a bound for a nonlinear composite by comparing its response with that of the linear composite. With this motivation, a "comparison linear composite", is introduced, with quadratic potentials V_{c} and ϕ_{c} but the same microgeometry and elastic modulus tensor as the actual composite. Assuming constant L, its effective potential $U^{\mathrm{eff}}_{\mathrm{c}}$ can be expressed like (4.1) with V^{eff} replaced by $V^{\mathrm{eff}}_{\mathrm{c}}$. Starting from definition (3.2), it follows that

$$\begin{aligned} U^{\text{eff}}(\bar{\varepsilon}_{ij},\bar{\varepsilon}^{\text{p}}_{ij}) = & \inf_{\varepsilon_{ij},\varepsilon^{\text{p}}_{ij}}\left\{\frac{1}{|D|}\left[\int_D\left(\frac{1}{2}(\varepsilon_{ij}-\varepsilon^{\text{p}}_{ij})L_{ijkl}(\varepsilon_{kl}-\varepsilon^{\text{p}}_{kl})+V_{\text{c}}(\varepsilon^{\text{p}}_{ij},\varepsilon^{\text{p}}_{ij,k})\right)\text{d}x\right.\right. \\ & +\int_D[V(\varepsilon^{\text{p}}_{ij},\varepsilon^{\text{p}}_{ij,k})-V_{\text{c}}(\varepsilon^{\text{p}}_{ij},\varepsilon^{\text{p}}_{ij,k})]\,\text{d}x \\ & \left.\left.+\int_{\Gamma_D}\phi_{\text{c}}(\varepsilon^{\text{p}}_{ij})\,\text{d}\Gamma+\int_{\Gamma_D}(\phi(\varepsilon^{\text{p}}_{ij})-\phi_{\text{c}}(\varepsilon^{\text{p}}_{ij})d\Gamma\right]\right\} \\ & \leqslant U^{\text{eff}}_{\text{c}}(\bar{\varepsilon}_{ij},\bar{\varepsilon}^{\text{p}}_{ij})+\frac{1}{|D|}\left[\int_D\max(V-V_{\text{c}})\,\text{d}x\right. \\ & \left.+\int_{\Gamma_D}\max(\phi-\phi_{\text{c}})\,\text{d}\Gamma\right], \end{aligned} \tag{4.11}$$

assuming that V and ϕ grow no faster than quadratically when their arguments are large, so that the maxima introduced here are finite. It follows, in the case of constant L, that

$$V^{\text{eff}}(\bar{\varepsilon}^{\text{p}}_{ij})\leqslant V^{\text{eff}}_{\text{c}}(\bar{\varepsilon}^{\text{p}}_{ij})+\frac{1}{|D|}\left[\int_D\max(V-V_{\text{c}})\,\text{d}x+\int_{\Gamma_D}\max(\phi-\phi_{\text{c}})\,\text{d}\Gamma\right]. \tag{4.12}$$

Optimising this inequality, for any chosen $\bar{\varepsilon}^{\text{p}}_{ij}$, with respect to the parameters in the comparison potentials generates a bound of the type first introduced by Ponte Castañeda (1991). No correspondingly elementary reasoning has lead to a refined lower bound for a composite with potentials with the type of growth postulated here (see Talbot and Willis, 1994a,b).

5. One-dimensional problems

Problems involving one spatial dimension may be realised, for example, by considering a bar under tension or compression, the properties of the bar varying only along its length, or by considering a laminate subjected to simple shear. In either case, there is just one relevant component of stress, displacement, total strain, plastic strain, and higher-order stress. It is appropriate therefore to drop all suffixes, and to let x denote the coordinate in which there is variation. The partial differential equations of Section 2 reduce to ordinary differential equations, derivable from the 1-D realisation of the variational principle (2.10). Likewise, the variational characterisation (3.2) of U^{eff} becomes, explicitly,

$$U^{\text{eff}}(\bar{\varepsilon},\bar{\varepsilon}^{\text{p}})=\inf_{\varepsilon,\varepsilon^{\text{p}}}\left\{\frac{1}{|D|}\left[\int_D\left(\frac{1}{2}L(\varepsilon-\varepsilon^{\text{p}})^2+V(\varepsilon^{\text{p}},\varepsilon^{\text{p}}_{,x})\right)\text{d}x+\sum_{x\in\Gamma_D}\phi(\varepsilon^{\text{p}})\right]\right\}. \tag{5.1}$$

The infimum with respect to ε is realised when $L(\varepsilon-\varepsilon^{\text{p}})=\bar{\sigma}$, constant. Hence, $\varepsilon-\varepsilon^{\text{p}}=L^{-1}\bar{\sigma}$ and so, by averaging, $\bar{\varepsilon}-\bar{\varepsilon}^{\text{p}}=(L_{\text{R}})^{-1}\bar{\sigma}$, where L_{R} is the

Reuss average

$$L_{\mathrm{R}} \equiv \left(\frac{1}{|D|}\int_D L^{-1}\,\mathrm{d}x\right)^{-1}. \tag{5.2}$$

It follows then that

$$U^{\mathrm{eff}}(\bar{\varepsilon},\bar{\varepsilon}^{\mathrm{p}}) = \tfrac{1}{2}L_{\mathrm{R}}(\bar{\varepsilon}-\bar{\varepsilon}^{\mathrm{p}})^2 + V^{\mathrm{eff}}(\bar{\varepsilon}^{\mathrm{p}}), \tag{5.3}$$

where

$$V^{\mathrm{eff}}(\bar{\varepsilon}^{\mathrm{p}}) = \inf_{\varepsilon^{\mathrm{p}}}\left\{\frac{1}{|D|}\left[\int_D V(\varepsilon^{\mathrm{p}},\varepsilon^{\mathrm{p}}_{,x})\,\mathrm{d}x + \sum_{x\in\Gamma_D}\phi(\varepsilon^{\mathrm{p}})\right]\right\}. \tag{5.4}$$

Result (5.4) is simpler than formula (4.4), which applies to any number of dimensions; it can be used even if the elastic constant L varies with x.

5.1. Periodic medium, linear response

As a first example, a single-phase medium with a linear response is considered; thus, V is assumed to be a quadratic function of both $\varepsilon^{\mathrm{p}},\varepsilon^{\mathrm{p}}_{,x}$

$$V(\varepsilon^{\mathrm{p}},\varepsilon^{\mathrm{p}}_{,x}) = \tfrac{1}{2}\beta[(\varepsilon^{\mathrm{p}})^2 + l^2(\varepsilon^{\mathrm{p}}_{,x})^2], \tag{5.5}$$

where β and l are constants.

If there were no interfaces, the solution of the infimum problem (5.4) would be $\varepsilon^{\mathrm{p}} = \bar{\varepsilon}^{\mathrm{p}}$, constant, and there would be no strain-gradient effect. Here, however, it is assumed that interfaces are distributed periodically with period $2L$. The interfacial energy term is taken to be a quadratic function of ε^{p} and hence the potential ϕ is given by

$$\phi(\varepsilon^{\mathrm{p}}) = \tfrac{1}{2}\alpha(\varepsilon^{\mathrm{p}})^2, \tag{5.6}$$

where α is a material parameter. For this, as for any similar problem for a periodic medium, it suffices to seek the infimum over plastic strain fields that are periodic with period $2L$. Various such examples were solved by Aifantis and Willis (2005). The governing equations are obtainable either directly from Eq. (5.4) or by specialising to one dimension the general equations (3.4)–(3.6). Explicitly, considering one period $(-L,L)$, with an interface situated at $x=0$, ε^{p} will be an even function of x and will satisfy, on the half-period $(0,L)$,

$$\begin{aligned}&\beta(\varepsilon^{\mathrm{p}} - l^2\varepsilon^{\mathrm{p}}_{,xx}) = \bar{\sigma}, \quad 0<x<L,\\ &\beta l^2\varepsilon^{\mathrm{p}}_{,x}(0) = \alpha\varepsilon^{\mathrm{p}}(0)/2, \quad \varepsilon^{\mathrm{p}}_{,x}(L) = 0.\end{aligned} \tag{5.7}$$

Strictly, the right-hand side of Eq. $(5.7)_1$ should be written $\sigma + s^*$, and s^* has to be chosen to deliver the correct value for $\bar{\varepsilon}^{\mathrm{p}}$. However, ultimately, to achieve the infimum in (3.1), $\bar{\varepsilon}^{\mathrm{p}}$ has to be such that $s^* = 0$, and σ is in any case constant and so equal to its mean value. The solution of system (5.7) is

$$\varepsilon^{\mathrm{p}}(x)=\frac{\overline{\sigma}}{\beta}\left[1-\frac{\cosh[(L-|x|)/l]}{\cosh(L/l)+(\beta l/\alpha)\sinh(L/l)}\right],\quad -L\leqslant x\leqslant L. \tag{5.8}$$

The simplest route to finding the effective potential V^{eff} is to average relation (5.8). This gives

$$\overline{\sigma}=\beta^{\mathrm{eff}}\overline{\varepsilon}^{\mathrm{p}}, \tag{5.9}$$

where

$$\beta^{\mathrm{eff}}=\beta\left\{\frac{1+(2\beta l/\alpha)\tanh(L/l)}{1+(2\beta l/\alpha-l/L)\tanh(L/l)}\right\}. \tag{5.10}$$

At the solution ($s^{*}=0$, as already assumed), the effective relations conform to the pattern of $(2.6)_2$ for non-strain-gradient material, and hence immediately

$$V^{\mathrm{eff}}(\overline{\varepsilon}^{\mathrm{p}})=\tfrac{1}{2}\beta^{\mathrm{eff}}(\overline{\varepsilon}^{\mathrm{p}})^2. \tag{5.11}$$

This same result can be obtained more laboriously by substituting Eq. (5.8) into Eq. (5.4), with $\overline{\sigma}=\beta^{\mathrm{eff}}\overline{\varepsilon}^{\mathrm{p}}$.

5.2. *Periodic linear medium, nonlinear interfacial response*

Next, the same linear hardening medium is considered but the periodically distributed interfaces are taken to respond according to the nonlinear potential

$$\phi(\varepsilon^{\mathrm{p}})=\gamma|\varepsilon^{\mathrm{p}}|. \tag{5.12}$$

This form of ϕ is not differentiable at $\varepsilon^{\mathrm{p}}=0$. The appropriate generalisation of the interface condition $(3.6)_2$ is $[\tau]\in\partial\phi(\varepsilon^{\mathrm{p}})$; that is,

$$\begin{aligned}[]
[\tau]&\in(-\gamma,\gamma)\quad \text{if } \varepsilon^{\mathrm{p}}=0,\\
&=\gamma\varepsilon^{\mathrm{p}}/|\varepsilon^{\mathrm{p}}|\quad \text{if } \varepsilon^{\mathrm{p}}\neq 0.
\end{aligned} \tag{5.13}$$

Physically, this says that the interfaces are impermeable to dislocations, and hence plastic strain cannot accumulate there, so long as the jump in the hyperstress, $[\tau]$, is smaller in magnitude than a critical value γ. The constant γ is a material parameter related to the tendency of dislocations to pile up at an interface until the applied stress reaches a level sufficient to generate a force on the leading dislocation large enough to drive it across (or else to activate a dislocation source on the interface). It will be seen below that the critical value γ of $|[\tau]|$ is first attained when the magnitude of the applied stress reaches a critical value σ_{c}. When the jump in τ reaches the critical value, the interface begins to deform plastically (i.e. the plastic strain there differs from zero). It then continues to deform (as long as $|\overline{\sigma}|>\sigma_{\mathrm{c}}$) in a perfectly plastic mode (in the sense that the condition $|[\tau]|=\gamma$ always holds true) such that plastic strain accumulates on both the grain boundary and the interior, through dislocation motion. Therefore, σ_{c} can be viewed as the interfacial yield stress. For definiteness in the equations to follow, $\overline{\sigma}$ is taken to be positive. The governing equations for ε^{p} are

$$\beta(\varepsilon^{\mathrm{p}} - l^2\varepsilon^{\mathrm{p}}_{,xx}) = \overline{\sigma}, \quad 0<x<L, \qquad \varepsilon^{\mathrm{p}}_{,x}(L) = 0 \tag{5.14}$$

(as previously), together with

$$\varepsilon^{\mathrm{p}}(0) = 0 \quad \text{so long as } \beta\varepsilon^{\mathrm{p}}_{,x}(0)<\gamma/2, \qquad \beta l^2\varepsilon^{\mathrm{p}}_{,x}(0) = \gamma/2 \quad \text{otherwise.}$$

These conditions define two linear problems, both easily solved to yield

$$\varepsilon^{\mathrm{p}}(x) = \begin{cases} \dfrac{\overline{\sigma}}{\beta}\left[1 - \dfrac{\cosh[(L-|x|)/l]}{\cosh(L/l)}\right], & \text{so long as } \overline{\sigma}<\sigma_{\mathrm{c}}, \\ \dfrac{\overline{\sigma}}{\beta} - \dfrac{\gamma\cosh[(L-|x|)/l]}{2\beta l\sinh(L/l)} & \text{otherwise } (\overline{\sigma}\geqslant\sigma_{\mathrm{c}}), \end{cases} \tag{5.16}$$

where the critical stress for interfacial yielding, σ_{c}, is given by

$$\sigma_{\mathrm{c}} = \frac{\gamma}{2l}\coth(L/l). \tag{5.17}$$

The corresponding relation between mean stress and mean plastic strain is obtained by averaging Eq. (5.16):

$$\overline{\sigma} = \begin{cases} \dfrac{\beta\overline{\varepsilon}^{\mathrm{p}}}{1-(l/L)\tanh(L/l)} & \text{if } |\overline{\varepsilon}^{\mathrm{p}}|<\varepsilon^{\mathrm{p}}_{\mathrm{c}}, \\ \beta\overline{\varepsilon}^{\mathrm{p}} + \dfrac{\gamma}{2L} & \text{otherwise,} \end{cases} \tag{5.18}$$

where

$$\varepsilon^{\mathrm{p}}_{\mathrm{c}} = \frac{\gamma}{2l\beta}\left\{\frac{1-(l/L)\tanh(L/l)}{\tanh(L/l)}\right\}. \tag{5.19}$$

The effective potential V^{eff} follows by integration:

$$V^{\mathrm{eff}}(\overline{\varepsilon}^{\mathrm{p}}) = \begin{cases} \dfrac{\beta(\overline{\varepsilon}^{\mathrm{p}})^2}{2[1-(l/L)\tanh(L/l)]} & \text{if } |\overline{\varepsilon}^{\mathrm{p}}|<\varepsilon^{\mathrm{p}}_{\mathrm{c}}, \\ \dfrac{\beta(\varepsilon^{\mathrm{p}}_{\mathrm{c}})^2}{2[1-(l/L)\tanh(L/l)]} + \dfrac{1}{2}\beta[(\overline{\varepsilon}^{\mathrm{p}})^2 - (\varepsilon^{\mathrm{p}}_{\mathrm{c}})^2] + \dfrac{\gamma}{2L}(|\overline{\varepsilon}^{\mathrm{p}}| - \varepsilon^{\mathrm{p}}_{\mathrm{c}}) & \text{if } |\overline{\varepsilon}^{\mathrm{p}}|\geqslant\varepsilon^{\mathrm{p}}_{\mathrm{c}}. \end{cases} \tag{5.20}$$

5.3. Use of comparison medium

An alternative approach for the problem of the preceding subsection is to employ the "comparison" method outlined in Section 4.2. Take the actual medium to be the one studied above, with interfacial potential ϕ given by Eq. (5.12), and employ the linear comparison medium with interfacial potential given by Eq. (5.6). The potential

V is the same for both the actual and the comparison medium. The inequality (4.12) reduces in this case to

$$V^{\text{eff}}(\bar{\varepsilon}^{\text{p}}) \leqslant \frac{1}{2}\beta^{\text{eff}}(\bar{\varepsilon}^{\text{p}})^2 + \frac{\gamma^2}{4L\alpha} \tag{5.21}$$

with β^{eff} given by Eq. (5.10). The best bound of this type, for any chosen $\bar{\varepsilon}^{\text{p}}$, is obtained by calculating the infimum with respect to α. The infimum is achieved either at the unique finite stationary point or by letting $\alpha \to \infty$. As $\alpha \to \infty$, the right-hand side of Eq. (5.21) has the asymptotic form

$$\frac{\beta}{2[1-(l/L)\tanh(L/l)]}\left\{1 - \frac{(2\beta l^2/L\alpha)\tanh^2(L/l)}{1-(l/L)\tanh(L/l)}\right\}(\bar{\varepsilon}^{\text{p}})^2 + \frac{\gamma^2}{4L\alpha}. \tag{5.22}$$

This expression decreases as α increases if $|\bar{\varepsilon}^{\text{p}}| < \varepsilon^{\text{p}}_{\text{c}}$; in this case, the best bound is obtained by letting $\alpha \to \infty$. If $|\bar{\varepsilon}^{\text{p}}| > \varepsilon^{\text{p}}_{\text{c}}$, the best bound is achieved at the stationary point. Completion of the calculation reproduces the exact result (5.20). The bound coincides with the exact solution because there was only a need to "match" the subgradient of the nonlinear potential ϕ at a single point.

6. Nonlinear material with periodic interfaces

This section addresses a problem in which a single-phase nonlinear medium contains a periodic array of interfaces, with period $2L$. The potential V of the medium is taken to be that employed by Fleck and Willis (2004):

$$V(\varepsilon^{\text{p}}, \varepsilon^{\text{p}}_{,x}) = \frac{\sigma_0 e_0}{n+1}\left(\frac{E_{\text{p}}}{e_0}\right)^{n+1}, \tag{6.1}$$

where $n < 1$ and

$$E_{\text{p}} = [(\varepsilon^{\text{p}})^2 + l^2(\varepsilon^{\text{p}}_{,x})^2]^{1/2}. \tag{6.2}$$

The interfacial potential is taken as that given by Eq. (5.12).

It is possible to compute the solution by solving the nonlinear ordinary differential equation, together with the boundary conditions that emerge by specialising equations (3.4)–(3.6). Explicitly, the differential equation is

$$\frac{1}{(E_{\text{p}})^{3/2}}\left\{\sigma_0 l^2\left(\frac{E_{\text{p}}}{e_0}\right)^n [nl^2(\varepsilon^{\text{p}}_{,x})^2\varepsilon^{\text{p}}_{,xx} + \varepsilon^{\text{p}}((n-1)(\varepsilon^{\text{p}}_{,x})^2 + \varepsilon^{\text{p}}_{,x}\varepsilon^{\text{p}}_{,xx})]\right\} - \frac{\sigma_0\varepsilon^{\text{p}}_{,x}}{e_0}(E_{\text{p}})^{n-1} = -\bar{\sigma}. \tag{6.3}$$

The boundary conditions are given by Eq. (5.13), with $[\tau] = 2\sigma_0 l^2(\varepsilon^{\text{p}}_{,x}/E_{\text{p}})(E_{\text{p}}/e_0)^n$, evaluated at $x = 0$. Fig. 1 gives plots of the effective stress–plastic strain response obtained from the computed solution[1] of the nonlinear differential equation (6.3),

[1]High accuracy was judged not to be necessary and the computation was performed with the aid of the program Mathematica.

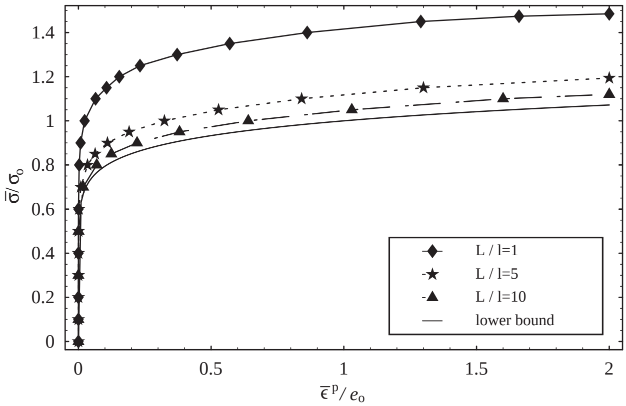

Fig. 1. Plots of normalised mean stress versus normalised mean plastic strain, for different values of L/l, for material with hardening exponent $n = 0.1$.

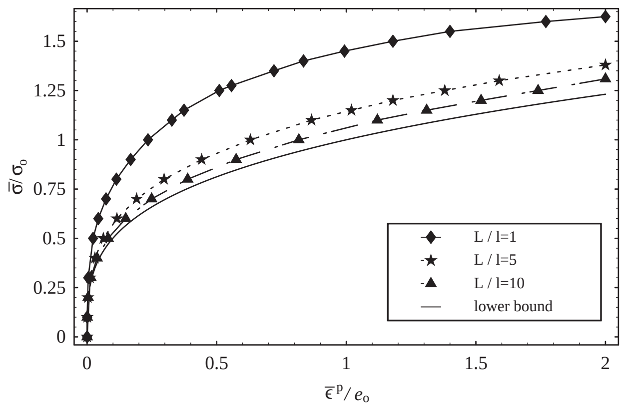

Fig. 2. Plots of normalised mean stress versus normalised mean plastic strain, for different values of L/l, for material with hardening exponent $n = 0.3$.

with $n = 0.1$, for a range of values of L/l. The plots are normalised, showing $\overline{\sigma}/\sigma_0$ versus $\bar{\varepsilon}^{\mathrm{p}}/e_0$, with $\gamma/(\sigma_0 l) = 2.2$.

Elementary upper and lower bounds for V^{eff}, V_V and V_{R} respectively, follow from Section 4.1. In this case,

$$V_{\mathrm{R}}(\bar{\varepsilon}^{\mathrm{p}}) \equiv \frac{\sigma_0 e_0}{n+1}\left(\frac{\bar{\varepsilon}^{\mathrm{p}}}{e_0}\right)^{n+1} \leqslant V^{\mathrm{eff}}(\bar{\varepsilon}^{\mathrm{p}}) \leqslant \frac{\sigma_0 e_0}{n+1}\left(\frac{\bar{\varepsilon}^{\mathrm{p}}}{e_0}\right)^{n+1} + \frac{\gamma|\bar{\varepsilon}^{\mathrm{p}}|}{2L} \equiv V_V(\bar{\varepsilon}^{\mathrm{p}}). \qquad (6.4)$$

The curve designated "lower bound" in Fig. 1 is obtained by differentiating V_{R}. It corresponds to the response of the material without interfaces and so provides the limiting case $L/l \to \infty$. Fig. 2 provides similar plots for a more strongly hardening material, with $n = 0.3$. For this, and for all subsequent plots, the value $\gamma/(\sigma_0 l) = 2.2$ was maintained. Figs. 1 and 2 are not directly comparable, being for different materials, but both show a trend of Hall–Petch type, with strength increasing as the "grain size" L decreases. For this simple single-medium case, the effect is entirely due to the interfacial potential.

A "refined" upper bound can be obtained by implementing the method of Section 4.2, taking the linear comparison medium to be that discussed in Section 5.1. The inequality (4.12) gives

$$V^{\mathrm{eff}}(\bar{\varepsilon}^{\mathrm{p}}) \leqslant \frac{1}{2}\beta^{\mathrm{eff}}(\bar{\varepsilon}^{\mathrm{p}})^2 + \frac{\sigma_0 e_0}{2}\left(\frac{1-n}{1+n}\right)\left(\frac{\sigma_0}{\beta e_0}\right)^{(1+n)/(1-n)} + \frac{\gamma^2}{4L\alpha}. \tag{6.5}$$

Optimising first with respect to α gives

$$V^{\mathrm{eff}}(\bar{\varepsilon}^{\mathrm{p}}) \leqslant V_0^{\mathrm{eff}}(\bar{\varepsilon}^{\mathrm{p}}) + \frac{\sigma_0 e_0}{2}\left(\frac{1-n}{1+n}\right)\left(\frac{\sigma_0}{\beta e_0}\right)^{(1+n)/(1-n)}, \tag{6.6}$$

where V_0^{eff} is the potential given by Eq. (5.20). The remaining optimisation, with respect to β, has to be performed numerically—at least, when $\bar{\varepsilon}^{\mathrm{p}}$ is large enough to require use of expression $(5.20)_2$.

Fig. 3 gives plots of $V^{\mathrm{eff}}/(\sigma_0 e_0)$ against $\bar{\varepsilon}^{\mathrm{p}}/e_0$, as deduced from the solution of the differential equation (here designated "exact"), together with the elementary bounds (6.4) and the "refined" bound obtained by optimising (6.6), all for the case $L/l = 5$, $n = 0.3$. The "refined" bound is very close to the "exact" solution. The same trend is shown in Fig. 4, which gives the corresponding approximations to the (normalised) effective stress–plastic strain relation, $\bar{\sigma} = \mathrm{d}V^{\mathrm{eff}}/\mathrm{d}\bar{\varepsilon}^{\mathrm{p}}$.

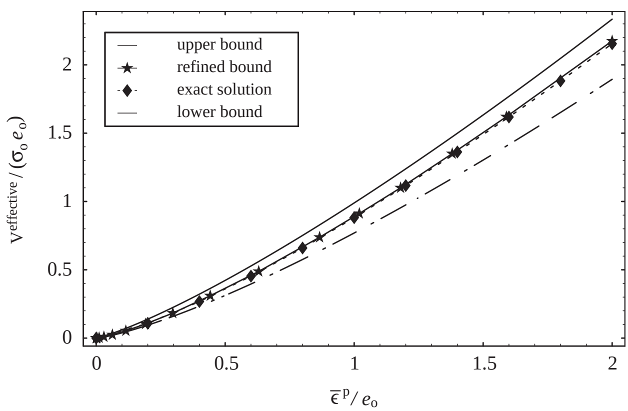

Fig. 3. Comparison of "exact solution" for $V^{\mathrm{eff}}(\bar{\varepsilon}^{\mathrm{p}})$ with bounds, when $L/l = 5$, for material with hardening exponent $n = 0.3$.

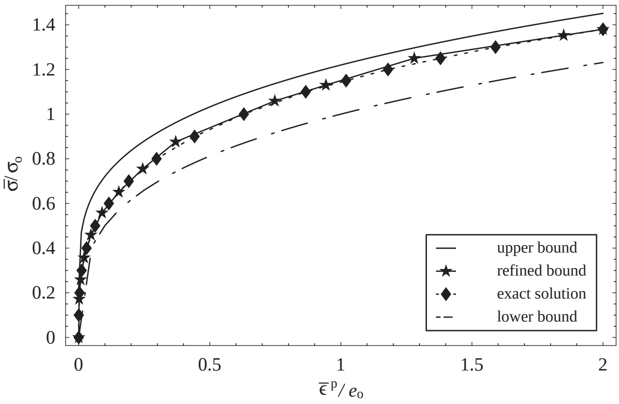

Fig. 4. Comparison of normalised mean stress versus normalised mean plastic strain, calculated "exactly" or estimated from bounds, when $L/l = 5$, for material with hardening exponent $n = 0.3$.

7. Simple examples for a random medium

All of the examples discussed so far could be approached directly by solving the governing differential equations. To that extent, the variational approach is not essential. It comes into its own when random media are considered: the problems cannot be solved exactly but the variational structure provides a framework for the development of systematic approximations. This is illustrated here by considering analogues of the problems addressed in the preceding sections. A single 1-D medium is considered. It is rendered heterogeneous by the presence of interfaces, but now the interfaces are taken to be distributed according to a Poisson process of intensity $\lambda = 1/(2L)$.

The "linear comparison medium" approach will be adopted. The first step, therefore, is to obtain an expression for the effective potential of a medium with properties as given in Section 5.1, except that the interfaces are randomly distributed. The exact effective constant β^{eff} cannot be found but an expression which takes account of the pairwise statistics of the interfaces through use of the "quasicrystalline approximation" of Lax (1952) is developed in the appendix. The result is

$$\beta^{\text{eff}} = \beta\left\{1 + \frac{l/L}{1 + (2l\beta/\alpha)}\right\}. \tag{7.1}$$

Equality is indicated here for convenience but it is emphasised that Eq. (7.1) represents an approximation which is, in fact, a lower bound; the proof will be given in a more general context elsewhere.

7.1. Linear medium, nonlinear interfacial response

As in Sections 5.2 and 5.3, let the medium be linear, with constant β, but take the interface potential to be (5.12). The "comparison" method follows the pattern described in Section 5.3. It requires the optimisation of inequality (5.22), now with β^{eff} given by Eq. (7.1). As $\alpha \to \infty$, the right-hand side of Eq. (5.22) (with Eq. (7.1)) takes the asymptotic form

$$\beta\left\{1+\frac{l}{L}-\frac{2\beta l^2}{L\alpha}\right\}(\bar{\varepsilon}^{\mathrm{p}})^2+\frac{\gamma^2}{4L\alpha} \tag{7.2}$$

and the supremum is approached as $\alpha \to \infty$ if $|\bar{\varepsilon}^{\mathrm{p}}|<\varepsilon_{\mathrm{c}}^{\mathrm{p}}$, where

$$\varepsilon_{\mathrm{c}}^{\mathrm{p}}=\frac{\gamma}{2l\beta}. \tag{7.3}$$

Otherwise, the supremum is attained at the stationary point. Completion of the details gives

$$V_0^{\mathrm{eff}}(\bar{\varepsilon}^{\mathrm{p}})=\begin{cases}\frac{1}{2}\beta\left(1+\frac{l}{L}\right)(\bar{\varepsilon}^{\mathrm{p}})^2 & \text{if } |\bar{\varepsilon}^{\mathrm{p}}|<\varepsilon_{\mathrm{c}}^{\mathrm{p}},\\ \frac{1}{2}\beta\left(1+\frac{l}{L}\right)(\varepsilon_{\mathrm{c}}^{\mathrm{p}})^2+\frac{1}{2}\beta\left((\bar{\varepsilon}^{\mathrm{p}})^2-(\varepsilon_{\mathrm{c}}^{\mathrm{p}})^2\right)+\frac{\gamma}{2L}\left(|\bar{\varepsilon}^{\mathrm{p}}|-\varepsilon_{\mathrm{c}}^{\mathrm{p}}\right) & \text{if } |\bar{\varepsilon}^{\mathrm{p}}|\geqslant\varepsilon_{\mathrm{c}}^{\mathrm{p}}.\end{cases} \tag{7.4}$$

7.2. Nonlinear medium, nonlinear interfacial response

Now consider the analogue of the problem discussed in Section 6: the response of the medium is defined by the Fleck–Willis potential (6.1) while the potential of the interfaces remains (5.12). As in Section 6, the optimisation over the parameters α, β can be done sequentially. First optimising with respect to α generates expression (6.6), except that now V_0^{eff} is the potential given by Eq. (7.4).

Sample results are shown in Figs. 5 and 6. There is no "exact" solution but the procedure based on the use of the linear "comparison" medium yields

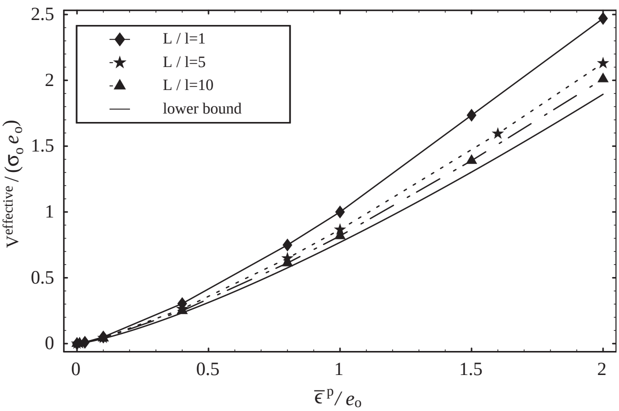

Fig. 5. Plots of normalised V^{eff} versus normalised mean plastic strain, for material with randomly placed interfaces with mean spacing L and hardening exponent $n=0.3$, for different values of L/l.

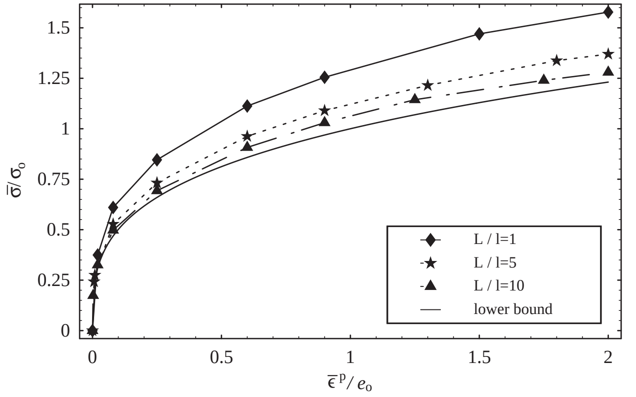

Fig. 6. Plots of normalised mean stress versus normalised mean plastic strain, for material with randomly placed interfaces with mean spacing L and hardening exponent $n = 0.3$, for different values of L/l.

approximations for the effective potential V^{eff}, and hence by differentiation to corresponding approximations for the effective stress–plastic strain relation. Fig. 5 shows plots of $V^{\mathrm{eff}}/(\sigma_0 e_0)$ versus $\bar{\varepsilon}^{\mathrm{p}}/e_0$ calculated by this procedure, for $n = 0.3$ and $\gamma/(\sigma_0 l) = 2.2$, for a range of values of L/l. The "lower bound" limit ($L/l \to \infty$) is the same as for the periodic case. Fig. 6 gives the corresponding plots for $\bar{\sigma}/\sigma_0$ versus $\bar{\varepsilon}^{\mathrm{p}}/e_0$. This figure is directly comparable to Fig. 2, the only difference being the distribution of the interfaces. Fig. 2 corresponds to "perfectly ordered" interfaces, with exactly uniform spacing $2L$, while Fig. 6 corresponds to "perfectly disordered" interfaces, with mean spacing $2L$. The "disorder" slightly reduces the sensitivity to scale. However, the trends are the same and the numbers are similar. Thus, the scale effects that are shown would appear to be robust.

8. Concluding remarks

The distinctive feature of this work is the recognition that the assumption of strain-gradient-sensitive constitutive behaviour carries with it the opportunity to incorporate physical properties of interfaces through the introduction of an interfacial potential. There is a natural coupling between the physics of the constituent media and the physics of the interfaces: only interfacial conditions which are compatible with mathematically consistent boundary or interfacial jump conditions can be imposed. The examples that have been presented here have been based on the Fleck and Willis (2004) structure for strain-gradient plasticity. In employing plastic strain as internal variable it leads to a relatively simple and convenient formulation for applications but it precludes the explicit consideration of dislocations and their motion. A desirable future development would be to obtain a corresponding formulation based on more detailed gradient-sensitive models. It is remarked, however, that many models will collapse down to the form of the present one, in the context of the 1-D problems considered here.

The examples that were presented display a sensitivity to length scale only through the presence of the interfacial potential: in its absence, the material would support uniform fields and hence the constitutive gradient-dependence would have no influence. Other problems, in which the material itself is heterogeneous, would display scale-dependence, as demonstrated, for instance, in the work of Fleck and Willis (2004). In such cases, the interfacial potential will lead to a more pronounced scale-dependence, no longer limited by the "Taylor upper bound".

Calculation of the effective response of any medium with periodic microstructure requires the solution of a problem for a periodic cell, and this can be done just as easily with an interfacial potential as without. Problems for a random medium cannot be solved exactly and it is for such problems that the variational formulation plays an essential role. Introduction of an interfacial potential induces the need to define surface–surface and surface–volume correlations that are consistent with the usual two-point (volume–volume) probabilities. A more complete study of such problems will be reported elsewhere.

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Appendix A. Approximation for a linear medium with randomly placed interfaces

The medium under consideration has potential (5.5) and interfacial potential (5.6), as in Section 5.1. The difference is that now the interfaces are distributed randomly, according to some stationary random process. One way to formulate the problem is to note that the differential equation $(5.7)_1$ (now applying for all x except interface points), together with the jump conditions

$$\beta l^2 [\varepsilon^{\mathrm{p}}_{,x}] = t \quad \text{across any interface} \tag{A.1}$$

can equivalently be stated

$$\beta(\varepsilon^{\mathrm{p}} - l^2 \varepsilon^{\mathrm{p}}_{,xx}) + \sum_{x' \in \Gamma_D} t(x')\delta(x - x') = \overline{\sigma}, \tag{A.2}$$

where

$$t(x') = \alpha \varepsilon^{\mathrm{p}}(x'). \tag{A.3}$$

Introduce the Green's function

$$G(x-x')=\frac{\exp(-|x-x'|/l)}{2l}. \tag{A.4}$$

This satisfies the differential equation

$$l^2\frac{d^2G}{dx^2}-G+\delta(x-x')=0. \tag{A.5}$$

Hence, the solution[2] of the differential equation (A.2) can be expressed in the form

$$\varepsilon^{\mathrm{p}}(x)=\frac{\overline{\sigma}}{\beta}-\frac{1}{\beta}\sum_{x'\in\Gamma_D}G(x-x')t(x'). \tag{A.6}$$

Evaluation of $\varepsilon^{\mathrm{p}}(x)$ for any $x\in\Gamma_D$ yields, together with relation (A.3), the system of equations

$$\varepsilon^{\mathrm{p}}(x)=\frac{\overline{\sigma}}{\beta}-\frac{\alpha}{\beta}\sum_{x'\in\Gamma_D}G(x-x')\varepsilon^{\mathrm{p}}(x'),\quad x\in\Gamma_D. \tag{A.7}$$

In the case of a periodic medium, $\varepsilon^{\mathrm{p}}(x)$ takes the same value ($\varepsilon^{\mathrm{p}}(0)$ say) at all interface points. Then, system (A.7) reduces to a single equation for $\varepsilon^{\mathrm{p}}(0)$. The sum over the periodically distributed interface points is easily calculated and the solution given in Section 5.1 can be reproduced.

For a random medium, however, what is required is an expression for the ensemble mean $\langle\varepsilon^{\mathrm{p}}\rangle$ which, for a statistically uniform medium, will coincide with the spatial mean of $\varepsilon^{\mathrm{p}}(x)$, in the "homogenisation limit" that $D/l\to\infty$, where D is the dimension of the sample. It follows by ensemble averaging equation (A.6) that

$$\langle\varepsilon^{\mathrm{p}}(x)\rangle=\frac{\overline{\sigma}}{\beta}-\frac{\alpha}{\beta}\int_{-\infty}^{\infty}G(x-x')p(x')\langle\varepsilon^{\mathrm{p}}(x')\rangle_{x'}\,\mathrm{d}x', \tag{A.8}$$

where $\langle\varepsilon^{\mathrm{p}}(x')\rangle_{x'}$ is the ensemble mean of $\varepsilon^{\mathrm{p}}(x')$, *conditional* on the presence of an interface point at x', and $p(x')$ is the probability density (assumed uniform, and so independent of x') for finding an interface point at x'. Now attempt to find an equation for $\langle\varepsilon^{\mathrm{p}}(x')\rangle_{x'}$ by conditionally averaging Eq. (A.6):

$$\langle\varepsilon^{\mathrm{p}}(x)\rangle_x=\frac{\overline{\sigma}}{\beta}-\frac{\alpha}{\beta}\int_{-\infty}^{\infty}G(x-x')p(x'|x)\langle\varepsilon^{\mathrm{p}}(x')\rangle_{x',x}\,\mathrm{d}x'. \tag{A.9}$$

Here, $p(x'|x)$ is the probability density for finding an interface at x', *conditional* on the presence of an interface point at x, and $\langle\varepsilon^{\mathrm{p}}(x')\rangle_{x',x}$ is the ensemble mean of $\varepsilon^{\mathrm{p}}(x')$, conditional on the presence of interfaces at x' and x. Evidently, following this course produces a hierarchy of equations for conditional means of ε^{p}. A simple expedient is to close the hierarchy by making the "quasicrystalline approximation" (QCA)

$$\langle\varepsilon^{\mathrm{p}}(x')\rangle_{x',x}=\langle\varepsilon^{\mathrm{p}}(x')\rangle_{x'}, \tag{A.10}$$

[2]This solution disregards end conditions which are not significant for the "effective medium" problem.

first introduced by Lax (1952), so-called because it becomes exact in the special case of a periodic medium. For a statistically uniform medium, $p(x'|x)$ is a function just of $(x'-x)$ and Eq. (A.9), together with the QCA (A.10), delivers a constant value for the conditional mean $\langle \varepsilon^{\mathrm{p}}(x')\rangle_{x'}$.

It is possible to eliminate $\overline{\sigma}$ between Eqs. (A.8) and (A.9) to yield together with the QCA,

$$\langle \varepsilon^{\mathrm{p}}(x)\rangle_x = \overline{\varepsilon}^{\mathrm{p}} - \frac{\alpha}{\beta}\int_{-\infty}^{\infty} G(x-x')(p(x'|0)-\lambda)\,\mathrm{d}x'\langle \varepsilon^{\mathrm{p}}(x)\rangle_x, \tag{A.11}$$

having written $p(x')=\lambda$, constant, equal to the number density of the interfaces, $\langle \varepsilon^{\mathrm{p}}(x)\rangle = \overline{\varepsilon}^{\mathrm{p}}$, and having exploited the translation invariance. The required solution (subject to the QCA) is thus

$$\langle \varepsilon^{\mathrm{p}}(x)\rangle_x = \frac{\overline{\varepsilon}^{\mathrm{p}}}{1+(\alpha/2l\beta)\int_{-\infty}^{\infty} \mathrm{e}^{-|x'|/l}(p(x'|0)-\lambda)\,\mathrm{d}x'}. \tag{A.12}$$

It follows by performing the elementary integration in (A.8) (with $p(x')=\lambda$ and $\left\langle \varepsilon^{\mathrm{p}}(x')\right\rangle_{x',x} = \left\langle \varepsilon^{\mathrm{p}}(x')\right\rangle_{x'}$, constant) that

$$\overline{\varepsilon}^{\mathrm{p}} = \frac{\overline{\sigma}}{\beta} - \frac{\alpha}{\beta}\lambda\langle \varepsilon^{\mathrm{p}}(x)\rangle_x. \tag{A.13}$$

Together with Eq. (A.12), this gives the effective stress–plastic strain relation

$$\overline{\sigma} = \beta^{\mathrm{eff}}\overline{\varepsilon}^{\mathrm{p}}, \tag{A.14}$$

where

$$\beta^{\mathrm{eff}} = \beta\left\{1 + \frac{\lambda\alpha/\beta}{1+(\alpha/2l\beta)\int_{-\infty}^{\infty} e^{-|x'|/l}(p(x'|0)-\lambda)\,\mathrm{d}x'}\right\}. \tag{A.15}$$

Specialise now to the case of interfaces generated by a Poisson process of intensity λ. Since interface points are placed independently, it follows that

$$p(x'|0) = \delta(x') + \lambda \tag{A.16}$$

(the delta function is present because it is *given* that there is an interface at 0). The integral in formula (A.15) reduces to 1, and this results in Eq. (7.1), upon setting $\lambda = 1/(2L)$.

It can be shown, in fact, that formula (A.15) provides a *lower bound* for β^{eff}, but this will be demonstrated elsewhere, in the context of a more comprehensive study of random media.

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