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NONLINEAR COMPOSITES AND MICROSTRUCTURE EVOLUTION

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Abstract Recently developed methods for estimating the effective behavior of nonlinear composites are reviewed. The methods follow from variational principles expressing the effective behavior of the given nonlinear composites in terms of the behavior of suitably chosen “linear comparison” composites. These methods allow the use of classical bounds and estimates (e.g. Hashin-Shtrikman, effective medium approximations) for linear materials to generate corresponding information for nonlinear ones. Comparisons are made with numerical simulations for metal-matrix composites, showing that the new methods are significantly more accurate than earlier ones, especially at high nonlinearity and heterogeneity contrast. The methods can be extended to incorporate evolution of the microstructure and its influence on the effective response under finite-strain conditions. An application to a forming process involving a porous metal is considered for illustrative purposes.

1. INTRODUCTION

In the context of linear elasticity, rigorous and reliable methods have been available for quite some time to estimate the effective or overall behavior of heterogeneous materials. These so-called homogenization methods include the variational methods of Hashin and Shtrikman (1962) and Beran (1965), both of which are particularly well suited to composites with *particulate* random microstructures. There is also the self-consistent approximation, which is known to be fairly accurate for polycrystals and other materials with *granular* microstructures. For a review, see e.g. Willis (1981).

For heterogeneous materials with *nonlinear* (e.g. plastic, viscoplastic) properties, rigorous methods have not been available until fairly recently, even though efforts along these lines have been going on for a long time, particularly in the context of ductile polycrystals. Following an extension of the Hashin-Shtrikman (HS) variational principles by Willis (1983), the first bounds of the HS type for nonlinear composites were derived by Talbot and Willis (1985). A more general approach consisting in the use of an optimally chosen “linear comparison composite” was proposed by Ponte Castañeda (1991), and, independently for the special case of power-law materials, by Suquet (1993). This approach not only is capable of delivering bounds of the HS type for nonlinear composites, but also can be used to generate bounds and estimates of other types, by making use of the corresponding bounds and estimates for the linear comparison composite. More recently, Ponte Castañeda (1996a) proposed an alternative approach making use of a more sophisticated linear comparison composite, which while not yielding bounds, appears to give more accurate results. In particular, this method gives the only general homogenization estimates to date capable of reproducing exactly to second order in the contrast the asymptotic expansions of Suquet and Ponte Castañeda (1993).

While the idea of using linear composites to estimate the effective behavior of nonlinear ones is quite old, the key feature in these novel linear comparison methods is the use of rigorous variational principles to determine the best possible choice of the linear comparison composite of a given type. Within the context of the “secant” approximation, first used by Chu and Hashin (1971), it follows from the work of Suquet (1995) (and, independently, Hu (1996)) that the optimal choice is that made in the variational method of Ponte Castañeda (1991), i.e. the secant moduli of the phases evaluated at the second moments of the relevant fields in the phases, and *not* at the phase averages, or first moments, as had been done previously in the classical secant approaches. Alternatively, within the context of “tangent”-type approximations, first used by Hill (1965) in his popular incremental method, the work of Ponte Castañeda and Willis (1999) shows that the optimal choice is, in some restricted sense, that made in the second-order procedure of Ponte Castañeda (1996a), i.e. the tangent moduli of the phases evaluated at the phase averages of the relevant fields in a more general *thermoelastic* comparison composite.

In this short review paper, we attempt to summarize these recent developments, focusing on applications and on comparisons with recent numerical simulations (Moulinec and Suquet (1998), Michel et al. (1999), Michel et al. (2000)). For more detailed reviews, concentrating on the

more theoretical aspects, the reader is referred to Ponte Castañeda and Suquet (1998) and Willis (2000).

2. EFFECTIVE BEHAVIOR

The assumption is made that the material is composed of N different phases, which are distributed randomly in a specimen occupying a volume Ω at a length scale that is much smaller than the size of the specimen and the scale of variation of the loading conditions. The constitutive behavior of the nonlinear phases will be characterized by convex energy functions $w^{(r)}$ ($r = 1, \dots, N$), such that the local stress-strain relation (Fig. 1(a)) is defined by

$$\sigma = \frac{\partial w}{\partial \epsilon}(\mathbf{x}, \epsilon), \quad w(\mathbf{x}, \epsilon) = \sum_{r=1}^N \chi^{(r)}(\mathbf{x}) w^{(r)}(\epsilon), \quad (1)$$

where the function $\chi^{(r)}$ is equal to 1 if the position vector \mathbf{x} is inside phase r (i.e. $\mathbf{x} \in \Omega^{(r)}$) and zero otherwise.

The relations (1) can be used to describe several constitutive models, including deformation theory of plasticity, in which case ϵ and σ

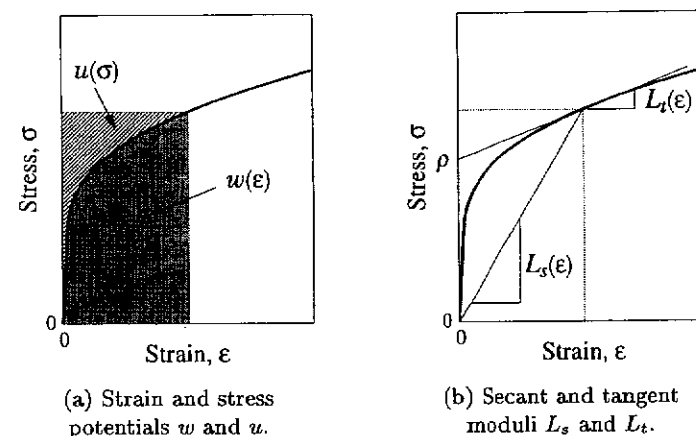


Figure 1 Constitutive relation.

are identified with the infinitesimal strain and stress, respectively. The relation applies equally well to viscoplastic materials, in which case the associated deformations are finite and ϵ and σ are associated with the Eulerian strain rate and Cauchy stress, respectively. A commonly used

form for $w^{(r)}$ is the isotropic, incompressible power-law form

$$w^{(r)}(\varepsilon) = \frac{\varepsilon_0 \sigma_0^{(r)}}{m+1} \left(\frac{\varepsilon_e}{\varepsilon_0} \right)^{m+1}, \quad (2)$$

where m is the rate-sensitivity parameter, such that $0 \leq m \leq 1$, $\sigma_0^{(r)}$ is the flow stress, ε_0 is a reference strain rate, and ε_e is the equivalent von Mises strain or strain rate.

Making use of the symbols $\langle \cdot \rangle$ and $\langle \cdot \rangle^{(r)}$ to denote volume averages over the composite (Ω) and over phase r ($\Omega^{(r)}$), respectively, we determine the effective behavior of the composite by the *effective energy function*

$$\widetilde{W}(\bar{\varepsilon}) = \inf_{\varepsilon \in \mathcal{K}} \langle w(\mathbf{x}, \varepsilon) \rangle = \inf_{\varepsilon \in \mathcal{K}} \sum_{r=1}^N c^{(r)} \langle w^{(r)}(\varepsilon) \rangle^{(r)}, \quad (3)$$

where the scalars $c^{(r)} = \langle \chi^{(r)} \rangle$ denote the volume fractions of the given phases and \mathcal{K} denotes the set of kinematically admissible strains ε , such that there is \mathbf{v} with $\varepsilon = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$ in Ω , $\mathbf{v} = \bar{\varepsilon} \mathbf{x}$ on $\partial\Omega$. Thus, \widetilde{W} physically corresponds to the energy stored in the composite when subjected to an affine displacement on the boundary with prescribed average strain $\bar{\varepsilon} = \langle \varepsilon \rangle$. It can be shown (Hill (1963)) that the *average stress* $\bar{\sigma} = \langle \sigma \rangle$ is then related to the average strain $\bar{\varepsilon}$ via

$$\bar{\sigma} = \frac{\partial \widetilde{W}}{\partial \bar{\varepsilon}}. \quad (4)$$

3. HOMOGENIZATION VIA LINEAR COMPARISON COMPOSITES

In this section, a brief introduction is given to the “linear comparison composite” methods. A linear composite is introduced with potential

$$w_0(\mathbf{x}, \varepsilon) = \frac{1}{2} \varepsilon \cdot \mathbf{L}_0(\mathbf{x}) \varepsilon, \quad \mathbf{L}_0(\mathbf{x}) = \sum_{r=1}^N \chi^{(r)}(\mathbf{x}) \mathbf{L}_0^{(r)}, \quad (5)$$

where the $\mathbf{L}_0^{(r)}$ are symmetric, positive definite, constant tensors.

Following Ponte Castañeda (1996b), we make use of the basic result that

$$\inf_{x \in A} \{f(x) + g(x)\} \geq \inf_{x \in A} \{f(x)\} + \inf_{x \in A} \{g(x)\}, \quad (6)$$

where the assumption has been made that the functions (or functionals) f and g are bounded below within the set A .

Noting that under the hypotheses associated with expression (2) the function $(w_0 - w)$ is bounded below, and applying the result (6) to the function $w_0 = w + (w_0 - w)$, we find that

$$\inf_{\varepsilon \in \mathcal{K}} \langle w_0(\mathbf{x}, \varepsilon) \rangle \geq \inf_{\varepsilon \in \mathcal{K}} \langle w(\mathbf{x}, \varepsilon) \rangle + \inf_{\varepsilon \in \mathcal{K}} \langle w_0(\mathbf{x}, \varepsilon) - w(\mathbf{x}, \varepsilon) \rangle, \quad (7)$$

and therefore that

$$\widetilde{W}(\bar{\varepsilon}) \leq \widetilde{W}_0(\bar{\varepsilon}) - \inf_{\varepsilon \in \mathcal{K}} \langle w_0(\mathbf{x}, \varepsilon) - w(\mathbf{x}, \varepsilon) \rangle, \quad (8)$$

where \widetilde{W}_0 is the effective potential associated with the linear elastic comparison composite with local potential given by (5):

$$\widetilde{W}_0(\bar{\varepsilon}) = \inf_{\varepsilon \in \mathcal{K}} \langle w_0(\mathbf{x}, \varepsilon) \rangle = \inf_{\varepsilon \in \mathcal{K}} \frac{1}{2} \sum_{r=1}^N c^{(r)} \langle \varepsilon \cdot \mathbf{L}_0^{(r)} \varepsilon \rangle^{(r)} = \frac{1}{2} \bar{\varepsilon} \cdot \tilde{\mathbf{L}}_0 \bar{\varepsilon}. \quad (9)$$

Here $\tilde{\mathbf{L}}_0$ is the effective modulus of the linear comparison composite.

Next, relaxing the constraint in the second term on the right of expression (8), we arrive at

$$\widetilde{W}(\bar{\varepsilon}) \leq \widetilde{W}_0(\bar{\varepsilon}) - \inf_{\varepsilon} \langle w_0(\mathbf{x}, \varepsilon) - w(\mathbf{x}, \varepsilon) \rangle. \quad (10)$$

Observing that this result must hold for any choice of the tensors $\mathbf{L}_0^{(r)}$, and bringing the infimum over ε inside of the averages, we find that

$$\widetilde{W}(\bar{\varepsilon}) \leq \inf_{\mathbf{L}_0^{(r)} > 0} \left\{ \widetilde{W}_0(\bar{\varepsilon}) - \sum_{r=1}^N c^{(r)} \inf_{\varepsilon^{(r)}} \left[w_0^{(r)}(\varepsilon^{(r)}) - w^{(r)}(\varepsilon^{(r)}) \right] \right\}. \quad (11)$$

It is noted that if the phases of the nonlinear composite are isotropic, the optimal choice of the comparison moduli $\mathbf{L}_0^{(r)}$ is also isotropic with bulk and shear moduli $\kappa_0^{(r)}$ and $\mu_0^{(r)}$, respectively.

Expression (11) is the bound first proposed by Ponte Castañeda (1991) in the context of nonlinear composites with general isotropic phases. A generalization for polycrystals was given by deBotton and Ponte Castañeda (1995). When it is used in conjunction with the upper bound of Hashin and Shtrikman (1963) for $\tilde{\mathbf{L}}_0$, the bounds of Talbot and Willis (1985) are recovered. However, there are pathological cases (not including the standard models of plasticity) for which the bounds generated by the Talbot–Willis procedure are superior (see Willis (1992); Talbot and Willis (1992)). On the other hand, the result (11) can be used together with any other bound (e.g. three-point bounds) or estimate (e.g. the

self-consistent estimates) for linear composites to generate corresponding estimates for nonlinear composites. For example, Ponte Castañeda (1992) used this procedure to compute three-point bounds. In addition, for the special case of power-law composites, an alternative, but equivalent, form has been given by Suquet (1993) using Hölder-type inequalities. The result is given by

$$\widetilde{W}(\bar{\epsilon}) \leq \inf_{\mu_0^{(r)} > 0} \left\{ \frac{\widetilde{W}_0(\bar{\epsilon})^{\frac{m+1}{2}}}{(m+1)\epsilon_0^m} \left[\sum_{r=1}^N c^{(r)} \left(\frac{3\mu_0^{(r)}}{2(\sigma_0^{(r)})^{\frac{2}{m+1}}} \right)^{\frac{m+1}{m-1}} \right]^{\frac{1-m}{2}} \right\}. \quad (12)$$

The effective constitutive relation for the nonlinear composite is obtained by making use of expression (11) for \widetilde{W} in expression (4) and enforcing the optimality condition in the variables $L_0^{(r)}$ to obtain

$$\bar{\sigma} = \widetilde{L}_0 \bar{\epsilon}. \quad (13)$$

This means that the effective constitutive relation for the nonlinear composite is precisely the same as that of the linear comparison composite, where the local properties of the linear comparison composite are determined as the solution of the procedure (11) for the optimized variables $\hat{L}_0^{(r)}$. Clearly, since these variables depend on the applied strain $\bar{\epsilon}$, the above relation is nonlinear in this variable, as expected. It is emphasized, however, that the microstructure of the linear comparison composite is identical to that of the nonlinear composite.

Finally, it is noted that the optimal choice of the variables $L_0^{(r)}$ can be given an interpretation in terms of the second moment of the strain field in the linear comparison composite. Full details about this derivation can be found in Suquet (1995), Suquet (1997), Ponte Castañeda and Suquet (1998); therefore, we limit ourselves here to simple heuristic arguments when the phases are isotropic.

The condition for the optimal choice of the variables $\epsilon^{(r)}$ in the inner infimum problem in (11) is given by

$$\frac{\partial w^{(r)}}{\partial \epsilon}(\hat{\epsilon}^{(r)}) = L_0^{(r)} \hat{\epsilon}^{(r)}, \quad (14)$$

which physically means that $L_0^{(r)}$ should be chosen to be the *secant* modulus tensor $L_s^{(r)}$ of nonlinear phase r (Fig. 1(b)). Assuming stationarity with respect to $L_0^{(r)}$, we generate the condition for the optimal choice of these variables by substituting the expression (9) for \widetilde{W}_0 in (11) to obtain

$$\hat{\epsilon}^{(r)} \otimes \hat{\epsilon}^{(r)} = \langle \epsilon \otimes \epsilon \rangle^{(r)}. \quad (15)$$

In other words, the modulus $L_0^{(r)}$ of phase r in the linear comparison composite is the nonlinear secant modulus evaluated at some "effective" strain $\hat{\epsilon}^{(r)}$ defined through relation (15), where the right-hand side is the second-order moment of the strain field over phase r of the linear comparison composite. It is emphasized that the expression (15) may not be satisfied in general. However, Suquet (1995) has remarked that, for the case of isotropic phases, this tensorial relation is not needed and that the optimal linear comparison composite can be defined using the second moment of the von Mises strain $\langle \epsilon_e^2 \rangle^{(r)}$. The more general case was considered in Ponte Castañeda and Suquet (1998) by making use of a suitable extension of the above ideas.

The important point to retain here is the following. As mentioned earlier, many attempts have been made to estimate the effective behavior of nonlinear composites in terms of the effective behavior of linear comparison composites—in particular, making use of secant-type approximations. However, because the strain field in the composite is highly nonuniform, it is not obvious what strain to use in the evaluation of the secant moduli for the phases of the linear comparison composite. In the past, ad hoc prescriptions have been tried, mostly making use of the average, or first moment, of the strain field in the phases of the composite. Expression (11) shows that the best choice—within the context of a rigorous variational principle—is the second moment of the strain field over the phases. As will be seen in the next section, this approach gives much better results than the classical schemes. It should be noted that Buryachenko and Lipanov (1989) were apparently to be the first to use second-moment type quantities in the context of their "multi-particle effective field scheme."

However, as already noted in the Introduction, the estimates (11) are not able to recover the perturbation estimates of Suquet and Ponte Castañeda (1993) for weakly inhomogeneous nonlinear materials, which are exact to second order in the heterogeneity contrast. This is in contrast with the Hashin-Shtrikman and self-consistent estimates for linear composites, which are known to be exact to second-order in the contrast. A homogenization method that has the capability to recover small-contrast results exactly to second order in the contrast was introduced recently by Ponte Castañeda (1996a). A full derivation of this result cannot be given here, but the result can be stated succinctly as

$$\widetilde{W}(\bar{\epsilon}) = \sum_{r=1}^N c^{(r)} \left\{ w^{(r)}(\bar{\epsilon}^{(r)}) + \frac{1}{2} \rho^{(r)} \cdot (\bar{\epsilon} - \bar{\epsilon}^{(r)}) \right\}, \quad (16)$$

where $\rho^{(r)} = \partial w^{(r)} / \partial \varepsilon(\varepsilon^{(r)})$, and $\bar{\varepsilon}^{(r)} = \langle \varepsilon \rangle^{(r)}$ is the average of the strain field over phase r in a linear thermoelastic composite with phase r defined by the constitutive relation

$$\sigma = \rho^{(r)} + \mathbf{L}_0^{(r)} (\varepsilon - \varepsilon^{(r)}), \quad (17)$$

where the modulus tensor $\mathbf{L}_0^{(r)}$ is defined by

$$\mathbf{L}_0^{(r)} = \frac{\partial^2 w^{(r)}}{\partial \varepsilon \partial \varepsilon}(\varepsilon^{(r)}). \quad (18)$$

It was shown by Ponte Castañeda and Willis (1999) that this “second-order” procedure follows from suitable approximations in the context of a rigorous variational principle. However, the principle is only *stationary* and therefore leads only to stationary estimates and not to bounds. It is further noted that this procedure leads naturally to the choice of the *tangent* modulus tensors $\mathbf{L}_t^{(r)}$ (Fig. 1(b)) for the linear comparison composite. But these should be evaluated at the phase averages of the strain—not at the second moments. As will be seen later, although the second-order estimates are not bounds, they are complementary to the bounds discussed earlier and appear to be more accurate.

Other recent developments in the field of nonlinear composites, which will not be reviewed here for lack of space, include the computation of the “hard” bounds by Talbot and Willis (1997), who made use of suitably chosen nonlinear comparison composites; bounds on the strain fields (as opposed to the energies) by Milton and Serkov (2000); an affine procedure due to Masson et al. (2000) that is closely related to the second-order method, but that also works for elastic-viscoplastic composites; new self-consistent estimates for polycrystals (Bornert and Ponte Castañeda (1998), Nebozhyn et al. (1999) and Gilormini et al. (2001)) showing dramatic improvements over the classical estimates; and applications of the second-order method in finite elasticity (Ponte Castañeda and Tiberio (2000)), where the relevant potentials are non-convex, leading to the failure of other methods.

4. SAMPLE RESULTS

Sample results are presented here for various special cases, including particle-reinforced composites and porous metals. For simplicity, all constituents are assumed to be governed by relation (2) with the same exponent m , but with different flow stresses $\sigma_0^{(r)}$. The microstructures are assumed to be statistically isotropic, so that the effective potentials \bar{W} of the nonlinear composite are isotropic functions of the (traceless)

strain $\bar{\varepsilon}$, thus depending only on its second and third invariants. They can therefore be written in the form

$$\bar{W}(\bar{\varepsilon}) = \frac{\varepsilon_0 \bar{\sigma}_0(\omega)}{m+1} \left(\frac{\bar{\varepsilon}_e}{\varepsilon_0} \right)^{m+1}, \quad (19)$$

where the *effective flow stress* $\bar{\sigma}_0$ is seen to be a function of the plastic phase angle ω , which in turn is related to the two invariants of $\bar{\varepsilon}$ through the relation $\cos(3\omega) = 4 \det(\bar{\varepsilon}) / \bar{\varepsilon}_e^3$. Note that the extreme values of the variable ω correspond to uniaxial tension ($\omega = 0$) and simple shear ($\omega = \pi/6$). Some of the results presented here are for two-dimensional composites with transverse isotropy subjected to plane-strain conditions, in which case a result analogous to (19) is generated, but where the equivalent strain $\bar{\varepsilon}_e$ has been suitably redefined. The corresponding effective flow stresses $\bar{\sigma}_0$ are constant (independent of $\bar{\varepsilon}$) in this case.

In the figures and discussion below, the following abbreviations will be used for simplicity: Hashin-Shtrikman (HS), self-consistent (SC), upper bound (UB), and lower bound (LB). Similarly, the following terminology will be used: “Variational” refers to the relation (11) of Ponte Castañeda (1991), or, equivalently, for power-law materials, relation (12) of Suquet (1993). “Second-order” refers to relation (16) of Ponte Castañeda (1996a). “Incremental” refers to the procedure first proposed by Hill (1965), in the form developed by Hutchinson (1976) for power-law viscous materials. “Secant” refers to the classical secant procedure, used by various authors, starting with Chu and Hashin (1971). “Tangent” refers to the procedure first proposed by Molinari, Canova, and Ahzi (1987) in its full anisotropic form (no further approximations). “Voigt” and “Reuss” will be used to denote the classical microstructure-independent upper (uniform strain) and lower (uniform stress) bounds. Finally, FEM and FFT will be used to denote the the results of the finite-element method and fast-Fourier-transform simulations of Moulinec and Suquet (1998), Michel et al. (1999), and Michel et al. (2000).

4.1. Particle-reinforced composites

In Fig. 2, the variational HS UB and the second-order HS estimate are compared against the classical Voigt UB and Reuss LB, the incremental, secant, and tangent procedures, and the FEM simulations of Michel et al. (1999) for two-phase, isotropic, rigid ideally plastic composites with 15% concentration of the harder phase, subjected to uniaxial tension. The effective flow stress $\bar{\sigma}_0$ is thus plotted as a function of the flow stress ratio of the two phases. It is emphasized that the FEM simulations are for composites with periodic microstructures and cylindrical unit cells, while all the HS estimates correspond to random microstructures with

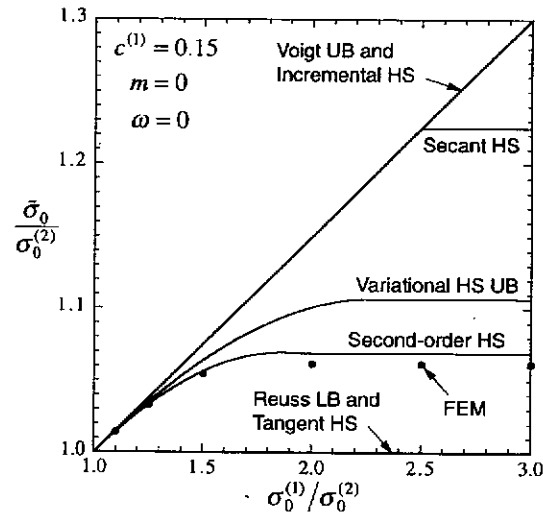


Figure 2 Rigidly reinforced, ideally plastic composites with statistically isotropic microstructures: Influence of the heterogeneity contrast.

overall isotropy. Therefore, the HS and FEM estimates are not expected to be in good agreement for general values of the volume fraction of the reinforcing phase. (In particular, the FEM predictions will not lead to exactly isotropic behavior.) However, for small enough volume fractions, the HS estimates would be expected to be in good agreement with the FEM simulations and hence the comparisons shown the figure at 15% concentration are considered to be meaningful.

The main observation in this figure is that the second-order HS estimate gives the best overall agreement with the FEM simulations, even at large contrast (within 1%). The variational HS result, which is an upper bound for all other HS estimates, is satisfied by the second-order and tangent estimates, but not by the secant and incremental estimates. However, the tangent prediction in this limiting case agrees exactly with the Reuss lower bound, which is believed to be too soft. In conclusion, for this extreme nonlinearity, essentially all the classical schemes break down and we are left with the variational bound and second-order estimates, which are complementary to each other and can be used to estimate the effective behavior of the composite fairly accurately.

4.2. Fiber-reinforced composites

Figure 3(a) depicts a comparison between yield surfaces computed with the variational procedure using the HS lower bounds to estimate

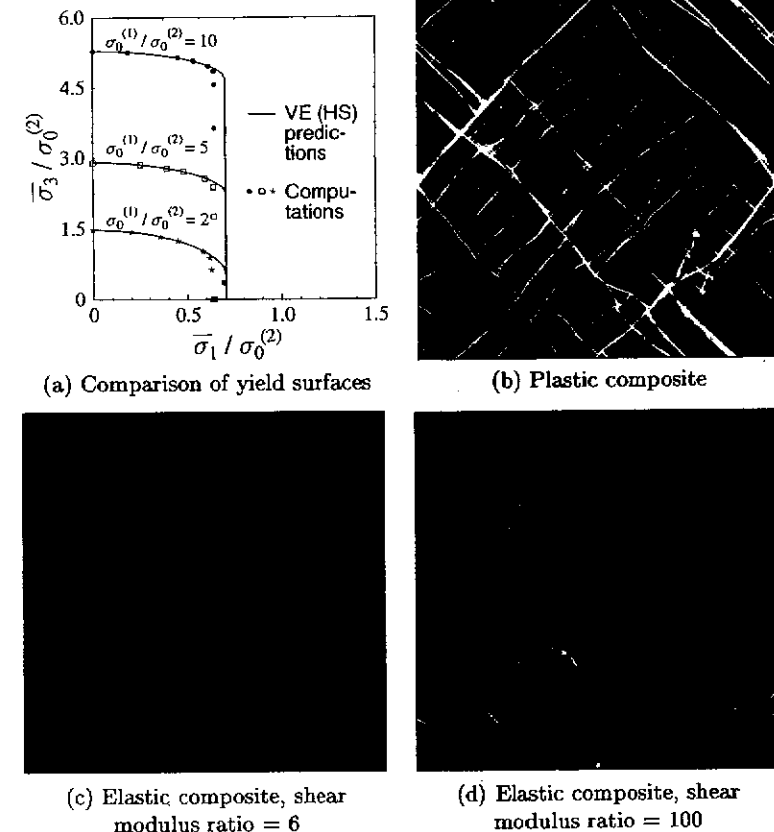


Figure 3 Effective flow surfaces and deformation maps for fiber-reinforced composites.

the properties of the linear comparison composite (continuous lines) and FFT simulations (various symbols) for generalized plane strain loading of a fiber-reinforced, ideally plastic composite. The fibers, which are aligned in the out-of-plane direction, are taken to be 2, 5, and 10 times stronger than the matrix. The horizontal axis ($\bar{\sigma}_1$) corresponds to in-plane shear loading of the form $\bar{\sigma}_1(e_1 \otimes e_1 - e_2 \otimes e_2)$, and the vertical axis ($\bar{\sigma}_3$) to out-of-plane axial loading. It can be seen that the agreement between the analytical predictions and the FFT simulations is quite good, at least in qualitative terms. The variational procedure is able to capture the "bimodal" character of the yield surfaces, which has also been observed experimentally (Dvorak and Bahei-El-Din (1987)).

Figure 3(b) presents strain intensity maps for transverse shear loading ($\bar{\sigma}_3 = 0$) of the plastic composite. Note that the microstructure in the

FFT simulations is taken to be periodic, with 64 fibers thrown at random in the unit cell. The shear bands (white lines) that develop through matrix channels between the hard fibers (black circles) are the source of the relatively “weak” behavior in this mode of deformation. For comparison purposes, results are also given in Figs. 3(c) and (d), for the same mode of deformation in linear elastic composites with the same microstructure and shear moduli ratios of 6 and 100, respectively. It is interesting to note that while strain intensification is also observed in the regions of close proximity between the fibers, shear bands going from one end of the specimen to the other end are not observed. It may then be surprising that the variational procedure, which uses the solution of a linear elastic problem to estimate the effective behavior of the nonlinear problem, does so well, in particular, capturing the strongly nonlinear “flat” sector on the yield surface. However, the important thing to remember here is that the variational principle is designed to select the optimal properties of the linear comparison composite to model as accurately as possible the effective behavior of the nonlinear composite, which is characterized in this case by the effective yield surfaces.

4.3. Effect of the third invariant: Particle-reinforced composites

In this section, the effect of the third invariant of the loading, as measured by the plastic angle ω , on the effective flow stress of two-phase, ideally plastic composites with overall isotropy is considered. Thus, in Fig. 4(a), a comparison is given between the variational and second-order procedures, used in conjunction with the HS lower bounds for the relevant linear comparison problem, and the FFT simulations carried out by Moulinec and Suquet (unpublished) for “quasi-random” microstructures, as defined by the unit cell with 15% reinforcement shown in Figure 4(b). The FFT simulations show dependence on ω , as expected from general considerations. This dependence is also captured by the second-order procedure quite well near the axisymmetric end ($\omega = 0$) and less well near the pure shear limit ($\omega = \pi/6$), where it tends to the flow stress of the matrix. The variational HS estimate is independent of ω , but on the other hand provides an upper bound for the effective flow stress.

Figures 4(c) and (d) provide deformation maps in the FFT simulations for the two extreme cases, axisymmetric tension and pure shear, respectively. As can be seen in the transverse diagonal planes highlighted in the figures, the deformation is distributed more uniformly in the matrix for axisymmetric tension, while it tends to become localized on shear bands passing through the matrix for pure shear, thus elucidating the

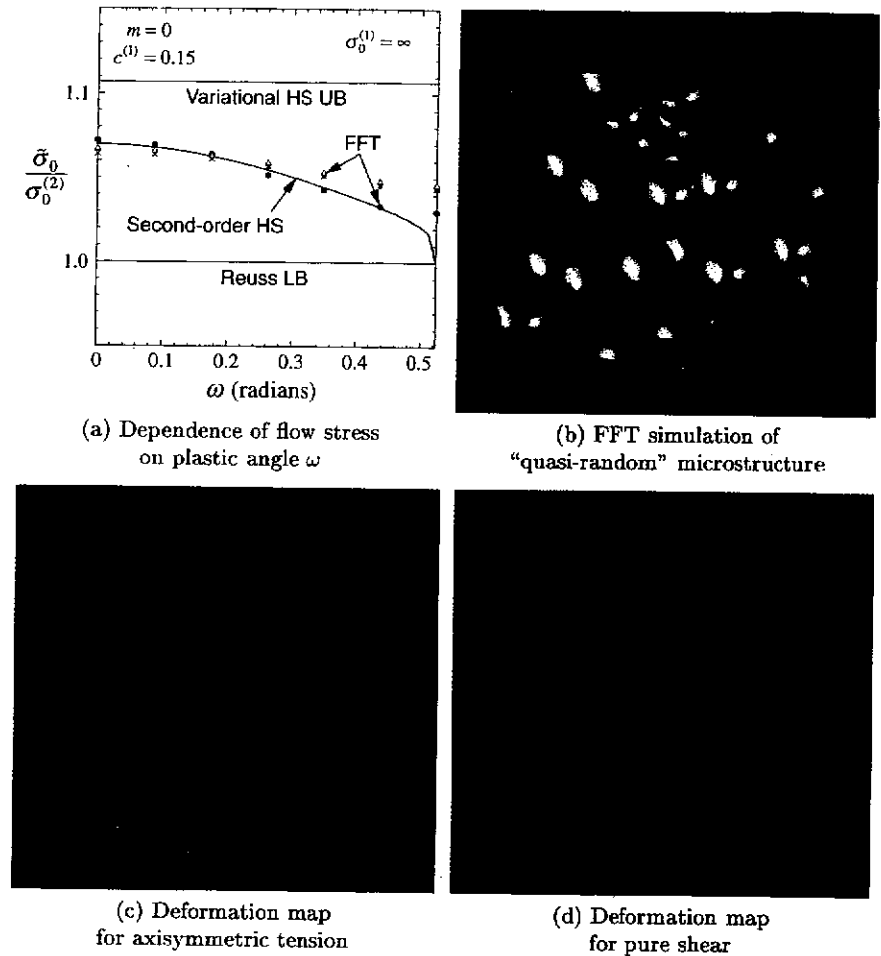


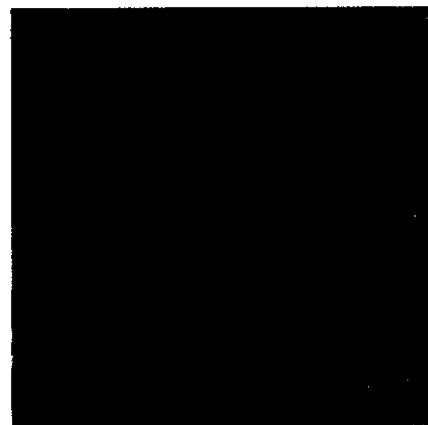
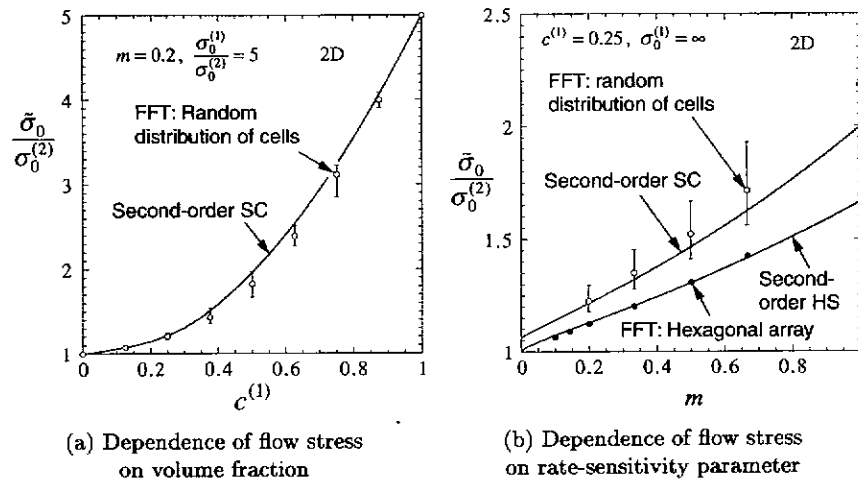
Figure 4 Rigidly reinforced, ideally plastic composites with statistically isotropic microstructures: Influence of the third invariant of the applied stress.

physical source of the dependence on the third invariant for strongly nonlinear composites.

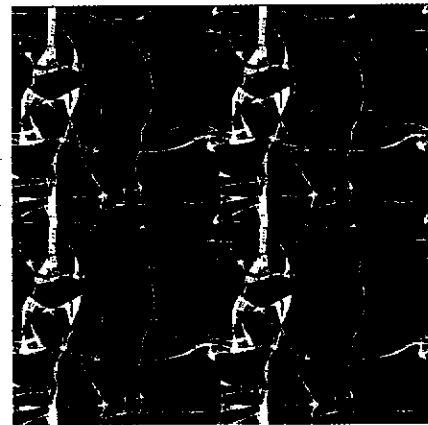
4.4. Cellular microstructures

In this section, two-phase composites with transversely isotropic cellular microstructures, subjected to plane strain loading, are considered. Comparisons are shown in Figs. 5(a) and (b) between the predictions of the second-order procedure, using the SC estimates for the linear

comparison composite, and FFT simulations for composites with ran-



(c) Unit cell for random distribution of hexagons



(d) Deformation map for a plastic matrix and reinforcement 5 times as strong

Figure 5 Two-dimensional composites with cellular microstructures: Effect of volume fraction and nonlinearity.

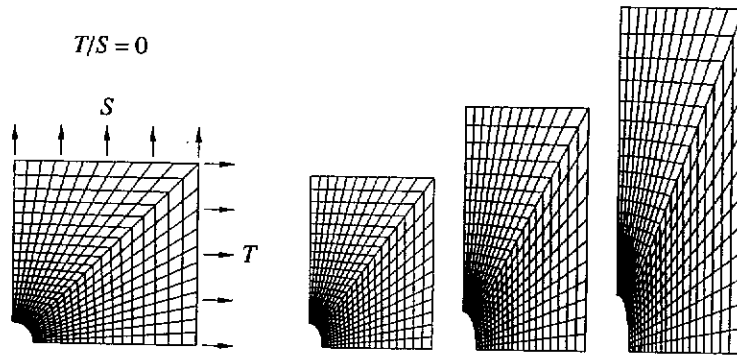
dom distributions of hexagons defined by unit cells of the type shown in Fig. 5(c) (25 configurations were used; the circles denote the average value, and the error bars the maximum and minimum values). It is known from earlier work in the context of linear elastic composites that these microstructures are well approximated by the self-consistent model, at least at finite heterogeneity contrast. It is thus seen in Fig. 5(a)

that the second-order SC estimates predict with fair accuracy the dependence on volume fraction at this moderate level of nonlinearity. (The results are not as good as the nonlinearity increases for intermediate values of the volume fraction.) Similarly, Fig. 5(b) shows relatively good agreement even at infinite contrast and high values of the nonlinearity (m tending to zero), for a volume fraction of 25% of the rigid phase. (Also shown in this figure are the corresponding second-order HS estimates, which are compared with periodic FFT results for a perfect lattice consisting of a hexagonal distribution of rigid hexagons in the matrix material.) Finally, Fig. 5(d) shows the deformation maps for the configuration defined by Fig. 5(c) with an ideally plastic matrix and reinforcement phase 5 times as strong. (The soft phase is shown in black in Fig. 5(c).) Note, once again, that shear bands develop passing through channels of the weaker phase.

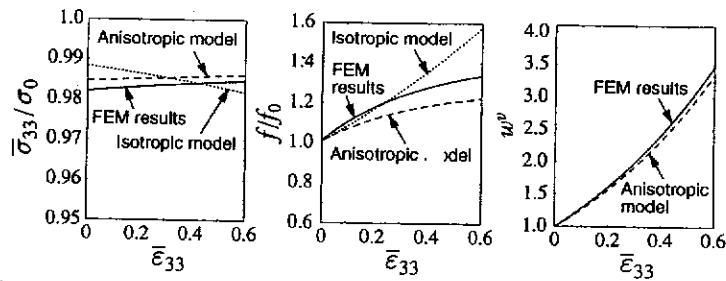
4.5. Microstructure evolution in porous materials

In forming processes involving porous metals, for example, the strains are large enough to cause the microstructure to evolve as a function of the deformation. An *isotropic* porous plasticity model that has been shown to work extremely well under nearly hydrostatic loading conditions was proposed by Gurson (1977). However, for processes involving lower triaxiality conditions, such as rolling and extrusion, the material is expected to develop anisotropy, even if its initial state is isotropic. An *anisotropic* model, which is based on the use of the HS variational estimates of Ponte Castañeda (1991) and Michel and Suquet (1992) for porous media, was proposed by Ponte Castañeda and Zaidman (1994) and Kailasam et al. (2000) to account for the evolution of pore shape and orientation.

In Fig. 6, a comparison is made between the predictions of the *anisotropic* model of Ponte Castañeda and Zaidman (1994) and finite-strain FEM simulations for a periodic composite with axisymmetric unit cell, as depicted in the figure. In addition, the predictions of an extension of the *isotropic* Gurson model, due to Găărăjeu et al. (2000), for a power-law viscoplastic matrix material are also shown. The initial porosity is $f_0 = 10^{-3}$, the strain-rate sensitivity is $m = 0.2$, and uniaxial tension is applied with triaxiality $X = 1/3$. It can be seen that the predictions of the *anisotropic* model—in contrast with those of the *isotropic* model—are at least in qualitative agreement with the FEM simulations at this level of triaxiality. In particular, the *anisotropic* model captures not only the evolution of the average shape of the voids (w^v), but, in addition,



(a) Finite-strain FEM simulations for a periodic composite with axisymmetric unit cell

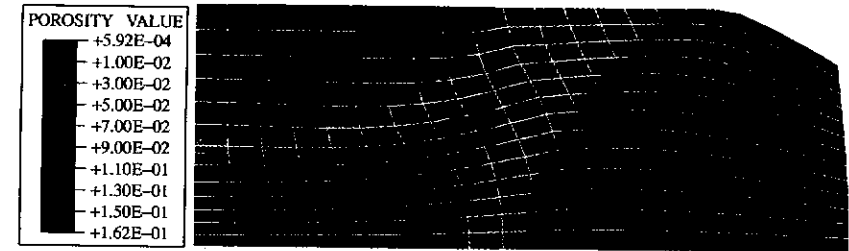


(b) Evolution of the axial stress $\bar{\sigma}_{33}$, porosity f , and average pore shape w^v as functions of the applied strain $\bar{\epsilon}_{33}$.

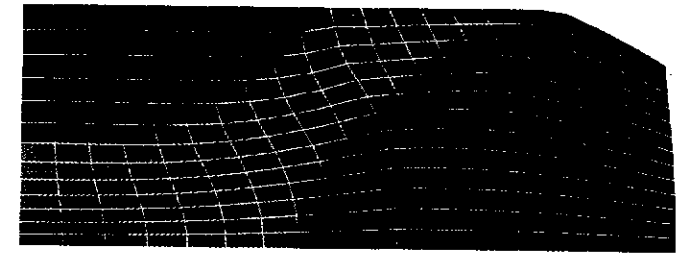
Figure 6 Porous materials subjected to uniaxial tension.

also predicts the gentler increases in the porosity f (which is found to saturate at large enough strain $\bar{\epsilon}_{33}$), as well as the overall hardening of the porous material (positive slope in the uniaxial stress-strain relation, as opposed to the negative slope predicted by the *isotropic* model). Analogous observations have been made for other low-triaxiality situations, including uniaxial compression, where the *anisotropic* model is found to predict full densification at around 70% strain, which is in much better agreement with numerical and experimental evidence than the value predicted by the Gurson-type models (around 250% strain). On the other hand, it should be emphasized that the Gurson-type models give the most accurate predictions for high triaxialities.

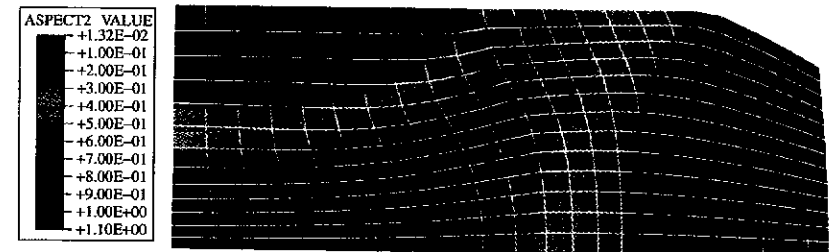
Finally, in Fig. 7, contour plots are given (Kailasam et al. (2000)) for the distribution of the porosity predicted by the *anisotropic* and Gurson models, as well as for the pore aspect ratios predicted by the *anisotropic* model, in a disk compaction experiment (Parteder et al.



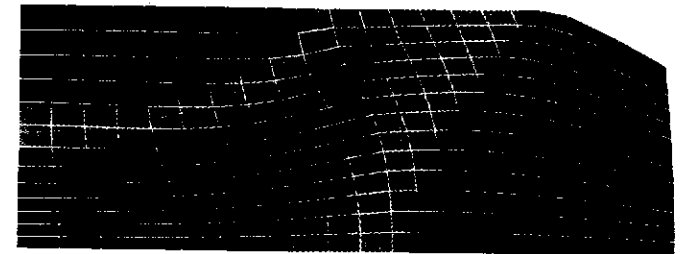
(a) Porosity distribution according to the anisotropic model



(b) Porosity distribution according to the Gurson model



(c) In-plane pore aspect ratios according to the anisotropic model



(d) Out-of-plane pore aspect ratios according to the anisotropic model

Figure 7 Compaction of a tapered disk with a height reduction of 37.5%.

(1999)). The initial porosity of the tapered axisymmetric disk (only one quarter of the cross-section of which is shown) is $f_0 = 15\%$, and the macroscopic height reduction is 37.5%. The main observation in the context of this figure is that the porosity reduction predicted by the *anisotropic* model (Fig. 7(a)) is considerably larger than that predicted by the Gurson model (Fig. 7(b)). More specifically, the size of the region where the porosity is less than 1% (inner dark region) is much larger for the *anisotropic* model than for the Gurson model. Also, in this region, the *anisotropic* model predicts that the pores have become nearly flat (i.e. they have become cracks) and are aligned with the horizontal direction (Fig. 7(c) and (d)). For more details on these simulations, the reader is referred to Kailasam et al. (2000).

5. CONCLUDING REMARKS

In this review, two nonlinear homogenization methods have been briefly described, the main ingredient in both being the use of linear comparison composites in the context of suitably designed variational principles. Their predictions for various types of composite material have been compared with the corresponding predictions of the classical schemes, as well as with numerical simulations. It is found that the "second-order" method, which makes use of the tangent moduli evaluated at the average strain in the phases, usually leads to the most accurate estimates, while the less accurate "variational" method, which makes use of secant moduli evaluated at the second moments of the strain, gives rigorous bounds. Thus, in some sense, they provide complementary information. The main advantage of these methods is their relative simplicity and computational efficiency. Explicit (or nearly so) expressions are available for most of the cases considered here, including rigidly reinforced composites and porous materials—see Ponte Castañeda and Suquet (1998) for the most comprehensive set of results. These results compare favorably with FEM and FFT simulations, which, while very accurate for the specific configurations chosen, are much more computationally intensive. It is important to emphasize that, by their very nature, these homogenization methods cannot be more accurate than the estimates that are used as input in the computation of the effective behavior of the relevant linear comparison composites. Thus far, reasonable accuracy has been achieved for composites that are modeled well by the Hashin-Shtrikman and self-consistent approximations. More accurate estimates, incorporating higher-order statistics, are likely to be needed for other types of microstructure and for improved performance. Concerning the nonlinear schemes themselves, improvements are still needed to be able to handle

the most extreme circumstances, usually involving very highly nonlinear behavior.

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