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Report AFOSR-89-0288

THE OVERALL RESPONSE OF COMPOSITE MATERIALS UNDERGOING LARGE ELASTIC DEFORMATIONS

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13 June 1990

Annual Technical Report for Period 1 April 1989 - 31 March 1990

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Abstract

The main goal of this project is to estimate theoretically the overall or effective constitutive properties of *nonlinear* composite materials undergoing *large* deformations. Two types of large deformations are of interest: large elastic deformations, and large viscous deformations. The proposed method is to apply variational principles that are under development to characterize the range of the effective properties given partial statistical information about the microstructure (such as the volume fractions of the phases). For some particular microstructures of interest exact estimates may be given. Significant progress was made over the first year with the development of a new variational principle allowing the estimation of the effective properties of a given nonlinear composite in terms of the effective properties of linear composites (which are assumed to be known). The potential significance of this work derives from its simplicity allowing the application of a large body of prior research on linear composites to nonlinear composites. This method has been applied to the case of large viscous deformations, and some results for particular materials systems have already been reported in the pertinent literature.

Research goals

The main goal of this project is to estimate the overall or effective constitutive properties of nonlinear composite materials undergoing large deformations. Two types of large deformations are of particular interest: large *elastic* deformations, corresponding to materials such as polymeric composites, rubber foams and solid rocket fuel composites; and large viscous deformations, corresponding to the high-temperature creeping, or to the dynamic plastic deformation of metals.

Background

The first and only available rigorous procedure thus far for estimating the overall constitutive properties of nonlinear random composites was given by Talbot & Willis (1985). This procedure is based on an extension of the well-known Hashin-Shtrikman Fer (HS) variational principles to a class of nonlinear materials. Ponte Castañeda & Willis ¹ (1988) applied this procedure to nonlinearly viscous materials, and gave the first rigorous dbounds and self-consistent (SC) estimates for the effective properties of composites in power-law creep. Ponte Castañeda (1989) extended the work of Talbot & Willis to finite elasticity, and used the resulting theory to provide the first bounds and estimates for 3n/2nonlinearly elastic composites. Avail and/or



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Progress in first year

Introduction

The research carried out under the sponsorship of AFOSR in the past year has brought about an important development, reported in Ponte Castañeda (1990a & b). In these works, a new variational structure is introduced that yields the following important result for the effective properties of *isotropic* nonlinear composites: given the overall properties of a "comparison" linear composite with the same microstructural distribution of phases as the nonlinear composite, it is possible to give an estimate (in the form of a bound) for the overall properties of the nonlinear isotropic composite. Thus, available bounds and estimates for linear composites can be "translated" into corresponding bounds and estimates for nonlinear composites. The new structure has the following advantages: it is more general than the corresponding structure of Talbot & Willis, because it not only yields HS bounds and SC estimates, but it generalizes to the nonlinear case any other type of bound or estimate that may be available for the linear composite; it is *easier* to implement, because it only requires the calculation of the extreme values of two appropriately defined functions; and, finally, it gives in some cases stronger (in other, identical) results than the method of Talbot & Willis.

The method has been applied to three different material systems. Porous and rigidly reinforced materials with pure-power law and Ramberg-Osgood matrix behaviors, respectively, are considered in Ponte Castañeda (1990a) and Ponte Castañeda and de Botton (1990). Alternatively, Ponte Castañeda (1990b) considered a family of brittle/ductile composites containing a linear and a nonlinear phase. In addition to low-temperature plasticity (in its deformation theory form), these results can also be re-interpreted in the context of high-temperature creep and high strain-rate viscoplasticity.

The method

Consider an *n*-phase composite occupying a domain Ω (normalized to have unit volume), with each phase occupying a sub-domain $\Omega^{(r)}$ (r = 1, 2, ..., n), and let the stress potential, $U(\sigma, \mathbf{x})$, be expressed in terms of the *n* homogeneous phase potentials, $U^{(r)}(\sigma)$, via

$$U(\boldsymbol{\sigma}, \mathbf{x}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) U^{(r)}(\boldsymbol{\sigma}), \qquad (1)$$

where

$$\chi^{(r)}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} \in \Omega^{(r)} \\ 0 & \text{otherwise} \end{cases}$$
(2)

is the indicator function of phase r. The phases are assumed to be isotropic, so that the potentials $U^{(r)}(\sigma)$ depend on the stress σ only through its three principal invariants. Here, we will further assume that the dependence is only through two of the invariants, namely,

the mean stress, $\sigma_m = \frac{1}{3} \text{tr} \sigma$, and the effective stress, $\sigma_e = \sqrt{\frac{3}{2} \mathbf{S} \cdot \mathbf{S}}$, where S is the deviator of σ .

The effective behavior of the composite material is defined in terms of the effective energy, $\tilde{U}(\bar{\sigma})$, that arises due to the uniform traction boundary condition

$$\sigma_{ii}n_i = \overline{\sigma}_{ii}n_i, \quad \mathbf{x} \in \partial\Omega, \tag{3}$$

where $\partial \Omega$ denotes the boundary of the composite, **n** is its unit outward normal, and $\overline{\sigma}$ is a given constant symmetric tensor. The average stress in the composite is then precisely $\overline{\sigma}$ and it follows from the principle of minimum complementary energy that

$$\tilde{U}(\overline{\mathbf{\sigma}}) = \min_{\mathbf{\sigma} \in S(\overline{\mathbf{\sigma}})} \tilde{U}(\mathbf{\sigma}), \tag{4}$$

where

$$\widehat{U}(\boldsymbol{\sigma}) = \int_{\Omega} U(\boldsymbol{\sigma}, \mathbf{x}) dV$$

is the complementary energy functional of the problem, and

$$S(\overline{\sigma}) = \{\sigma | \sigma_{ij,j} = 0 \text{ in } \Omega, \text{ and } \sigma_{ij}n_j = \overline{\sigma}_{ij}n_j \text{ on } \partial\Omega \}$$

is the set of statically admissible stresses. Thus, if $\vec{\epsilon}$ denotes the average strain over the composite, it can be readily shown that

$$\bar{\varepsilon}_{ij} = \frac{\partial \bar{U}}{\partial \sigma_{ij}}(\bar{\sigma}), \qquad (5)$$

which yields an effective constitutive relation for the composite in terms of the average variables $\overline{\sigma}$ and $\overline{\epsilon}$. Given this connection between the effective potential for the composite $\tilde{U}(\overline{\sigma})$ and the effective stress/strain relation, it makes sense to seek information on $\tilde{U}(\overline{\sigma})$. Next we make use of a linear heterogeneous "comparison" material, with effective properties that can be characterized in terms of bounds and estimates, to obtain corresponding bounds and estimates for the effective properties of a nonlinear composite. To this end, we introduce the quadratic potential

$$\hat{U}(\sigma, \mathbf{x}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) \hat{U}^{(r)}(\sigma) = \frac{1}{6\hat{\mu}(\mathbf{x})} \sigma_{\sigma}^{2} + \frac{1}{2\hat{\kappa}(\mathbf{x})} \sigma_{m}^{2}, \qquad (6)$$

such that $\hat{\mu}(\mathbf{x}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) \hat{\mu}^{(r)} > 0$, and $\hat{\kappa}(\mathbf{x}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) \hat{\kappa}^{(r)} > 0$, with the $\hat{\mu}^{(r)}$ and $\hat{\kappa}^{(r)}$

constant, corresponding to a linear isotropic composite with the same phase distribution (the same indicator functions) as the nonlinear composite.

Then, if the nonlinearity in the potential of the original composite is stronger than quadratic as the norm of the stress becomes large, it makes sense to define the set of functions

$$V^{(r)}(\hat{\mu}^{(r)}, \hat{\kappa}^{(r)}) = \max_{\sigma} \{ \hat{U}^{(r)}(\sigma) - U^{(r)}(\sigma) \}.$$
(7)

It follows that,

$$\tilde{U}(\overline{\mathbf{\sigma}}) \ge \max_{\hat{\mu}^{(\nu)}, \hat{\kappa}^{(\nu)} > 0} \{ \tilde{\tilde{U}}(\overline{\mathbf{\sigma}}) - \overline{V}(\hat{\mu}, \hat{\kappa}) \}.$$
(8)

where

$$\tilde{\hat{U}}(\overline{\mathbf{\sigma}}) = \min_{\boldsymbol{\sigma} \in S(\overline{\mathbf{\sigma}})} \overline{\hat{U}}(\mathbf{\sigma})$$
(9)

is the effective potential of the linear composite, and

$$\bar{V}(\hat{\mu},\hat{\kappa}) = \sum_{r=1}^{n} c^{(r)} V^{(r)}(\hat{\mu}^{(r)},\hat{\kappa}^{(r)}), \qquad (10)$$

is expressed in terms of the volume fractions of each phase,

$$c^{(r)} = \int_{\Omega} \chi^{(r)}(\mathbf{x}) \, dV.$$

The details of the derivation of this result are given in Appendix A (Ponte Castañeda 1990a) in pages 6 through 9. We note however that expression (8) allows the estimation of the effective properties of the nonlinear composite in terms of the effective properties of a family of linear composites with elastic moduli $\hat{\mu}^{(r)}$ and $\hat{\kappa}^{(r)}$.

Usually, however, it is not possible to find $\hat{\hat{U}}(\overline{\sigma})$ explicitly, but instead bounds and estimates may be available for $\tilde{\hat{U}}(\overline{\sigma})$. If we have a lower bound (such as a Hashin-Shtrikman lower bound) $\tilde{\hat{U}}_{-}(\overline{\sigma})$ for $\tilde{\hat{U}}(\overline{\sigma})$, such that

$$\hat{\hat{U}}(\overline{\mathbf{\sigma}}) \ge \hat{\hat{U}}_{_}(\overline{\mathbf{\sigma}}), \tag{11}$$

then, replacing $\tilde{\hat{U}}(\overline{\sigma})$ by $\tilde{\hat{U}}_{-}(\overline{\sigma})$ in equation (8) for $\tilde{U}_{-}(\overline{\sigma})$ yields a lower bound for $\tilde{U}(\overline{\sigma})$.

On the other hand, if we only have an estimate (such as a self-consistent estimate) $\hat{U}_{\epsilon}(\overline{\sigma})$ for $\tilde{U}(\overline{\sigma})$, then

$$\tilde{U}_{\epsilon}(\overline{\boldsymbol{\sigma}}) = \max_{\hat{\mu}^{(\nu)}, \hat{\kappa}^{(\nu)} > 0} \{ \tilde{\tilde{U}}_{\epsilon}(\overline{\boldsymbol{\sigma}}) - \bar{V}(\hat{\mu}, \hat{\kappa}) \}$$
(12)

would provide only an estimate for $\tilde{U}(\overline{\sigma})$.

We note that the prescriptions (8) and (12) lead to convex expressions for the bounds and estimates of the effective potential of the nonlinear composite, provided that the corresponding bounds and estimates for the linear composite are convex, which is in turn guaranteed assuming that $\hat{\mu}$ and $\hat{\kappa} > 0$. This is a desirable feature, because the effective potential of the composite is known to be convex.

An alternative derivation, and a stronger version, of this variational procedure is given in Appendix C (Ponte Castañeda 1990b) in pages 4 to 6. The advantage of the alternative derivation is that it allows the characterization of the circumstances under which the inequality in equation (8) turns into equality. This idea is important in the context of assessing the strength of the bounds.

Results

The general procedure was applied in Ponte Castañeda (1990a) to an isotropic porous material with incompressible behavior for the matrix with potential described by

$$U^{(1)}(\boldsymbol{\sigma}) = f(\boldsymbol{\sigma}_{\boldsymbol{\epsilon}}). \tag{13}$$

The result of this calculation are a Hashin-Shtrikman (H-S) lower bound for $\tilde{U}(\overline{\sigma})$, given by

$$\tilde{U}_{-}(\overline{\mathbf{\sigma}}) = c^{(1)}f(s), \tag{14a}$$

with

$$s = \frac{1}{c^{(1)}} \sqrt{(1 + \frac{2}{3}c^{(2)})} \overline{\sigma}_{e}^{2} + \frac{9}{4}c^{(2)} \overline{\sigma}_{m}^{2}, \qquad (14b)$$

and a self-consistent (S-C) estimate given by

$$\tilde{U}_{\epsilon}(\overline{\mathbf{\sigma}}) = c^{(1)}f(s), \tag{15a}$$

$$s = \sqrt{\frac{1}{c^{(1)}} \left(\frac{1 - c^{(2)}/3}{1 - 2c^{(2)}} \right) \left(\overline{\sigma}_{e}^{2} + \frac{9}{4} \frac{c^{(2)}}{c^{(1)}} \overline{\sigma}_{m}^{2} \right)}.$$
 (15b)

The details of the derivation of these results is given in pages 9 to 12 of Appendix A. Results are also given in this reference for a rigidly reinforced material with matrix behavior characterized by relation (13), and for a general two-phase incompressible composite. The above results are also specialized in Ponte Castañeda (1990a) to pure power-law behavior for f. Results for appropriately defined low-triaxiality "shear" and high-triaxiality "bulk" moduli for the porous material are given in Figures 2 and 3 of Appendix A for representative values of the hardening parameter n as functions of the porosity. Analogous results are given in Figures 3 and 4 for the effective "shear" modulus of the two-phase incompressible composite and the rigidly reinforced material, respectively. The new results are compared with previously available results such as dilute and self-consistent estimates. For the porous material, the bounds are found to be the best bounds available (better than the corresponding bounds of Ponte Castañeda and Willis, 1988 obtained using the nonlinear extension of the Hashin-Shtrikman variational principle of Talbot and Willis, 1984). In addition to their intrinsic value, these bounds are also essential in characterizing the range of validity of numerical calculations based on the dilute approximation. Thus, it is found (see Figures 2) that the dilute calculations of Duva and Hutchinson (1984) for the low-triaxiality modulus are reasonably good for porosities up to 40%. On the other hand, their corresponding calculations for the high-triaxiality bulk modulus (Figures 3) have a very small range of validity (less than 1% for practically important values of the hardening parameter). In Figure 4, the new self-consistent estimates for the rigidly reinforced material compare favorably with the corresponding differential self-consistent estimates of Duva (1984).

In Ponte Castañeda and de Botton (1990), the above procedure is specialized to a porous material with "linear plus power hardening" (Ramberg-Osgood) behavior for the nonlinear phase. Results are given for the effective potential of the composite as a function of the average stress and for representative stress/strain relations for the porous material in Figures 1 and 2 of Appendix B for different values of the hardening parameter and the porosity. The results are compared with results by Willis (1990), and the new results are found to be superior. In particular, the physically unrealistic discontinuous behavior of Willis' model between the linear and nonlinear domains at the larger values of the triaxiality

with

(see the continuous lines in Figure 1d) is not observed in the new results (there is a smooth transition between the linear and plastic domains for the dashed lines).

Finally, in Ponte Castañeda (1990b) results in the form of Hashin-Shtrikman bounds are given for composites containing linear and nonlinear (c.f. equation (13)) phases. As it turns out, some of these bounds can be shown to be optimal (best possible bounds given the volume fractions of each phase) in some cases. This is accomplished by identifying special microstructures (called sequentially laminated composites) attaining the bounds. Results specialized to pure power-law behavior for the nonlinear material are given in Figures 2 and 3 of Appendix C. Figures 2 give bounds for an appropriately normalized form of the effective energy of the composite versus an appropriately normalized measure of the average stress for representative values of the hardening parameter n at small enough stress levels. Figures 3 give the corresponding results for larger values of the average stress. In Figures 4, some results are given for a linear plus power (Ramberg-Osgood) behavior for the nonlinear phase. These results for the bounds are the first of its kind, and thus we have not been able to compare them with other results.

Research plans for next year

Encouraged by the above results, we plan to generalize the work in two ways. First, we would like to address anisotropic composites, and then later nonlinearly elastic (with finite deformations) composites. The extension to anisotropic composites is already in progress, with the assistance of one of my graduate students, Mr. Gal de Botton. This work is expected to yield important new results without too much difficulty, and it will serve to introduce Mr. de Botton to this area of research. Additionally, another graduate student, Mr. F.-Y. Huang (to be replaced by Mr. G. Li), will attempt to compare the results predicted by the new procedure with those predicted by the mathematical theory of homogenization for the special case of periodic composites, where exact results can be obtained by numerical computation. These latter results would serve to further characterize the strength of the proposed variational structure. Finally, the non-trivial extension to nonlinearly elastic composites is expected to occupy our efforts for the most part of the next two years (04/01/90 to 03/31/92). The complications in this last problem are related to the strong nonlinearities that arise due to the large deformation kinematics, but it is expected that the ideas developed in Ponte Castañeda (1989) will also be useful in this work, leading to improved results for the effective properties of such composites.

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Other recent publications

Ponte Castañeda, P. and Mataga, P.A. (1990) "Stable crack growth along a brittle/ductile interface. Part I – Near-tip fields." *International Journal of Solids and Structures*, in press.

Presentations

Session on Homogenization Theory and Effective Properties of Inhomogeneous Elastic Solids, Symposium on Constitutive Issues in Finite Elasticity, ASME Winter Annual Meeting, Dallas, to be held November 25-30, 1990 (invited presentation).

""The effective properties of incompressible brittle/ductile composites," *IUTAM Symposium on Inelastic Deformation of Composite Materials*, Rensselaer Polytechnic Institute, Troy, May 29-June 1, 1990 (invited presentation).

"Bounds and estimates for the effective properties of nonlinear composites," 11th U.S. National Congress of Applied Mechanics, University of Arizona, Tucson, May 21-25, 1990.

"Variational estimates for the effective properties of porous Ramberg-Osgood materials," 15th Southeastern Conference on Theoretical and Applied Mechanics, Georgia Institute of Technology, Atlanta, March 22-23, 1990 (invited presentation).

Invited seminars

Department of Mathematica Sciences, University of Delaware, Wilmington, April 13, 1989.

Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, February 15, 1990.

Department of Mechanical Engineering, Stanford University, Palo Alto, March 5, 1990.

Department of Materials Science and Mineral Engineering, University of California, Berkeley, March 6, 1990.

Instituto de Investigaciones en Matematicas Applicadas y en Systemas, Universidad Nacional Autonoma de Mexico, Mexico City, July 1990.

Graduate students

Gal de Botton, B.S., M.S. (supported by AFOSR) Fu-Ying Huang, B.S. (leaving July 1990) Guan Li, M.S. (supported by Mechanical Engineering Department) Appendix A.

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THE EFFECTIVE MECHANICAL PROPERTIES OF NONLINEAR ISOTROPIC COMPOSITES

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(Received 2 January 1990)

ABSTRACT

A NEW variational structure is proposed that yields a prescription for the effective energy potentials of nonlinear composites in terms of the corresponding energy potentials for linear composites with the same microstructural distributions. The prescription can be used to obtain bounds and estimates for the effective mechanical properties of nonlinear composites from any bounds and estimates that may be available for the effective properties of linear composites. The main advantages of the procedure are the simplicity of its implementation, the generality of its applications and the strength of its results. The general prescription is applied to three special nonlinear composites : a porous material, a two-phase incompressible composite and a rigidly reinforced material. The results are compared with previously available results for the special case of power-law constitutive behavior.

1. INTRODUCTION

THE PREDICTION of the *effective*, or *overall*, constitutive behavior of composite solid materials is both a practically and theoretically important problem, which draws input from many different disciplines, including material science, mechanics and mathematics. This paper deals with the theoretical prediction of the effective mechanical properties of heterogeneous materials with *nonlinear* phases that are perfectly bonded to each other, and isotropic. To make sense of the notion of effective properties for the composite, the size of the typical heterogeneity is generally assumed to be small compared to the size of the specimen and the scale of variation of the applied loads. It is further assumed that the effect of the interfaces is negligible, so that the effective properties of the composite are essentially derived from the bulk behavior of the constituent phases.

The corresponding theory for linear composites is fairly well developed, including different approaches to the problem with varying degrees of mathematical sophistication and physical relevance. Thus, exact estimates have been determined for the effective properties of *ad hoc* models of composites; rigorous variational bounds have been given for the properties of *random* composites; and precise definitions and explicit "homogenization" formulae have been proposed for the properties of *periodic* composites. Appropriate, but by no means exhaustive, references dealing with the linear theories are provided by the review articles of WILLIS (1982, 1983) and KOHN (1989), and by the monographs of CHRISTENSEN (1979) and SANCHEZ-PALENCIA

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(1980). By contrast, in the context of nonlinear composites, most of the results are based on ad hoc models, such as dilute and self-consistent models. For instance, DUVA and HUTCHINSON (1984) (referred to as DH fin the sequel) gave dilute estimates for the effective properties of a nonlinear porous material, and DUVA (1984) proposed self-consistent estimates of the differential type for a rigidly reinforced, nonlinear material. To the knowledge of the author, the first and only contribution so far dealing with the calculation of rigorous bounds for the effective properties of nonlinear composites is provided by the work of TALBOT and WILLIS (1985) (referred to as TW), which was introduced in WILLIS (1983). These authors extended the well-known Hashin-Shtrikman variational principles to include nonlinear constitutive behavior, and their methods have been applied to a number of examples in different physical contexts. For example, PONTE CASTANEDA and WILLIS (1988) (referred to as PCW), and more recently WILLIS (1989), have determined bounds and estimates for the effective properties of nonlinearly viscous (or infinitesimally elastic) materials. Also, PONTE CASTAÑEDA (1989) provided extensions of the minimum complementary energy and the Talbot-Willis variational principles to finite elasticity, that allowed the calculation of bounds and estimates for the effective properties of a broad class of nonlinearly elastic composites. Additional developments are provided by appropriate extensions of the periodic homogenization formula by MARCELLINI (1978) for problems with convex energy densities, and by MULLER (1987) for finite elasticity (with a non-convex energy density).

In this work, we propose an alternative variational structure that allows the estimation of the effective energy densities of nonlinear composites in terms of the corresponding information for linear composites with the same microstructural distribution. Although the procedure has application to problems in other physical contexts that have a variational characterization (see PONTE CASTANEDA, 1990, for an application in conductivity), here we will study the specific application of the theory to composite materials with constitutive behavior characterized by nonlinear viscosity, or by the mathematically analogous theory of nonlinear infinitesimal elasticity. Effective properties are defined in Section 2 by means of the principle of minimum potential energy, and its dual counterpart, the principle of minimum complementary energy. The new structure is developed in Section 3, where it is shown that a general bound (or, alternatively, an estimate) for the linear composite can be translated into a bound (or estimate) for the nonlinear composite. In Section 4, the general procedure is applied to three particular cases of general interest: a porous material, a two-phase incompressible composite and a material reinforced by rigid inclusions. For each of these composites, we give bounds and estimates for their effective properties. In Section 5, the results are specialized further to phases with a power-law type of constitutive behavior, and the results are discussed and compared with previously available results. Finally, in Section 6 some general conclusions are drawn.

2. EFFECTIVE PROPERTIES

We are interested in estimating the effective, or overall, properties of composites with nonlinear material behavior. By a "composite" we mean an idealized material

Effective properties of nonlinear composites

that corresponds to the limit of a sequence of heterogeneous materials with two distinct length scales : one microscopic *l* corresponding to the size of the heterogeneity, and one macroscopic *L* corresponding to the size of the specimen of interest and the scale of variation of the boundary conditions. The effective behavior of the composite is then obtained by considering the limit of the behavior of the sequence of materials as the ratio of scales $\varepsilon = l/L$ tends to zero. The study of the definition and existence of such limit properties is called homogenization theory, and it is an area of current interest in the general mathematics community (KOHN, 1989). However, for the purposes of this work, it will not be necessary to introduce this formalism; we can always rely on our physical intuition to understand the concept of effective properties, and in the analysis that follows, it will suffice to take our composite to be a heterogeneous material with very small, but finite microscale. The effective properties are then understood in an approximate sense.

Consider an *n*-phase composite occupying a domain Ω , with each phase occupying a sub-domain $\Omega^{(r)}$ (r = 1, 2, ..., n), and let the stress potential, $U(\sigma, x)$, be expressed in terms of the *n* homogeneous phase potentials, $U^{(r)}(\sigma)$, via

$$U(\sigma, \mathbf{x}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) U^{(r)}(\sigma), \qquad (2.1)$$

where

$$\chi^{(\prime)}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} \in \Omega^{(\prime)} \\ 0 & \text{otherwise} \end{cases}$$
(2.2)

is the characteristic function of phase r. The phases are assumed to be isotropic, so that the potentials $U^{(r)}(\sigma)$ depend on the stress σ only through its three principal invariants. Here, we will further assume that the dependence is only through two of the invariants, namely, the mean stress

$$\sigma_m = \frac{1}{3} \mathrm{tr} \, \sigma,$$

and the effective stress

$$\sigma_{c} = \sqrt{\frac{1}{2} \mathbf{S} \cdot \mathbf{S}},$$

where S is the deviator of σ .

Then, the strain tensor (or the strain-rate tensor, depending on whether we are dealing with nonlinear infinitesimal elasticity or viscosity) ε , which is required to satisfy the compatibility relations

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

in terms of the displacement (or velocity field) u, is related to the stress σ , satisfying the equilibrium equations

$$\sigma_{ijj} = 0, \tag{2.4}$$

via the constitutive relation

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$$\varepsilon_{ij} = \frac{\partial U}{\partial \sigma_{ij}}(\sigma, \mathbf{x}).$$
 (2.5)

The commas in (2.3) and (2.4) denote differentiation, and the summation convention has also been used in (2.4). We assume that the phases are perfectly bonded, so that the displacement (or velocity) is continuous across the interphase boundaries. However, the strains and, therefore, the stresses may be discontinuous across such boundaries, and hence (2.4) must be interpreted in a weak sense, requiring continuity of the traction components of the stress across the interphase boundaries. Also, at least one of the phase potentials is assumed to be non-quadratic in the stress, so that the constitutive response of the material as given by (2.5) is genuinely nonlinear.

The statement of the problem is completed by the selection of an appropriate boundary condition:

$$\sigma_{ij}n_j = \hat{\sigma}_{ij}n_j, \quad \mathbf{x} \in \partial\Omega, \tag{2.6}$$

where $\partial\Omega$ denotes the boundary of the composite, n is its unit outward normal, and σ is a given constant symmetric tensor. This uniform constraint condition has some useful properties, discovered by HILL (1963). Let

$$\bar{\sigma} = \int_{\Omega} \sigma(\mathbf{x}) \, \mathrm{d}V, \qquad (2.7)$$

and

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$$\bar{\varepsilon} = \int_{\Omega} \varepsilon(\mathbf{x}) \, \mathrm{d} V \tag{2.3}$$

denote the respective averages of the *actual* stress and strain fields in the composite. Here, the scale of Ω has been normalized to have unit volume. Then, we have that

$$\ddot{\sigma} = \dot{\sigma}, \tag{2.9}$$

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and

$$\tilde{\boldsymbol{\varepsilon}} = \frac{1}{2} \int_{in} \left(\mathbf{u} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u} \right) dS.$$
 (2.10)

This means that the average stress $\bar{\sigma}$ in the composite is precisely $\dot{\sigma}$, and that the average strain $\bar{\varepsilon}$ can be "measured" in terms of the boundary displacements.

The third property makes use of the principle of minimum complementary energy, which is a variational characterization of the above problem, described by (2.3) to (2.5), and was first introduced by HILL (1956), under the assumption of strict convexity of the nonlinear potential $U(\sigma, x)$. Thus, we define the effective energy for the composite via the relation

$$\vec{U}(\vec{\sigma}) = \inf_{\sigma \in S(\vec{\sigma})} \vec{U}(\sigma), \qquad (2.11)$$

where

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$$\bar{U}(\sigma) = \int_{\Omega} U(\sigma, \mathbf{x}) \,\mathrm{d}V$$

is the complementary energy functional of the problem at hand, and

$$S(\bar{\sigma}) = \{\sigma | \sigma_{ij,j} = 0 \text{ in } \Omega, \text{ and } \sigma_{ij} n_j = \bar{\sigma}_{ij} n_j \text{ on } \partial \Omega \}$$

is the set of statically admissible stresses. Then, if $\vec{U}(\vec{\sigma})$ is assumed to be differentiable, it can be readily shown that

$$\bar{\varepsilon}_{ij} = \frac{\partial \bar{U}}{\partial \bar{\sigma}_{ij}}(\bar{\sigma}), \qquad (2.12) \qquad \text{over set}$$

which yields an effective constitutive relation for the composite in terms of the average variables $\bar{\sigma}$ and $\bar{\epsilon}$. Given this connection between the effective potential for the composite $\bar{U}(\bar{\sigma})$ and the effective stress/strain relation, it makes sense to seek information on $\bar{U}(\bar{\sigma})$. Notice that, under the above assumptions, $\bar{U}(\bar{\sigma})$ is convex (refer to, for instance, Appendix A of PCW).

A dual formulation can be given by means of the principle of minimum potential energy in terms of the strain potential $W(\varepsilon, x)$, which is obtained from the stress potential $U(\sigma, x)$ via the Legendre (Fenchel) transformation

$$W(\varepsilon, \mathbf{x}) = \sup_{\underline{\sigma}} \left\{ \sigma \cdot \varepsilon - U(\sigma, \mathbf{x}) \right\}.$$
(2.13)

Thus, if we define the effective strain potential of the composite via

$$\tilde{W}(\tilde{\varepsilon}) = \inf_{\substack{\varepsilon \in K(t) \\ \varepsilon \in K(t)}} \tilde{W}(\varepsilon), \qquad (2.14)$$

where $\bar{W}(\varepsilon)$ is the pertinent potential energy functional, and

$$K(\bar{z}) = \{ z | z_{ij} = 1/2(u_{i,j} + u_{j,j}) \text{ in } \Omega, \text{ and } u_i = \bar{z}_{ij} x_j \text{ on } \partial \Omega \}$$

is the set of kinematically admissible strains satisfying a uniform strain boundary condition, we have an effective stress/strain relation for the composite, expressed by

$$\bar{\sigma}_{ij} = \frac{\partial \bar{W}}{\partial \bar{\varepsilon}_{ij}}(\bar{\varepsilon}), \qquad (2.15) \qquad \text{out-BAN}$$

where now \bar{s} , representing the average strain in the composite, is equal to the prescribed uniform strain on the boundary, and $\bar{\sigma}$, representing the average stress, can be "measured" in terms of the traction on the boundary. Notice that $\tilde{W}(\bar{s})$ is also convex.

The above development suggests that $\tilde{W}(\bar{z})$ and $\tilde{U}(\bar{\sigma})$ could also be related through the Legendre transformation:

$$\tilde{W}(\bar{\varepsilon}) = \sup_{\tilde{\omega}} \left\{ \bar{\sigma} \cdot \bar{\varepsilon} - \tilde{U}(\bar{\sigma}) \right\}.$$
(2.16)

However, this is certainly not true for a general heterogeneous material, since the boundary conditions associated with the two formulations are different (uniform traction versus uniform strain), and hence $\tilde{U}(\bar{\sigma})$ and $\tilde{W}(\bar{s})$ would correspond to the solutions of different problems. In fact, WILLIS (1990) has shown that replacing the uniform traction boundary condition in $S(\bar{\sigma})$ by the condition that the stresses have

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mean value $\tilde{\sigma}$ gives exact duality. This implies that, in general, the equality (=) in (2.16) must be replaced by an inequality (\geq). On the other hand, it seems reasonable that in the limit of the microscale tending to zero (the homogenized limit), the response of the composite would be the same for both types of boundary conditions, and thus $\hat{U}(\hat{\sigma})$ and $\hat{W}(\hat{\epsilon})$ are expected to be Legendre duals in that limit. A rigorous proof of this fact, however, would involve a more rigorous definition of the homogenized limit than we have utilized, and is beyond the scope of this work.

At this point, a few remarks are in order. First of all, it should be noted that the three properties (2.9), (2.10) and (2.12) (or the corresponding ones in the dual formulation) hold true for any heterogeneous material, whether it is a "composite" in the sense described above, or not. However, $\tilde{U}(\tilde{\sigma})$ is expected to represent the effective properties of some idealized homogeneous material, obtained as an appropriately defined mathematical limit of a sequence of heterogeneous materials with vanishingly small microscale. Now, if the microstructure of the composite is deterministic as in a periodic composite, $\tilde{U}(\bar{\sigma})$ can (in principle) be determined uniquely in terms of the solution of a nonlinear boundary problem on a unit cell with periodic boundary conditions (MARCELLINI, 1978). On the other hand, if the microstructure of the composite is random, usually only partial statistical information is available in the form of the volume fractions of the phases, or, less frequently, some higher-order information such as overall isotropy for the composite. It is then not possible to determine the effective properties of any given composite precisely, and it is essential to refinterpret $\tilde{U}(\bar{\sigma})$ as the set of effective energies of a family of composites with some prescribed statistics of the microstructure. In any event, whether the composite is periodic and its effective properties are difficult to find, or random so that its properties are not deterministic, it makes sense to attempt to delimit the effective behavior of composites by specifying bounds for $\overline{U}(\vec{\sigma})$ in terms of some prescribed microstructural information. In some cases, as when the bounds are too far apart to be useful, it may be possible to identify a special solution, called an estimate, that in some sense best characterizes the properties of a certain family of composites. In this work, we will only be interested in the case of composites for which the volume fractions of the constituent phases are specified, and that are, in addition, isotropic in an overall sense. In the sequel, we will attempt to specify bounds and estimates for the effective properties of this class of nonlinear composites.

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3. THE NEW VARIATIONAL STRUCTURE

In this section, we make use of a linear heterogeneous "comparison" material, with effective properties that can be characterized in terms of bounds and estimates, to obtain corresponding bounds and estimates for the effective properties of a nonlinear composite. To this end, we introduce the following quadratic potential

$$\hat{U}(\sigma, \mathbf{x}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) \hat{U}^{(r)}(\sigma) = \frac{1}{6\hat{\mu}(\mathbf{x})} \sigma_{e}^{2} + \frac{1}{2\hat{\kappa}(\mathbf{x})} \sigma_{m}^{2}, \qquad (3.1)$$

where

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$$\hat{\mu}(\mathbf{x}) = \sum_{i=1}^{n} \chi^{(i)}(\mathbf{x}) \hat{\mu}^{(i)} > 0$$
, and $\hat{\kappa}(\mathbf{x}) = \sum_{i=1}^{n} \chi^{(i)}(\mathbf{x}) \hat{\kappa}^{(i)} > 0$,

with the $\mu^{(n)}$ and $\kappa^{(n)}$ constant, corresponding to a linear isotropic composite with the same phase distribution (the same characteristic functions) as the nonlinear composite.

Then, if the nonlinearity in the potential of the original composite is stronger than quadratic as the norm of the stress becomes large, it makes sense to define the set of functions

$$V^{(\prime)}(\dot{\mu}^{(\prime)}, \dot{\kappa}^{(\prime)}) = \sup_{\mathcal{L}} \{ \hat{U}^{(\prime)}(\sigma) - U^{(\prime)}(\sigma) \}, \qquad (3.2)$$

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such that

$$V(\hat{\mu}, \hat{\kappa}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) V^{(r)}(\hat{\mu}^{(r)}, \hat{\kappa}^{(r)}) = \sup_{\sigma} \{ \hat{U}(\sigma, \mathbf{x}) - U(\sigma, \mathbf{x}) \}.$$
(3.3)

It follows that, for all $\hat{\mu}^{(r)}$, $\hat{\kappa}^{(r)} > 0$ (r = 1, ..., n) and σ , at each $x \in \Omega$

$$U(\sigma, \mathbf{x}) \ge \tilde{U}(\sigma, \mathbf{x}) - V(\hat{\mu}, \hat{\kappa}),$$

and hence that for all $\dot{\mu}^{(r)}$, $\dot{\kappa}^{(r)} > 0$ (r = 1, ..., n), and for every $\bar{\sigma}$

$$\tilde{U}(\bar{\sigma}) \ge \tilde{U}(\bar{\sigma}) - \vec{V}(\hat{\mu}, \hat{\kappa}), \qquad (3.4)$$

where

$$\tilde{\tilde{U}}(\bar{\sigma}) = \inf_{\sigma \in S(d)} \tilde{\tilde{U}}(\sigma) \tag{3.5}$$

is the effective potential of the linear composite, and

$$\bar{V}(\hat{\mu}, \hat{x}) = \sum_{r=1}^{n} c^{(r)} V^{(r)}(\hat{\mu}^{(r)}, \hat{x}^{(r)}),$$

expressed in terms of the volume fractions of each phase,

 $c^{(r)} = \int_{\Omega} \chi^{(r)}(\mathbf{x}) \,\mathrm{d} V.$

Thus, if we could compute $\tilde{U}(\bar{\sigma})$ for the linear composite in terms of $\hat{\mu}^{(\prime)}$ and $\hat{\kappa}^{(\prime)}$, expression (3.4) yields a family of bounds for the effective potential of the nonlinear composite, $\bar{U}(\bar{\sigma})$, for every choice of the set of parameters $\hat{\mu}^{(\prime)}$, $\hat{\kappa}^{(\prime)} > 0$. This family of bounds can be optimized by considering

$$\vec{U}_{-}(\vec{\sigma}) = \sup_{\vec{\mu}^{m}, \vec{\kappa}^{m} > 0} \{ \vec{\tilde{U}}(\vec{\sigma}) - \vec{\mathcal{V}}(\vec{\mu}, \vec{\kappa}) \}.$$
(3.6)

Then, evidently,

$$\tilde{U}(\bar{\sigma}) \ge \tilde{U}_{-}(\bar{\sigma}). \tag{3.7}$$

Usually, however, it is not possible to find $\tilde{U}(\tilde{\sigma})$ explicitly, but instead bounds and estimates may be available for $\tilde{U}(\tilde{\sigma})$. If we have a lower bound (such as a Hashin-Shtrikman lower bound) $\tilde{U}_{-}(\tilde{\sigma})$ for $\tilde{U}(\tilde{\sigma})$, such that

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 $\vec{U}(\vec{a}) \ge \vec{U}_{\perp}(\vec{a}),$ (3.8)

then, replacing $\hat{U}(\bar{\sigma})$ by $\hat{U}_{-}(\bar{\sigma})$ in (3.6) for $\hat{U}_{-}(\bar{\sigma})$, still yields a lower bound for $\tilde{U}(\bar{\sigma})$; alternatively, an upper bound for $\tilde{U}(\bar{\sigma})$ is not useful in terms of obtaining an upper bound for $\tilde{U}(\bar{\sigma})$. On the other hand, if we only have an estimate (such as a selfconsistent estimate) $\tilde{U}_{+}(\bar{\sigma})$ for $\tilde{U}(\bar{\sigma})$, then

$$\tilde{U}_{\epsilon}(\tilde{\sigma}) = \sup_{\tilde{\mu}^{m}, \tilde{\kappa}^{m} > 0} \left\{ \tilde{\tilde{U}}_{\epsilon}(\tilde{\sigma}) - \tilde{V}(\hat{\mu}, \hat{\kappa}) \right\}$$
(3.9)

would provide only an estimate for $\tilde{U}(\bar{\sigma})$.

We note that the prescriptions (3.6) and (3.9) lead to convex expressions for the bounds and estimates of the effective potential of the nonlinear composite, provided that the corresponding bounds and estimates for the linear composite are convex, which is in turn guaranteed assuming that $\hat{\mu}$ and $\hat{\kappa} > 0$. This is a desirable feature, because the effective potential of the composite is known to be convex, and it follows directly from the convexity of $\hat{U}(\vec{\sigma})$ in $\vec{\sigma}$ (the supremum of a family of convex functions is convex).

Although this will not apply to the present work, it is possible that, in other physical contexts, the nonlinearity of the potential for the composite will be weaker than quadratic. In this case, upper bounds $\vec{U}_+(\vec{\sigma})$ of the form (3.6) and estimates $\vec{U}_e(\vec{\sigma})$ of the form (3.9) would be obtained for $\vec{U}(\vec{\sigma})$, if we replaced the suprema by infima in the definitions (3.2), and the expressions (3.6) for the bound, and (3.9) for the estimate, respectively. In either case, it is important to note that the given prescriptions for the bounds and estimates involve only the evaluation of the extreme values of some multidimensional functions, assuming that the corresponding information is available for the linear comparison material.

Before we apply the general procedure developed in this section to some special cases, we show that there is no *duality gap* in our procedure. This is unlike the procedure of TW, which sometimes leads to different bounds and estimates for the effective energy of the nonlinear composite, depending on whether a formulation based on the principle of minimum complementary energy, or on the principle of minimum potential energy is selected.

Using a procedure completely analogous to the above procedure, but starting with the minimum potential energy formulation, instead of the minimum complementary energy formulation, we are led to the following upper bound for the effective potential $\tilde{W}(\tilde{s})$:

$$\tilde{W}_{+}(\tilde{\varepsilon}) = \inf_{\mu^{(m_{\chi},\kappa^{(m)})} \in \emptyset} \left\{ \tilde{W}(\tilde{\varepsilon}) + \tilde{V}(\hat{\mu},\hat{\kappa}) \right\}, \tag{3.10}$$

where

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$$\vec{\tilde{W}}(\vec{\epsilon}) = \inf_{\epsilon \in K(\ell)} \vec{\tilde{W}}(\epsilon), \qquad (3.11)$$

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and

$$\mathcal{V}(\hat{\mu}, \hat{\kappa}) = \sup \left\{ \mathcal{W}(\boldsymbol{\varepsilon}, \mathbf{x}) - \hat{\mathcal{W}}(\boldsymbol{\varepsilon}, \mathbf{x}) \right\}.$$
(3.12)

Notice that the use of the same notation for the difference function $V(\hat{\mu}, \hat{\kappa})$ is justified,

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because, as the following development shows, this present definition of $V(\hat{\mu}, \hat{\kappa})$ is in exact agreement with the prior definition (3.3) of $V(\hat{\mu}, \hat{\kappa})$. Thus,

$$V(\hat{\mu}, \hat{\kappa}) = \sup_{t} \left\{ \sup_{t} \{ \sigma \cdot \varepsilon - U(\sigma, x) \} - \hat{W}(\varepsilon, x) \right\}$$
$$= \sup_{t} \left\{ \sup_{t} \{ \sigma \cdot \varepsilon - \hat{W}(\varepsilon, x) \} - U(\sigma, x) \right\}$$
$$= \sup_{t} \{ \hat{U}(\sigma, x) - U(\sigma, x) \},$$

where we have used the fact that the order of suprema may be interchanged.

To demonstrate that there is no duality gap in the above procedure, we start with the upper bound for the effective strain potential of the composite

$$\bar{W}(\bar{\varepsilon}) \leqslant \bar{W}_{+}(\bar{\varepsilon}). \tag{3.13}$$

Then, applying the Legendre transformation to both sides of this inequality, we get (see VAN TIEL, 1984, Section 6.3a)

$$\tilde{U}(\hat{\sigma}) \ge \sup \left\{ \hat{\sigma} \cdot \tilde{\varepsilon} - \tilde{W}_{+}(\tilde{\varepsilon}) \right\},$$

where we have made use of (2.16), and the fact that both $\tilde{W}(\tilde{\epsilon})$ and $\tilde{U}(\tilde{\sigma})$ are convex. Next note, from (3.6), that

where we have made use of some of the properties of infima and suprema, and assumed that duality in the form of (2.16) also applies for the linear composite. Thus, we conclude that the two bounds obtained above for the effective energy of the nonlinear composite (one arising from the potential energy principle, and the other from the complementary energy principle) are equivalent, and hence there is no duality gap. More generally, we can apply the same ideas to the specialized versions of the bounds, and again we would obtain exact duality of the bounds, even for a general (not necessarily a "composite") heterogeneous material. For instance, if we replace $\tilde{U}(\bar{\sigma})$ by its linear HS lower bound, and $\tilde{W}(\bar{s})$ by its linear HS upper bound, then the exact duality of the linear HS bounds translates into exact duality for the nonlinear bounds. A more formal development of these ideas, with some additional results, is given in PONTE CASTAÑEDA (1990).

4. APPLICATIONS

4.1. The porous composite

In this sub-section, we apply the general procedure of Section 3 to a two-phase isotropic composite with one vacuous phase. We take the other phase to be incompressible, with potential P. P. CASTANEDA

$$U^{(1)}(\sigma) = f(\sigma_{\epsilon}), \tag{4.1}$$

where f is a strictly convex function of its argument with stronger than quadratic growth as the argument becomes large. Then, the stress/strain relation for this phase is given by

$$\varepsilon_{ij} = \frac{3}{2} \frac{f'(\sigma_i)}{\sigma_i} S_{ij}, \qquad (4.2)$$

so the the effective strain, $\varepsilon_r = \sqrt{\frac{1}{2}e \cdot e}$ (e is the deviator of ε), is related to the effective stress via

 $\varepsilon_{\epsilon} = \frac{1}{2}f'(\sigma_{\epsilon}).$

On the other hand, the potential of the vacuous phase is given by

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 $U^{(2)}(\sigma) = \delta_0(\sigma_c) + \delta_q(\sigma_m)$ (4.3) $\delta_0(x) = \begin{cases} 0 & \text{if } x = 0 \\ \infty & \text{otherwise.} \end{cases}$

Now, if we let

 $\hat{U}^{(1)}(\sigma) = \frac{1}{6\hat{\mu}^{(1)}}\sigma_{e}^{2}$ (4.4)

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where

 $\hat{U}^{(2)}(\sigma) = \delta_0(\sigma_{e})_{\mu} + \frac{\delta_0(\sigma_{me})}{1 + \delta_0(\sigma_{me})}$ (4.5)

$$V^{(1)}(\hat{\mu}^{(1)}) = \frac{1}{2}\sigma f'(\sigma) - f(\sigma), \qquad (4.6)$$

where σ is some function of $\hat{\mu}^{(1)}$ determined by the optimization problem (3.2), and also that

$$V^{(2)}(\hat{\mu}^{(2)}) = 0. \tag{4.7}$$

It follows from (3.6) that

$$\tilde{U}_{-}(\hat{\sigma}) = \sup_{\vec{\mu}^{(0)} = 0} \{ \tilde{\tilde{U}}(\tilde{\sigma}) - c^{(1)} V^{(1)}(\hat{\mu}^{(1)}) \}, \qquad (4.8)$$

provides a general lower bound for $\tilde{U}(\sigma)$ given $\tilde{U}(\sigma)$. As discussed previously, in general, we do not know $\tilde{U}(\sigma)$ precisely. Here, we will make use of the Voigt and lower Hashin-Shtrikman (HS) bounds for $\tilde{U}(\sigma)$ to obtain corresponding bounds for $\tilde{U}(\sigma)$. Additionally, we will provide a self-consistent (SC) estimate for $\tilde{U}(\sigma)$ in terms of the well-known SC estimate for $\tilde{U}(\sigma)$.

4.1.1. Voigt bound. For the linear composite with one vacuous phase, it is known that

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$$\vec{\tilde{U}}(\vec{\sigma}) \geqslant \frac{1}{6\dot{\mu}_{r}}\vec{\sigma}_{r}^{2},$$

where $\hat{\mu}_{\nu} = c^{(1)}\hat{\mu}^{(1)}$. Therefore, from relation (4.8), we have that

$$\tilde{\mathcal{D}}(\bar{\sigma}) \ge c^{(1)} \sup_{\mu^{(1)} > 0} \left\{ \frac{1}{6\bar{\mu}^{(1)}} s^2 - \mathcal{V}^{(1)}(\bar{\mu}^{(1)}) \right\}$$
$$= c^{(1)} f(s), \qquad (4.9)$$

where

$$s = \bar{\sigma}_e / c^{(1)}, \qquad (4.10)$$

and where we have made use of the result of the Appendix, and hence we must further assume that F(x) = f(s) is a convex function of $x = s^2 > 0$. The result expressed by (4.9) and (4.10) is precisely the nonlinear Voigt bound, which could alternatively be obtained from the principle of minimum potential energy by assuming a uniform strain field throughout the composite, and dualizing the result. Thus, at least in this simple case, the new procedure reproduces the "right" result, exactly.

4.1.2. Hashin-Shtrikman bound. For linear isotropic composites, HASHIN and SHTRIKMAN (1962) found upper and lower bounds that are tighter than the Voigt/ Reuss bounds. The lower bound for our particular example specializes to

$$\tilde{\tilde{U}}(\bar{\sigma}) \geq \frac{1}{6\hat{\mu}_{HS}}\bar{\sigma}_{\epsilon}^2 + \frac{1}{2\hat{\kappa}_{HS}}\bar{\sigma}_{m}^2,$$

where

$$\hat{\mu}_{HS} = \frac{c^{(1)}\hat{\mu}^{(1)}}{1+\frac{2}{3}c^{(2)}}$$
 and $\hat{\kappa}_{HS} = \frac{4}{3}\frac{c^{(1)}}{\mathbf{f}c^{(2)}}\hat{\mu}^{(1)}$.

Then, a bound of the form (4.9) applies, where now

$$s = \frac{1}{c^{(1)}} \sqrt{(1 + \frac{2}{3}c^{(2)})\bar{\sigma}_{e}^{2} + \frac{9}{4}c^{(2)}\bar{\sigma}_{m}^{2}},$$
 (4.11)

and again we have made use of the result of the Appendix. Because this bound was derived from the linear HS bound, we refer to it as the nonlinear HS bound. Note that, unlike the Voigt bound, it predicts overall compressibility for the composite, as expected physically.

4.1.3. Self-consistent estimate. For linear isotropic composites, BUDIANSKY (1965) and HILL (1965) provided the so-called SC estimates for the effective moduli. In this particular case, these estimates specialize to

$$\tilde{\vec{U}}(\bar{\sigma}) \approx \frac{1}{6\hat{\mu}_{sc}} \bar{\sigma}_{e}^{2} + \frac{1}{2\hat{\kappa}_{sc}} \bar{\sigma}_{m}^{2},$$

where

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$$\dot{\mu}_{sc} = \frac{(1-2c^{(2)})}{(1-c^{(2)}/3)}\dot{\mu}^{(1)}, \text{ and } \dot{\kappa}_{sc} = \frac{4}{3}\frac{c^{(1)}}{c^{(2)}}\frac{(1-2c^{(2)})}{(1-c^{(2)}/3)}\dot{\mu}^{(1)}.$$

Then

$$\vec{U}(\vec{\sigma}) \approx c^{(1)} f(s),$$

where now

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$$s = \sqrt{\frac{1}{c^{(1)}}} \frac{4}{c^{(2)}} \left(\frac{1 - c^{(2)}/3}{1 - 2c^{(2)}} \right) \left(\bar{\sigma}_r^2 + \frac{9}{4} \frac{c^{(2)}}{c^{(1)}} \bar{\sigma}_m^2 \right)}, \tag{4.12}$$

and once again we have made use of the Appendix. We refer to this result as the nonlinear SC estimate.

4.2. The two-phase incompressible composite

In this sub-section, we consider a general two-phase composite with isotropic, incompressible and nonlinear phases such that

$$U^{(r)}(\sigma) = f^{(r)}(\sigma_e), \quad (r = 1, 2),$$
 (4.13)

where the $f^{(r)}$ satisfy the same convexity conditions of the previous section. Then if we let

$$\hat{U}^{(r)}(\sigma) = \frac{1}{6\mu^{(r)}}\sigma_{\epsilon}^{2}, \qquad (4.14)$$

we have that

$$Y^{(r)}(\hat{\mu}^{(r)}) = \frac{1}{2}\sigma^{(r)}f^{(r)}(\sigma^{(r)}) - f^{(r)}(\sigma^{(r)}), \qquad (4.15)$$

where the $\sigma^{(r)}$ are some functions of the $\hat{\mu}^{(r)}$ that are determined by the solution of the optimization problem (3.2). It follows that

$$\tilde{U}_{-}(\tilde{\sigma}) = \sup_{\vec{\mu}^{(1)}, \vec{\mu}^{(2)} > 0} \left\{ \tilde{\tilde{U}}(\tilde{\sigma}) - c^{(1)} V^{(1)}(\hat{\mu}^{(1)}) - c^{(2)} V^{(2)}(\hat{\mu}^{(2)}) \right\}$$
(4.16)

is a general lower bound for $\tilde{U}(\sigma)$, given $\tilde{\tilde{U}}(\sigma)$. As in the previous sub-section, we use this result to obtain the Voigt bound, a HS bound and a SC estimate for the effective potential of the nonlinear composite in terms of the corresponding results for the linear composite.

4.2.1. Voigt bound. In this case, it is more convenient to consider the dual formulation. For the linear composite, we have that

$$\hat{W}(\tilde{\varepsilon}) \leq \frac{2}{3} \hat{\mu}_{F} \tilde{\varepsilon}_{e}^{2} + \delta_{0}(\tilde{\varepsilon}_{m}), \qquad (4.17)$$

where $\hat{\mu}_r = c^{(1)}\hat{\mu}^{(1)} + c^{(2)}\hat{\mu}^{(2)}$. Then, it can easily be shown that

$$\bar{W}(\bar{s}) \leq c^{(1)} W^{(1)}(\bar{s}) + c^{(2)} W^{(2)}(\bar{s}), \qquad (4.18)$$

where we have made use of the appropriate specialization of (3.10), and a dual version

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of the result of the Appendix. As in the previous example, this result agrees exactly with the nonlinear Voigt bound.

4.2.2. Hashin-Shirikman bounds. For the linear composite, we have

$$\vec{U}(\vec{\sigma}) \ge \frac{1}{6\hat{\mu}_{HS}} \vec{\sigma}_{\epsilon}^2, \qquad (4.19)$$

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where

$$\hat{\mu}_{HS} = \frac{c^{(1)}\hat{\mu}^{(1)}(6\hat{\mu}^{(2)}+9\hat{\mu}) + c^{(2)}\hat{\mu}^{(2)}(6\hat{\mu}^{(1)}+9\hat{\mu})}{c^{(1)}(6\hat{\mu}^{(2)}+9\hat{\mu}) + c^{(2)}(6\hat{\mu}^{(1)}+9\hat{\mu})}$$

and $\hat{\mu} = \max{\{\hat{\mu}^{(1)}, \hat{\mu}^{(2)}\}} = \hat{\mu}^{(1)}$ (by assumption). Then, it follows that

$$\tilde{U}(\bar{\sigma}) \ge \sup_{\mu^{(1)}, \mu^{(2)} > 0} \left\{ \frac{1}{6\bar{\mu}_{HS}} \bar{\sigma}_{e}^{2} - c^{(1)} V^{(1)}(\bar{\mu}^{(1)}) - c^{(2)} V^{(2)}(\bar{\mu}^{(2)}) \right\}$$
(4.20)

but, unfortunately, no further simplification is possible in general, due to the coupling of $\hat{\mu}^{(1)}$ and $\hat{\mu}^{(2)}$ in the term involving $\hat{\mu}_{HS}$. Later we will apply this result to a special case where $f^{(1)}, f^{(2)}$ have a simple power-law form.

4.2.3. Self-consistent estimates. The results for the SC estimates have the same forms (4.19) and (4.20) as the HS bounds, but with $\dot{\mu}_{HS}$ replaced by $\dot{\mu}_{SC}$, given by the positive root of the expression

$$3\hat{\mu}_{sc}^{2} + \{(2-5c^{(1)})\hat{\mu}^{(1)} + (2-5c^{(2)})\hat{\mu}^{(2)}\}\hat{\mu}_{sc} - 2\hat{\mu}^{(1)}\hat{\mu}^{(2)} = 0.$$
(4.21)

As was the case for the HS bound, these results cannot be simplified further without specifying in more detail the constitutive behavior of the phase materials.

4.3. The composite reinforced by rigid inclusions

This is a special case of the previous material with $f^{(1)}(\sigma_r) = 0$, corresponding to the case where phase #1 is rigid. Then, the choice $\tilde{U}^{(1)}(\sigma) = 0$ leads to $\mathcal{V}^{(1)}(\hat{\mu}^{(1)}) = 0$, and we have the following general lower bound for the effective energy of the composite:

$$\tilde{U}(\bar{\sigma}) \ge \sup_{\mu^{2} \to 0} \{ \tilde{U}(\bar{\sigma}) - c^{(2)} V^{(2)}(\mu^{(2)}) \}.$$
(4.22)

In this case, however, it is clear that the lower bounds are trivial, and we will only be able to give estimates for the effective energy of the composite. We will consider the standard SC estimate, as well as a differential self-consistent (DSC) estimate.

4.3.1. Self-consistent estimate. For the linear composite, it is known that

$$\tilde{\vec{U}}(\vec{\sigma}) \approx \frac{1}{6\hat{\mu}_{sc}} \, \vec{\sigma}_{\epsilon}^2, \tag{4.23}$$

where

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 $\hat{\mu}_{SC} = \frac{\hat{\mu}^{(2)}}{(1 - \frac{1}{2}c^{(1)})} \quad (c^{(1)} < \frac{1}{5}).$

Using this result in the general expression (4.22) induces a nonlinear SC estimate for the effective energy

$$\tilde{U}(\vec{\sigma}) \approx c^{(2)} f^{(2)}(s),$$
 (4.24)

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where

$$s = \left(\frac{1 - \frac{5}{2}c^{(1)}}{c^{(2)}}\right)^{1/2} \bar{\sigma}_{\epsilon}, \tag{4.25}$$

and once again we have made use of the result in the Appendix.

4.3.2. Differential self-consistent estimate. The DSC estimates of BOUCHER (1974), and MCLAUGHLIN (1975) for linear elastic composites specialize in this case to expression (4.23), with $\hat{\mu}_{SC}$ replaced by

$$\hat{\mu}_{DSC} = \frac{\hat{\mu}^{(2)}}{(c^{(2)})^{5/2}}.$$
(4.26)

This induces a nonlinear DSC estimate via (4.22) that reduces to an expression similar to (4.24), where now

$$s = (c^{(2)})^{3/4} \bar{\sigma}_e. \tag{4.27}$$

5. RESULTS FOR POWER-LAW MATERIALS

In this section, we specialize further the calculations of the previous section by taking the constitutive behavior of the phases to be governed by a power law relation

$$f^{(r)}(\sigma_{e}) = \frac{1}{3} \left(\frac{2}{n+1} \right) \frac{1}{(2\mu^{(r)})^{n}} \sigma_{e}^{n+1}.$$
 (5.1)

This class of functions clearly satisfies all the assumptions invoked in Sections 3 and 4, including the convexity assumption of the Appendix. Additionally, we compare the new results for the bounds and estimates with previously available results.

5.1. The porous material

In this case, our results for the Voigt bound, the HS bound and the SC estimate all take the simple form of expression (4.9), with s given by (4.10), (4.11) and (4.12), respectively. We compare these results with the results of PCW for the same material. We note, however, that WILLIS (1989) has given a HS bound and several SC estimates for the general case considered in Section 4.1, but the form of his results is more complicated than our new results. For this reason, and because we expect the comparison of the power-law results to be fairly representative, we do not make a more

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general comparison between our new results and those of WILLIS (1989). There are two domains of particular interest: the low-triaxiality range corresponding to $\omega = |\tilde{\sigma}_m/\bar{\sigma}_r| \ll 1$, and the high-triaxiality range corresponding to $\omega \gg 1$.

For low-triaxiality, all the results for the bounds and estimates take the form

$$\bar{U}(\bar{\sigma}) \approx \frac{1}{3} \left(\frac{2}{n+1} \right) \frac{1}{(2\bar{\mu})^n} [1 + b(c^{(2)}, n)\omega^2] \bar{\sigma}_r^{n+1}, \qquad (5.2)$$

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and it suffices to compare all the corresponding values of the low-triaxiality modulus $\tilde{\mu}$, as functions of $\mu^{(1)}$, $c^{(2)}$ and *n*. We give the results below, where we identify the source of the results in parentheses:



The last expression corresponds to a dilute concentration of voids, and was carried out by DH, who made use of the results of BUDIANSKY *et al.* (1982). The values of f^* , k and x^* as functions of n are taken from that reference.

In the linear limit (n = 1), all the above results agree with the well-known results from the linear theory. For small volume fractions of the vacuous phase $(c^{(2)})$, the HS, SC and dilute results agree to first order, and for larger volume fractions the dilute result lies between the HS upper bound and the SC estimate. Figure 1 gives the results for the bounds and estimates of the effective low-triaxiality moduli $\tilde{\mu}$ as functions of $c^{(2)}$, for two distinct nonlinear cases (n = 3 and 10). These results are similar to the linear results, with the HS upper bounds lying below the Voigt bound, and the SC estimates close to the dilute results for moderate volume fractions, but approaching the same percolation limit $(c^{(2)} = 1/2)$ as the corresponding linear results. Comparing the *new* bound and estimate with those of PCW, we observe that the new results lie slightly below the old results. For the bound, this has the implication that the new bound is an *improvement* on the old bound, at least in the low-triaxiality range. P. P. CASTANEDA





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For high triaxiality, all the results for the bounds and estimates take the form

$$\vec{U}(\vec{\sigma}) \approx \frac{1}{3} \left(\frac{2}{n+1} \right) \frac{1}{(2\vec{\gamma})^n} \left| \frac{3}{2} \vec{\sigma}_m \right|^{n+1}, \qquad (5.4)$$

and thus we express all the results in terms of the high-triaxiality moduli $\tilde{\gamma}$, so that

$$(Voigt) \qquad \frac{\tilde{\gamma}_{V}}{\mu^{(1)}} = \int^{\infty} \int$$

In the linear limit (n = 1), the expressions for the HS bounds and SC estimates reduce to the linear results, and, additionally, they agree in the dilute limit $(\bar{y} \sim (c^{(2)})^{-1})$. Figure 2 depicts plots of the HS bounds and SC and dilute estimates of the hightriaxiality modulus appropriately normalized $((c^{(2)})^{(n+1)/2n}\tilde{\gamma})$ versus the volume fraction of the void phase $(c^{(2)})$ for two values of the nonlinearity parameter (n = 3 and)10). By comparison with the results of PCW, we find that the new results provide a significant improvement over the old results, since the new bounds lie significantly below the old bounds, and are hence tighter. Similarly, the old SC estimate violates the new bound, and must be discarded in favor of the new SC estimate. The dilute result of DH lies below the HS bound for small volume fractions of the void phase $(\tilde{\gamma}_D \sim (c^{(2)})^{-(1/n)})$, whereas $\tilde{\gamma}_{HS} \sim (c^{(2i)})^{-(n+1)/2n}$, but it is clear from the plots that the range of validity of the dilute result is severely limited for larger values of n. On the other hand, we should emphasize that the *new* expressions for y are not valid for small values of $c^{(2)}$. This is because the original expression for $\overline{U}(\overline{\sigma})$, from which they derive, is indeterminate in the limit as $\omega \to \infty$ and $c^{(2)} \to 0$. A better comparison of the new results with the dilute results is accomplished by making use of the original expression for $\vec{U}(\vec{\sigma})$ in the form

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FIG. 2. Bounds and estimates for the high-triaxiality modulus of the porous material as functions of the volume fraction of voids. The continuous lines correspond to the *new* HS upper bound and SC estimate; the long-dash lines correspond to the HS upper bound and SC estimate of PCW; and the short-dash line corresponds to the dilute calculation of DH. Case (a) is for n = 3, and (b) for n = 10.

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$$\tilde{U}(\bar{\sigma}) = \frac{1}{3} \left(\frac{2}{n+1} \right) \frac{1}{(2\bar{\mu}^*)^n} \bar{\sigma}_r^{n+1},$$
(5.6)

where now μ^* is a function of $c^{(2)}$, *n* and ω . Thus, we have that

$$\frac{\tilde{\mu}_{NS}^{*}}{\mu^{(1)}} = \frac{c^{(1)}}{\left[1 + c^{(2)}(\frac{2}{3} + \frac{2}{3}\omega^2)\right]^{(n+1)/2n}},$$
(5.7)

and

$$\frac{\tilde{\mu}_{0}^{*}}{\mu^{(1)}} = \frac{1}{\left[1 + c^{(2)}(n+1)f(\omega, n)\right]^{1/n}},$$
(5.8)

where $f(\omega, n)$ is taken from the work DH.

Written in this form, it is clear that both expressions for the effective energy of the composite are indeterminate in the limit as $\omega \to \infty$ and $c^{(2)} \to 0$. The first expression, however, is general, whereas the second assumes that $c^{(2)} \ll 1$, and its range of validity is not known. Figure 3 shows a comparison of these two results as functions of ω for two values of n (3 and 10) and three values of $c^{(2)}$ (0.1, 0.01 and 0.001). It is apparent that the dilute approximation of DH is acceptable (although this is not a proof that it is correct) for very small values of $c^{(2)}$ in the sense that it does not violate the new bound, but unacceptable for values of $c^{(2)}$ in the order of 1 to 10%, or larger, depending on the specific value of n. On the other hand, it appears that the new bound could conceivably be subject to improvement for very small values of $c^{(2)}$.

. 5.2. The two-phase incompressible composite

In the case when $f^{(1)}$ and $f^{(2)}$ have the same form of (5.1), but with different moduli $\mu^{(1)}$ and $\mu^{(2)}$, respectively, all the results of Section 4.2 take the form

$$\bar{U}(\bar{\sigma}) = \frac{1}{3} \left(\frac{2}{n+1} \right) \frac{1}{(2\bar{\mu})^n} \bar{\sigma}_e^{n+1},$$
(5.9)

and it suffices to compare the bounds and estimates for the effective modulus $\tilde{\mu}$. The Voigt bound is obtained from (4.18), and is given by

$$\frac{\tilde{\mu}_{\mathbf{v}}}{\mu^{(1)}} = c^{(1)} + c^{(2)} \frac{\mu^{(2)}}{\mu^{(1)}}.$$
(5.10)

The new HS bound is obtained by solving the optimization problem given in (4.20); the result is

$$\frac{\tilde{I}_{HS}}{\mu^{(1)}} = \left[c^{(1)} \frac{\tilde{S}_{n+1}}{(1)} + c^{(2)} \left(\frac{\mu^{(1)}}{\mu^{(2)}} \right)^n \frac{\tilde{S}_{n+1}}{(2)} \right]^{-(1/n)}, \qquad (5.11)$$

where $S_{(1)}$ and $S_{(2)}$ satisfy the relations

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$$S - (2 + 3c^{(2)})S_{(2)}]\overline{S_{(1)}}^{-1} = 3c^{(1)} \left(\frac{\mu^{(1)}}{\mu^{(2)}}\right)S_{(2)}^{-1}$$

and

$$15c^{(1)}S^{2}_{(1)} = 6c^{(1)}S_{(2)} + \frac{1}{c^{(1)}}[3 + c^{(2)}(2 - 5S_{(2)})][5 - (2 + 3c^{(2)})S_{(2)}], \quad (5.12)$$

subject to the restriction that

$$\left(\frac{S_{(2)}}{S_{(1)}}\right) > \left(\frac{\mu^{(1)}}{\mu^{(2)}}\right)^{\mu(n-1)}$$

The SC estimate \tilde{y}_{SC} is obtained from (4.20), and the result has the same form as (5.11), but now $S_{(1)}$ and $S_{(2)}$ satisfy

$$c^{(1)}S^{2}_{(1)} + c^{(2)}\frac{\hat{\mu}^{(1)}}{\hat{\mu}^{(2)}}S^{2}_{(2)} = \frac{\hat{\mu}^{(1)}}{\hat{\mu}_{sc}}$$

and

$$\left[3\frac{\hat{\mu}_{sc}}{\hat{\mu}^{(1)}} + (2-5c^{(1)})\right]\frac{\hat{\mu}^{(2)}}{\hat{\mu}^{(1)}} = c^{(2)}\left[6\frac{\hat{\mu}_{sc}}{\hat{\mu}^{(1)}} + (2-5c^{(1)}) + (2-5c^{(2)})\frac{\hat{\mu}^{(2)}}{\hat{\mu}^{(1)}}\right]\frac{\hat{\mu}_{sc}}{\hat{\mu}^{(1)}}S^{2}_{(2)},$$
(5.13)

where

$$\frac{\hat{\mu}^{(1)}}{\hat{\mu}^{(2)}} = \left(\frac{\mu^{(1)}}{\mu^{(2)}}\right)^{n} \left(\frac{S_{(2)}}{S_{(1)}}\right)^{n-1}$$

and $\hat{\mu}_{SC}$ is the positive root of (4.21). Additionally, for this problem we have a non-trivial Reuss lower bound (if $\mu^{(2)} > 0$) given by

$$\frac{\tilde{\mu}_{R}}{\mu^{(1)}} = \left[c^{(1)} + c^{(2)} \left(\frac{\mu^{(1)}}{\mu^{(2)}} \right)^{n} \right]^{-(1/n)}.$$
(5.14)

In the linear limit (n = 1), the above results reduce to the well-known results from the linear theory and additionally there is a HS lower bound for $\tilde{\mu}$. The HS bounds are nested within the Reuss/Voigt bounds, and the SC estimate lies within the HS bounds, agreeing with the HS upper bound for small volume fractions of phase #2 ($c^{(1)}$), and with the HS lower bound for small volume fractions of phase #1 ($c^{(1)} = 1 - c^{(2)}$). As the ratio $\mu^{(2)}/\mu^{(1)}$ becomes smaller, the bounds spread out until eventually (when $\mu^{(2)}/\mu^{(1)} = 0$) the lower bounds become trivial and the SC estimate

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reaches a percolation limit at $c^{(2)} = 3/5$. Figure 4 depicts the corresponding results (except the HS lower bound) for the two usual values of n (3 and 10). By comparison with the linear results (not shown), they roughly show the same trends. However, the following comparisons can be established: the Voigt bound is unaffected; the SC estimate is shifted up for low values of $c^{(2)}$, and down slightly for low values of $c^{(1)}$, with larger values of n; and the Reuss bound is shifted down significantly with larger values of n to the point of being nearly without practical value for large n. Extrapolating from the linear theory, and according to the new results, we expect the SC estimates to be good at predicting the effective moduli of the composite, if $\mu^{(2)}/\mu^{(1)}$ is not too small.

-5.3. The composite reinforced by rigid inclusions

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In this case, as in the previous one, all the results take the form of relation (5.1), where now we no longer have bounds for $\bar{\mu}$, but only estimates, including a SC as well as a DSC estimate.

The SC estimate is obtained from expressions (4.24) and (4.25) and is given by

$$\frac{\bar{\mu}_{sc}}{\mu^{(2)}} = \frac{(c^{(2)})^{(n-1)/2n}}{(1-\frac{1}{2}c^{(1)})^{(n+1)/2n}}.$$
(5.15)

The corresponding result from PCW is given by

$$\frac{\bar{u}_{5C}}{\frac{\bar{u}_{5C}}{c}} = \frac{\left(1 - \frac{7n - 3}{4n}c^{(1)}\right)}{\left(1 - \frac{5}{2}c^{(1)}\right)(c^{(2)})^{1/n}}.$$
(5.16)

Our DSC estimate is obtained from the corresponding linear estimate via expression (4.24), together with (4.27) and is given by

$$\frac{\bar{\mu}_{osc}}{\mu^{(2)}} = \frac{1}{(c^{(2)})^{(3n+7)/4n}}.$$
(5.17)

 D_{UVA} (1984) has also provided a DSC estimate, based on computations for an isolated rigid inclusion in an infinite power-law viscous matrix. The result of his calculation can also be represented in the form of (5.1), with

$$\frac{\tilde{\mu}_{DSC}}{\mu^{(2)}} = \frac{1}{(c^{(2)})^{g(n)/n}},$$
(5.18)

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where g(n) is given in the above reference. From the plot of this function, we obtain that g(1) = 5/2, $g(3) \approx 3.3$ and $g(10) \approx 6.6$.

As before our new results reduce to the linear results in the limit as *n* approaches unity. Figure 5 gives results for the above estimates of the effective modulus for the two usual values of *n* (3 and 10). Note that the plot is given in terms of $\mu^{(2)}/\bar{\mu}$ as a function of $c^{(2)}$, so that $\mu^{(2)}/\bar{\mu}$ tends to zero as $c^{(2)}$ tends to unity. Our SC estimate is slightly lower than the prior result of PCW; this is probably due to the fact that if we had an upper bound, it would also appear lower in our plot. On the other hand, our



Fig. 4. Bounds and estimates for the effective modulus of the two-phase incompressible composite as functions of the volume fractions of phase $\neq 2$ for three different ratios of the moduli of the two phases. The continuous lines correspond to the *new* HS upper bound and SC estimate, and the dotted lines correspond to the Voigt/Reuss bounds. Case (a) is for n = 3, and (b) for n = 10.

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DSC estimate lies somewhat above the DSC of DUVA (1984). This is not too surprising since we expect our procedure in general to **an investimate** the energy of the composite $\tilde{W}(\bar{z})$. For the linear case, it has been shown (MILTON, 1985; AVELLANEDA, 1987) that the DSC estimates can be attained by particular microstructures. Then, we could expect our procedure to give an upper bound for the actual $\tilde{W}(\bar{z})$ of the corresponding nonlinear material. Thus, the present example could be used to assess the efficiency of our method infestimating the exact effective properties of nonlinear composites with deterministic microstructure, such as periodic composites. This idea will be tested elsewhere, but if the indications of the present example are upheld, we would conclude that our prescription performs rather well given its simplicity.

6. CONCLUDING REMARKS

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The main contribution of this work is the establishment of a new variational structure that allows the estimation of the effective properties of nonlinear composites in terms of the corresponding properties for linear composites with the same micro-structural distribution of phases. Assuming that the exact effective energy density is available for the linear composite, and depending on the growth conditions of the phase potentials, the new estimate will either be an upper bound, or a lower bound for the actual effective energy density of the nonlinear composite. Alternatively, if only an estimate or a bound of the right type (an upper bound if the estimate is an upper bound, or vice versa) is available for the linear composite, the new estimate for the nonlinear composite will also be either only an estimate, or a bound (of the same type). In this respect, the present variational structure has the same limitation as the structure proposed by TW in that only one-sided bounds will result in general.

In the context of specific results, we note that the nonlinear bounds, corresponding to the linear Voigt bounds, proposed by the new prescription turn out to be precisely the nonlinear Voigt bounds obtained directly from the principle of minimum potential energy. On the other hand, the nonlinear bounds corresponding to the Hashin-Shtrikman bounds for the linear isotropic composite turn out to be superior in some cases to the Talbot-Willis bounds for the same material, and identical in other cases (see PONTE CASTAÑEDA, 1990, for an example). Finally, whereas the Talbot-Willis structure leads to some ambiguity in the prescription of self-consistent estimates, the new structure leads to a unique prescription for a self-consistent estimate, as well as to a straightforward generalization of other types of estimates, including differential and dilute estimates. The main advantages of the new structure are the simplicity of its implementation and the generality of its potential applications. Clearly, these are features that could make the proposed structure of great practical, as well as theoretical value. A more abstract derivation of this structure is given in PONTE CASTAÑEDA (1990), and some of the potential applications to other types of composites will be addressed elsewhere.

ACKNOWLEDGEMENTS

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Appendix: Exact Duality Between f and $V^{(i)}$

Here we demonstrate that

$$f(s) = \sup_{\mu^{(1)} > 0} \left\{ \frac{1}{6\hat{\mu}^{(1)}} s^2 - \mathcal{V}^{(1)}(\hat{\mu}^{(1)}) \right\}, \qquad (A1)$$

given that

Effective properties of nonlinear composites

$$V^{(1)}(\vec{\mu}^{(1)}) = \sup_{s \to 0} \left\{ \frac{1}{6\vec{\mu}^{(1)}} s^2 - f(s) \right\}.$$
 (A2)

Proof: Let $x = s^2$, and assume that F(x) = f(s) is a convex function of its argument. Then, if we define G(y) via the Legendre transform

$$G(y) = \sup_{x > 0} \{xy - F(x)\},$$
 (A3)

we have by Fenchel duality (VAN TIEL, 1984, Corollary to Section 6.11a) that

$$F(x) = \sup_{y>0} \{xy - G(y)\}.$$
 (A4)

Now, if we let $y = 1/6\hat{\mu}^{(1)}$, (A2) and (A3) imply that

$$G(y) = V^{(1)}(\hat{\mu}^{(1)}),$$
 (A5)

and therefore it follows from (A4) that (1) holds.

Estonse: This result is a special case of a more general result derived in PONTE CASTANEDA (1990).

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Appendix B.

VARIATIONAL ESTIMATES FOR THE EFFECTIVE PROPERTIES OF A POROUS RAMBERG-OSGOOD MATERIAL

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<u>Abstract</u>

A new variational procedure recently developed by Ponte Castañeda [1] for estimating and bounding the effective properties of nonlinear composite materials is applied to an incompressible isotropic matrix containing an isotropic distribution of voids. The uniaxial stress-strain behavior of the matrix is linear up to the *yield* stress, and "linear plus power-hardening" for stresses exceeding the yield level. The solution procedure exploits a useful "comparison" between the effective potential of the nonlinear porous material and that of an appropriately chosen inhomogeneous, linear material. It is important to note that the proposed procedure is different from the procedure advocated by Talbot & Willis [2], which makes use of a linear, but homogeneous comparison material to accomplish the same goal. Results are given in the form of a rigorous lower bound and a self-consistent estimate for the effective potential of the porous material. The results are compared with the results of Willis [3] for the same problem.

Introduction

The theory of linear composites is fairly well developed, including different approaches to the problem. Thus, exact estimates have been determined for the effective properties of ad hoc models for composites; rigorous variational bounds have been given for the properties of random composites; and explicit formulae have been given for the properties of *periodic* composites. Appropriate, but by no means exhaustive, references dealing with the linear theories are provided by [4-6]. By contrast, the theory of nonlinear composites is not very well developed, and most of the results are based on ad hoc models, such as dilute and self-consistent models. For instance, dilute estimates are given in [7] for the effective properties of a nonlinear porous material. The first contribution dealing with the calculation of rigorous bounds for the effective properties of nonlinear composites is provided by the work of Talbot and Willis [2]. These authors extended the well-known Hashin-Shrikman [8] variational principles to include nonlinear constitutive behavior, and their methods have been applied to a number of examples in different physical contexts. For example, bounds and estimates for the effective properties of nonlinearly viscous (or deformationtheory plastic) materials are determined in [3] and [9]. A new variational procedure for estimating the effective properties of nonlinear composite materials was developed recently by Ponte Castañeda [1]. This procedure can be used directly to obtain bounds and estimates for the effective properties of nonlinear composites from any corresponding bounds and estimates that may be available for the effective properties of linear composites with the same distribution of phases. The main advantages of the new procedure over the procedure given by [2] are the simplicity of its implementation, the generality of its potential applications and the strength of the results. In reference [1], the general procedure is also applied to an incompressible isotropic matrix containing

an isotropic distribution of voids, and specific results in the form of a Hashin-Shtrikman bound and a self-consistent estimate are provided for pure-power law behavior for the matrix material. The results for the bounds are found to be stronger than the corresponding bounds given in [9]. In this work, we consider the application of the general result for a porous material for the special case of stress-strain behavior for the matrix which is linear up to the yield stress and linear plus power-hardening for stresses exceeding the yield level. The new results are discussed and compared with the corresponding results of Willis [3].

New Nonlinear Hashin-Shtrikman Bounds and Self-Consistent Estimates

We are interested in estimating the effective properties of composites with nonlinear material behavior. By a "composite" we mean an idealized material that corresponds to the limit of a sequence of heterogeneous materials with two distinct length scales: one microscopic l corresponding to the size of the heterogeneity, and one macroscopic L corresponding to the size of the scale of variation of the boundary conditions. The effective behavior of the composite is then obtained by considering the limiting behavior of the sequence of materials as the ratio of scales $\varepsilon = l/L$ tends to zero.

Consider an *n*-phase composite occupying a domain Ω (normalized to have unit volume), with each phase occupying a sub-domain $\Omega^{(r)}$ (r = 1, 2, ..., n), and let the stress potential,

 $U(\sigma, \mathbf{x})$, be expressed in terms of the *n* homogeneous phase potentials, $U^{(r)}(\sigma)$, via

$$U(\sigma, \mathbf{x}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) U^{(r)}(\sigma), \qquad (1)$$

where

$$\chi^{(r)}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} \in \Omega^{(r)} \\ 0 & \text{otherwise} \end{cases}$$
(2)

is the indicator function of phase r. The phases are assumed to be isotropic, so that the potentials $U^{(r)}(\sigma)$ depend on the stress σ only through its three principal invariants. Here, we will further assume that the dependence is only through two of the invariants, namely, the mean stress,

$$\sigma_m = \frac{1}{3} \text{tr} \sigma$$
, and the effective stress, $\sigma_n = \sqrt{\frac{3}{2} S \cdot S}$, where S is the deviator of σ .

The effective behavior of the composite material is defined, following [10], in terms of the effective energy, $\bar{U}(\bar{\sigma})$, that arises due to the uniform traction boundary condition

$$\sigma_{ij}n_j = \overline{\sigma}_{ij}n_j, \quad \mathbf{x} \in \partial\Omega, \tag{3}$$

where $\partial \Omega$ denotes the boundary of the composite, n is its unit outward normal, and $\overline{\sigma}$ is a given constant symmetric tensor. The average stress in the composite is then precisely $\overline{\sigma}$ and it follows from the principle of minimum complementary energy that

$$\tilde{U}(\overline{\mathbf{\sigma}}) = \min_{\boldsymbol{\sigma} \in S(\overline{\mathbf{\sigma}})} \overline{U}(\mathbf{\sigma}), \tag{4}$$

where

$$\overline{U}(\boldsymbol{\sigma}) = \int_{\boldsymbol{\Omega}} U(\boldsymbol{\sigma}, \mathbf{x}) \, dV$$

is the complementary energy functional of the problem, and

$$S(\overline{\sigma}) = {\sigma | \sigma_{ij,j} = 0 \text{ in } \Omega, \text{ and } \sigma_{ij} n_j = \overline{\sigma}_{ij} n_j \text{ on } \partial \Omega}$$

is the set of statically admissible stresses. Thus, if $\overline{\epsilon}$ denotes the average strain over the composite, it can be readily shown that

$$\bar{\varepsilon}_{ij} = \frac{\partial \tilde{U}}{\partial \sigma_{ij}}(\bar{\sigma}), \tag{5}$$

which yields an effective constitutive relation for the composite in terms of the average variables $\overline{\sigma}$ and $\overline{\epsilon}$. Given this connection between the effective potential for the composite $\tilde{U}(\overline{\sigma})$ and the effective stress/strain relation, it makes sense to seek information on $\tilde{U}(\overline{\sigma})$. Notice that $\tilde{U}(\overline{\sigma})$ is convex.

Next, following [1], we make use of a linear heterogeneous "comparison" material, with effective properties that can be characterized in terms of bounds and estimates, to obtain corresponding bounds and estimates for the effective properties of a nonlinear composite. To this end, we introduce the quadratic potential

$$\hat{U}(\sigma, \mathbf{x}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) \hat{U}^{(r)}(\sigma) = \frac{1}{6\hat{\mu}(\mathbf{x})} \sigma_{*}^{2} + \frac{1}{2\hat{\kappa}(\mathbf{x})} \sigma_{*}^{2},$$
(6)

such that $\hat{\mu}(\mathbf{x}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) \hat{\mu}^{(r)} > 0$, and $\hat{\kappa}(\mathbf{x}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) \hat{\kappa}^{(r)} > 0$, with the $\hat{\mu}^{(r)}$ and $\hat{\kappa}^{(r)}$

constant, corresponding to a linear isotropic composite with the same phase distribution (the same indicator functions) as the nonlinear composite.

Then, if the nonlinearity in the potential of the original composite is stronger than quadratic as the norm of the stress becomes large, it makes sense to define the set of functions

$$W^{(r)}(\hat{\mu}^{(r)}, \hat{\kappa}^{(r)}) = \max_{\sigma} \{ \hat{U}^{(r)}(\sigma) - U^{(r)}(\sigma) \},$$
(7)

such that

$$V(\hat{\mu}, \hat{\kappa}) = \sum_{r=1}^{n} \chi^{(r)}(\mathbf{x}) V^{(r)}(\hat{\mu}^{(r)}, \hat{\kappa}^{(r)}) = \max_{\sigma} \{ \hat{U}(\sigma, \mathbf{x}) - U(\sigma, \mathbf{x}) \}.$$
 (8)

It follows that, for all $\hat{\mu}^{(r)}$, $\hat{\kappa}^{(r)} > 0$ (r = 1, ..., n) and σ , at each $x \in \Omega$

$$U(\sigma,\mathbf{x}) \geq \hat{U}(\sigma,\mathbf{x}) - V(\hat{\mu},\hat{\kappa}),$$

and hence that for all $\hat{\mu}^{(r)}$, $\hat{\kappa}^{(r)} > 0$ (r = 1, ..., n), and for every $\overline{\sigma}$

$$\tilde{U}(\overline{\sigma}) \ge \hat{U}(\overline{\sigma}) - \bar{V}(\hat{\mu}, \hat{\kappa}), \tag{9}$$

where

$$\tilde{\hat{U}}(\overline{\boldsymbol{\sigma}}) = \min_{\boldsymbol{\sigma} \in S(\overline{\boldsymbol{\sigma}})} \overline{\hat{U}}(\boldsymbol{\sigma})$$
(10)

is the effective potential of the linear composite, and

$$\bar{V}(\hat{\mu},\hat{\kappa}) = \sum_{r=1}^{n} c^{(r)} V^{(r)}(\hat{\mu}^{(r)},\hat{\kappa}^{(r)}),$$

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expressed in terms of the volume fractions of each phase,

$$c^{(r)} = \int_{\Omega} \chi^{(r)}(\mathbf{x}) dV.$$

Thus, if we could compute $\tilde{U}(\overline{\sigma})$ for the linear composite in terms of $\hat{\mu}^{(r)}$ and $\hat{\kappa}^{(r)}$, expression (9) yields a family of bounds for the effective potential of the nonlinear composite, $\tilde{U}(\overline{\sigma})$, for every choice of the set of parameters $\hat{\mu}^{(r)}$, $\hat{\kappa}^{(r)} > 0$. This family of bounds can be optimized by considering

$$\vec{U}_{-}(\vec{\sigma}) = \max_{\hat{\mu}^{(\nu)}, \hat{\kappa}^{(\nu)} > 0} \{ \tilde{\vec{U}}(\vec{\sigma}) - \vec{V}(\hat{\mu}, \hat{\kappa}) \}.$$
(11)

Then, evidently,

$$\tilde{U}(\overline{\sigma}) \ge \tilde{U}_{-}(\overline{\sigma}).$$
 (12)

Usually, however, it is not possible to find $\hat{U}(\overline{\sigma})$ explicitly, but instead bounds and estimates may be available for $\tilde{U}(\overline{\sigma})$. If we have a lower bound (such as a Hashin-Shtrikman lower bound) $\tilde{U}(\overline{\sigma})$ for $\tilde{U}(\overline{\sigma})$, such that

$$\tilde{\hat{U}}(\overline{\sigma}) \ge \tilde{\hat{U}}_{-}(\overline{\sigma}), \tag{13}$$

then, replacing $\tilde{\hat{U}}(\overline{\sigma})$ by $\tilde{\hat{U}}_{-}(\overline{\sigma})$ in equation (11) for $\tilde{U}_{-}(\overline{\sigma})$, still yields a lower bound for $\bar{U}(\overline{\sigma})$; alternatively, an upper bound for $\tilde{\hat{U}}(\overline{\sigma})$ is not useful in terms of obtaining an upper bound for $\tilde{\hat{U}}(\overline{\sigma})$. On the other hand, if we only have an estimate (such as a self-consistent estimate) $\tilde{\hat{U}}_{\epsilon}(\overline{\sigma})$ for $\tilde{\hat{U}}(\overline{\sigma})$, then

$$\tilde{U}_{\epsilon}(\overline{\sigma}) = \max_{\hat{\mu}^{(\prime)}, \hat{\kappa}^{(\prime)} > 0} \{ \tilde{\tilde{U}}_{\epsilon}(\overline{\sigma}) - \overline{V}(\hat{\mu}, \hat{\kappa}) \}$$
(14)

would provide only an estimate for $U(\overline{\sigma})$.

We note that the prescriptions (11) and (14) lead to convex expressions for the bounds and estimates of the effective potential of the nonlinear composite, provided that the corresponding bounds and estimates for the linear composite are convex, which is in turn guaranteed assuming that $\hat{\mu}$ and $\hat{\kappa} > 0$. This is a desirable feature, because the effective potential of the composite is known to be convex.

In reference [1], this general procedure was applied to an isotropic porous material with incompressible behavior for the matrix with potential

$$U^{(1)}(\boldsymbol{\sigma}) = f(\boldsymbol{\sigma}_{s}), \tag{15}$$

where f is assumed to satisfy the condition that F(x) = f(s) be a convex function of $x = s^2 > 0$.

The result of this calculation are a Hashin-Shtrikman (H-S) lower bound for $\tilde{U}(\overline{\sigma})$, given by

$$\tilde{U}_{-}(\overline{\sigma}) = c^{(1)}f(s), \tag{16a}$$

with

$$s = \frac{1}{c^{(1)}} \sqrt{(1 + \frac{\gamma_3}{c^{(2)}})} \overline{\sigma}_{\bullet}^2 + \frac{\gamma_4}{c^{(2)}} \overline{\sigma}_{m}^2}, \qquad (16b)$$

and a self-consistent (S-C) estimate given by

$$\bar{U}_{\epsilon}(\overline{\sigma}) = c^{(1)}f(s), \qquad (17a)$$

with

$$s = \sqrt{\frac{1}{c^{(1)}} \left(\frac{1 - c^{(2)}/3}{1 - 2c^{(2)}} \right) \left(\vec{\sigma}_e^2 + \frac{9}{4} \frac{c^{(2)}}{c^{(1)}} \vec{\sigma}_m^2 \right)}.$$
 (17b)

New Results for the Porous Ramberg-Osgood Material

In this section, we specialize further the results of the previous section by taking the constitutive behavior of the matrix, as given by equation (15), to be described by the relation

$$f(s) = \int_0^s f'(s) \, ds$$

where

$$f'(s) = \varepsilon_o \left\{ \frac{s}{\sigma_o} + \left[\left(\frac{s}{\sigma_o} \right)^n - \left(\frac{\sigma_y}{\sigma_o} \right)^n \right] H(s - \sigma_y) \right\}.$$
 (18)

Here, H is the unit step function, n > 1, σ_{v} is the yield stress, and σ_{o} and ε_{o} are used to

normalize the stresses and strains, respectively, such that the ratio σ_o/ε_o corresponds to the Young's modulus of the material. Then, the uniaxial stress/strain relation for the matrix material is linear up to the yield level, and linear plus power-hardening for stress levels in excess of the yield value. Note that this function satisfies the convexity assumption invoked above.

Thus, the H-S bound and S-C estimate for the effective energy of the porous material are given by expressions (16) and (17), respectively, where f is specified by equation (18). From these expressions, we can also determine, via equation (5), effective stress/strain relations for the porous material of the form

$$\bar{\varepsilon}_{\epsilon} = \frac{3}{2} c^{(1)} f'(s) \frac{\partial s}{\partial \bar{\sigma}_{\epsilon}}, \qquad (19)$$

where s is given by either (16b) for the H-S bound, or by (17b) for the S-C estimate.

We compare the new results with the results of reference [3] for the same material in Figures 1. All the results correspond to $\sigma_y/\sigma_o = 0.2$, n = 10 and porosity, $c^{(2)} = 0.3$. Figure 1a shows normalized plots of the H-S lower bounds and the S-C estimates for the effective energy \bar{U} as functions of the average effective stress, $\bar{\sigma}_e$, for a fixed value of the average hydrostatic stress, $\bar{\sigma}_m/\sigma_o = 0.25$. The dashed lines correspond to the new results given by equations (16) and (17), and the continuous lines correspond to the "best" results^{*} of [3]. The H-S lower bounds lie below

^{*} The raw data of [3] was not available, and the plots of these results in Figure 1 was accomplished by graphical methods. Thus, there may be some small error in the representation of the results of [3] in Figures 1.

the S-C estimates, as they should. It is seen that, for this case, corresponding to relatively low triaxialities, the new results are not very different from the results of [3], but the new bound lies slightly above the bound of [3], and hence it is better. Figure 1b shows similar normalized plots

for the case where $\bar{\sigma}_m/\sigma_o = 1.0$. In this case, corresponding to higher triaxialities, the improvement in the H-S lower bound is more dramatic, with the new bound lying well above the bound of [3]. The new S-C estimate also lies well above the bounds and S-C estimate of reference [3] (outside the range depicted in the graph). This is not surprising, however, because for such large values of n the differences in results are being exaggerated by the stress energies (which are

proportional to the stress to the n+1 power!). Figures 1c and 1d show plots of $\overline{\sigma}_{e}$ versus $\overline{\varepsilon}_{e}$, according to equation (19), corresponding to the bounds and estimates given in Figures 1a and 1b, respectively. The S-C estimates, being less stiff, lie below the H-S bounds. It is interesting to note that the new results do not show the complicated structure of the results of [3] for the larger value of the average hydrostatic stress. This is because for the new results, a large enough average bydrostatic stress will saturate the linear response of the material, in such a way that additional average shear stress leads to a less stiff power-type response. By contrast, the stress/strain relation predicted by [3] does not seem to be influenced significantly in its initial stages by the level of applied average hydrostatic stress, showing an unrealistically stiff initial behavior.

Figures 2a and 2b show normalized plots of the H-S bounds for the effective energy \tilde{U} as functions of the average effective stress, $\overline{\sigma}_{e}$, in the low-triaxiality range corresponding to

 $\omega = \left| \overline{\sigma}_{n} / \overline{\sigma}_{n} \right| << 1$, for values of n = 3 and 10, respectively. The three curves correspond to values of $c^{(2)} = 0.25$, 0.1 and 0.01, and a value of $\sigma_y/\sigma_o = 0.2$. Higher porosity naturally leads to less stiff behavior. Figures 2c and 2d show normalized plots of the H-S bounds for the effective energy \bar{U} as functions of the average hydrostatic stress, $\bar{\sigma}_{\pi}$, in the high-triaxiality range corresponding to $\omega >> 1$, for values of n = 3 and 10, respectively. The two curves correspond to values of $c^{(2)} = 0.25$, and 0.1.

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Fig. 1 Normalized plots of (a) & (b) H-S bounds and S-C estimates for \vec{U} against $\vec{\sigma}_{e}$, and of (c) & (d) $\vec{\sigma}_{e}$ against $\vec{\epsilon}_{e}$ computed from the H-S bounds and S-C estimates, for the two values of $\vec{\sigma}_{e}/\sigma_{e} = 0.25$ and 1.0, respectively. The dashed lines correspond to the new results, and the continuous lines correspond to the results of [3].



Fig. 2 Normalized plots of (a) and (b) H-S bounds for \overline{U} against $\overline{\sigma}_{e}$ in the low-triaxiality range, and of (c) & (d) H-S bounds for \overline{U} against $\overline{\sigma}_{e}$ in the high-triaxiality range, for the two values of n = 3, 10, respectively. The different curves correspond to three different values of the porosity $c^{(2)} = 0.25$, 0.1 and 0.01, with the higher porosities lying lower in the graph.

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Appendix C.

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The Effective Properties of Brittle/Ductile Incompressible Composites

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Abstract

A new variational method for estimating the effective properties of nonlinear composites in terms of the corresponding properties of linear composites with the same microstructural distributions of phases is applied to an isotropic, incompressible composite material containing a brittle (linear) and a ductile (nonlinear) phase. More specifically, in this particular work the prescription is used to obtain bounds of the Hashin-Shtrikman type for the effective properties of the nonlinear composite in terms of the well-known linear bounds. It can be shown that in some cases the method leads to optimal bounds.

Introduction

PONTE CASTAÑEDA (1990a) has proposed a new procedure for estimating the effective properties of composite materials with phases exhibiting nonlinear constitutive behavior. The procedure, which is straightforward to implement, expresses the effective properties of the nonlinear composite in terms of the effective properties of a family of linear composites with the same distribution

of phases as the nonlinear composite. Appropriate references for the linear theory of composites are given by the review article of WILLIS (1982) and by the monograph of CHRISTENSEN (1979). The new procedure was applied in the above reference to materials containing a nonlinear matrix either weakened by voids or reinforced by rigid particles. Estimates and rigorous bounds were obtained for the effective properties of such materials. The Hashin-Shtrikman bounds (obtained via the new method from the linear Hashin-Shtrikman bounds) were found to be an improvement over the corresponding bounds obtained by PONTE CASTAÑEDA and WILLIS (1988) for the same class of materials using an extension of the Hashin-Shtrikman variational principle to nonlinear problems proposed by TALBOT and WILLIS (1985). Recently, WILLIS (1990) has shown that the Hashin-Shtrikman bounds obtained via the new method can also be obtained by the method of TALBOT and WILLIS (1985) with an optimal choice of the comparison material. More generally, however, the new procedure can make use of linear higher-order bounds and estimates to yield corresponding bounds and estimates for nonlinear materials. In fact, the new procedure can be shown to yield exact results for a certain class of nonlinear composites. This is discussed in detail by PONTE CASTANEDA (1990b).

In this paper we apply the general procedure to a composite containing a brittle (linear) and a ductile (nonlinear) phase. We assume that the phases are perfectly bonded to each other, incompressible and isotropic. Additionally, the size of the typical heterogeneity is assumed to be small compared to the size of the specimen and the scale of variation of the applied loads. It is further assumed that the effect of the interfaces is negligible, so that the effective properties of the composite are essentially derived from the bulk behavior of the constituent phases. Both upper and lower bounds of the Hashin-Shtrikman type are given for the isotropic composite as functions of the properties and volume fractions of the phases. Specific results are given when the behavior of the nonlinear phase is linear plus power-law, including the pure power-law case. Some of the bounds are shown to be *optimal* (i.e., microstructures can be given attaining these bounds).

Effective Properties

Consider a two-phase composite occupying a region of unit volume Ω , with each phase occupying a subregion $\Omega^{(r)}$ (r = 1, 2), and let the stress potential, $U(\sigma, \mathbf{x})$, be expressed in terms of the homogeneous phase potentials, $U^{(r)}(\sigma)$, via

$$U(\sigma, \mathbf{x}) = \sum_{r=1}^{2} \chi^{(r)}(\mathbf{x}) U^{(r)}(\sigma), \qquad (1)$$

$$\chi^{(r)}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} \in \Omega^{(r)} \\ 0 & \text{otherwise} \end{cases}$$
(2)

is the characteristic function of phase r. The phases are assumed to be incompressible and isotropic, so that the potentials $U^{(r)}(\sigma)$ can be assumed to depend on the stress σ only through the effective stress

$$\sigma_{n}=\sqrt{\frac{3}{2}\mathbf{S}\cdot\mathbf{S}}\,,$$

where S is the deviator of σ . Thus, we assume that there exist scalar-valued functions $f^{(\prime)}$ such that

$$U^{(r)}(\sigma) = f^{(r)}(\sigma_{\epsilon}).$$

Then, the stress field σ , satisfying the equilibrium equations

$$\sigma_{\psi,j} = 0, \tag{3}$$

is related to the strain field ε , related to the displacement field u via

$$\varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}), \qquad (4)$$

through the constitutive relation

$$\varepsilon_{ij} = \frac{\partial U}{\partial \sigma_{ij}}(\sigma, \mathbf{x}). \tag{5}$$

The commas in equations (3) and (4) denote differentiation, and the summation convention has also been used in equation (3). We assume that the phases are perfectly bonded, so that the displacement is continuous across the interphase boundaries. However, the strains and, therefore, the stresses may be discontinuous across such boundaries, and hence equation (3) must be interpreted in a weak sense, requiring continuity of the traction components of the stress across the interphase boundaries.

We note that if we let ε represent the rate-of-deformation tensor and u the velocity field, the above equations can be used to model high-temperature creep, as well as high-rate viscoplastic deformations. Here we will present our work in the context of time-independent plasticity (deformation theory), but in view of the above comment the results could be given appropriate interpretations in nonlinear creep and viscoplasticity.

To define the effective properties of the heterogeneous material we introduce, following HILL (1963), the uniform constraint boundary condition

$$\sigma_{ij} n_j = \overline{\sigma}_{ij} n_j, \ \mathbf{x} \in \partial \Omega, \tag{6}$$

where $\partial \Omega$ denotes the boundary of the composite, n is its unit outward normal, and $\overline{\sigma}$ is a given constant symmetric tensor. Then, the average stress is precisely $\overline{\sigma}$, i.e.

where

$\overline{\sigma} = \int_{\sigma} \sigma(\mathbf{x}) dV$

(7)

and we define the average strain in a similar manner by

$$\vec{\varepsilon} = \int_{\Omega} \varepsilon(\mathbf{x}) dV. \tag{8}$$

The effective behavior of the composite, or the relation between the average stress and the average strain then follows from the principle of minimum complementary energy, which can be stated in the form

$$\bar{U}(\bar{\sigma}) = \min_{\sigma \neq s(\bar{\sigma})} \bar{U}(\sigma), \qquad (9)$$

where

$$\overline{U}(\sigma) = \int_{\sigma} U(\sigma, \mathbf{x}) \, dV$$

is the complementary energy functional of the problem,

$$S(\overline{\sigma}) = \{\sigma | \sigma_{ij,j} = 0 \text{ in } \Omega, \text{ and } \sigma_{ij}n_j = \overline{\sigma}_{ij}n_j \text{ on } \partial\Omega \}$$

is the set of statically admissible stresses, and where we have assumed convexity of the nonlinear potential $U(\sigma, x)$. Thus, we have that

$$\vec{\varepsilon}_{ij} = \frac{\partial \tilde{U}}{\partial \sigma_{ij}} (\vec{\sigma}).$$
(10)

Our task will be to determine bounds and estimates for $\tilde{U}(\overline{\sigma})$, which, under the above assumptions, is known to be convex.

Bounds and Estimates

A new variational principle for determining bounds and estimates for the effective properties of nonlinear composites in terms of the effective properties of linear composites was proposed by PONTE CASTAÑEDA (1990a,b). In this section, we specialize the derivation given in PONTE CASTAÑEDA (1990b) for the case where both phases are incompressible, and phase #2 is linear so that

$$U^{(2)}(\sigma) = \frac{1}{6\mu^{(2)}}\sigma_{\epsilon}^{2}.$$

The new variational principle is based on a representation of the potential of the nonlinear material in terms of the potentials of a family of linear *comparison* materials. Thus, for a homogeneous nonlinear material with "stronger than quadratic" growth in its potential, $U(\sigma)$, we have that

$$U(\sigma) \ge \max\{U_{\bullet}(\sigma) - V(\mu)\},\tag{11}$$

where

$$V(\mu) = \max_{\sigma} \{ U_{\sigma}(\sigma) - U(\sigma) \}$$
(12)

and

$$U_{\bullet}(\sigma) = \frac{1}{6\mu} \sigma_{\bullet}^2 \tag{13}$$

is the the potential of the comparison linear material.

To demonstrate this result, let

$$U(\sigma) = \phi(s), \tag{14}$$

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where $s = \sigma_{e}^{2}$. Then, the Legendre-Fenchel transform of the scalar-valued function ϕ is given by

$$\phi^{*}(\alpha) = \max\{\alpha s - \phi(s)\}, \qquad (15)$$

where α is assumed to be positive. A well-known result in convex analysis (VAN TIEL 1984, §6.3) is that

$$\phi(s) \ge \max\{s\alpha - \phi^{*}(\alpha)\}, \qquad (16)$$

with equality if ϕ is a convex function of its argument. With the identifications $s = \sigma_e^2$ and $\alpha = (6\mu)^{-1}$, we can see that (11) and (12) are but simple restatements of (16) and (15), respectively. In particular,

$$V(\mu) = \phi^{\bullet} \left(\frac{1}{6\mu}\right). \tag{17}$$

To derive the new variational principle, we apply (11) to the nonlinear phase #1, and make use of the result in the complementary energy principle (9). Thus, after some manipulations, we find that

$$\tilde{U}(\overline{\sigma}) \ge \max_{\mu^{(1)}(\mathbf{x})} \left\{ \tilde{U}_{\bullet}(\overline{\sigma}) - \int_{\Omega^{*}} V^{(1)}(\mu^{(1)}) dV \right\},$$
(18)

where

$$\bar{U}_{\bullet}(\overline{\sigma}) = \min_{\sigma \in \mathfrak{s}(\overline{\sigma})} \overline{U}_{\bullet}(\sigma), \qquad (19)$$

$$U_{\bullet}(\sigma,\mathbf{x}) = \sum_{r=1}^{2} \chi^{(r)}(\mathbf{x}) U_{\bullet}^{(r)}(\sigma)$$

and

$$U_{\bullet}^{(r)}(\sigma) = \frac{1}{6\mu^{(r)}}\sigma_{\bullet}^2$$

Note that the comparison linear material agrees with the actual material in phase # 2 (which is linear). In the above derivation, we note that the comparison moduli $\mu^{(1)}$ are functions of x, since the stress field σ will also in general be a function of x within phase #1. If we assume that $U^{(1)}(\sigma)$ is "strongly convex" (i.e. if ϕ is convex), then we have equality in (11), and hence, usually, equality in (18). However, if the conditions for equality are not met, relation (18) still provides a useful lower bound for $\tilde{U}(\overline{\sigma})$. An detailed derivation of this result, discussing the precise conditions for equality, is given in PONTE CASTANEDA (1990b).

The variational principle described by (18) roughly corresponds to solving a completely linear problem for a heterogeneous material with arbitrary moduli variation within the nonlinear phase, and then optimizing with respect to the variations in moduli within the nonlinear phase. Thus, one can think of the nonlinear material as a "linear" material with variable moduli that are determined by prescription (18) in such a way that its properties agree with those of the nonlinear material.

This suggests that if the fields happen to be constant over the nonlinear phase, then the variable moduli $\mu^{(1)}(x)$ can be replaced by constant moduli $\mu^{(1)}$. More generally, however, we have the following lower bound for $\overline{U}(\overline{\sigma})$

$$\tilde{U}_{\bullet}(\vec{\sigma}) = \max_{\mu^{(0)} \to 0} \{ \tilde{U}_{\bullet}(\vec{\sigma}) - c^{(1)} V^{(1)}(\mu^{(1)}) \},$$
(20)

where $c^{(1)}$ is the volume fraction of phase #1. The result in this form is a special case of a more general result first derived by PONTE CASTAÑEDA (1990a), when only one of the phases is nonlinear, and the other one is linear.

We note that the prescriptions (18) and (20) lead to convex expressions for the bounds and estimates of the effective potential of the nonlinear composite, provided that the corresponding bounds and estimates for the linear composite are convex. This is a desirable feature, because the effective potential of the composite is known to be convex.

Application to Hashin-Shtrikman Bounds

HASHIN and SHTRIKMAN (1962) prescribed bounds for the effective moduli of linear-elastic, isotropic composites, depending only on the volume fractions of the phases. When there are only two phases, these bounds have been shown to be optimal (i.e., microstructures can be given that simultaneously attain the bounds for the shear and bulk modulus) by FRANCFORT and MURAT (1987).

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δ << ε

Figure 1. Rank-2 laminate.

Their construction made use of *iterated* laminates for which the effective properties can be computed exactly. Such materials are obtained by layering the two constituent phases to obtain a rank-1 laminate; the resulting material is once again layered (in an arbitrary direction) with one of the original phases in a smaller lengthscale. This procedure can obviously be iterated n times to obtain a rank-n laminate. In general such materials will be anisotropic, but by choosing appropriately the layer orientations at the different layering operations, it is possible to obtain an isotropic composite, and its properties coincide with one of the Hashin-Shtrikman (H-S) bounds depending on which constituent phase is selected to play the role of the matrix material. Figure 1 depicts a rank-2 laminate (not to scale) with phase #2 as the matrix phase.

For the special case of incompressible materials, when there is only one modulus for the composite, the H-S upper bound for the effective shear modulus can be expressed in the form

$$\tilde{\mu}_{+} = \begin{cases} \frac{\mu^{(1)}}{\alpha(\mu^{(1)},\mu^{(2)})} & \text{if } \mu^{(1)} \ge \mu^{(2)} \\ \frac{\mu^{(2)}}{\beta(\mu^{(1)},\mu^{(2)})} & \text{if } \mu^{(1)} \le \mu^{(2)} \end{cases}$$
(21)

where

$$\alpha(\mu^{(1)},\mu^{(2)}) = \frac{2c^{(1)}\mu^{(2)} + (3+2c^{(2)})\mu^{(1)}}{(2+3c^{(2)})\mu^{(2)} + 3c^{(1)}\mu^{(1)}}$$
(22)

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and

$$\mathcal{G}(\mu^{(1)},\mu^{(2)}) = \frac{2c^{(2)}\mu^{(1)} + (3+2c^{(1)})\mu^{(2)}}{(2+3c^{(1)})\mu^{(1)} + 3c^{(2)}\mu^{(2)}} .$$
(23)

The corresponding H-S lower bound is obtained by interchanging the expressions in (21) for the upper bound (and keeping the conditions on the shear moduli $\mu^{(1)}$ and $\mu^{(2)}$ fixed).

The above H-S upper bound for the effective shear modulus yields a lower bound for the potential of the linear material \tilde{U}_{\bullet} . This information can be used in combination with prescription (20) to yield a H-S lower bound for the potential of the nonlinear material \tilde{U} . On the other hand, upper bounds for \tilde{U}_{\bullet} do not necessarily generate upper bounds for \tilde{U} .

The result for the lower bound on \tilde{U} depends on which of the two branches of (21) is used in conjunction with (20). If $\mu^{(1)} > \mu^{(2)}$, then the average effective stress $\overline{\sigma}$, must be such that the condition

$$3\mu^{(2)}f'(\overline{\sigma}_{\epsilon}) < \overline{\sigma}_{\epsilon}, \tag{24}$$

is satisfied (usually when the average shear stress is small enough). Here, for simplicity, we have made the identification $f^{(1)} = f$. The corresponding form of the bound is then

$$\vec{U}_{-}(\vec{\sigma}) = f_{1}(\vec{\sigma}_{i}), \qquad (25)$$

where

$$\bar{f}_{1}(\bar{\sigma}_{\epsilon}) = c^{(1)}f(s) + \mu^{(2)} \left[\frac{(2+3c^{(2)})}{2} - \left(\frac{\bar{\sigma}_{\epsilon}}{s}\right)^{2} \right] (f'(s))^{2}$$
(26)

and s solves the equation

$$c^{(1)} + \mu^{(2)} \left(2 + 3c^{(2)}\right) \frac{f'(s)}{s} = \frac{5}{3} \left[\frac{\left(2 + 3c^{(2)}\right) \left(s/\overline{\sigma}_{s}\right)^{2} - 2}{3c^{(2)}} \right]^{1/2}.$$
 (27)

On the other hand, if $\mu^{(1)} < \mu^{(2)}$, then the average effective stress $\overline{\sigma}_{\epsilon}$ must be such that the condition

$$3\mu^{(2)}f'(\overline{\sigma}_{*}) > \overline{\sigma}_{*}, \tag{28}$$

is satisfied (i.e., when the average shear stress is large enough), and

$$\tilde{U}_{-}(\overline{\sigma}) = \bar{f}_{2}(\overline{\sigma}_{*}), \qquad (29)$$

where

$$\bar{f}_{2}(\bar{\sigma}_{*}) = c^{(1)}f(s) + \frac{(3+2c^{(1)})\bar{\sigma}_{*}^{2} + c^{(1)}(2+3c^{(1)})s^{2} - 10c^{(1)}s\bar{\sigma}_{*}}{18c^{(2)}\mu^{(2)}},$$
(30)

and s solves the equation

$$9c^{(2)}\mu^{(2)}f'(s) = 5\overline{\sigma}_{s} - (2+3c^{(1)})s.$$
 (31)

The corresponding stress/strain relations have the form

$$\boldsymbol{\varepsilon} = \frac{3}{2} \tilde{f}'(\boldsymbol{\overline{\sigma}}_{\star}) \mathbf{S}, \qquad (32)$$

1

where

$$\tilde{f}_{2}'(\overline{\sigma}_{e}) = \frac{2}{3} \frac{(3+2c^{(1)})\overline{\sigma}_{e} - 5c^{(1)}s}{6c^{(2)}\mu^{(2)}},$$
(33)

but $f_i(\overline{\sigma}_i)$ does not have a simple expression.

In general, we do not expect the above lower bounds for \overline{U} to be optimal. In fact, expression (25) does not yield an optimal bound if condition (24) is satisfied. However, it is shown in PONTE CASTANEDA (1990b) that if condition (28) is satisfied, then the bound (29) is optimal. This is because the same microstructure attaining the linear bounds can be also shown to attain the nonlinear bound; the reason being that the fields are constant in the (nonlinear) inclusion phase, and hence expressions (20) and (18) are identical. Similar observations have been made by KOHN (1990) in a similar context (starting from the Talbot-Willis nonlinear variational principle) and, independently, by PONTE CASTANEDA (1990c) in the context of conductivity.

Conversely, in general, we do not expect that interchanging conditions (24) and (28) would turn expression (25) and (29) into upper bounds for the nonlinear potential \tilde{U} . This is contrary to the corresponding operation for the linear composite. All that can be said, however, is that expression (29) is an estimate for the upper bound for \tilde{U} if condition (24) is satisfied and that expression (25) is an estimate for the upper bound for \tilde{U} if condition (24) is satisfied. Both of these estimates are expected to get progressively better with weaker nonlinearities.

Application to Power-Law Behavior

In this section, we specialize further the calculations of the previous section by taking the constitutive behavior of the nonlinear phase to be governed by a linear plus power relation

$$f(\sigma_{\epsilon}) = \frac{1}{3} \left[\frac{1}{2\mu} + \left(\frac{1}{n+1} \right) \frac{1}{\eta} \sigma_{\epsilon}^{n-1} \right] \sigma_{\epsilon}^{2}.$$
(34)

Note that the case $\mu \to \infty$ corresponds to pure power-law behavior, and the limits $n \to 1$ (in addition to $\mu \to \infty$) or $\eta \to \infty$ correspond to linear behavior.

The conditions (24) and (28) determining the appropriate branch of the bound specialize to

$$\frac{\mu^{(2)}}{\mu} + \frac{\mu^{(2)}}{\eta} \overline{\sigma}_{e}^{n-1} < 1$$
(35)

and the opposite inequality, respectively. The first condition guaranteeing that (25) is a lower bound (and correspondingly that (29) is an estimate for the upper bound) corresponds to small enough average stress on the composite. Alternatively, the second condition (with > instead of <) corresponds to sufficiently large average stress. Note that, if $\mu^{(2)}/\mu > 1$, condition (35) can never be satisfied and, conversely, the alternative condition is always satisfied. This condition ensures that the difference between the potential of phase #1 and that of phase #2 is convex. Here, we will consider two cases: one case, meeting this condition, with $\mu^{(2)}/\mu = 2$, and the other with $\mu^{(2)}/\mu = 0$, corresponding to the pure power-law case.

The results for the bounds (25) and (29) specialized to the case when (34) holds can be expressed in the form:

$$\frac{\bar{U}(\bar{\sigma})}{U^{(2)}(\bar{\sigma})} = F\left\{\frac{\mu^{(2)}}{\eta} \overline{\sigma}_{e}^{n-1}; \frac{\mu^{(2)}}{\mu}, c^{(2)}, n\right\},$$
(36)

where the precise form of F depends on whether (25) or (29) applies, and $(\mu^{(2)}/\eta)\overline{\sigma}_{\epsilon}^{n-1}$ plays the role of the independent variable, with $\mu^{(2)}/\mu$, $c^{(2)}$ and n, serving as parameters.

Results for the upper and lower bounds for \overline{U} are given in Figures 2 and 3 for the case where $\mu^{(2)}/\mu = 0$, and in Figure 4 for the case where $\mu^{(2)}/\mu = 2$. In the first case, condition (35) determining whether (29) is an estimate for the upper bound or an optimal lower bound, and whether (25) is an estimate for the upper bound, or a non-optimal lower bound, simply reduces to the condition of

whether the independent variable $(\mu^{(2)}/\eta)\overline{\sigma}_{\bullet}^{n-1}$ is less or greater than unity. For that reason, we give results emphasizing the small stress and large stress domains, separately, in Figures 2 and 3, respectively.

In each plot we have three sets of curves corresponding to three values of $c^{(2)}$ (0.1, 0.5 and 0.9). Additionally, we show the limiting cases corresponding to $c^{(2)} = 0$ and $c^{(2)} = 1$. These limiting curves appear as straight lines, one with with variable slope depending on the value of *n* and $\mu^{(2)}/\mu$, and the other with



Figure 2(a). Plots of the bounds for the effective energy of the composite as functions of the average stress (appropriately normalized) for $\mu^{(n)}/\mu = 0$ and n = 3 (small stress).

zero slope (value equal to unity), respectively. The intermediate sets of curves correspond to the upper and lower bounds.

In Figure 2, depicting results for two values of the nonlinearity parameter (n = 3 and 10), the continuous line corresponds to the estimate for the upper bound (for \overline{U}), and the dashed line corresponds to the rigorous lower bound. In Figure 3, showing also results for the same two values of the nonlinearity parameter, the continuous line corresponds to the optimal lower bound, and the dashed line is an estimate for the upper bound. For this value of $\mu^{(2)}/\mu$, the upper and lower bound coalesce when the value of the independent variable



Figure 2(b). Plots of the bounds for the effective energy of the composite as functions of the average stress (appropriately normalized) for $\mu^{(n)}/\mu = 0$ and n = 10 (small stress).

 $(\mu^{(2)}/\eta)\overline{\sigma_{\bullet}^{n-1}}$ approaches unity. In the linear case, this behavior corresponds to the limit of the moduli of the phases approaching each other. More generally, assuming that $\mu^{(2)}/\mu$ is less than unity, there is a value of the independent variable (i.e., an average stress level) at which the bounds are equal, and hence the effective energy of the composite is known exactly. This phenomenon is related to the lack of convexity of the difference between the potentials of the nonlinear and linear phases.

In Figure 4, depicting results for the same two values of the nonlinearity parameter, the continuous line corresponds to the optimal lower bound (for \overline{U}), and the dashed line corresponds to the estimate for the upper bound. In this case,



Figure 3(a). Plots of the bounds for the effective energy of the composite as functions of the average stress (appropriately normalized) for $\mu^{(1)}/\mu = 0$ and n = 3 (large stress)

with a convex difference between the nonlinear and linear potentials, there is no value of the independent variable for which the upper and lower bound are equal.

Both in Figures 3 and 4, we observe that the lower bound approaches a straight line with zero slope and the upper bound approaches a straight line with slope depending on the value of n (smaller for larger n). This is consistent with the following asymptotic behaviors for the lower and upper bounds

$$\frac{\bar{U}(\bar{\sigma})}{U^{(2)}(\bar{\sigma})} \approx \frac{(1+3/c^{(1)})}{c^{(2)}},$$
(37)



Figure 3(b). Plots of the bounds for the effective energy of the composite as functions of the average stress (appropriately normalized) for $\mu^{(2)}/\mu = 0$ and n = 10 (large stress)

and

, **`**

$$\frac{\tilde{U}(\overline{\sigma})}{U^{(2)}(\overline{\sigma})} = \frac{2}{n+1} \frac{1}{\omega^n} \frac{\mu^{(2)}}{\eta} \overline{\sigma}_e^{n-1},$$
(38)

with

$$\omega = \frac{\left(1 + \frac{1}{2}c^{(2)}\right)^{\frac{1}{2}}}{\left(c^{(1)}\right)^{\frac{1}{2}}} = 1 + \left(\frac{3n+7}{4n}\right)c^{(2)} \quad \text{as } c^{(2)} \to 0$$
(39)



Figure 4(a). Plots of the bounds for the effective energy of the composite as functions of the average stress (appropriately normalized) for $\mu^{(n)}/\mu = 2$ and n = 3.

respectively. These two behaviors correspond physically to the cases of a linear matrix with voids and a power-law matrix with rigid inclusions (studied by PONTE CASTAÑEDA, 1990a), respectively. The reason for these behaviors is that the lower bound (for \overline{U}) corresponds to putting the stiffer material in the matrix phase and the less stiff material in the inclusion phase (and viceversa for the upper bound). Clearly, for large enough stresses, the linear phase is stiffer than the nonlinear phase.

We note that accurate numerical calculations of the potential of a power-law matrix with spherical rigid inclusion have yielded results of the form (38) with

$$\omega = 1 + \left(\frac{g(n)}{n}\right) c^{(2)} \quad \text{as } c^{(2)} \to 0, \tag{40}$$



Figure 4(b). Plots of the bounds for the effective energy of the composite as functions of the average stress (appropriately normalized) for $\mu^{(n)}/\mu = 2$ and $n \approx 10$.

where g(n) is such that g(1) = 5/2, g(3) = 3.21 and g(10) = 6.09 (LEE and MEAR, 1990), and $g(n) \rightarrow 0.38n$ as $n \rightarrow \infty$ (HUTCHINSON, 1990). These results do not compare very favorably with the corresponding results from (39): 5/2, 4.00, 9.25 and 0.75n, but it should be recalled that these results correspond to the case for which we do not have a rigorous bound (it is simply an estimate of the bound). None the less, the results of (38) with (39) may provide reasonable estimates for larger values of the volume fraction of the linear phase.

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