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SOME SIMPLE EXPLICIT BOUNDS FOR THE OVERALL BEHAVIOUR OF NONLINEAR COMPOSITES

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Abstract—Variational expressions developed over the last few years provide bounds for the overall energy functions of a range of nonlinear composite materials. The evaluation of a bound requires the solution of a system of nonlinear algebraic equations and this generally involves a computation. There are, however, certain simple composites, comprising a nonlinear matrix containing either rigid inclusions or cavities, for which very simple explicit formulae can be given. These formulae are displayed here, at a level of generality greater than in any previous presentation. The energy density function of the matrix is arbitrary and the microgeometry of the composite appears through an expression which bounds the energy of a linear composite with the same geometry. To the extent that such linear bounds can be developed making allowance for any amount of statistical information on the composite, the new nonlinear bounds reflect this. New results, at the level of employing bounds of Hashin–Shtrikman type for the linear problem, are given for an incompressible matrix reinforced by aligned rigid platelets or weakened by aligned cracks. In the course of the work, a recently-derived formula, more general than any available previously, is presented and developed explicitly for any two-phase composite.

1. INTRODUCTION

The problem to be addressed is that of bounding (when possible) the overall, or effective, energy density function of a composite, made up from materials of n different types, firmly bonded across interfaces. Material of type r has energy density function $W_r(e)$, which is taken to be a convex function of the infinitesimal strain tensor e. The energy density function for the composite depends on position x and can be written

$$W(e,x) = \sum_{r=1}^{n} W_r(e)f_r(x), \tag{1}$$

where $f_r(x)$ represents the characteristic function of the region occupied by material of type r. The composite occupies a domain Ω and, for convenience, units of length are chosen so that Ω has unit volume. The overall energy function, $\tilde{W}(\bar{e})$, is then defined as the mean energy density, when the composite is subjected to a mean strain $\bar{e}$, through application of the displacement boundary conditions

$$u_i = \bar{e}_{ij}x_j, \quad x \in \partial\Omega. \tag{2}$$

The minimum energy principle allows $\tilde{W}$ to be characterized as

$$\tilde{W}(\bar{e}) = \inf_{e} \int_{\Omega} W(e,x)\,\mathrm{d}x, \tag{3}$$

the infimum being taken over strain fields e that are derived from displacements conforming to the boundary conditions (2).

The same mathematics applies to problems involving steady-state creep. Then, u is interpreted as velocity, e as strain rate and the energy density functions are interpreted as stress potentials.

The ideas that are employed in this work stem from a generalization to nonlinear problems of the Hashin–Shtrikman variational principle (Hashin and Shtrikman, 1962, 1963), developed in Willis (1983, 1986) and Talbot and Willis (1985). In general, explicit results require a computation; the most extensive study to date is that reported in Dendievel *et al.* (1991) for the overall creep behaviour of a polycrystal. There are, however, certain configurations, of some practical interest, for which bounds can be given in simple closed forms. It is the purpose of this note to place these bounds on record. An additional novel feature of the work is that a general bound expression is given, which can make allowance for statistical information of any order; the germ of the idea was exposed in Willis (1991a) but here it is developed and simplified in the case of any two-phase composite, and given yet more explicit forms in the cases of a matrix containing either rigid inclusions or cavities.

2. THE BASIC VARIATIONAL STRUCTURE

The energy density function of the composite depends on position x and corresponds to nonlinear material behaviour; the exact value of $\tilde{W}$, defined in (3), is correspondingly hard to find. It proves fruitful to introduce a "comparison" material, with energy density $W_0(e)$, and to define

$$(W-W_0)^*(\tau) = \sup_e [\tau\cdot e-(W-W_0)(e)]. \tag{4}$$

Here, the dependence of W on x is not acknowledged explicitly but it is still present. Then,

$$W(e) \geqslant W_0(e)+\tau\cdot e-(W-W_0)^*(\tau) \tag{5}$$

for any e, τ and it follows, from (3) and (5), that

$$\tilde{W}(\bar{e}) \geqslant \inf_e \int_\Omega [W_0(e)+\tau\cdot e-(W-W_0)^*(\tau)]\,\mathrm{d}x, \tag{6}$$

the infimum still being over the set of strain fields that are admissible for (3). The inequality (6) embodies the variational principle of Hashin and Shtrikman (1962), generalized to nonlinear material behaviour.

The function W_0 is usually taken to be quadratic, corresponding to linear material behaviour, and independent of x. Neither of these are essential, however. Suppose now that W_0 is taken, instead, to be a *comparison linear composite*, with the same microgeometry as the given nonlinear composite: to distinguish this from the more usual case, the comparison energy function is now called $\hat{W}$. Then, (6) yields the bound

$$\tilde{W}(\bar{e}) \geqslant \sup_{\hat{W}} \left\{\inf_e \int_\Omega [\hat{W}(e)+\tau\cdot e-(W-\hat{W})^*(\tau)]\,\mathrm{d}x\right\}. \tag{7}$$

This bound, as well as (6), is simple enough to be useful if τ is taken to have the piecewise constant form

$$\tau(x) = \sum_{r=1}^{n} \tau_r f_r(x), \tag{8}$$

in correspondence with the expression (1) for $W(e, x)$. Then, awkward nonlinear averages are avoided.

When τ has the form (8), the problem of finding

$$\tilde{W}_T(\bar{e};\tau) = \inf_e \int_\Omega [\hat{W}(e)+\tau\cdot e]\,\mathrm{d}x \tag{9}$$

is analogous to finding the energy of a *linear thermoelastic composite*: call the temperature 1, let the thermal stress tensor be $-\tau$ and suppose the heat capacity at constant strain is zero.

A simple consequence of (7) is obtained by setting $\tau = 0$. This gives

$$\tilde{W}(\bar{e}) \geqslant \sup_{\hat{W}} \left\{ \hat{W}_B(\bar{e}) + \int_\Omega \min(W-\hat{W})\,\mathrm{d}x \right\}, \tag{10}$$

where $\hat{W}_B$ is *any lower bound to the overall energy function of the linear comparison composite*. This bound was introduced by Ponte Castañeda (1991). Generally, this bound is not as good as (7), but it can be in particular cases. The idea of employing a comparison linear composite was introduced in Ponte Castañeda (1991) and, in a somewhat different context, in Dendievel *et al.* (1991). The relative merits of (10) and (6) have been discussed in Willis (1991, in press).

It should be noted that the bounds (6), (7) and (10) are nontrivial only so long as $(W-W_0)^*$ or $(W-\hat{W})^*$ is finite; considering the former quantity, this requires that

$$(W-W_0)(e)/\|e\| \to +\infty \quad \text{as} \quad \|e\| \to \infty.$$

If, alternatively,

$$(W^*-W_0^*)(\sigma)/\|\sigma\| \to +\infty \quad \text{as} \quad \|\sigma\| \to \infty,$$

an exactly similar formulation starting from the complementary energy principle provides bounds for

$$\tilde{W}^*(\bar{\sigma}) = \inf_\sigma \int_\Omega W^*(\sigma)\,\mathrm{d}x, \tag{11}$$

the infimum being taken over divergence-free fields σ with prescribed mean value $\bar{\sigma}$. There are also cases for which one of these conditions is satisfied for some values of x, while the other condition is satisfied elsewhere; no bounds are then known, apart from the elementary ones which follow directly by substitution of constant fields into the integrals in (3), (10), to yield

$$(\bar{W}^*)^*(\bar{e}) \leqslant \tilde{W}(\bar{e}) \leqslant \bar{W}(\bar{e}). \tag{12}$$

Here,

$$\bar{W}(\bar{e}) = \int_\Omega W(\bar{e},x)\,\mathrm{d}x = \sum_{r=1}^{n} c_r W_r(\bar{e}),$$

where c_r denotes the volume fraction of material of type r, and $\bar{W}^*(\bar{\sigma})$ is defined similarly.

3. A TWO-PHASE COMPOSITE

In the particular case of a two-phase composite, the "linear thermoelastic" problem (9) can be solved explicitly, in terms of the corresponding purely mechanical problem (Levin, 1967; Laws, 1973). Introduce the notation

$$\hat{W}_1(e) = \tfrac{1}{2}eL_1e, \quad \hat{W}_2(e) = \tfrac{1}{2}eL_2e. \tag{13}$$

The comparison linear composite then has tensor of overall moduli $\tilde{L}$, say, and corresponding energy function

$$\tilde{W}(\bar{e}) = \tfrac{1}{2}e\tilde{L}e. \tag{14}$$

Manipulation of formulae given in Levin (1967) and Laws (1973) then yields

$$\tilde{W}_T(\bar{e};\tau) = \tfrac{1}{2}\bar{e}\tilde{L}\bar{e}+\bar{e}\bar{\tau}-\tfrac{1}{2}[\bar{e}+(L_1-L_2)^{-1}(\tau_1-\tau_2)](\bar{L}-\tilde{L})[\bar{e}+(L_1-L_2)^{-1}(\tau_1-\tau_2)]. \tag{15}$$

A lower bound is obtained by replacing $\tilde{L}$ by any lower bound L_B in (15); the bound formula (7) then becomes explicit.

4. A NONLINEAR MATRIX CONTAINING RIGID INCLUSIONS OR CAVITIES

Let the matrix have energy function $W_1(e)$ and let phase 2 be rigid. The linear comparison composite is similarly defined by a tensor of moduli L_1, while $L_2 \to \infty$. The expression (15) simplifies drastically and the bound corresponding to (7) becomes

$$\tilde{W}(\bar{e}) \geqslant \sup_{L_1}\sup_{\tau_1}[\tfrac{1}{2}\bar{e}L_B\bar{e}+\bar{e}\tau_1-c_1(W_1-\hat{W}_1)^*(\tau_1)],$$

or, upon evaluating the supremum over τ_1,

$$\tilde{W}(\bar{e}) \geqslant \sup_{L_1}\left[\tfrac{1}{2}\bar{e}L_B\bar{e}+c_1(W_1-\hat{W}_1)^{**}\left(\frac{\bar{e}}{c_1}\right)\right]. \tag{16}$$

Here, L_B is *any* lower bound for $\tilde{L}$. The bound formula (16) is the most general that is known for this type of composite: no assumption such as isotropy has been made, either in relation to material behaviour or microgeometry. It is free of the deficiency of (10), noted in Willis (1991c), that the bound need not *always* be as good as the older bound, (6). When L_B is taken as the Hashin–Shtrikman bound, (16) can also be derived directly from (6), identifying W_0 with $\hat{W}_1$. This direct derivation was given in Willis (1991b).

For a matrix weakened by cavities, the formula corresponding to (16) follows from the dual formulation based on (11). The result is

$$\tilde{W}^*(\bar{\sigma}) \geqslant \sup_{M_1}\left[\tfrac{1}{2}\bar{\sigma}M_B\bar{\sigma}+c_1(W_1^*-\hat{W}_1^*)^{**}\left(\frac{\bar{\sigma}}{c_1}\right)\right], \tag{17}$$

where Ms denote compliance tensors, inverse to the corresponding Ls.

5. SOME SPECIAL CASES

The formulae listed below were all derived by making the replacements

$$(W_1-\hat{W}_1)^{**} \to \min(W_1-\hat{W}_1), \quad (W_1^*-\hat{W}_1^*)^{**} \to \min(W_1^*-\hat{W}_1^*). \tag{18}$$

The bounds that result are thus based on (10) and are *only* as good as bounds based on (7) when the replacements listed above have no adverse effect. This is often the case in practice; conditions are discussed in Willis (1991b, in press).

(a) *Rigid inclusions in an incompressible matrix*

Here, the linear bound L_B can be *any* bound for an isotropic incompressible matrix, with shear modulus $\hat{\mu}_1$, containing rigid inclusions. It has the form

$$L_B = \hat{\mu}_1 B, \tag{19}$$

say, where the tensor B depends on the geometrical arrangement only. Having made the replacement (18), $\hat{\mu}_1$ appears linearly and the required saddle point follows directly. The bound is

$$\tilde{W}(\bar{e}) \geq \min_e c_1 W_1(e), \tag{20}$$

where e is restricted so that its associated equivalent shear strain has the value

$$e_e^2 = \frac{\bar{e}B\bar{e}}{3c_1}. \tag{21}$$

An expression of Hashin–Shtrikman type for B is known, for any microgeometry, from work of Willis (1981, 1982). For a linear matrix with general tensor of moduli L_1,

$$L_B = L_1 + \frac{c_2}{c_1} P^{-1}, \tag{22}$$

where P is a tensor which depends on points in the composite, taken two at a time. In the special case that the composite has a "spheroidal" symmetry, which can be thought of as having been realized by subjecting a composite with isotropic microgeometry to a stretch in one direction, the tensor P is known explicitly (see Willis (1977) for the first proof); one source for the detailed formulae, in the case of isotropic L_1, is Willis (1990). When B is obtained from a Hashin–Shtrikman bound, the following results may be derived, as special cases of a composite with spheroidal symmetry.

Spherical rigid inclusions. The bound is (20), subject to the restriction

$$c_1 e_e^2 = \left(\frac{2+3c_2}{2c_1}\right)\bar{e}_e^2. \tag{23}$$

Aligned platelets, radius a, number density n.

$$\tilde{W}(\bar{e}) \geq \min_e W_1(e), \tag{24}$$

where

$$e_e^2 = \bar{e}_e^2 + \frac{32na^3}{27}\left[\frac{3}{2}(\bar{e}_{11}^2 + \bar{e}_{22}^2) - \bar{e}_{11}\bar{e}_{22} + 4\bar{e}_{12}^2\right]. \tag{25}$$

(b) *Rigid spheres in a compressible matrix*

Here, the linear Hashin–Shtrikman bound is used and the matrix is taken to have energy function

$$W_1(e) = \tfrac{9}{2}\kappa_1 e_m^2 + W_e(e_e). \tag{26}$$

The bound is

$$\tilde{W}(\bar{e}) \geq \frac{9\kappa_1}{2c_1}\bar{e}_m^2 + \frac{5\kappa_1\mu_0^2}{2(\kappa_1+2\mu_0)^2}\frac{c_2}{c_1}\bar{e}_e^2 + c_1 W_e(e_e), \tag{27}$$

where

$$\mu_0 = \frac{W_e'(e_e)}{3e_e} \tag{28}$$

and

$$c_1 e_e^2 = \bar{e}_e^2\left[\frac{5c_2}{6c_1}\left(\frac{3\kappa_1+4\mu_0}{\kappa_1+2\mu_0} - \frac{2\kappa_1\mu_0}{(\kappa_1+2\mu_0)^2}\right)+1\right] + \frac{4c_2}{c_1}\bar{e}_m^2. \tag{29}$$

This result still requires the solution of the nonlinear equation (29) and demonstrates how rapidly complications can set in.

(c) *Cavities in an incompressible matrix*

Here, the linear bound for the compliance tensor of the comparison composite (which contains cavities) has the form

$$M_B = B^*/\mu_1. \tag{30}$$

The bound is

$$\tilde{W}^*(\bar{\sigma}) \geqslant \min_{\sigma} c_1 W_1^*(\sigma), \tag{31}$$

where σ is restricted so that

$$c_1\sigma_e^2 = 3\bar{\sigma}B^*\bar{\sigma}. \tag{32}$$

The linear Hashin–Shtrikman bound can be given in the form

$$M_B = M_1 + \frac{c_2}{c_1}Q^{-1}, \tag{33}$$

where

$$Q = L_1 - L_1PL_1 \tag{34}$$

and so is known explicitly when the matrix is isotropic and the composite has spheroidal symmetry. When this is employed, there are the following results.

Spherical cavities. The restriction (32) becomes

$$c_1\sigma_e^2 = \frac{9c_2}{4c_1}\bar{\sigma}_m^2 + \left(\frac{3+2c_2}{3c_1}\right)\bar{\sigma}_e^2. \tag{35}$$

Aligned cracks, radius a, number density n.

$$\tilde{W}^*(\bar{\sigma}) \geqslant \min_{\sigma} W_1^*(\sigma), \tag{36}$$

where

$$\sigma_e^2 = \bar{\sigma}_e^2 + 4na^3[\tfrac{4}{3}(\bar{\sigma}_{13}^2+\bar{\sigma}_{23}^2)+\bar{\sigma}_{33}^2]. \tag{37}$$

6. CONCLUDING REMARKS

The formulations given in Section 2 are the only ones known for the systematic production of bounds more refined than the elementary bounds (12). In particular, the result (7) is the best that is known. The general two-phase bounds obtained by combining (7), (9) and (15) have not been presented before. The bounds (16) and (17) are likewise new. They cannot easily be simplified for general energy function W_1 but, when the replacements (18) are acceptable, very simple explicit formulae result. They follow from Ponte Castañeda's bound formula (10) but have not been obtained at this level of generality before. Even at the level of employing linear bounds of Hashin–Shtrikman type, the expressions (24) and (37), for a matrix containing rigid platelets or cracks, have not been given previously. Limitations of space preclude the presentation of results for further special cases; the ones that have been given were selected for their particular simplicity. It is remarked, however, that other results, such as for a nonlinear matrix reinforced by linear fibres (Talbot and Willis, 1991), have been reproduced from the present style of reasoning.

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