BOUNDS FOR EXPANSION COEFFICIENTS OF COMPOSITES

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Summary
A method is suggested to bound the anisotropic effective stiffness and extension tensors of a multiphase composite made of expandable materials. The bounds are valid for composites of any microstructure. It is shown that the expansion coefficients vary an ellipsoid which parameters depend on properties of the phases, their fractions, and the effective stiffness of a composite. The obtained tensorial inequalities generalize bounds by Schapery, Rozen and Hashin, and Gibiansky and Torquato. Particularly, the bounds for the mixtures with voids are obtained.

INTRODUCTION

This paper suggests a method for bounds for a anisotropic effective compliance S_* and anisotropic extension tensor α_* of a composite. One meets these problems dealing with composites made of materials that experience phase transition or thermal expansion. The bounds are independent of the structure of a composite and depend only on the moduli of the phases and their volume fractions. The bounds for S_* are independent of the extension tensors of the phases, but the bounds for α_* depend on the compliance and expansion coefficients of the phases and on the effective compliance tensor S_* of a composite.

The bounds for effective compliance tensor S_* are well-studied starting from the classical bounds by Reiss, Voigt, and Hill, they where tighten for isotropic materials by Hashin and Shtrikman and Walpole, then by Cherkaev and Gibiansky. The bound were tighten by exploring the differential constraints on the stress and strain tensors; the method for accounting for these constraints is now called the translation method [5].

The bounds for expansion coefficients are much less developed. The existing bounds [1, 2, 3] deal with the isotropic case, and the bounds by Gibiansky and Torquato [3] are extremely close to the results of numerical optimization by Sigmund and Torquato [4]. The complicated algebraic structure of the isotropic bounds makes their generalization for general anisotropic case not too attractive. However, we show that the general bounds are given by rather elegant tensorial expressions of a clear algebraic structure.

Study of anisotropic multiphase thermal expansion is important for applications. Most composites (such as the laminates) are anisotropic. The bounds for anisotropic expansion estimates the maximum and minimum of the effective expansion in any direction; they can be used in structural optimization.

THE PROBLEM

The constitutive relation for an expandable material subject to a transformation and an elastic load is described as

$$\epsilon = S : \sigma + \alpha, \quad \nabla \cdot \sigma = 0, \quad \nabla \times (\nabla \times \epsilon)^T = 0 \tag{1}$$

where ϵ is the stress tensor, σ is the stress tensor, S is the fourth-order tensor of elastic compliance (the inverse to the stiffness tensor C, $S = C^{-1}$, and (:) is the convolution. The expansion tensor α is a symmetric second rank tensor of deformation due to the temperature change or the phase transition. The equation (1) is normalized with respect to the temperature change. For isotropic thermo-elastic materials, α is a spherical tensor; for materials under austenite-martensite transformation, α is close to a deviatoric tensor. The energy of the expandable material can be presented in two mutually dual forms

$$W_\epsilon(C, \alpha, \epsilon) = \frac{1}{2}\epsilon : C : \epsilon - \epsilon : C : \alpha + c_v, \quad W_\sigma(S, \alpha, \sigma) = \frac{1}{2}\sigma : S : \sigma + \sigma : \alpha - c_p$$

where the difference between the parameters c_v and c_p is given by $c_v - c_p = \alpha : C : \alpha$ due to the duality relations.

A composite with perfect bonds between phases is characterized by the effective relation between volume averaged stress $\langle\sigma\rangle$ and stain $\langle\sigma\rangle$ that is similar to (1) while the tensors S and α are replaced by the tensors of effective moduli S_* and α_*, respectively. The expression for the energy changes accordingly. The effective tensors depend on the moduli and expansion coefficients of the mixed materials and on microstructure, but are independent of the acting fields.

The bounds for the effective moduli are independent of the microstructure; they are represented by the inequalities of the type

$$\mathcal{G}(S_*, \alpha_*, S_{ph}, \alpha_{ph}, m_{ph}) \geq 0$$

where $m_{ph} = \{m_1, \dots m_N\}$ are the volume fractions of the phases in the composite, $S_{ph} = \{S_1, \dots S_N\}$ and $\alpha_{ph} = \{\alpha_1, \dots \alpha_N\}$ are the moduli of the phases. In order to obtain the bound, we deal with the following questions: (i) What functional should be estimated? (ii) What expression bound the functional from below? (iii) How to pass from the bound on the functional to the bounds on the effective coefficients? (iv) What are the bounds when void is presented in the mixture?

THE METHOD

We estimate from below the sum $W_\sigma + W_\epsilon$ of the energy and its dual form by using the translation method [5]. Namely, we neglect the differential constraints in (1) replacing them with inequalities of the type $\langle \sigma : T_\sigma : \sigma \rangle \geq \langle \sigma \rangle : T_\sigma : \langle \sigma \rangle$ which are considered as algebraic constraints. Here, T_σ is the matrix translator (for explicit form of T, see [5]): A nonpositively defined matrix that nevertheless provides the above inequality due to differential constraints on the field σ. The minimization problem becomes algebraic, and the standard minimization procedure yields to the inequality

$$W_\sigma(C_*, \alpha_*, \langle\sigma\rangle) + W_\epsilon(S_*, \alpha_*, \langle\epsilon\rangle) \geq \frac{1}{2} z^T P_B z + q_B^T z + r_B, \quad \forall z = (\langle\sigma\rangle, \langle\epsilon\rangle)^T \tag{2}$$

where the tensors $P_B = P_B(m_{ph}, C_{ph})$ and $q_B = q_B(m_{ph}, C_{ph}, \alpha_{ph})$ of the fourth and second rank, respectively, and the constant $r_B = r_B(m_{ph}, C_{ph}, \alpha_{ph})$ are explicitly calculated. The left-hand side of the (2) is also a quadratic function of averaged fields z which coefficients are effective properties C_*, α_* of the composite. Eliminating the dependence of z, we obtain the bounds for the effective properties as it is described below.

NEW BOUNDS

The inequality (2) yields to the following inequalities for the effective coefficients. A matrix inequality

$$\begin{pmatrix} S_* + T_\sigma & T_{\epsilon\sigma} \\ T_{\epsilon\sigma} & C_* + T_\epsilon \end{pmatrix} - P_B \geq 0 \quad \forall T : \begin{pmatrix} S_i + T_\sigma & T_{\epsilon\sigma} \\ T_{\epsilon\sigma} & C_i + T_\epsilon \end{pmatrix} \geq 0, \quad P_B = \left\langle \begin{pmatrix} S + T_\sigma & T_{\epsilon\sigma} \\ T_{\epsilon\sigma} & C + T_\epsilon \end{pmatrix}^{-1} \right\rangle^{-1}, \tag{3}$$

where $i = 1, \ldots, N$ and $T_{\epsilon\sigma}$ and T_ϵ are the translators similar to T_σ, is obtained from (2) when $\|z\| \to \infty$. Inequality (3) does not depend on α_{ph} and coincides with the translation bound for the effective elastic tensor. It contains, as particular cases, the Hill bounds and the Hashin-Shtrikman-Walpole bounds for isotropic S_*. Notice that tensorial inequality (3) naturally includes both the upper and lower bounds for S_*.

The range of α_* is determined by the scalar inequality

$$(\alpha_* - \alpha_E(T)) : P_E(T) : (\alpha_* - \alpha_E(T)) \leq r_E(T) \quad \forall T \text{ as in (3)}. \tag{4}$$

It is obtained from the requirement that the minimum of the difference between the left- and right-hand sides of (2) over z is nonnegative. The explicitly calculated coefficients: fourth-rank tensor P_E, the second-order tensor α_E, and the scalar r_E depend on the properties of the phases, volume fractions, and effective tensor S_*. For each admissible tensor T, the coefficients of the effective tensor α_* are bounded by an ellipsoid centered at $\alpha_E(T)$, and the bound (4) states that they belong to the intersection of all such ellipsoids.

Special cases

The results for the mixtures with voids are easily obtained. This case poses difficulties for previously suggested bounds, see [4]. In this case, the coefficients in (4) are simplified to

$$P_E = \left(\tilde{S}_* - \langle \tilde{S}^{-1} \rangle^{-1}\right)^{-1}, \quad \alpha_E = \langle \tilde{S}^{-1} \rangle^{-1} : \langle S^{-1} : \alpha \rangle, \quad r_E = \langle \alpha : S^{-1} : \alpha \rangle - \langle \alpha : S^{-1} \rangle : \langle \tilde{S}^{-1} \rangle^{-1} : \langle S^{-1} : \alpha \rangle$$

where $\tilde{S} = S + T_\sigma$.

The previously obtained bounds by Schapery [1], Rozen and Hashin [2], and Gibiansky and Torquato [3] (see also Sigmund and Torquato [4] follow from our bounds. Particularly, for the two-phase mixtures, the constant r_E vanishes which leads to the explicit relation $\alpha_* = \alpha_E$, which agrees with the result by Rozen and Hashin [2]. If the effective tensor S_* approaches its bound, some eigenvalues of tensor P_E go to infinity and the effective expansion coefficients tends to the coefficients of α_E, which agrees with the result by Gibiansky and Torquato [3].

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References

[1] Schapery R.A.: Thermal Expansion Coefficients of Composite Materials based on Energy Principles. *J. Comp. Mat* **2**:380–404, 1968.

[2] Rozen B.W. and Hashin Z.: Effective Thermal Expansion Coefficients and Specific Heats of Composite Materials. *Int. J. Engng. Sci.* **8**:157–173, 1970.

[3] Gibiansky L. V. and Torquato S. Thermal Expansion of Isotropic Multiphase Composites and Polycrystals. *J. Mech. Phys. Solids* **45**(7):1223–1252, 1997.

[4] Sigmund O. and Torquato S. Design of Materials with Extreme Thermal Expansion using Three-Phase Topology Optimization Method. *J. Mech. Phys. Solids* **45**(6):1037–1067, 1997.

[5] Cherkaev A. Variational Methods for Structural Optimization. Springer, NY, 2000.