Pergamon

J. Mech. Phys. Solids, Vol. 45, No. 7, pp. 1223 1252, 1997
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0022-5096/97 $17.00+0.00

PII: S0022-5096(96)00129-9

THERMAL EXPANSION OF ISOTROPIC MULTIPHASE COMPOSITES AND POLYCRYSTALS

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(*Received* 13 *June* 1996)

ABSTRACT

Sharp bounds on the effective thermal expansion coefficients of isotropic multiphase composites and isotropic polycrystals are obtained by using classical variational principles and the translation method. Our bounds are appreciably narrower than the known Schapery–Rosen–Hashin bounds. Conditions are formulated that guarantee a one-to-one correspondence between the bulk modulus and thermal expansion coefficient of a polycrystal. All of our results can be readily applied to the poroelasticity problem. Generalizations of the results to treat anisotropic composites comprised of anisotropic phases are discussed.

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Keywords: A. thermomechanical processes, B. inhomogeneous material, B. polycrystalline material, B. thermal expansion, C. variational calculus.

1. INTRODUCTION

Elastic properties of composites and polycrystals have been studied extensively. The first rigorous bounds on the effective elastic moduli of multiphase composites and polycrystals were obtained by Hill (1952). He proved that the arithmetic and harmonic means of the phase moduli are respectively upper and lower bounds on the moduli of the composite. These results are sometime called Reuss–Voigt bounds, owing to the fact that Reuss and Voigt used the arithmetic and harmonic mean averages of the phase properties as approximations for the effective moduli. Subsequently, Hashin and Shtrikman (1962, 1963) introduced new variational principles that allowed them to improve the bounds on the effective moduli of isotropic elastic composites significantly. The recent development of the translation method has enabled one to derive even tighter bounds for two-phase isotropic elastic composites [Cherkaev and Gibiansky (1993); see also Gibiansky and Cherkaev (1984, 1987)] and for isotropic elastic polycrystals (Avellaneda and Milton, 1989; Avellaneda *et al.*, 1996).

The literature dealing with the thermal expansion of elastic composites is not nearly as rich as that for the pure elasticity problem. By using an elegant method proposed by Levin (1967) and Cribb (1968), one can show that for two-phase composites the thermal expansion coefficient is determined solely by the effective elastic tensor of the same composite. Generalizations of Levin's (1967) idea to more complicated structures followed. For example, Hashin (1984) and Schulgasser (1987, 1989a, b) found a similar correspondence between the elastic moduli and thermal expansion of a polycrystal in cases when the elastic tensor of the original crystal possesses some special symmetries. Dvorak (1986) obtained similar relations for two-phase thermoelastic–plastic composites. Dvorak and Chen (1989) studied the thermoelastic behavior of three-phase fiber-reinforced composites and Benveniste (1996) examined the thermoelastic properties of fiber-reinforced polycrystals.

For general multiphase composites, the effective elastic tensor does not determine the effective thermal expansion coefficients. Schapery (1968) and Rosen and Hashin (1970) used variational principles describing the thermoelastic problem (analogous to the classical principles for pure elasticity) to derive the simplest Reuss–Voigt-type bounds on the thermal expansion coefficients. In contrast to the pure elasticity problem, more advanced methods (like the Hashin–Shtrikman or translation methods) have not been used to improve these results. In this paper we fill this gap by applying the translation method to derive tight bounds on the effective thermal expansion coefficient of isotropic composites and polycrystals. Our new bounds are much stronger than the earlier known bounds.

We treat the problem in two and three spatial dimensions. The two-dimensional setting also describes the transverse moduli of a transversely isotropic composite with cylindrical phase geometries, i.e. when phase boundaries are parallel to the axial direction.

Despite significant improvement over known bounds, our results still allow for exotic isotropic composites having negative thermal expansion coefficients that are made of phases with positive thermal expansion coefficients. Indeed, the numerical experiments of Sigmund and Torquato (1996, 1997) provide the first evidence that such composites can be found. Their examples also show that our new bounds are not only tight but may even be optimal for the phase moduli and volume fractions that they chose for their numerical investigation.

For polycrystals, our upper and lower bounds on the thermal expansion coefficient as a function of the effective bulk modulus coincide for some groups of symmetry of the original crystal. In such cases the effective thermal expansion tensor is uniquely determined by the effective stiffness tensor, even for anisotropic polycrystals. Conditions are derived that specify these groups of symmetry and guarantee one-to-one correspondence between the bulk modulus and thermal expansion coefficient of the polycrystal. These conditions agree with similar results from Hashin (1984) and Schulgasser (1987, 1989a, b). In fact, these symmetry conditions and the derivation leading to them follow the arguments of Schulgasser (1989a) very closely, although our results are slightly more general. When the derived conditions are not satisfied, our bounds provide significant improvement over the previously known results of Rosen and Hashin (1970) for the two-dimensional problem. In the three-dimensional polycrystal problem, the translation method leads to the earlier results of Rosen and Hashin.

All our results can be applied directly to three-dimensional composites in which the effective stiffness tensor has cubic symmetry, and to two-dimensional composites with square symmetry. Biot (1956) and Rice and Cleary (1976) have shown that the equations of thermoelasticity are equivalent to those of poroelasticity [see also

Berryman and Milton (1991), Norris (1992) for applications of this equivalency]. Therefore, all of our results can be immediately applied to the poroelasticity problem.

The remainder of the paper is organized as follows: in Section 2 we describe the basic equations of thermoelasticity and reformulate variational principles in a form that is convenient for our use. We derive the simplest bounds on the thermal expansion coefficients similar to ones given by Schapery (1968), and Rosen and Hashin (1970) but in a form that allows for simple improvement of the procedure by using the translation method. In Section 3 we outline the basic idea behind the translation method, provide some necessary tools to apply this method to the problem under study, and finally use it to derive bounds on the effective thermal expansion of isotropic multiphase composites and polycrystals. In Section 4 we apply the general formulas of Section 3 to the important case in which the isotropic composite possesses isotropic phases, and then compare our results with previously known bounds. In Section 5 we derive thermal expansion bounds for isotropic polycrystals, and obtain conditions that guarantee a one-to-one correspondence between the bulk modulus and effective thermal expansion coefficient of isotropic polycrystal. When these conditions are not satisfied, we show that known thermal expansion bounds can be improved in two dimensions. In Section 5 we discuss how our results can be extended to the general case of anisotropic composites with anisotropic phases. Finally, we discuss how our results translate immediately into equivalent results for the poroelasticity problem.

2. PRELIMINARIES

2.1. *Constitutive equations and homogenization*

We consider the linear thermoelastic problem with a state law defined by the equations

$$\boldsymbol{\varepsilon} = \mathbf{S} : \boldsymbol{\tau} + \boldsymbol{\alpha}\theta,$$

$$\zeta = \boldsymbol{\alpha} : \boldsymbol{\tau} + \frac{c_p \theta}{T_0}, \tag{2.1}$$

or in the matrix form

$$\begin{pmatrix} \boldsymbol{\varepsilon} \\ \zeta \end{pmatrix} = \begin{pmatrix} \mathbf{S} & \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^{\mathrm{T}} & c_p/T_0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\tau} \\ \theta \end{pmatrix}, \tag{2.2}$$

where $\theta = T - T_0$ is the infinitesimal change in temperature T measured from some base temperature T_0, $\boldsymbol{\tau}$ is the stress tensor that satisfies equilibrium conditions

$$\nabla \cdot \boldsymbol{\tau} = \mathbf{0}, \quad \boldsymbol{\tau} = \boldsymbol{\tau}^{\mathrm{T}}, \tag{2.3}$$

(superscript T denotes transpose tensor); $\boldsymbol{\varepsilon}$ is the strain tensor equal to a symmetric part of the gradient of the displacement vector $\mathbf{u}$, i.e.

$$\boldsymbol{\varepsilon} = \tfrac{1}{2}[\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}]; \tag{2.4}$$

$\mathbf{S} = \mathbf{C}^{-1}$ is the compliance tensor, $\mathbf{C}$ is the stiffness tensor, $\boldsymbol{\alpha}$ is the thermal expansion tensor, ζ is the increase in the entropy per unit volume over the entropy of the state where $\boldsymbol{\tau} = \mathbf{0}$ and $\theta = 0$, and c_p is the specific heat per unit volume at constant stress. The symbol : denotes a contraction over two indices, so that

$$\mathbf{a}:\mathbf{A}:\mathbf{a} = \sum_{i=1}^{d}\sum_{j=1}^{d}\sum_{k=1}^{d}\sum_{l=1}^{d} A_{ijkl}a_{ji}a_{lk}, \quad \mathbf{a}:\mathbf{b} = \sum_{i=1}^{d}\sum_{j=1}^{d} a_{ij}b_{ji}, \tag{2.5}$$

and

$$\mathbf{b} = \mathbf{A}:\mathbf{a} \quad \text{if and only if } b_{ij} = \sum_{k=1}^{d}\sum_{l=1}^{d} A_{ijkl}a_{lk}, \tag{2.6}$$

where d is the spatial dimension.

Alternatively, the thermoelastic state of the composite can be described by the equations in the form

$$\begin{pmatrix} \tau \\ -\zeta \end{pmatrix} = \begin{pmatrix} \mathbf{C} & \mathbf{\Gamma} \\ \mathbf{\Gamma}^{\mathrm{T}} & -c_v/T_0 \end{pmatrix} \begin{pmatrix} \varepsilon \\ \theta \end{pmatrix}, \tag{2.7}$$

where

$$\mathbf{\Gamma} = -\mathbf{C}:\boldsymbol{\alpha} \tag{2.8}$$

is the thermal stress tensor, and

$$c_v = c_p - \boldsymbol{\alpha}:\mathbf{C}:\boldsymbol{\alpha}T_0 \tag{2.9}$$

is the specific heat at constant strain.†

For a homogeneous body, the thermal expansion tensor $\boldsymbol{\alpha}$ is the first derivative of the strain with respect to temperature in a stress-free material ($\boldsymbol{\tau} = \mathbf{0}$). The thermal stress tensor $\mathbf{\Gamma}$ is the first derivative of the stress with respect to temperature in a strain-free material ($\boldsymbol{\varepsilon} = \mathbf{0}$).

Consider now an N-phase composite in d dimensions with volume fractions f_n, $n = 1, \ldots, N$:

$$\sum_{n=1}^{N} f_n = 1. \tag{2.10}$$

Each phase is characterized by its elastic tensor $\mathbf{C}_n = \mathbf{S}_n^{-1}$, thermal expansion tensor $\boldsymbol{\alpha}_n$, and specific heat $(c_p)_n$, $n = 1, \ldots, N$. Then the equations (2.2)–(2.4) describe the local strains and stresses in the thermoelastic composite if we substitute the quantities

$$\mathbf{C}(\mathbf{x}) = \sum_{n=1}^{N} \chi_n(\mathbf{x})\mathbf{C}_n, \quad \boldsymbol{\alpha}(\mathbf{x}) = \sum_{n=1}^{N} \chi_n(\mathbf{x})\boldsymbol{\alpha}_n, \tag{2.11}$$

where

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† Note that here and throughout the paper all the terms including specific heats c_p and c_v have opposite signs compared with the paper by Rosen and Hashin (1970). We follow Christensen (1979) who in his book reviewed the works of Schapery (1968) and Rosen and Hashin (1970).

$$\chi_n(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x} \in \text{phase } n, \\ 0, & \text{otherwise}, \end{cases} \qquad n = 1, \ldots, N, \tag{2.12}$$

is the characteristic function of the region occupied by the phase n. Note that

$$\langle \chi_n(\mathbf{x}) \rangle = f_n, \tag{2.13}$$

where angular brackets denote a volume average. We note that all of the ensuing results are valid in any space dimension d, but obviously the cases of physical significance are $d = 2$ or 3.

In the polycrystal problem, the stiffness and the thermal expansion tensors of different grains differ only by orientation, i.e.

$$\mathbf{C}(\mathbf{x}) = \mathcal{R}(\phi(\mathbf{x})) : \mathbf{C} : \mathcal{R}^{\mathrm{T}}(\phi(\mathbf{x})), \quad \boldsymbol{\alpha}(\mathbf{x}) = \mathcal{R}(\phi(\mathbf{x})) : \boldsymbol{\alpha}, \tag{2.14}$$

where $\mathcal{R}(\phi(\mathbf{x}))$ is a tensor of rotation by the angle $\phi(\mathbf{x})$, which depends on the point, and $\mathbf{C}$ and $\boldsymbol{\alpha}$ are the constant tensors that characterize the original crystal.

When the size of the periodic cell or inhomogeneities are much smaller than the size of the sample and the characteristic wavelength of the applied fields, then the composite behaves as a homogeneous body. The behavior of the composite can be described by the homogenized system

$$\begin{pmatrix} \langle \boldsymbol{\varepsilon} \rangle \\ \langle \zeta \rangle \end{pmatrix} = \begin{pmatrix} \mathbf{S}^* & \boldsymbol{\alpha}^* \\ (\boldsymbol{\alpha}^*)^{\mathrm{T}} & c_p^*/T_0 \end{pmatrix} \begin{pmatrix} \langle \boldsymbol{\tau} \rangle \\ \theta \end{pmatrix}, \tag{2.15}$$

or, equivalently, by the system

$$\begin{pmatrix} \langle \boldsymbol{\tau} \rangle \\ \langle -\zeta \rangle \end{pmatrix} = \begin{pmatrix} \mathbf{C}^* & \boldsymbol{\Gamma}^* \\ (\boldsymbol{\Gamma}^*)^{\mathrm{T}} & -c_v^*/T_0 \end{pmatrix} \begin{pmatrix} \langle \boldsymbol{\varepsilon} \rangle \\ \theta \end{pmatrix}, \tag{2.16}$$

where

$$\boldsymbol{\Gamma}^* = -\mathbf{C}^* : \boldsymbol{\alpha}^*, \tag{2.17}$$

$$c_v^* = c_p^* - \boldsymbol{\alpha}^* : \mathbf{C}^* : \boldsymbol{\alpha}^* T_0, \tag{2.18}$$

and $\mathbf{C}^*$, $\mathbf{S}^*$, $\boldsymbol{\alpha}^*$, $\boldsymbol{\Gamma}^*$, c_p^*, and c_v^* are the corresponding effective properties of the composite or polycrystal.

2.2. *Variational principles*

Our main interest in this paper is to derive bounds on the effective thermal expansion tensor $\boldsymbol{\alpha}^*$. As in pure elasticity, the thermoelasticity problem permits a variational description. A set of variational principles that describes the behavior of multiphase composites and defines the effective tensors follows immediately from the formulations (2.15)–(2.17). These principles were introduced by Schapery (1968) and Rosen (1970). We will use two of them which can be formulated as follows:

$$\begin{pmatrix} \boldsymbol{\varepsilon}_0 \\ \theta \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \mathbf{C}^* & \boldsymbol{\Gamma}^* \\ (\boldsymbol{\Gamma})^{\mathrm{T}} & -c_v^*/T_0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\varepsilon}_0 \\ \theta \end{pmatrix} = \inf_{\substack{\boldsymbol{\varepsilon} : \langle \boldsymbol{\varepsilon} \rangle = \boldsymbol{\varepsilon}_0 \\ \boldsymbol{\varepsilon} = \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}}{2}}} \left\langle \begin{pmatrix} \boldsymbol{\varepsilon}(\mathbf{x}) \\ \theta \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \mathbf{C}(\mathbf{x}) & \boldsymbol{\Gamma}(\mathbf{x}) \\ \boldsymbol{\Gamma}^{\mathrm{T}}(\mathbf{x}) & -c_v(\mathbf{x})/T_0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\varepsilon}(\mathbf{x}) \\ \theta \end{pmatrix} \right\rangle \tag{2.19}$$

and

$$\begin{pmatrix} \boldsymbol{\tau}_0 \\ \theta \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \mathbf{S}^* & \boldsymbol{\alpha}^* \\ (\boldsymbol{\alpha}^*)^{\mathrm{T}} & c_p^*/T_0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\tau}_0 \\ \theta \end{pmatrix} = \inf_{\substack{\boldsymbol{\tau} : \langle \boldsymbol{\tau} \rangle = \boldsymbol{\tau}_0 \\ \boldsymbol{\tau} = \boldsymbol{\tau}^{\mathrm{T}},\, \nabla \cdot \boldsymbol{\tau} = 0}} \left\langle \begin{pmatrix} \boldsymbol{\tau}(\mathbf{x}) \\ \theta \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \mathbf{S}(\mathbf{x}) & \boldsymbol{\alpha}(\mathbf{x}) \\ \boldsymbol{\alpha}^{\mathrm{T}}(\mathbf{x}) & c_p(\mathbf{x})/T_0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\tau}(\mathbf{x}) \\ \theta \end{pmatrix} \right\rangle. \tag{2.20}$$

The first one states that the energy stored in the composite medium is equal to the minimum of the average stored energy over the admissible strain fields for a given average strain. The second principle states that the complementary energy of the composite medium is equal to the minimum of the average complementary energy over the admissible stress fields for a given average stress. Each of these variational principles can be considered to be a definition of the effective tensors. These definitions (2.19) and (2.20) are equivalent to each other and to the homogenized systems (2.15)–(2.16).

It is important to note that the arguments $\boldsymbol{\varepsilon}$ or $\boldsymbol{\tau}$ and the temperature rise θ play different roles in the variational principles (2.19)–(2.20). The temperature rise θ is given and constant throughout the body, while the strain and the stress fields are to be found from the above variational principles.

2.3. *Previous bounds*

Schapery (1968) and Rosen and Hashin (1970) have used variational principles to get bounds on the thermal expansion coefficients. In this section we will show how to derive their results. We will present the derivation for the case of isotropic composites. The general case will be discussed in the last section of the paper. The procedure that we use differs slightly from the one used in the original papers, but employs the same ideas and leads to the same results. It is important that we discuss this procedure here because it allows for simple improvement by the use of the translation method that we describe in the next section.

Immediately from the variational definition (2.19) of the effective properties we get the bound

$$\frac{\boldsymbol{\varepsilon}_0 : \mathbf{C}^* : \boldsymbol{\varepsilon}_0}{2} + \boldsymbol{\Gamma}^* : \boldsymbol{\varepsilon}_0 \theta - \frac{c_v^* \theta^2}{2T_0} \geqslant \inf_{\boldsymbol{\varepsilon} : \langle \boldsymbol{\varepsilon} \rangle = \boldsymbol{\varepsilon}_0} \left\langle \frac{\boldsymbol{\varepsilon} : \mathbf{C}(\mathbf{x}) : \boldsymbol{\varepsilon}}{2} + \boldsymbol{\Gamma}(\mathbf{x}) : \boldsymbol{\varepsilon} \theta - \frac{c_v(\mathbf{x}) \theta^2}{2T_0} \right\rangle, \tag{2.21}$$

Indeed, the variational problem (2.21) is identical to one in (2.19) except for relaxing the conditions on the admissible field $\boldsymbol{\varepsilon}$, which is no longer required to be a deformation field. Therefore, the minimum in the variational problem (2.21) is lower than in (2.19), thus leading to the bound (2.21). The value of the right-hand side of the inequality

(2.21) can be easily evaluated explicitly. One can replace this variational problem by the simplest variational problem:

$$\inf_{\boldsymbol{\varepsilon}:\langle\boldsymbol{\varepsilon}\rangle=\boldsymbol{\varepsilon}_0}\left\langle\frac{\boldsymbol{\varepsilon}:\mathbf{C}(\mathbf{x}):\boldsymbol{\varepsilon}}{2}+\boldsymbol{\Gamma}(\mathbf{x}):\boldsymbol{\varepsilon}\theta-\frac{c_v(\mathbf{x})\theta^2}{2T_0}\right\rangle$$

$$=\sup_{\boldsymbol{\sigma}}\inf_{\boldsymbol{\varepsilon}}\left\langle\frac{\boldsymbol{\varepsilon}:\mathbf{C}(\mathbf{x}):\boldsymbol{\varepsilon}}{2}+\boldsymbol{\Gamma}(\mathbf{x}):\boldsymbol{\varepsilon}\theta-\frac{c_v(\mathbf{x})\theta^2}{2T_0}-\boldsymbol{\sigma}:(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_0)\right\rangle, \qquad (2.22)$$

where $\boldsymbol{\sigma}$ is the constant matrix Lagrange multiplier under the condition

$$\langle\boldsymbol{\varepsilon}\rangle=\boldsymbol{\varepsilon}_0. \qquad (2.23)$$

The stationary condition [derivative of the functional (2.22) over the tensor variable $\boldsymbol{\varepsilon}$]

$$\mathbf{C}(\mathbf{x}):\boldsymbol{\varepsilon}(\mathbf{x})+\boldsymbol{\Gamma}(\mathbf{x})\theta-\boldsymbol{\sigma}=0 \qquad (2.24)$$

defines the tensor field $\boldsymbol{\varepsilon}(\mathbf{x})$:

$$\boldsymbol{\varepsilon}(\mathbf{x})=-\mathbf{C}^{-1}(\mathbf{x}):(\boldsymbol{\Gamma}(\mathbf{x})\theta-\boldsymbol{\sigma}). \qquad (2.25)$$

Substituting (2.25) into the equality (2.23), gives the Lagrange multiplier $\boldsymbol{\sigma}$ as

$$\boldsymbol{\sigma}=\langle\mathbf{C}^{-1}(\mathbf{x})\rangle^{-1}:(\langle\mathbf{C}^{-1}(\mathbf{x}):\boldsymbol{\Gamma}(\mathbf{x})\rangle\theta+\boldsymbol{\varepsilon}_0). \qquad (2.26)$$

By substituting (2.25) and (2.26) into the functional (2.21), we derive the bound

$$\frac{\boldsymbol{\varepsilon}_0:\mathbf{C}^*:\boldsymbol{\varepsilon}_0}{2}+\boldsymbol{\Gamma}^*:\boldsymbol{\varepsilon}_0\theta-\frac{c_v^*\theta^2}{2T_0}\geqslant\frac{\boldsymbol{\varepsilon}_0:\mathbf{C}_{\mathrm{h}}:\boldsymbol{\varepsilon}_0}{2}+\langle\mathbf{C}^{-1}:\boldsymbol{\Gamma}\rangle:\mathbf{C}_{\mathrm{h}}:\boldsymbol{\varepsilon}_0\theta-\frac{\langle c_v\rangle\theta^2}{2T_0}$$

$$-\frac{\langle\boldsymbol{\Gamma}:\mathbf{C}^{-1}:\boldsymbol{\Gamma}\rangle\theta^2}{2}+\frac{\langle\mathbf{C}^{-1}:\boldsymbol{\Gamma}\rangle:\mathbf{C}_{\mathrm{h}}:\langle\mathbf{C}^{-1}:\boldsymbol{\Gamma}\rangle\theta^2}{2}, \qquad (2.27)$$

where

$$\mathbf{C}_{\mathrm{h}}=\langle\mathbf{C}^{-1}\rangle^{-1}. \qquad (2.28)$$

In fact, we found the stationary value of the functional (2.22); this corresponds to the true minimum if the second derivative of this functional over the variable $\boldsymbol{\varepsilon}$ is positive, i.e. if $\mathbf{C}\geqslant 0$. In our case, the stiffness tensor is always positive definite. The condition $\mathbf{C}(\mathbf{x})\geqslant 0$ will play an important role in the translation method that we will discuss in the next section. Note that $\mathbf{C}^{-1}:\boldsymbol{\Gamma}=-\boldsymbol{\alpha}$, but we will keep the form (2.27) of the bounds for future use.

The bound (2.27) is independent of the microgeometry of the composite. Indeed, the right-hand side of (2.27) depends only on the phase properties and volume fractions.

Similarly, by using variational principle (2.20), instead of (2.19), one can get the bound

$$\frac{\boldsymbol{\tau}_0:\mathbf{S}^*:\boldsymbol{\tau}_0}{2}+\boldsymbol{\alpha}^*:\boldsymbol{\tau}_0\theta+\frac{c_p^*\theta^2}{2T_0}\geqslant\frac{\boldsymbol{\tau}_0:\mathbf{S}_{\rm h}:\boldsymbol{\tau}_0}{2}+\langle\mathbf{S}^{-1}:\boldsymbol{\alpha}\rangle:\mathbf{S}_{\rm h}:\boldsymbol{\tau}_0\theta+\frac{\langle c_p\rangle\theta^2}{2T_0}$$

$$-\frac{\langle\boldsymbol{\alpha}:\mathbf{S}^{-1}:\boldsymbol{\alpha}\rangle\theta^2}{2}+\frac{\langle\mathbf{S}^{-1}:\boldsymbol{\alpha}\rangle:\mathbf{S}_{\rm h}:\langle\mathbf{S}^{-1}:\boldsymbol{\alpha}\rangle\theta^2}{2},\qquad(2.29)$$

where

$$\mathbf{S}_{\rm h}=\langle\mathbf{S}^{-1}\rangle^{-1}.\qquad(2.30)$$

Let us now assume that the composite is isotropic, i.e.

$$\mathbf{C}^*=\kappa_*\delta_{ij}\delta_{kl}+\mu_*\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{d}\delta_{ij}\delta_{kl}\right),\qquad(2.31)$$

and

$$\boldsymbol{\alpha}^*=\alpha_*\delta_{ij}=\alpha_*\mathbf{I},\quad\boldsymbol{\Gamma}^*=\Gamma_*\delta_{ij}=\Gamma_*\mathbf{I},\qquad(2.32)$$

where κ_* and μ_* are the effective bulk and shear moduli of the composite, α_* is the effective thermal expansion coefficient, $\Gamma_*=-d\kappa_*\alpha_*$ is the effective thermal stress coefficient, δ_{ij} is the Kronecker delta, and $\mathbf{I}$ is the d-dimensional unit tensor. Let the average strain and stress fields in the variational bounds (2.27) and (2.29) be proportional to the unit tensor

$$\boldsymbol{\varepsilon}_0=\varepsilon_0\mathbf{I},\quad\boldsymbol{\tau}_0=\tau_0\mathbf{I}.\qquad(2.33)$$

Then, the bound (2.27) leads to the inequality

$$\frac{\kappa_*-A_1}{2}\left(\frac{\varepsilon_0}{\theta}\right)^2-(\kappa_*\alpha_*+B_1)\left(\frac{\varepsilon_0}{\theta}\right)+(C_1+\gamma)\geqslant 0,\qquad(2.34)$$

where

$$A_1=\frac{I:C_{\rm h}:I}{d^2},\quad B_1=\frac{\langle\mathbf{C}^{-1}:\boldsymbol{\Gamma}\rangle:\mathbf{C}_{\rm h}:\mathbf{I}}{d^2},$$

$$C_1=\frac{\langle\boldsymbol{\Gamma}:\mathbf{C}^{-1}:\boldsymbol{\Gamma}\rangle}{2d^2}-\frac{\langle\mathbf{C}^{-1}:\boldsymbol{\Gamma}\rangle:\mathbf{C}_{\rm h}:\langle\mathbf{C}^{-1}:\boldsymbol{\Gamma}\rangle}{2d^2},\qquad(2.35)$$

and

$$\gamma=-\frac{c_v^*-\langle c_v\rangle}{2d^2T_0}.\qquad(2.36)$$

Similarly, the bound (2.29) leads to the inequality

$$\frac{1}{2}\left(\frac{1}{\kappa_*}-A_2\right)\left(\frac{\tau_0}{\theta}\right)^2+d(\alpha_*-B_2)\left(\frac{\tau_0}{\theta}\right)+d^2\left(\frac{\kappa_*\alpha^2{}_*}{2}+C_2-\gamma\right)\geqslant 0,\qquad(2.37)$$

where

$$A_2=\mathbf{I}:\mathbf{S}_{\rm h}:\mathbf{I},\quad B_2=\frac{\langle\mathbf{S}^{-1}\boldsymbol{\alpha}\rangle:\mathbf{S}_{\rm h}:\mathbf{I}}{d},$$

$$C_2 = \frac{\langle \boldsymbol{\alpha} : \mathbf{S}^{-1} : \boldsymbol{\alpha} \rangle}{2d^2} - \frac{\langle \boldsymbol{\alpha} : \mathbf{C} : \boldsymbol{\alpha} \rangle}{2d^2} - \frac{\langle \boldsymbol{\alpha} : \mathbf{S}^{-1} \rangle : \mathbf{S}_{\mathrm{h}} : \langle \boldsymbol{\alpha} : \mathbf{S}^{-1} \rangle}{2d^2}. \tag{2.38}$$

In (2.37) we have used the specific heat formulas (2.9) and (2.18) to obtain

$$\frac{c_p^* - \langle c_p \rangle}{2T_0} = \frac{c_v^* - \langle c_v \rangle}{2T_0} + \frac{d^2 \kappa_* \alpha^2{}_*}{2} - \frac{\langle \boldsymbol{\alpha} : \mathbf{C} : \boldsymbol{\alpha} \rangle}{2}. \tag{2.39}$$

Note that the sum of the first two terms in the expression for the C_2 coefficient is equal to zero:

$$\frac{\langle \boldsymbol{\alpha} : \mathbf{S}^{-1} : \boldsymbol{\alpha} \rangle}{2} - \frac{\langle \boldsymbol{\alpha} : \mathbf{C} : \boldsymbol{\alpha} \rangle}{2} = 0, \tag{2.40}$$

because $\mathbf{C} = \mathbf{S}^{-1}$. In the more general translation bounds that will be developed in Section 3, the difference of similar terms will be non-zero.

Observe that the quadratic equations (2.34) and (2.37) are positive for all values of the variables ε_0/θ and τ_0/θ. Therefore, the quadratic and constant terms are positive, and the discriminants are negative, i.e.

$$\kappa_* - A_1 \geqslant 0, \quad (\kappa_* \alpha_* + B_1)^2 - 2(\kappa_* - A_1)(\gamma + C_1) \leqslant 0, \quad \gamma + C_1 \geqslant 0, \tag{2.41}$$

and

$$\frac{1}{\kappa_*} - A_2 \geqslant 0, \quad (\alpha_* - B_2)^2 - 2\left(\frac{1}{\kappa_*} - A_2\right)\left(\frac{\kappa_* \alpha^2{}_*}{2} + C_2 - \gamma\right) \leqslant 0,$$

$$\frac{\kappa_* \alpha^2{}_*}{2} + C_2 - \gamma \geqslant 0. \tag{2.42}$$

The conditions (2.41)–(2.42) provide bounds on the effective bulk modulus, thermal expansion coefficient, and specific heats.

Specifically, the first inequalities in (2.41) and (2.42) lead to Hill's (1952) bulk modulus bounds

$$\kappa_{\mathrm{H}}^{\mathrm{l}} \leqslant \kappa_* \leqslant \kappa_{\mathrm{H}}^{\mathrm{u}}, \quad \kappa_{\mathrm{H}}^{\mathrm{l}} = A_1 = \frac{\mathbf{I} : \langle \mathbf{C}^{-1} \rangle^{-1} : \mathbf{I}}{d^2}, \quad \kappa_{\mathrm{H}}^{\mathrm{u}} = \frac{1}{A_2} = \frac{1}{\mathbf{I} : \langle \mathbf{S}^{-1} \rangle^{-1} : \mathbf{I}}. \tag{2.43}$$

Using the translation method, we will obtain in Section 3 the Hashin–Shtrikman (1963) bulk modulus bounds in the case of isotropic composites having isotropic phases.

The second inequalities in (2.41) and (2.42) are quadratic functions of the effective thermal expansion coefficient α_*. For a given value of the effective bulk modulus κ_*, each of them defines a parabola in the α_*–γ plane with an axis that is parallel to the γ-axis. Two intersections of these parabolas, which are given by the solution of the system

$$(\kappa_* \alpha_* + B_1)^2 - 2(\kappa_* - A_1)(\gamma + C_1) = 0,$$

$$(\alpha_* - B_2)^2 - 2\left(\frac{1}{\kappa_*} - A_2\right)\left(\frac{\kappa_* \alpha^2{}_*}{2} + C_2 - \gamma\right) = 0, \tag{2.44}$$

as functions of γ and α_*, define the bounds on α_*. They are given by the inequalities

$$\alpha^- \leqslant \alpha_* \leqslant \alpha^+, \tag{2.45}$$

where

$$\alpha^\pm = \frac{1}{\kappa_*(\kappa_H^u - \kappa_H^l)}(-B_1(\kappa_H^u - \boldsymbol{\kappa}_*) + B_2\kappa_H^u(\kappa_* - \kappa_H^l) \pm \Psi^{1/2}(\kappa_* - \kappa_H^l)^{1/2}(\kappa_H^u - \kappa_*)^{1/2}), \tag{2.46}$$

and

$$\Psi = 2(C_1 + C_2)(\kappa_H^u - \kappa_H^l) - B_1^2 - 2\kappa_H^u B_1 B_2 - \kappa_H^l \kappa_H^u B_2^2. \tag{2.47}$$

As we will see, these bounds are equivalent to the ones given by Schapery (1968) and Rosen and Hashin (1970) for isotropic multiphase composites having isotropic phases.

The third condition in each of the systems (2.41) and (2.42), as well as the ones that we just studied, lead to the restriction on the $\gamma = -(c_v^* - \langle c_v \rangle)/(2d^2 T_0)$ coefficient, i.e. restrictions on the specific heat of the composite. However in this paper, we will concentrate only on bounds on the effective thermal expansion coefficients.

In summary, in this section we evaluated explicit bounds on the bulk modulus and effective thermal expansion coefficient of isotropic composites of any number of anisotropic phases. The bounds (2.43) on the effective bulk modulus are Hill's (1952) bounds, which can be improved. The bounds on the effective thermal expansion coefficient (2.45)–(2.47) correspond to the known Schapery–Rosen–Hashin bounds, which we will show can also be improved.

In Section 3 of the paper we will modify the procedure by using the translation method. We will be able directly to use the formulas for the bounds (2.45)–(2.47) with some modification of the coefficients in the expressions. The new procedure will provide us with improved bounds on both the bulk modulus and the thermal expansion coefficient.

We will end this section with an explicit evaluation of the bounds (2.43)–(2.47) for the isotropic composites having isotropic phases. In this case, we have

$$A_1 = \frac{1}{\langle \kappa^{-1} \rangle}, \quad B_1 = -\frac{\langle \alpha \rangle}{\langle \kappa^{-1} \rangle}, \quad C_1 = \frac{\langle \kappa \alpha^2 \rangle}{2} - \frac{\langle \alpha \rangle^2}{2\langle \kappa^{-1} \rangle}; \tag{2.48}$$

and

$$A_2 = \frac{1}{\langle \kappa \rangle}, \quad B_2 = \frac{\langle \kappa \alpha \rangle}{\langle \kappa \rangle}, \quad C_2 = -\frac{\langle \kappa \alpha \rangle^2}{2\langle \kappa \rangle}. \tag{2.49}$$

Then the bulk modulus bounds

$$\langle \kappa^{-1} \rangle^{-1} \leqslant \kappa_* \leqslant \langle \kappa \rangle, \tag{2.50}$$

coincide with the Hill's (1952) bounds. The thermal expansion bounds

$$\alpha^{\pm} = \frac{1}{\langle 1/\kappa\rangle - 1/\langle\kappa\rangle}\left\{\langle\alpha\rangle\left(\frac{1}{\kappa_*} - \frac{1}{\langle\kappa\rangle}\right) + \frac{\langle\kappa\alpha\rangle}{\langle\kappa\rangle}\left(\left\langle\frac{1}{\kappa}\right\rangle - \frac{1}{\kappa_*}\right)\right.$$
$$\left. \pm\Psi^{1/2}\left(\left\langle\frac{1}{\kappa}\right\rangle - \frac{1}{\kappa_*}\right)^{1/2}\left(\frac{1}{\kappa_*} - \frac{1}{\langle\kappa\rangle}\right)^{1/2}\right\}, \quad (2.51)$$

where

$$\Psi = \left(\left\langle\frac{1}{\kappa}\right\rangle - \frac{1}{\langle\kappa\rangle}\right)\left(\langle\kappa\alpha^2\rangle - \frac{\langle\kappa\alpha\rangle^2}{\langle\kappa\rangle}\right) - \left(\langle\alpha\rangle - \frac{\langle\kappa\alpha\rangle}{\langle\kappa\rangle}\right)^2, \quad (2.52)$$

coincide with the Schapery (1968) and Rosen and Hashin (1970) bounds.

One can check that $\Psi = 0$ for two-phase composites and hence expression (2.51) uniquely determines the thermal expansion given the effective bulk modulus of the composite [see, e.g., Levin (1967), and Rosen and Hashin (1970) and references therein].

3. TRANSLATION BOUNDS

The translation method is a powerful tool for obtaining bounds on the effective moduli of composite materials. It was introduced by Lurie and Cherkaev (1984, 1986a, b), Murat and Tartar (1985), and Tartar (1978, 1985), who found optimal bounds on the conductivity tensor of two-phase composites. The method was used to regularize the optimal design problem for elastic bars and plates by Lurie *et al.* (1982). It was further developed and applied to a variety of problems by Milton (1990a, b), Cherkaev and Gibiansky (1992, 1993), and Gibiansky and Torquato (1995a, 1996a). Here we will use the energy bounding procedure that was developed for the elasticity problem by Gibiansky and Cherkaev (1984, 1987) in connection with structural optimization problems. Among other works on this subject, one should mention the papers by Allaire and Kohn (1993), Gibiansky and Milton (1993), Gibiansky and Torquato (1995b, 1996b), Avellaneda *et al.* (1996), and Bhattacharya and Kohn (1997) all of which deal with different aspects of the translation method and its applications.

Out goal is to improve the bounds (2.27) and (2.29) on the energy functionals (2.19) and (2.20). To get the bound (2.27), we enlarged the space of the admissible deformation field ε by removing the differential conditions $\varepsilon = [\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}}]/2$ that reflect the compatibility conditions. This allowed us to evaluate the minimum in (2.21), but at the cost: the bounds (2.27) are too wide in most cases and can be improved. The translation procedure enables us to improve these bounds by still removing the differential restrictions, but exploiting the existence of so-called quasiconvex functions.

3.1. *Quasiconvex quadratic forms*

Consider an arbitrary second-order tensor $\mathbf{e}$ and a fourth-order tensor $\mathcal{T}$. The quadratic form

$$\phi(\mathbf{e}) = \mathbf{e} : \mathscr{T} : \mathbf{e} \tag{3.1}$$

is convex if and only if the inequality

$$\langle \mathbf{e} : \mathscr{T} : \mathbf{e} \rangle - \langle \mathbf{e} \rangle : \mathscr{T} : \langle \mathbf{e} \rangle \geqslant 0 \tag{3.2}$$

holds for any tensor field $\mathbf{e}(\mathbf{x})$. The inequality (3.2) holds for any tensor field $\mathbf{e}(\mathbf{x})$ if an only if the corresponding tensor $\mathscr{T}$ is positive semi-definite.

In the problem under study we are interested in the similar properties of the quadratic forms of the strain and stress fields. The strain tensor is not arbitrary, but can be expressed as a symmetric part of the gradient of the displacement vector $\mathbf{u}$. The stress tensor is a symmetric divergence-free tensor. These additional properties allow us to ease the conditions on the tensor $\mathscr{T}$ that guarantee that the "convexity inequality" (3.2) holds. We will call the quadratic form $\phi_\varepsilon(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon} : \mathscr{T}_\varepsilon : \boldsymbol{\varepsilon}$ of the strain field $\boldsymbol{\varepsilon}$ quasiconvex, if

$$\langle \boldsymbol{\varepsilon} : \mathscr{T}_\varepsilon : \boldsymbol{\varepsilon} \rangle - \boldsymbol{\varepsilon}_0 : \mathscr{T}_\varepsilon : \boldsymbol{\varepsilon}_0 \geqslant 0, \tag{3.3}$$

for any strain field $\boldsymbol{\varepsilon}$ such that

$$\boldsymbol{\varepsilon} = \tfrac{1}{2}[\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}], \quad \langle \boldsymbol{\varepsilon} \rangle = \boldsymbol{\varepsilon}_0. \tag{3.4}$$

Similarly, we will call the quadratic form $\phi_\tau(\boldsymbol{\tau}) = \boldsymbol{\tau} : \mathscr{T}_\tau : \boldsymbol{\tau}$ of the stress field $\boldsymbol{\tau}$ quasiconvex, if

$$\langle \boldsymbol{\tau} : \mathscr{T}_\tau : \boldsymbol{\tau} \rangle - \boldsymbol{\tau}_0 : \mathscr{T}_\tau : \boldsymbol{\tau}_0 \geqslant 0, \tag{3.5}$$

for any stress field $\boldsymbol{\tau}$ such that

$$\nabla \cdot \boldsymbol{\tau} = 0, \quad \boldsymbol{\tau} = \boldsymbol{\tau}^{\mathrm{T}}, \quad \langle \boldsymbol{\tau} \rangle = \boldsymbol{\tau}_0. \tag{3.6}$$

Such functions are sometimes called A-quasiconvex [see Dacorogna (1982) for definitions, discussion, and references].

Quadratic quasiconvex forms that we need in this paper are given by the following statements:

Statement 1: The quadratic form $\boldsymbol{\varepsilon} : \mathscr{T}_\varepsilon : \boldsymbol{\varepsilon}$ of the strain field (3.4) satisfies the quasiconvexity inequality (3.3) if the corresponding fourth-order tensor $\mathscr{T}_\varepsilon(t_1)$ is given by

$$\mathscr{T}_\varepsilon = \mathscr{T}_\varepsilon(t_1) = -\frac{2(d-1)t_1}{d}\delta_{ij}\delta_{kl} + t_1\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{d}\delta_{ij}\delta_{kl}\right) \tag{3.7}$$

and the parameter t_1 is non-negative,

$$t_1 \geqslant 0. \tag{3.8}$$

Note that the tensor $\mathscr{T}_\varepsilon(t_1)$ is the stiffness tensor of an isotropic material with a *negative* bulk modulus $-2(d-1)t_1/d$ and a shear modulus t_1 [cf. (2.31) and (3.7)].

Statement 2: The quadratic form $\boldsymbol{\tau} : \mathscr{T}_\tau : \boldsymbol{\tau}$ of the stress field (3.6) satisfies the quasiconvexity inequality (3.5) if the corresponding fourth-order tensor $\mathscr{T}_\tau(t_2)$ is given by

$$\mathcal{T}_\tau = \mathcal{T}_\tau(t_2) = -\frac{t_2}{2d(d-1)}\delta_{ij}\delta_{kl} + \frac{t_2}{4}\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{d}\delta_{ij}\delta_{kl}\right) \tag{3.9}$$

and the parameter t_2 is non-negative,

$$t_2 \geqslant 0, \quad \text{if } d \geqslant 3, \tag{3.10}$$

or has any (positive or negative) value for the two-dimensional problem ($d = 2$).

Note that the tensor $\mathcal{T}_\tau(t_2)$ is equal to the compliance tensor of the material with a bulk modulus $-2(d-1)/(dt_2)$ and a shear modulus $1/t_2$ [cf. (2.31) and (3.9)].

Statement 2 in two dimensions has been independently discovered by Lurie *et al.* (1982) who used it to regularize the optimal design problem of bars and plates, and by Kohn and Strang (1986) who applied it to the plane elasticity problem. Statement 1 in two dimensions, and the three-dimensional variants of Statements 1 and 2 were found by Gibiansky and Cherkaev (1984, 1987). One can find elementary proofs of all these inequalities in the paper by Gibiansky and Milton (1993).

3.2. *New bounds*

We are now in a position to prove the new bounds. We start with the variational principle (2.19), which we express in the form

$$\begin{aligned}\frac{\boldsymbol{\varepsilon}_0:(\mathbf{C}^*-\mathcal{T}_\varepsilon(t_1)):\boldsymbol{\varepsilon}_0}{2} &+ \boldsymbol{\Gamma}^*:\boldsymbol{\varepsilon}_0\theta - \frac{c_v^*\theta^2}{2T_0}\\ = \inf_{\substack{\boldsymbol{\varepsilon}:\langle\boldsymbol{\varepsilon}\rangle=\boldsymbol{\varepsilon}_0\\ \boldsymbol{\varepsilon}=\frac{\nabla\mathbf{u}+(\nabla\mathbf{u})^T}{2}}} &\left\langle \frac{\boldsymbol{\varepsilon}:(\mathbf{C}(\mathbf{x})-\mathcal{T}_\varepsilon(t_1)):\boldsymbol{\varepsilon}}{2} + \boldsymbol{\Gamma}(\mathbf{x}):\boldsymbol{\varepsilon}\theta - \frac{c_v(\mathbf{x})\theta^2}{2T_0}\right.\\ &\left. + \frac{\boldsymbol{\varepsilon}:\mathcal{T}_\varepsilon(t_1):\boldsymbol{\varepsilon}}{2}\right\rangle - \frac{\boldsymbol{\varepsilon}_0:\mathcal{T}_\varepsilon(t_1):\boldsymbol{\varepsilon}_0}{2}.\end{aligned} \tag{3.11}$$

Here we have subtracted the term $\frac{1}{2}\boldsymbol{\varepsilon}_0:\mathcal{T}_\varepsilon(t_1):\boldsymbol{\varepsilon}_0$ from both sides of (3.11) and added and subtracted the quasiconvex quadratic form $\frac{1}{2}\boldsymbol{\varepsilon}:\mathcal{T}_\varepsilon(t_1):\boldsymbol{\varepsilon}$ on the right-hand side of this equation. The difference between the last two terms on the right-hand side of the equality (3.11) is positive, due to the quasiconvexity of the quadratic form $\boldsymbol{\varepsilon}:\mathcal{T}_\varepsilon(t_1):\boldsymbol{\varepsilon}$ (see Statement 1). Therefore, we can neglect these terms, thus reducing the value of the right-hand side of (3.11). The following bound immediately follows:

$$\begin{aligned}\frac{\boldsymbol{\varepsilon}_0:(\mathbf{C}^*-\mathcal{T}_\varepsilon(t_1)):\boldsymbol{\varepsilon}_0}{2} &+ \boldsymbol{\Gamma}^*:\boldsymbol{\varepsilon}_0\theta - \frac{c_v^*\theta^2}{2T_0}\\ \geqslant \inf_{\boldsymbol{\varepsilon}:\langle\boldsymbol{\varepsilon}\rangle=\boldsymbol{\varepsilon}_0} &\left\langle \frac{\boldsymbol{\varepsilon}:(\mathbf{C}(\mathbf{x})-\mathcal{T}_\varepsilon(t_1)):\boldsymbol{\varepsilon}}{2} + \boldsymbol{\Gamma}(\mathbf{x}):\boldsymbol{\varepsilon}\theta - \frac{c_v(\mathbf{x})\theta^2}{2T_0}\right\rangle,\end{aligned} \tag{3.12}$$

where we also enlarged the space of admissible tensor fields $\boldsymbol{\varepsilon}$.

The value of the parameter t_1 is restricted by the quasiconvexity requirement $t_1 \geqslant 0$ for the quadratic form (3.3). In the process of deriving the bound (2.34), we also have used the fact that the stiffness tensor $\mathbf{C}(\mathbf{x})$ is non-negative, $\mathbf{C}(\mathbf{x}) \geqslant 0$. Therefore, we will also require

$$\mathbf{C}(\mathbf{x})-\mathscr{T}_{\varepsilon}(t_1) \geqslant 0, \quad t_1 \geqslant 0 \tag{3.13}$$

at any point in the composite. For example, for the case of a multiphase composite with isotropic phases,

$$t_1 \in [0, \mu_{\min}], \tag{3.14}$$

where $\mu_{\min} = \min\{\mu_1, \ldots, \mu_N\}$ is the minimal of the phase shear moduli. Indeed, comparing the representation of the elastic isotropic tensor (2.31) and the translation tensor $\mathscr{T}_{\varepsilon}(t_1)$ (3.7), one can see that the condition (3.14) guarantees inequality (3.13). Furthermore, we will omit the arguments $\mathbf{x}$ and t_1 to simplify the notation.

Literally following the procedure described in Section 3, we obtain the following inequality:

$$\frac{\kappa_* - A'_1}{2}\left(\frac{\varepsilon_0}{\theta}\right)^2 - (\kappa_*\alpha_* + B'_1)\left(\frac{\varepsilon_0}{\theta}\right) + (C'_1 + \gamma) \geqslant 0, \tag{3.15}$$

where

$$A'_1 = \frac{\mathbf{I}:\langle(\mathbf{C}-\mathscr{T}_{\varepsilon})^{-1}\rangle^{-1}:\mathbf{I}}{d^2} - \frac{2(d-1)t_1}{d},$$

$$B'_1 = \frac{\langle(\mathbf{C}-\mathscr{T}_{\varepsilon})^{-1}:\boldsymbol{\Gamma}\rangle:\langle(\mathbf{C}-\mathscr{T}_{\varepsilon})^{-1}\rangle^{-1}:\mathbf{I}}{d^2},$$

$$C'_1 = \frac{\langle\boldsymbol{\Gamma}:(\mathbf{C}-\mathscr{T}_{\varepsilon})^{-1}:\boldsymbol{\Gamma}\rangle}{2d^2} - \frac{\langle(\mathbf{C}-\mathscr{T}_{\varepsilon})^{-1}:\boldsymbol{\Gamma}\rangle:\mathbf{C}_{\mathrm{h}}:\langle(\mathbf{C}-\mathscr{T}_{\varepsilon}):\boldsymbol{\Gamma}\rangle}{2d^2}, \tag{3.16}$$

which is valid for any value ε_0 of the hydrostatic average strain field $\boldsymbol{\varepsilon}_0 = \varepsilon_0\mathbf{I}$.

Now one can appreciate our decision not to simplify the expressions for the coefficients B_1 and C_1. Indeed, the bounds (2.21) and (3.12) formally differ by replacing the $\mathbf{C}$-tensors in (2.21) by the $[\mathbf{C}-\mathscr{T}_{\varepsilon}(t_1)]$-tensors in (3.12). Therefore, we were able to skip all of the intermediate steps and make similar substitutions in the final formulas (2.34), thus obtaining the inequality (3.15). Note that the effective bulk modulus κ_* should be replaced by the expression $\kappa_* + 2(d-1)t_1/d$ in the quadratic term (2.34), the thermal stress tensor is still equal to $\boldsymbol{\Gamma} = -\mathbf{C}:\boldsymbol{\alpha}$, but the stiffness tensor $\mathbf{C}$ in the expressions (2.35) should be replaced by the "translated" stiffness tensor $\mathbf{C}-\mathscr{T}_{\varepsilon}$.

Similarly, from the variation principle (2.20) and Statement 2, one can get the bound

$$\frac{1}{2}\left(\frac{1}{\kappa_*} - A'_2\right)\left(\frac{\tau_0}{\theta}\right)^2 + d(\alpha_* - B'_2)\left(\frac{\tau_0}{\theta}\right) + d^2\left(\frac{\kappa_*\alpha_*^2}{2} + C'_2 - \gamma\right) \geqslant 0, \tag{3.17}$$

where

$$A'_2 = \mathbf{I}:\langle(\mathbf{S}-\mathscr{T}_{\tau})^{-1}\rangle^{-1}:\mathbf{I} - \frac{dt_2}{2(d-1)},$$

$$B'_2 = \frac{1}{d}\langle(\mathbf{S}-\mathcal{T}_\tau)^{-1}:\boldsymbol{\alpha}\rangle:\langle(\mathbf{S}-\mathcal{T}_\tau)^{-1}\rangle^{-1}:\mathbf{I},$$

$$C'_2 = \frac{\langle\boldsymbol{\alpha}:(\mathbf{S}-\mathcal{T}_\tau)^{-1}:\boldsymbol{\alpha}\rangle}{2d^2} - \frac{\langle\boldsymbol{\alpha}:\mathbf{C}:\boldsymbol{\alpha}\rangle}{2d^2}$$
$$- \frac{\langle\boldsymbol{\alpha}:(\mathbf{S}-\mathcal{T}_\tau)^{-1}\rangle:\langle(\mathbf{S}-\mathcal{T}_\tau)^{-1}\rangle^{-1}:\langle\boldsymbol{\alpha}:(\mathbf{S}-\mathcal{T}_\tau)^{-1}\rangle}{2d^2}. \tag{3.18}$$

This is obtained from (2.37) by replacement of the $\mathbf{S}$ tensor by the difference $\mathbf{S}-\mathcal{T}_\tau$. The inequality (3.17) is valid for any value of the stress field amplitude τ and for the values of the parameter t_2 which satisfy the condition

$$\mathbf{S}-\mathcal{T}_\tau(t_2) \geqslant 0, \quad \begin{cases} \forall t_2, & d=2, \\ t_2 \geqslant 0, & d \geqslant 3. \end{cases} \tag{3.19}$$

Therefore, for the case of isotropic composites having isotropic phases,

$$t_2 \in \left[-\frac{1}{\kappa_{\max}}, \frac{1}{\mu_{\max}}\right], \quad d=2, \tag{3.20}$$

for the two-dimensional problem, and

$$t_2 \in \left[0, \frac{1}{\mu_{\max}}\right], \quad d \geqslant 3, \tag{3.21}$$

in three dimensions.

Literally repeating the procedure that leads to the bounds (2.43) and (2.46)–(2.47), we obtain the new bulk modulus bounds

$$\kappa_t^{\mathrm{l}} \leqslant \kappa_* \leqslant \kappa_t^{\mathrm{u}}, \quad \kappa_t^{\mathrm{l}} = A'_1, \quad \kappa_t^{\mathrm{u}} = 1/A'_2; \tag{3.22}$$

and the new thermal expansion bounds

$$\alpha_t^- \leqslant \alpha_* \leqslant \alpha_t^+, \tag{3.23}$$

where

$$\alpha_t^{\pm} = \frac{1}{\kappa_*(\kappa_t^{\mathrm{u}}-\kappa_t^{\mathrm{l}})}\left(-B'_1(\kappa_t^{\mathrm{u}}-\kappa_*)+B'_2\kappa_t^{\mathrm{u}}(\kappa_*-\kappa_t^{\mathrm{l}}) \pm \Psi^{1/2}(\kappa_*-\kappa_t^{\mathrm{l}})^{1/2}(\kappa_t^{\mathrm{u}}-\kappa_*)^{1/2}\right), \tag{3.24}$$

and

$$\Psi = 2(C'_1+C'_2)(\kappa_t^{\mathrm{u}}-\kappa_t^{\mathrm{l}}) - B'^2_1 - 2\kappa_t^{\mathrm{u}}B'_1B'_2 - \kappa_t^{\mathrm{l}}\kappa_t^{\mathrm{u}}(B'_2)^2. \tag{3.25}$$

Each of these bounds depends on the choice of the parameters t_1 and t_2 subjected to the restrictions (3.13) and (3.19). For zero values of the parameters $t_1 = 0$ and $t_2 = 0$ the bounds (3.22) and (3.23)–(3.25) coincide with (2.43) and (2.45)–(2.47). Optimization over these parameters yields better bounds. The optimal choice of the parameters strongly depend on the phase properties. In the next section we will obtain bounds on the effective moduli of isotropic composites of isotropic phases. In Section 5 we consider the polycrystal problem.

4. MULTIPHASE ISOTROPIC COMPOSITES WITH ISOTROPIC PHASES

In this section we optimize the bounds (3.22)–(3.25) for the important case of a macroscopically isotropic composite consisting of N isotropic phases.

The stiffness and thermal expansion tensors of the nth isotropic phase can be expressed as

$$\mathbf{C}_n = \kappa_n\delta_{ij}\delta_{kl}+\mu_n\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{d}\delta_{ij}\delta_{kl}\right), \quad \boldsymbol{\alpha}_n = \alpha_n\delta_{ij}. \tag{4.1}$$

The volume averages of the properties for the multiphase composite are given by formulas similar to the following bulk modulus averaging:

$$\langle\kappa\rangle = \left\langle \sum_{n=1}^{N}\chi_n(\mathbf{x})\kappa_n \right\rangle = \sum_{n=1}^{N} f_n\kappa_n. \tag{4.2}$$

Recall that the index n is reserved only to indicate the phase type.

After straightforward calculations, one can obtain the relations

$$\begin{aligned}
A'_1 &= \left\langle \frac{d}{d\kappa+2(d-1)t_1} \right\rangle^{-1} - \frac{2(d-1)t_1}{d}, \\
B'_1 &= -\left\langle \frac{d\kappa\alpha}{d\kappa+2(d-1)t_1} \right\rangle^{2}\left\langle \frac{d}{d\kappa+2(d-1)t_1} \right\rangle^{-1}, \\
C'_1 &= \frac{1}{2}\left\langle \frac{d\kappa^2\alpha^2}{d\kappa+2(d-1)t_1} \right\rangle - \frac{1}{2}\left\langle \frac{d\kappa\alpha}{d\kappa+2(d-1)t_1} \right\rangle^{2}\left\langle \frac{d}{d\kappa+2(d-1)t_1} \right\rangle^{-1},
\end{aligned} \tag{4.3}$$

$$\begin{aligned}
A'_2 &= \left\langle \frac{2(d-1)}{2(d-1)\kappa^{-1}+dt_2} \right\rangle^{-1} - \frac{dt_2}{2(d-1)}, \\
B'_2 &= \left\langle \frac{2(d-1)\alpha}{2(d-1)\kappa^{-1}+dt_2} \right\rangle\left\langle \frac{2(d-1)}{2(d-1)\kappa^{-1}+dt_2} \right\rangle^{-1} \\
C'_2 &= \frac{1}{2}\left\langle \frac{2(d-1)\alpha^2}{2(d-1)\kappa^{-1}+dt_2} \right\rangle - \frac{\langle\kappa\alpha^2\rangle}{2} \\
&\quad - \frac{1}{2}\left\langle \frac{2(d-1)\alpha}{2(d-1)\kappa^{-1}+dt_2} \right\rangle^{2}\left\langle \frac{2(d-1)}{2(d-1)\kappa^{-1}+dt_2} \right\rangle^{-1}.
\end{aligned} \tag{4.4}$$

In the light of these relations, the bulk modulus bounds (3.22) can be rewritten as

$$\kappa_* \geqslant \max_{t_1 \in [0,\mu_{\min}]} \left[\left\langle \frac{d}{d\kappa + 2(d-1)t_1} \right\rangle^{-1} - \frac{2(d-1)t_1}{d} \right],$$

$$\frac{1}{\kappa_*} \geqslant \max_{t_2 \in [-\kappa_{\max}^{-1},\mu_{\max}^{-1}]} \left[\left\langle \frac{2(d-1)}{2(d-1)\kappa^{-1} + dt_2} \right\rangle^{-1} - \frac{dt_2}{2(d-1)} \right], \quad \text{if } d = 2,$$

$$\frac{1}{\kappa_*} \geqslant \max_{t_2 \in [0,\mu_{\max}^{-1}]} \left[\left\langle \frac{2(d-1)}{2(d-1)\kappa^{-1} + dt_2} \right\rangle^{-1} - \frac{dt_2}{2(d-1)} \right], \quad \text{if } d \geqslant 3. \tag{4.5}$$

One can check that the inequalities (4.5) are the most restrictive when

$$t_1 = \mu_{\min}, \quad t_2 = 1/\mu_{\max}. \tag{4.6}$$

For such values of the parameters t_1 and t_2, the inequalities (4.5) lead to the bounds

$$\kappa_{\rm HS}^{\rm l} \leqslant \kappa_* \leqslant \kappa_{\rm HS}^{\rm u}, \tag{4.7}$$

where

$$\kappa_{\rm HS}^{\rm l} = \left\langle \frac{d}{d\kappa + 2(d-1)\mu_{\min}} \right\rangle^{-1} - \frac{2(d-1)\mu_{\min}}{d}, \tag{4.8}$$

$$\kappa_{\rm HS}^{\rm u} = \left\langle \frac{d}{d\kappa + 2(d-1)\mu_{\max}} \right\rangle^{-1} - \frac{2(d-1)\mu_{\max}}{d}. \tag{4.9}$$

Not surprisingly, these bounds coincide with the Hashin–Shtrikman (1963) bounds on the bulk modulus of multiphase composites, explaining the notation used in (4.8) and (4.9). Such a proof of the Hashin–Shtrikman bounds (4.7) was first presented by Gibiansky and Cherkaev (1984, 1987) and Francfort and Murat (1986).

We will now use the same optimal values of the parameters t_1 and t_2 in the thermal expansion bounds (3.23)–(3.25). Indeed, it is natural to expect that for such optimal values, the thermal expansion bounds will also be the most restrictive, because they are obtained from the same functional as the bulk modulus bounds. We also numerically checked that this choice of the parameters is the best for all of the examples that we studied.

Substituting (4.3), (4.4), and (4.6) into (3.24)–(3.25), we obtain bounds

$$\begin{aligned} \alpha^{\pm} = \frac{1}{\kappa_*(\kappa_{\rm HS}^{\rm u} - \kappa_{\rm HS}^{\rm l})} \Bigg\{ & (\kappa_{\rm HS}^{\rm u} - \kappa_*) \left\langle \frac{d}{d\kappa + 2(d-1)\mu_{\min}} \right\rangle^{-1} \\ & \times \left\langle \frac{d\alpha\kappa}{d\kappa + 2(d-1)\mu_{\min}} \right\rangle + (\kappa_* - \kappa_{\rm HS}^{\rm l}) \left\langle \frac{d}{d\kappa + 2(d-1)\mu_{\max}} \right\rangle^{-1} \\ & \times \left\langle \frac{d\alpha\kappa}{d\kappa + 2(d-1)\mu_{\max}} \right\rangle \pm \sqrt{\Psi(\kappa_{\rm HS}^{\rm u} - \kappa_*)(\kappa_* - \kappa_{\rm HS}^{\rm l})} \Bigg\}, \end{aligned} \tag{4.10}$$

where

$$\begin{aligned}\hat{\Psi} = {} & -\left(\kappa^{\mathrm{u}}_{\mathrm{HS}} + \frac{2(d-1)\mu_{\max}}{d}\right)\left(\kappa^{\mathrm{l}}_{\mathrm{HS}} + \frac{2(d-1)\mu_{\min}}{d}\right) \\ & \times\left[\left\langle \frac{d\alpha\kappa}{d\kappa+2(d-1)\mu_{\min}} \right\rangle - \left\langle \frac{d\alpha\kappa}{d\kappa+2(d-1)\mu_{\max}} \right\rangle\right]^2 \\ & + \frac{2(d-1)(\mu_{\max}-\mu_{\min})}{d}\left[\left\langle \frac{d}{d\kappa+2(d-1)\mu_{\min}} \right\rangle^{-1} \right. \\ & \times \left\langle \frac{d\alpha\kappa}{d\kappa+2(d-1)\mu_{\min}} \right\rangle^2 - \left\langle \frac{d}{d\kappa+2(d-1)\mu_{\max}} \right\rangle^{-1} \\ & \left. \times \left\langle \frac{d\alpha\kappa}{d\kappa+2(d-1)\mu_{\max}} \right\rangle^2 \right] + (\kappa^{\mathrm{u}}_{\mathrm{HS}} - \kappa^{\mathrm{l}}_{\mathrm{HS}})\left[\left\langle \frac{2(d-1)\mu_{\max}\alpha^2\kappa}{d\kappa+2(d-1)\mu_{\max}} \right\rangle \right. \\ & \left. - \left\langle \frac{2(d-1)\mu_{\min}\alpha^2\kappa}{d\kappa+2(d-1)\mu_{\min}} \right\rangle \right]. \end{aligned} \tag{4.11}$$

For composites with extremal bulk modulus $\kappa = \kappa^{\mathrm{l}}_{\mathrm{HS}}$ or $\kappa = \kappa^{\mathrm{u}}_{\mathrm{HS}}$, the thermal expansion coefficient is uniquely defined by the relations (4.10), since the upper and lower bounds on α_* coincide for these points. They also coincide for the two-phase composite that corresponds to the results of Levin (1967). If $\mu_{\min} = 0$ and $\mu_{\max} = \infty$, then $t_1 = t_2 = 0$ and the Hashin–Shtrikman bulk modulus bounds (4.6) coincide with Hill's bounds (2.50) and the inequalities (4.9)–(4.10) are identical to the bounds (2.51)–(2.52).

Note that the bounds (4.9)–(4.10) can be rewritten in terms of the effective thermal stress coefficient $\Gamma^* = -d\kappa_*\alpha_*$

$$-d\kappa_*\alpha^+ \leqslant \Gamma_* \leqslant -d\kappa_*\alpha^-, \tag{4.12}$$

where α^+ and α^- are given by (4.9).

Recently, Sigmund and Torquato (1996, 1997) applied a topology optimization method to find two-dimensional, three-phase composites with extremal thermal expansion or thermal stress coefficients. They chose to use the phases with the following properties and volume fractions:

$$\begin{aligned} &\kappa_1 = 0.65\times 10^{-4}, \quad \mu_1 = 0.35\times 10^{-4}, \quad \alpha_1 = 1, \quad f_1 = 0.5, \\ &\kappa_2 = 0.65, \quad \mu_2 = 0.35, \quad \alpha_2 = 1, \quad f_2 = 0.25, \\ &\kappa_3 = 0.65, \quad \mu_3 = 0.35, \quad \alpha_3 = 10, \quad f_3 = 0.25. \end{aligned} \tag{4.13}$$

In fact, they actually studied three-phase composites consisting of two phases and a void. For numerical reasons, the void was replaced by a very soft phase 1 in their calculations. The bounds (4.9)–(4.10) on the effective thermal expansion coefficient α_* for such a composite are illustrated in Fig. 1. The corresponding bounds on the effective thermal stress coefficient Γ_* are given in Fig. 2. The bold curves correspond to our bounds (4.9)–(4.10) and the dashed curves show the Schapery–Rosen–Hashin

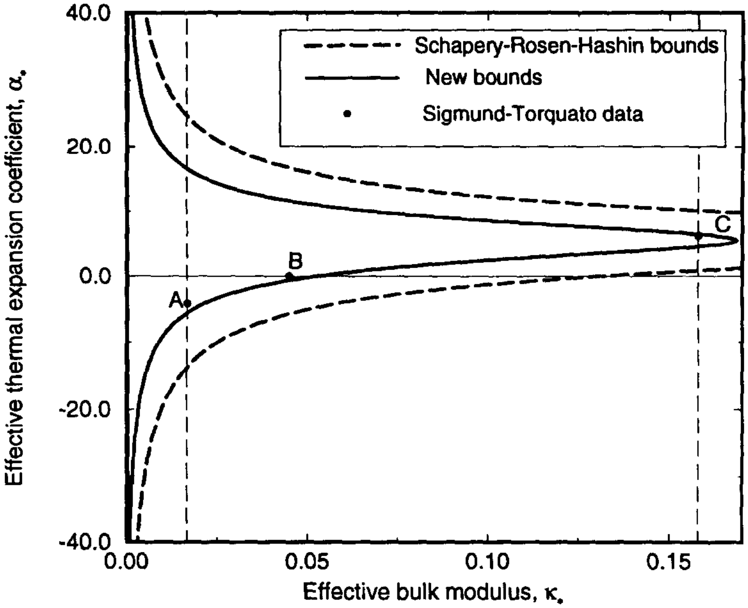

Fig. 1. Thermal expansion coefficient bounds for macroscopically isotropic two-dimensional composites consisting of three isotropic phases. The phase moduli are given by (4.13). The data *A*, *B*, and *C* are described in the text.

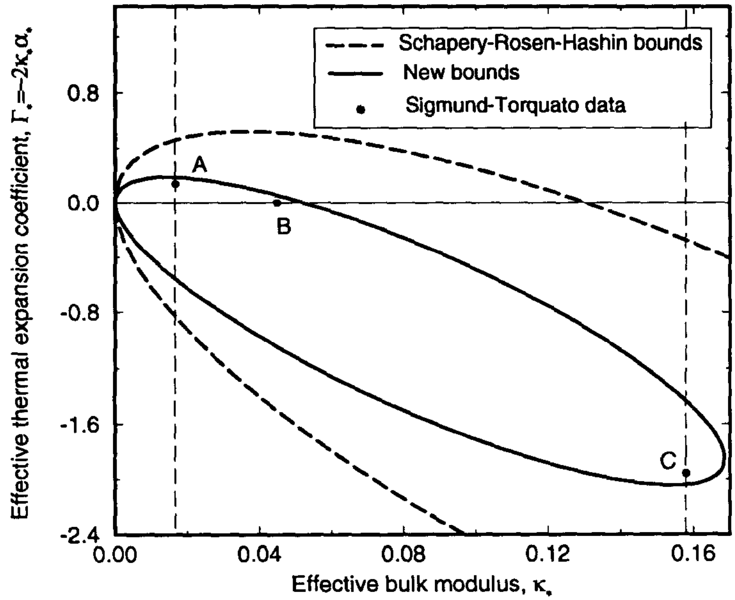

Fig. 2. Thermal stress coefficients bounds for macroscopically isotropic two-dimensional composites consisting of three isotropic phases. The phase moduli are given by (4.13). The data *A*, *B*, and *C* are described in the text.

bounds (2.51)–(2.52). Note that for the given values of the phase parameters (4.13), the bounds on α_* change rapidly in the small neighborhood of the lower bound on the effective bulk modulus κ_*.

The points A, B, and C on each of these figures correspond to the composites found by Sigmund and Torquato (1996, 1997). The point A corresponds to a composite which was found when they looked for a minimal thermal expansion coefficient for a specified bulk modulus value $\kappa_* = 0.1\kappa^{\mathrm{u}}_{\mathrm{HS}} = 0.0168$. The points B correspond to a composite with maximal bulk modulus for a specified value of the thermal expansion $\alpha_* = 0$. The points C correspond to a composite with minimal thermal stress coefficient $\Gamma_* = -2\kappa_*\alpha_*$ (bulk modulus $\kappa_* = 0.158$ at that point). One can see that our bounds provide significant improvement over the known results. They are very sharp or may even be optimal for the phase properties (4.13).

5. POLYCRYSTALS

In this section we examine the bounds (2.45)–(2.47) and (3.23)–(3.25) as applied to macroscopically isotropic polycrystals. We start with the simplest bounds on the effective thermal expansion and analyse the conditions when they coincide, thus uniquely defining the effective thermal expansion as a function of the effective bulk modulus. Then we will show how to improve the bounds on the thermal expansion of an isotropic *two-dimensional* polycrystal. We show that for the *three-dimensional* polycrystal the translation bounds coincide with the simplest ones.

5.1. *Simplest bounds*

Let us evaluate the bounds (2.45)–(2.47) for a polycrystal. We will assume that the polycrystal is random, meaning that all of the averages in the expressions (2.35) and (2.38) are isotropic tensors. Then, from (2.35) and (2.38), we have

$$A_1 = \kappa^{\mathrm{l}}_{\mathrm{H}}, \quad B_1 = -\frac{\mathrm{Tr}\,[\boldsymbol{\alpha}]}{d}\kappa^{\mathrm{l}}_{\mathrm{H}}, \quad C_1 = \frac{\boldsymbol{\alpha}:\mathbf{C}:\boldsymbol{\alpha}}{2d^2} - \frac{\mathrm{Tr}^2\,[\boldsymbol{\alpha}]}{2d^2}\kappa^{\mathrm{l}}_{\mathrm{H}}, \tag{5.1}$$

$$A_2 = \frac{1}{\kappa^{\mathrm{u}}_{\mathrm{H}}}, \quad B_2 = \frac{\mathrm{Tr}\,[\mathbf{C}:\boldsymbol{\alpha}]}{d^2\kappa^{\mathrm{u}}_{\mathrm{H}}}, \quad C_2 = -\frac{\mathrm{Tr}^2\,[\mathbf{C}:\boldsymbol{\alpha}]}{2d^4\kappa^{\mathrm{u}}_{\mathrm{H}}}, \tag{5.2}$$

where

$$\kappa^{\mathrm{l}}_{\mathrm{H}} = \frac{1}{\mathbf{I}:\mathbf{S}:\mathbf{I}}, \quad \kappa^{\mathrm{u}}_{\mathrm{H}} = \frac{\mathbf{I}:\mathbf{C}:\mathbf{I}}{d^2}, \tag{5.3}$$

$\mathbf{C} = \mathbf{S}^{-1}$, $\boldsymbol{\alpha}$ are the corresponding tensors for the single crystal, and

$$\mathrm{Tr}\,[\boldsymbol{\alpha}] = \mathbf{I}:\boldsymbol{\alpha} = \sum_{i=1}^{d} \alpha_{ii}. \tag{5.4}$$

The bulk modulus bounds (2.43) have the form

$$\kappa^{\mathrm{l}}_{\mathrm{H}} \leqslant \kappa_* \leqslant \kappa^{\mathrm{u}}_{\mathrm{H}}, \tag{5.5}$$

which coincide with Hill's bounds for the elastic polycrystal. The thermal expansion coefficient bounds (2.45)–(2.47) are equal to

$$\alpha^{\pm} = \frac{1}{\kappa_*(\kappa_{\mathrm{H}}^{\mathrm{u}} - \kappa_{\mathrm{H}}^{\mathrm{l}})}\left(X(\kappa_{\mathrm{H}}^{\mathrm{u}} - \kappa_*) + Y(\kappa_* - \kappa_{\mathrm{H}}^{\mathrm{l}}) \pm \Psi^{1/2}(\kappa_* - \kappa_{\mathrm{H}}^{\mathrm{l}})^{1/2}(\kappa_{\mathrm{H}}^{\mathrm{u}} - \kappa_*)^{1/2}\right) \qquad (5.6)$$

where

$$X = \frac{\mathrm{Tr}[\boldsymbol{\alpha}]}{d}\kappa_{\mathrm{H}}^{\mathrm{l}}, \quad Y = \frac{\mathrm{Tr}\,[\mathbf{C}:\boldsymbol{\alpha}]}{d^2}, \qquad (5.7)$$

$$\Psi = \frac{\boldsymbol{\alpha}:\mathbf{C}:\boldsymbol{\alpha}}{d^2}(\kappa_{\mathrm{H}}^{\mathrm{u}} - \kappa_{\mathrm{H}}^{\mathrm{l}}) - \frac{\mathrm{Tr}^2\,[\boldsymbol{\alpha}]}{d^2}\kappa_{\mathrm{H}}^{\mathrm{l}}\kappa_{\mathrm{H}}^{\mathrm{u}} + 2\kappa_{\mathrm{H}}^{\mathrm{l}}\frac{\mathrm{Tr}\,[\boldsymbol{\alpha}]\,\mathrm{Tr}\,[\mathbf{C}:\boldsymbol{\alpha}]}{d^3} - \frac{\mathrm{Tr}^2\,[\mathbf{C}:\boldsymbol{\alpha}]}{d^4}. \qquad (5.8)$$

These can be simplified by using the relation

$$\boldsymbol{\alpha} = \boldsymbol{\alpha}^{\mathrm{s}} + \frac{\mathrm{Tr}\,[\boldsymbol{\alpha}]}{d}\mathbf{I}, \qquad (5.9)$$

where $\boldsymbol{\alpha}^{\mathrm{s}}$ is the deviatoric part of the thermal expansion tensor. Substituting this expression into (5.6)–(5.8), one finds that

$$\alpha^{\pm} = \frac{\mathrm{Tr}\,[\boldsymbol{\alpha}]}{d} + \frac{\mathrm{Tr}\,[\mathbf{C}:\boldsymbol{\alpha}^{\mathrm{s}}]\kappa_{\mathrm{H}}^{\mathrm{l}}}{d^2(\kappa_{\mathrm{H}}^{u} - \kappa_{\mathrm{H}}^{l})}\left(\frac{1}{\kappa_{\mathrm{H}}^{l}} - \frac{1}{\kappa_*}\right) \pm \frac{\Psi^{1/2}(\kappa_* - \kappa_{\mathrm{H}}^{\mathrm{l}})^{1/2}(\kappa_{\mathrm{H}}^{\mathrm{u}} - \kappa_*)^{1/2}}{\kappa_*(\kappa_{\mathrm{H}}^{u} - \kappa_{\mathrm{H}}^{l})}, \qquad (5.10)$$

where

$$\Psi = \frac{\boldsymbol{\alpha}^{\mathrm{s}}:\mathbf{C}:\boldsymbol{\alpha}^{\mathrm{s}}}{d^2}(\kappa_{\mathrm{H}}^{\mathrm{u}} - \kappa_{\mathrm{H}}^{\mathrm{l}}) - \frac{\mathrm{Tr}^2\,[\mathbf{C}:\boldsymbol{\alpha}^{\mathrm{s}}]}{d^4}. \qquad (5.11)$$

An important and interesting question is when the upper and lower bounds on the effective thermal coefficient coincide, i.e. when does $\Psi = 0$? We first give arguments consistent with the ideas of Levin (1967), Cribb (1968), and Schulgasser (1989a) and then check them by explicit evaluation of the coefficient Ψ (5.8).

Let us assume that the deviatoric part of the crystal thermal expansion tensor is proportional to the deviatoric part of the tensor $\mathbf{S}:\mathbf{I}$, i.e.

$$\boldsymbol{\alpha}^{\mathrm{s}} = \boldsymbol{\alpha} - \frac{\mathrm{Tr}\,[\boldsymbol{\alpha}]}{d}\mathbf{I} = -\eta\left(\mathbf{S}:\mathbf{I} - \frac{\mathrm{Tr}\,[\mathbf{S}:\mathbf{I}]}{d}\mathbf{I}\right), \quad \text{or } \mathbf{R}:(\eta\mathbf{S}:\mathbf{I} + \boldsymbol{\alpha}) = 0, \qquad (5.12)$$

where η is some constant, and $\mathbf{R}$ is any trace-free tensor, i.e. such that $\mathbf{I}:\mathbf{R} = 0$. Then for any constant temperature rise $\hat{\theta}$, one can find the constant stress field $\boldsymbol{\tau} = \eta\hat{\theta}\mathbf{I}$ such that the stress and the deformation of the single crystal

$$\boldsymbol{\tau} = \eta\hat{\theta}\mathbf{I}, \quad \boldsymbol{\varepsilon} = (\eta\mathbf{S}:\mathbf{I} + \boldsymbol{\alpha})\hat{\theta}, \qquad (5.13)$$

are purely hydrostatic, i.e.

$$\mathbf{R}:\boldsymbol{\varepsilon} = \mathbf{R}:(\eta\mathbf{S}:\mathbf{I} + \boldsymbol{\alpha})\hat{\theta} = 0, \qquad (5.14)$$

due to (5.12). The strain and stress fields (5.13) are rotationally invariant and thus, one can combine such crystals with different orientations in a polycrystal without jumps in the stress and strain fields across the grain boundaries. Therefore, the local stress and strain fields in the polycrystal subject to temperature rise $\hat{\theta}$ and hydrostatic stress field $\boldsymbol{\tau} = \eta\hat{\theta}\mathbf{I}$ also satisfy (5.13). Note that although each of the terms on the right-hand side of the second equation (5.13) is not rotationally invariant, their sum is proportional to the unit tensor, i.e. it is rotationally invariant. Consequently, we have the identities $\boldsymbol{\varepsilon} = \langle\boldsymbol{\varepsilon}\rangle$ and $\boldsymbol{\tau} = \langle\boldsymbol{\tau}\rangle$, i.e.

$$\langle\boldsymbol{\varepsilon}\rangle = (\eta\mathbf{S}_* : \mathbf{I} + \boldsymbol{\alpha}_*)\hat{\theta} = \langle\eta\mathbf{S} : \mathbf{I} + \boldsymbol{\alpha}\rangle\hat{\theta} = (\eta\mathbf{S} : \mathbf{I} + \boldsymbol{\alpha})\hat{\theta}, \tag{5.15}$$

or, equivalently,

$$\boldsymbol{\alpha}_* = \langle\boldsymbol{\alpha}\rangle + \eta(\langle\mathbf{S}\rangle - \mathbf{S}_*) : \mathbf{I} = \boldsymbol{\alpha} + \eta(\mathbf{S} - \mathbf{S}_*) : \mathbf{I}. \tag{5.16}$$

For isotropic composites this reduces to the equality

$$\alpha_* = \frac{\mathrm{Tr}[\boldsymbol{\alpha}]}{d} + \frac{\eta}{d}\left(\frac{1}{\kappa_{\mathrm{H}}^{\mathrm{l}}} - \frac{1}{\kappa_*}\right), \tag{5.17}$$

where the constant η is defined by (5.12). Note that the final expression does not depend on the particular trial fields because the effective moduli are independent of the loading conditions.

The value of the constant η can easily be found by multiplying (5.12) by the stiffness tensor $\mathbf{C}$ and taking the trace, leading to the equality

$$\eta = \frac{\kappa_{\mathrm{H}}^{\mathrm{l}}\,\mathrm{Tr}\,[\mathbf{C} : \boldsymbol{\alpha}^{\mathrm{s}}]}{d(\kappa_{\mathrm{H}}^{\mathrm{u}} - \kappa_{\mathrm{H}}^{\mathrm{l}})}. \tag{5.18}$$

Substituting relation (5.12) into (5.11) enables one to prove that the coefficient Ψ is equal to zero when (5.12) holds. Then the bounds (5.10) coincide and are equal to the expressions (5.17).

The results of this section agree with the findings of Hashin (1984) and Schulgasser (1987) who discovered a relationship between the effective thermal expansion and effective compliance tensor of a polycrystal of a hexagonal, tetragonal, and trigonal crystal. The arguments follow the ideas of Cribb (1968) and Schulgasser (1989a). However, the general condition (5.12) and the relations (5.15)–(5.18) are new for thermoelastic composites of general symmetry.

Note that the tensor equality (5.12) is equivalent to a system of $[d(d+1)/2-1]$ scalar conditions (equal to the number of independent elements in the d-dimensional trace-free matrix). This system contains only one free parameter η, which should be chosen to satisfy all of these conditions. Therefore, the tensor equality (5.12) is equivalent to $[d(d+1)/2-2]$ relations among the crystal moduli. This number is equal to 1 for the plane problem, and equal to 4 for the three-dimensional problem. Comparing the number of scalar equations, one can see that for the plane problem, the tensor condition (5.12) is equivalent to the scalar equality $\Psi = 0$ [see (5.11)]. In three dimensions, the condition (5.12) is sufficient for the equality $\Psi = 0$ to be valid. The field arguments show that it is also a necessary condition for the bounds to coincide. Indeed, the bounds are valid as equalities if the constant trial strain or stress fields (proportional to the identity tensors) are the solutions of the elasticity problem for the polycrystal of any structure. Therefore, both the local strain and stress fields in each of the grains should be proportional to the unit tensor. This immediately leads to the equality (5.12). However, we were not able to give an algebraic proof that the scalar equality $\Psi = 0$ leads to the tensor equality (5.12).

The simplest bulk modulus bounds (5.5) are optimal for a three-dimensional polycrystal: polycrystals with bulk moduli that correspond to both the lower and upper bounds (5.5) were found by Avellaneda and Milton (1989). By contrast, in two dimensions, only the lower bound (5.5) is optimal. The upper bulk modulus bound for the plane elastic polycrystal was improved by using the translation method [see Avellaneda and Milton (1989), Avellaneda *et al.* (1996)].

The bounds for the thermal expansion coefficient follow from the same functionals as the bulk modulus bounds. One expects that for the three-dimensional problem, the thermal expansion coefficient bounds would not improve upon the simplest bounds. However, one can expect improved bounds in two dimensions, which are obtained in the next section.

5.2. *Translation bounds*

This section deals with the evaluation of the translation bounds (3.23)–(3.25) for a polycrystal. We start with a simpler problem and evaluate the optimal values (i.e. the values that give the sharpest inequalities) of the translation parameters t_1 and t_2 for the bulk modulus bounds (3.22).

One can verify that for the bulk modulus problem the parameters t_1 and t_2 should be as small as the restrictions (3.8), (3.10), (3.13), and (3.19) will allow. This means that the optimal choice of the parameter t_1 is trivially $t_1 = 0$, and the optimal choice of the parameters t_2 is trivially $t_2 = 0$ for $d \geqslant 3$. However, in two dimensions the value of the parameter t_2 can be negative. The optimal value for $d = 2$ is given by the negative root t_2^* of the equation

$$\det(\mathbf{S} - \mathbf{T}_\tau(t_2)) = 0. \tag{5.19}$$

Therefore, for $d \geqslant 3$, the translation bulk modulus bounds coincide with the simplest bounds, because $t_1 = t_2 = 0$. However in two dimensions, $t_2^* \neq 0$, and the translation upper bulk modulus bound improves upon the simplest one. The bulk modulus bounds (3.22) in two dimensions are given by the inequalities

$$\kappa_{\mathrm{H}}^{\mathrm{l}} \leqslant \kappa_* \leqslant \kappa_{\mathrm{T}}^{\mathrm{u}}, \quad \kappa_{\mathrm{T}}^{\mathrm{u}} = -\frac{1}{t_2^*}, \quad d = 2, \tag{5.20}$$

[see Avellaneda and Milton (1989)].

We will use the same values t_1 and t_2 in the thermal expansion bounds when applying them to the polycrystal problem. This means that the translation bounds on the effective thermal expansion coefficient improve upon the simplest bounds *only in two dimensions*. In the rest of this section we will assume that $d = 2$ in all the formulas.

The new effective thermal expansion coefficient bounds (3.23)–(3.25) can be expressed as

$$\alpha^{\pm} = \frac{1}{\kappa_*(\kappa_T^u-\kappa_H^l)}\left(\kappa_H^l\frac{\operatorname{Tr}[\boldsymbol{\alpha}]}{2}(\kappa_T^u-\kappa_*)+\kappa_T^u B_2'(\kappa_*-\kappa_H^l)\right.$$
$$\left.\pm\Psi^{1/2}(\kappa_*-\kappa_H^l)^{1/2}(\kappa_T^u-\kappa_*)^{1/2}\right), \quad (5.21)$$

where

$$\Psi = X(\kappa_T^u-\kappa_H^l)-\left(\kappa_H^l\frac{\operatorname{Tr}[\boldsymbol{\alpha}]}{2}\right)^2-(B_2')^2\kappa_T^u\kappa_H^l+\kappa_H^l\operatorname{Tr}[\boldsymbol{\alpha}]B_2'\kappa_T^u, \quad (5.22)$$

and

$$X=\frac{1}{4}\left(\boldsymbol{\alpha}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\boldsymbol{\alpha}-\frac{(\mathbf{I}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\boldsymbol{\alpha})^2}{\mathbf{I}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\mathbf{I}}-\kappa_H^l\operatorname{Tr}^2[\boldsymbol{\alpha}]\right), \quad (5.23)$$

$$B_2'=\frac{\mathbf{I}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\boldsymbol{\alpha}}{\mathbf{I}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\mathbf{I}}. \quad (5.24)$$

Here we have employed the formulas (3.23)–(3.25) using the values of the parameters $A_1'=A_1$, $B_1'=B_1$, and $C_1'=C_1$ given by (5.1), and the values of the parameters A_2', B_2', and C_2' given by (3.18). Note that one of the eigenvalues of the matrix $\mathbf{S}-\mathcal{T}_\tau(t_2^*)$ is equal to zero. Therefore, one has to be careful in evaluating the coefficients in (5.21)–(5.24). We will treat these equations as limits of the corresponding equations when the value of the parameter t_2 tends to t_2^*. As we will see, these limits exist and are finite.

Simplifying the expressions (5.22)–(5.24) by using the representation (5.9) of the thermal expansion tensor we obtain

$$\alpha^{\pm}=\frac{\operatorname{Tr}[\boldsymbol{\alpha}]}{d}+\frac{\kappa_T^u(\kappa_*-\kappa_H^l)}{\kappa_*(\kappa_T^u-\kappa_H^l)}\frac{\mathbf{I}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\boldsymbol{\alpha}^s}{\mathbf{I}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\mathbf{I}}\pm\Psi^{1/2}(t_2^*)\frac{(\kappa_*-\kappa_H^l)^{1/2}(\kappa_T^u-\kappa_*)^{1/2}}{\kappa_*(\kappa_T^u-\kappa_H^l)}, \quad (5.25)$$

where

$$\Psi(t_2^*)=\frac{\kappa_T^u-\kappa_H^l}{4}\left(\boldsymbol{\alpha}^s:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\boldsymbol{\alpha}^s-\frac{[\mathbf{I}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\boldsymbol{\alpha}^s]^2}{\mathbf{I}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\mathbf{I}}\right)$$
$$-\kappa_H^l\kappa_T^u\left[\frac{\mathbf{I}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\boldsymbol{\alpha}^s}{\mathbf{I}:(\mathbf{S}-\mathcal{T}_\tau(t_2^*))^{-1}:\mathbf{I}}\right]^2. \quad (5.26)$$

Now we need to evaluate the coefficients in the expressions (5.25)–(5.26). Let us assume that the matrix $\mathbf{S}-\mathcal{T}_\tau(t_2^*)$ has the eigenvalues λ_1, λ_2, and $\lambda_3=0$ and the corresponding eigentensors $\mathbf{s}_1$, $\mathbf{s}_2$, and $\mathbf{s}_3$, so that

$$\mathbf{S}-\mathcal{T}_\tau(t_2)=\lambda_1\mathbf{s}_1\mathbf{s}_1+\lambda_2\mathbf{s}_2\mathbf{s}_2. \quad (5.27)$$

Then

$$\lim_{t_2 \to t_2^*} \frac{\mathbf{I} : (\mathbf{S} - \mathcal{T}_\tau(t_2))^{-1} : \boldsymbol{\alpha}^{\mathrm{s}}}{\mathbf{I} : (\mathbf{S} - \mathcal{T}_\tau(t_2))^{-1} : \mathbf{I}} = \frac{\mathbf{s}_3 : \boldsymbol{\alpha}^{\mathrm{s}}}{\mathbf{s}_3 : \mathbf{I}}, \tag{5.28}$$

and

$$\lim_{t_2 \to t_2^*} \Psi(t_2) = \frac{\kappa_{\mathrm{T}}^{\mathrm{u}} - \kappa_{\mathrm{H}}^{\mathrm{l}}}{4(\mathbf{I} : \mathbf{s}_3)^2} \left[\frac{(\mathbf{I} : (\mathbf{s}_2\mathbf{s}_3 - \mathbf{s}_3\mathbf{s}_2) : \boldsymbol{\alpha}^{\mathrm{s}})^2}{\lambda_2} + \frac{(\mathbf{I} : (\mathbf{s}_1\mathbf{s}_3 - \mathbf{s}_3\mathbf{s}_1) : \boldsymbol{\alpha}^{\mathrm{s}})^2}{\lambda_1} \right] - \kappa_{\mathrm{T}}^{\mathrm{u}} \kappa_{\mathrm{H}}^{\mathrm{l}} \frac{(\boldsymbol{\alpha}^{\mathrm{s}} : \mathbf{s}_3)^2}{(\mathbf{I} : \mathbf{s}_3)^2}. \tag{5.29}$$

As we see, these expressions have finite values, thus giving meaning to the bounds (5.25).

In order to obtain explicit expressions for the bounds (5.25), we introduce the matrix representation of the stiffness and compliance tensors, and also thermal expansion and thermal stress tensors. Namely, in two dimensions,

$$\mathbf{C} = \begin{pmatrix} c_{1111} & c_{1122} & \sqrt{2}c_{1112} \\ c_{1122} & c_{2222} & \sqrt{2}c_{2212} \\ \sqrt{2}c_{1112} & \sqrt{2}c_{2212} & 2c_{1212} \end{pmatrix}, \quad \mathbf{S} = \mathbf{C}^{-1} = \begin{pmatrix} s_{1111} & s_{1122} & \sqrt{2}s_{1112} \\ s_{1122} & s_{2222} & \sqrt{2}s_{2212} \\ \sqrt{2}s_{1112} & \sqrt{2}_{2212} & 2s_{1212} \end{pmatrix}, \tag{5.30}$$

$$\boldsymbol{\alpha} = \begin{pmatrix} a_{11} \\ a_{22} \\ \sqrt{2}a_{12} \end{pmatrix}, \quad \boldsymbol{\Gamma} = \begin{pmatrix} \Gamma_{11} \\ \Gamma_{22} \\ \sqrt{2}\Gamma_{12} \end{pmatrix}, \tag{5.31}$$

where c_{ijkl}, s_{ijkl}, a_{ij}, and Γ_{ij} are the usual Cartesian elements of the corresponding tensors in some fixed basis. For isotropic composites in two dimensions, we have that

$$c_{1111} = c_{2222} = \kappa + \mu, \quad c_{1122} = \kappa - \mu, \quad c_{1112} = c_{2212} = 0, \quad c_{1212} = \mu,$$

$$s_{1111} = s_{2222} = \frac{\kappa + \mu}{4\kappa\mu}, \quad s_{1122} = \frac{\mu - \kappa}{4\kappa\mu}, \quad s_{1112} = s_{2212} = 0, \quad s_{1212} = \frac{1}{4\mu}, \tag{5.32}$$

$$\alpha_{11} = \alpha_{22} = \alpha, \quad \alpha_{12} = 0, \quad \Gamma_{11} = \Gamma_{22} = -2\kappa\alpha, \quad \Gamma_{12} = 0. \tag{5.33}$$

The tensor $\mathcal{T}_\tau(t_2)$ has the following matrix representation:

$$\mathcal{T}_\tau(t_1) = \begin{pmatrix} 0 & -t_2/2 & 0 \\ -t_2/2 & 0 & 0 \\ 0 & 0 & t_2/2 \end{pmatrix}. \tag{5.34}$$

Consider the crystal with the moduli given by

$$c_{1111} = 33, \quad c_{2222} = 34, \quad c_{1122} = -11, \quad c_{1112} = 0, \quad c_{2212} = -13/\sqrt{2},$$

$$c_{1212} = 13, \quad \alpha_{11} = 1, \quad \alpha_{22} = 2, \quad \alpha_{12} = 1/7, \tag{5.35}$$

in some Cartesian basis. These values have no particular physical meaning, i.e. they

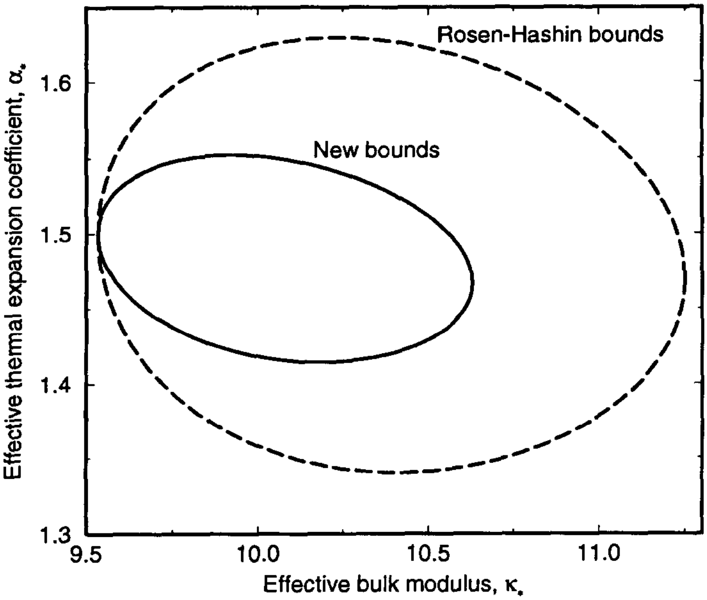

Fig. 3. Thermal expansion coefficient bounds for macroscopically isotropic two-dimensional polycrystals. The crystal moduli are given by (5.35).

do not correspond to any single crystal moduli and are chosen only for purposes of illustration. For such a situation, (5.19) has only one negative root:

$$t_2^* = -0.09408. \tag{5.36}$$

For such values of the parameters, the bulk modulus bounds (5.20) are given by

$$\kappa_{\mathrm{H}}^{\mathrm{l}} = 143/15 = 9.533, \quad \kappa_{\mathrm{T}}^{\mathrm{u}} = 10.63, \tag{5.37}$$

(compare with Hill's upper bounds $\kappa_{\mathrm{H}}^{\mathrm{u}} = 11.25$), and the bounds on the effective thermal expansion are given by the formula

$$\alpha^{\pm} = 1.179 + 3.060\frac{1}{\kappa_*} \pm \frac{1.228\sqrt{(\kappa_* - 9.533)(10.63 - \kappa_*)}}{\kappa_*}. \tag{5.38}$$

The bounds are depicted by solid curves in Fig. 3. The dashed curves are the simplest bounds (5.10)–(5.11) that correspond to the Rosen–Hashin bounds for this case. One can see that the translation bounds are much more restrictive for the chosen values of the parameters. The corresponding bounds on the effective stress coefficient $\Gamma_* = -2\kappa_*\alpha_*$ are shown in Fig. 4.

6. GENERALIZATIONS AND DISCUSSION

The bulk modulus bounds (3.22) and the thermal expansion bounds (3.23)–(3.25) are valid for the general case of a macroscopically isotropic composite comprised of an arbitrary number of anisotropic phases. The only non-trivial part is again the

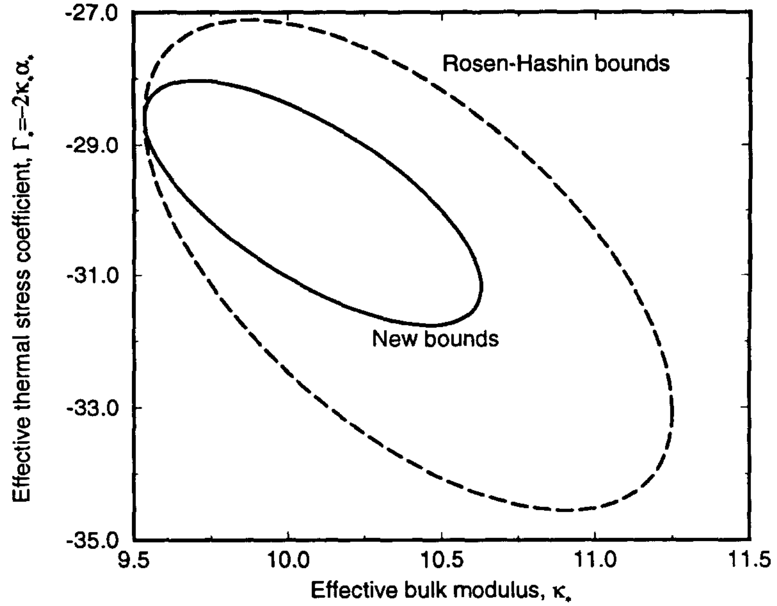

Fig. 4. Thermal stress coefficient bounds for macroscopically isotropic two-dimensional polycrystals. The crystal moduli are given by (5.35).

optimal choice of the parameters t_1 and t_2. As we saw in the previous sections, this choice is very different for the multiphase composite with isotropic phases and for the polycrystal. As a possible strategy for choosing these parameters, one can numerically investigate the dependence of the bulk modulus bounds on the values of t_1 and t_2 within the admissible range of these parameters, find the optimal values, and then use them for the thermal expansion inequalities.

It is an open question whether the obtained bounds can be further improved. It is known that the bounds on the effective bulk modulus of a polycrystal are exact: there exist composites with bulk moduli equal to the upper and lower bounds (5.5) (in three dimensions) or (5.20) (in two dimensions) [see Avellaneda and Milton (1989), Avellaneda *et al.* (1996)]. The thermal expansion bounds are obtained from the same functional as that used to obtain the bulk modulus bounds. Therefore, one may conjecture that these bounds are also optimal, but this remains an open question.

The bulk modulus bounds (4.7) for isotropic multiphase composites consisting of isotropic phases are optimal only for a sufficiently high volume fraction of the materials with minimal or maximal shear modulus [see Milton (1981)]. Therefore, thermal expansion bounds also may be optimal only for such values of the parameters; but the question of optimality of these bounds (even with the additional assumptions about the phase moduli and volume fractions) has not been studied.

By using our method, one can also derive bounds on the thermal expansion tensor of an anisotropic composite. To do this, one should use non-hydrostatic average trial fields, similar to the procedure used by Rosen and Hashin (1970). Moreover, in three dimensions one needs to use anisotropic translation tensors. Gibiansky and Cherkaev (1987) found such tensors and showed that each of them depends on three translation parameters. Again, the main and open question is how to find optimal values of these parameters in the translation bounds. One can do it either analytically or numerically, but it is a rather tedious problem.

All of the results obtained in the present paper are valid for cubic symmetric composites or square symmetric composites in two dimensions. Indeed, in the simplification of the expressions for the effective coefficients we relied only on the facts that the thermal expansion tensor is proportional to the unit tensor and that the unit tensor is the eigentensor of the elastic tensors. This is also true for the cubic (square) symmetric elasticity tensors.

Another possible application of our results is connected with the poroelasticity problem. The equations of poroelasticity describe the average fluid and solid displacement in a fluid-filled porous medium subject to external stress and variations in the fluid pressure. The constitutive relations take the form

$$\begin{pmatrix} \boldsymbol{\varepsilon}_{\mathrm{s}} \\ -\zeta \end{pmatrix} = \begin{pmatrix} \mathbf{S} & \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^{\mathrm{T}} & c \end{pmatrix} \begin{pmatrix} \boldsymbol{\tau}_{\mathrm{c}} \\ -p_{\mathrm{f}} \end{pmatrix}, \tag{6.1}$$

$$\boldsymbol{\varepsilon}_{\mathrm{s}} = \tfrac{1}{2}[\nabla \mathbf{u}_{\mathrm{s}} + (\nabla \mathbf{u}_{\mathrm{s}})^{\mathrm{T}}], \quad \nabla \cdot \boldsymbol{\tau} = 0, \quad \boldsymbol{\tau} = \boldsymbol{\tau}^{\mathrm{T}}, \tag{6.2}$$

where $\mathbf{u}_{\mathrm{s}}$ is the microscopic displacement of solid, ζ is the increment of fluid content that measures the net fluid flow in or out of a region $\boldsymbol{\tau}_{\mathrm{c}}$ is the confining stress tensor, p_{f} is the constant fluid pressure, $\mathbf{S}$ is the compliance tensor of the drained porous frame, $\boldsymbol{\alpha}$ is the tensor of expansion due to fluid pressure (at constant confining stress), and c is the coefficient relating the increment of fluid content to the fluid pressure (at constant confining pressure) [see, e.g., Berryman and Milton 1991, Norris 1992]. By comparing (2.2)–(2.4) and (6.1)–(6.2), it is clear that the equations of poroelasticity are mathematically analogous to the equations of thermal expansion. Therefore, all of the results obtained in this paper translate immediately into equivalent results for the poroelasticity problem with appropriate changes in notation.

ACKNOWLEDGEMENTS

The authors thank Ole Sigmund for very helpful discussions. We are also grateful to the creators of the MAPLE V (1981) program which we used heavily during the work on this project. We gratefully acknowledge the support of the Army Research Office under MURI Grant DAAH04-95-1-0102.

REFERENCES

Allaire, G. and Kohn, R., (1993) Optimal bounds on the effective behavior of a mixture of two well-ordered elastic materials. *Q. Appl. Math.* **51,** 643–674.

Avellaneda, M. and Milton, G. W. (1989) Optimal bounds on the effective bulk modulus of polycrystals. *SIAM J. Appl. Math.* **49,** 824–837.

Avellaneda, M., Cherkaev, A. V., Gibiansky, L. V., Milton, G. W. and Rudelson, M. (1996) On the effective conductivity of polycrystals and a three-dimensional phase-interchange inequality. *J. Mech. Phys. Solids* **44**(7), 1179–1218.

Benveniste, Y. (1996) Thermal expansion of polycrystalline aggregates consisting of elongated crystals and containing cylindrical pores or inclusions. *J. Mech. Phys. Solids* **44**(1), 137–153.

Berryman, J. and Milton, G. W. (1991) Exact results for generalized Gassman's equations in composite porous media with two constituents. *Geophysics* **56**, 1950–1960.

Bhattacharya, K. and Kohn, R. V. (1997) Elastic energy minimization and the recoverable strains of polycrystalline shape-memory materials. *Arch. Rat. Mech. Anal.*, in press.

Biot, M. A. (1956) Thermoelasticity and irreversible thermodynamics. *J. Appl. Phys.* **27**, 240–253.

Cherkaev, A. V. and Gibiansky, L. V. (1992) The exact coupled bounds for effective tensors of electrical and magnetic properties of two-component two-dimensional composites. *Proc. R. Soc. Edinburgh* **122A**, 93–125.

Cherkaev, A. V. and Gibiansky, L. V. (1993) Coupled estimates for the bulk and shear moduli of a two-dimensional isotropic elastic composite. *J. Mech. Phys. Solids* **41**, 937–980.

Christensen, R. M. (1979) *Mechanics of Composite Materials*. Wiley & Sons Inc., New York.

Cribb, J. L. (1968) Shrinkage and thermal expansion of a two-phase material. *Nature* **220**, 576–577.

Dacorogna, B. (1982) *Weak Continuity and Weak Lower Semicontinuity of Non-linear Functionals*. Lecture Notes in Math. 922. Springer-Verlag, Berlin.

Dvorak, G. . (1986) Thermal expansion of elastic plastic composite materials. *ASME J. Appl. Mech.* **53**, 737–743.

Dvorak, G. J. and Chen, T. (1989) Thermal expansion of three-phase composite materials. *ASME J. Appl. Mech.* **56**, 418–422.

Francfort, G. A. and Murat, F. (1986) Homogenization and optimal bounds in linear elasticity. *Arch. Rat. Mech. Anal.* **94**, 307–334.

Gibiansky, L. V. and Cherkaev, A. V. (1984) Design of composite plates of extremal rigidity. Ioffe Physico-Technical Institute, preprint #914, Leningrad. English translation in: A. V. Cherkaev and R. Kohn (eds) (1997) *Topics in the Mathematical Modeling of Composite Materials*. Birkhausen, New York.

Gibiansky, L. V. and Cherkaev, A. V. (1987) Microstructures of composites of extremal rigidity and exact estimates of provided energy density. Ioffe Physico-Technical Institute, preprint #1115, Leningrad. English translation in: A. V. Cherkaev and R. Kohn (eds) (1997) *Topics in the Mathematical Modeling of Composite Materials*. Birkhausen, New York.

Gibiansky, L. V. and Milton, G. W. (1993) On the effective viscoelastic moduli of two-phase media: I. Rigorous bounds on the complex bulk modulus. *Proc. R. Soc. Lond.* **A440**, 163–188.

Gibiansky, L. V. and Torquato, S. (1995a) Rigorous link between the conductivity and elastic moduli of fiber reinforced materials. *Phil. Trans. R. Soc. Lond.* **A452**, 253–283.

Gibiansky, L. V. and Torquato, S. (1995b) Geometrical-parameter bounds on the effective moduli of composites. *J. Mech. Phys. Solids* **43**(10), 1587–1613.

Gibiansky, L. V. and Torquato, S. (1996a) Connection between the conductivity and bulk modulus of isotropic composite materials. *Proc. R. Soc. Lond.* **A353**, 243–278.

Gibiansky, L. V. and Torquato, S. (1996b) Phase-interchange relations for the elastic moduli of two-phase composites. *Int. J. Engng Sci.* **34**(7), 739–760.

Hashin, Z., (1984) Thermal expansion of polycrystalline aggregates: I. Exact analysis. *J. Mech. Phys. Solids* **32**(2), 149–157.

Hashin, Z. and Shtrikman, S. (1962) A variational approach to the theory of the elastic behavior of polycrystals, *J. Mech. Phys. Solids* **10**, 343–352.

Hashin, Z. and Shtrikman, S. (1963) A variational approach to the theory of the elastic behavior of multiphase materials. *J. Mech. Phys. Solids* **11**, 127–140.

Hill, R. (1952) The elastic behavior of a crystalline aggregate. *Proc. Phys. Soc. Lond.* **A65**, 349–354.

Kohn, R. V. and Strang, G. (1986) Optimal design and relaxation of variational problems I, II, III. *Comm. Pure Appl. Math.* **39**, 113–137, 139–182, 353–377.

Levin, V. M. (1967) On the coefficients of thermal expansion of heterogeneous materials. *Mekhanika Tverdogo Tela* **2**, 88–94 (in Russian).

Lurie, K. A. and Cherkaev, A. V. (1984) Exact estimates of conductivity of composites formed by two isotropically conducting media taken in prescribed proportion. *Proc. R. Soc. Edinburgh* **A99,** 71–87.

Lurie, K. A. and Cherkaev, A. V. (1986a) Exact estimates of the conductivity of a binary mixture of isotropic materials. *Proc. R. Soc. Edinburgh* **A104,** 21–38.

Lurie, K. A. and Cherkaev, A. V. (1986b) The effective characteristics of composite materials and optimal design of constructions. *Advances in Mechanics* (*Poland*) **9,** 3–81.

Lurie, K. A., Cherkaev, A. V. and Fedorov, A. V. (1982) Regularization of optimal problems of design of bars and plates and solving the contradiction in a system of necessary conditions of optimality. *J. Opt. Th. Appl.* **37**(4), 499–522 (part 1), 523–542 (part 2).

MAPLE V (1981) Release 2, Princeton University, Copyright (©) 1981–1992 by the University of Waterloo.

Milton, G. W. (1981) Concerning bounds on the transport and mechanical properties of multicomponent composite materials. *Appl. Phys.* **A26,** 125.

Milton, G. W. (1990a) On characterizing the set of possible effective tensors of composites: the variational method and the translation method, *Comm. Pure Appl. Math.* **XLIII,** 63–125.

Milton, G. W. (1990b) A brief review of the translation method for bounding effective elastic tensors of composites. In *Continuum Models and Discrete Systems*, ed. G. A. Maugin, Vol. 1, pp. 60–74. Wiley, New York.

Murat, F. and Tartar, L. (1985) Calcul des variations et homogeneisation. *Les Methodes de l'Homogeneisation*: *Theorie et Applications en Physique*, *Coll. de la Dir. des Etudes et Recherches de Electr. de France*. Eyrolles, Paris, pp. 319–370.

Norris, A. (1992) On the correspondence between poroelasticity and thermoelasticity. *J. Appl. Phys.* **71,** 1138–1141.

Rice, J. R. and Cleary, M. P. (1976) Some basic stress diffusion solutions for fluid-saturated elastic porous media with compressible constituents. *Rev. Geophys. Space Phys.* **14,** 227–241.

Rosen, B. W. (1970) Thermoelastic energy functions and minimum energy principles for composite materials. *Int. J. Engng Sci.* **8**(1), 5–18.

Rosen, B. W. and Hashin, Z. (1970) Effective thermal expansion coefficients and specific heats of composite materials. *Int. J. Engng Sci.* **8,** 157–173.

Schapery, R. A. (1968) Thermal expansion coefficients of composite materials based on energy principles. *J. Comp. Mat.* **2,** 380–404.

Schulgasser, K. (1987) Thermal expansion of polycrystalline aggregates with texture. *J. Mech. Phys. Solids* **35**(1), 35–42.

Schulgasser, K. (1989a) Thermal expansion of polycrystals. *J. Mater. Sci. Lett.* **8,** 228–229.

Schulgasser, K. (1989b) The relationship between stiffness and thermal expansion of carbon fibers. *Mater. Sci. Engng* **A-110,** L35–L37.

Sigmund, O. and Torquato, S. (1996) Design of materials with extreme thermal expansion using three-phase topology optimization method. *Appl. Phys. Lett.* **69,** 3203–3205.

Sigmund, O. and Torquato, S. (1997) Design of materials with extreme thermal expansion using three-phase topology optimization method. *J. Phys. Mech. Solids* **45**(6), 1037–1067.

Tartar, L. (1978) Estimation de coefficients homogeneises. In *Computing Methods in Applied Sciences and Engineering*, Lecture Notes in Math. 704, 364–373. Springer-Verlag, Berlin.

Tartar, L. (1985) Estimations fines des coefficients homogeneises. In *Ennio de Giorgi Colloquium*, ed. P. Kree, Pitman Research Notes in Math. pp. 125, 168–187. Wiley, New York.