ON EFFECTIVE THERMAL EXPANSION COEFFICIENTS OF COMPOSITES WITH ANISOTROPIC PHASES

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Abstract—Bounds on thermal expansion coefficients of composite materials with anisotropic phases are derived using extremum principles of thermoelasticity. Numerical results are presented for two-phase composites with isotropic and orthotropic phases.

NOMENCLATURE

- a_{ij} Coefficients of deformation of phases
- A_{ij} coefficients of deformation of composites
- b_{ij} moduli of elasticity of phases
- k_i linear expansion coefficients of phases
- K_t linear expansion coefficients of composites
- T_i applied surface traction
- *u*₁ surface displacement
- V potential energy
- $-V_c$ complementary energy
- σ_i stress components
- $\bar{\sigma}_i$ applied stresses
- ε_t strain components
- $\bar{\varepsilon}_t$ average strains in composite specimen
- v_i volume fractions
- θ temperature.

INTRODUCTION

The problem of expressing effective thermal expansion coefficients of a composite in terms of its constituent properties was considered in the past by several investigators[1–5]. The problem for the general case of a composite with an arbitrary number of different constituents and arbitrary phase geometry was studied by Schapery[6] who used the extremum principles of thermoelasticity to derive the bounds on effective thermal expansion coefficients. Schapery presented the results for the composites with isotropic phases. In view of the fact that composites made of anisotropic phases are nowadays gaining importance, e.g. graphite reinforced composites, the present paper derives the results for the composites with anisotropic phases.

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ANALYSIS

Let the composite under consideration be composed of N phases and be statistically homogeneous. A unit representative volume of the composite is considered in the form of a rectangular parallelopiped with edges parallel to the coordinate axes. The solutions for effective thermal expansion coefficients will now be derived by applying the minimum potential and complementary energy principles to this composite specimen.

For convenience, normal stresses and strains in x, y and z directions are denoted by the subscripts 1, 2 and 3. Shearing stresses and strains in yz, zx and xy directions are denoted by subscripts 4, 5 and 6; that is,

$$\varepsilon_x = \varepsilon_1, \qquad \sigma_x = \sigma_1$$

 $\varphi_{xy} = \varepsilon_6, \qquad \sigma_{yz} = \sigma_4, \text{ etc.}$ (1)

It is assumed that the entire surface is subjected to tractions that are constant on each face of the composite specimen. The body forces are omitted and the temperature θ is considered to be spacewise uniform.

The generalized Hook's Law including the thermal effect is given by[7],

$$\sigma_i = \sum_{j=1}^6 b_{ij} \varepsilon_j - C_i \theta.$$
⁽²⁾

The inversion of equation (2) yields

$$\varepsilon_i = \sum_{j=1}^6 a_{ij} \sigma_j + k_i \theta.$$
(3)

The matrix a_{ij} is the inverse of the matrix b_{ij} . Also,

$$k_{i} = \sum_{j=1}^{6} a_{ij} C_{j}, \qquad C_{i} = \sum_{j=1}^{6} b_{ij} k_{j}.$$
(4)

The potential energy of the composite specimen is given by[7],

$$V = U + \Omega \tag{5}$$

where, U is the strain energy and Ω is the potential energy due to external load.

The expression for potential energy of the specimen is given by

$$V = \int_{v=1}^{6} \left[\frac{1}{2} \sum_{i=1}^{6} \sum_{j=2}^{6} b_{ij} \varepsilon_i \varepsilon_j - \sum_{i=1}^{6} C_i \theta \varepsilon_i \right] \mathrm{d}v - \int_s T_i u_i \,\mathrm{d}s \tag{6}$$

and the negative of complementary energy of the specimen can be expressed as[7],

$$V_{c} = -\int_{v=1}^{6} \left[\frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} a_{ij} \sigma_{i} \sigma_{j} + \sum_{i=1}^{6} k_{i} \sigma_{i} \theta \right] \mathrm{d}v.$$
(7)

From equations (2, 4, 6 and 7) it can be shown with the help of divergence theorem,

$$V_{c} = V + \frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} (b_{ij}k_{i}k_{j})^{a}\theta^{2}$$
(8)

where, $(b_{ij}k_ik_j)^a = \int_{v=1}^{v} b_{ij}k_ik_j dv$. For homogeneous phases n = 1 to N, each having a volume fraction v_n ,

$$(b_{ij}k_ik_j)^a = (b_{ij}k_ik_j)_1v_1 + (b_{ij}k_ik_j)_2v_2 + \cdots + (b_{ij}k_ik_j)_Nv_N.$$
(9)

Let the stress-strain relations in terms of gross elastic properties of composite be given by,

$$\bar{\varepsilon}_i = \sum_{j=1}^{6} A_{ij} \bar{\sigma}_j + K_i \theta.$$
⁽¹⁰⁾

Therefore, the negative of complementary strain energy density in terms of gross elastic properties is,

$$V_{c} = -\frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} A_{ij} \bar{\sigma}_{i} \bar{\sigma}_{j} - \sum_{i=1}^{6} K_{i} \bar{\sigma}_{i} \theta + C$$
(11)

where C is a function of temperature θ . The function C represents the energy arising from internal thermal stresses which develop when the phases have different thermal expansion coefficients.

The potential energy is a minimum with respect to all continuous displacements which satisfy boundary conditions, and the negative of complementary energy is a maximum when exact stresses are used. From these extremum properties it follows,

$$V_{c}^{a} \leq -\frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} A_{ij} \bar{\sigma}_{i} \bar{\sigma}_{j} - \sum_{i=1}^{6} K_{i} \bar{\sigma}_{i} \theta + C$$
(12a)

and

$$V^{a} + \frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} (b_{ij} k_{i} k_{j})^{a} \theta^{2} \ge -\frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} A_{ij} \bar{\sigma}_{i} \bar{\sigma}_{j} - \sum_{i=1}^{6} K_{i} \bar{\sigma}_{i} \theta + C$$
(12b)

where, superscript "a" on V and V_c stands for approximate values. The bounds on thermal expansion coefficients K_i 's can now be derived considering these inequalities.

To derive the approximate expression for the potential energy V^a of the composite specimen, a state of constant strain is assumed. Let this strain be represented by e_i . Substituting these strains in equation (6) and integrating throughout the volume,

$$V^{a} = \frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} b^{a}_{ij} e_{i} e_{j} - \sum_{i=1}^{6} \sum_{j=1}^{6} (b_{ij} k_{j})^{a} e_{i} \theta - \sum_{i=1}^{6} e_{i} \bar{\sigma}_{i}$$
(13)

where

$$b_{ij}^{a} = (b_{ij})_{1}v_{1} + (b_{ij})_{2}v_{2} + \cdots + (b_{ij})_{N}v_{N}.$$
(14)

Subscripts 1, 2, etc. indicate the phases and v_1 , v_2 , etc. denote their volume fractions.

The value of V^a can now be minimized with respect to the strain e_i . The minimized expression for V^a is given by,

$$V^{a} = -\frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} \sum_{k=1}^{6} \sum_{l=1}^{6} (b_{ij}k_{j})^{a} B_{ik} (b_{kl}k_{l})^{a} \theta^{2} - \sum_{i=1}^{6} \sum_{j=1}^{6} \sum_{k=1}^{6} (b_{ij}k_{j})^{a} B_{ik} \bar{\sigma}_{k} \theta$$
$$-\frac{1}{2} \sum_{i=1}^{6} \sum_{k=1}^{6} B_{ik} \bar{\sigma}_{i} \bar{\sigma}_{k} \quad (15)$$

where B_{ij} is the inverse of the matrix b_{ij}^a .

Now a constant stress distribution is assumed in the composite specimen for which approximate negative value of complementary energy V^a is given by,

$$V_{c}^{a} = -\frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} \bar{a}_{ij} \sigma_{i} \bar{\sigma}_{j} - \sum_{j=1}^{6} \bar{k}_{j} \bar{\sigma}_{j} \theta$$
(16)

where

$$\vec{a}_{ij} = (a_{ij})_1 v_1 + (a_{ij})_2 v_2 + \cdots + (a_{ij})_N v_N$$

and

$$\bar{k}_j = (k_j)_1 v_1 + (k_j)_2 v_2 + \cdots + (k_j)_N v_N.$$
(17)

To find the linear expansion coefficient in x direction, $\bar{\sigma}_1$ is set equal to σ and all other $\bar{\sigma}_i$'s are made zero. It may be noted that for the thermal coefficients in y or yz directions, $\bar{\sigma}_2$ or $\bar{\sigma}_4$ is to be set equal to σ instead of $\bar{\sigma}_1$. Substituting these values in equation (15) and (16),

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$$V^a = -\frac{1}{2}\sigma^2 \bar{a}_{11} - \bar{k}_1 \sigma \theta - N_1 \theta^2 \tag{18}$$

where

$$\overline{a}_{11} = B_{11}$$

$$\overline{k}_1 = \sum_{i=1}^6 \sum_{j=1}^6 (b_{ij} k_j)^a B_{i1}$$

$$N_1 = \frac{1}{2} \sum_{i=1}^6 \sum_{j=1}^6 \sum_{k=1}^6 \sum_{l=1}^6 (b_{ij} k_j)^a B_{ik} (b_{kl} k_l)^a$$
(19)

and

$$V_c^a = -\frac{1}{2}\bar{a}_{11}\sigma^2 - \bar{k}_1\sigma\theta.$$
⁽²⁰⁾

From inequalities (12a) and (12b)

$$\frac{1}{2}\sigma^2(A_{11} - \bar{a}_{11}) + \sigma\theta(K_1 - \bar{k}_1) \le C$$
(21a)

and

$$\frac{1}{2}\sigma^2(A_{11} - \bar{a}_{11}) + \sigma\theta(K_1 - \bar{k}_1) - N_1\theta^2 + \frac{1}{2}\sum_{i=1}^6\sum_{j=1}^6(b_{ij}k_ik_j)^a\theta^2 \ge C.$$
 (21b)

Maximizing the L.H.S. of equation (21a) and minimizing the L.H.S. of equation (21b) with respect to σ and subtracting one from the other the following inequality is obtained,

$$(K_1 - d)(K_1 - e) \le 0 \tag{22}$$

where

$$\mathbf{d} = \bar{k}_1 + (\bar{k}_1 - \bar{k}_1) \frac{(\bar{a}_{11} - \bar{A}_{11})}{(\bar{a}_{11} - \bar{a}_{11})} - h$$
(23)

$$e = \bar{k}_1 + (\bar{k}_1 - \bar{k}_1) \frac{(\bar{a}_{11} - \bar{A}_{11})}{(\bar{a}_{11} - \bar{a}_{11})} + h$$
(24)

$$h = \frac{(\bar{a}_{11} - A_{11})^{1/2} (A_{11} - \bar{a}_{11})^{1/2}}{(\bar{a}_{11} - \bar{a}_{11})} \left\{ (\bar{a}_{11} - \bar{a}_{11}) \times \left(\frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} (b_{ij} k_i k_j)^a - N_1 \right) - (\bar{k}_1 - \bar{k}_1)^2 \right\}^{1/2}.$$
(25)

Thus, the bounds on thermal expansion coefficients of the composite can be obtained once the properties of its phases, their volume fractions and gross elastic properties of the composite are known.

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It may be noted from inequalities (21a) and (21b), by setting θ equal to zero, that the coefficient of deformation of the composite in x direction A_{11} is bounded by,

$$\bar{a}_{11} \le A_{11} \le \bar{a}_{11}. \tag{26}$$

If the coefficient of deformation of the composite A_{11} is equal to its upper bound \bar{a}_{11} , then *h* in equation (25) becomes zero, and the linear expansion coefficient is given by the simple equation,

$$K_1 = \bar{k}_1 \tag{27}$$

which is the rule of mixture.

When A_{11} is equal to its lower bound \bar{a}_{11} , then

$$K_1 = \bar{k}_1. \tag{28}$$

NUMERICAL EXAMPLES AND DISCUSSION

In the first example, composites made of two constituent phases are considered. Table 1 shows the properties of the constituent phases. Phase 1 is isotropic while phase 2 is ortho-tropic. The ratio $(a_{11})_{\text{phase 1}}$; $(a_{11})_{\text{phase 2}}$ is 9.80:0.44.

Table 1								
Phase	a_{22}/a_{11}	a33/a11	<i>a</i> 12/ <i>a</i> 11	<i>a</i> 13/ <i>a</i> 11	a23/a11	k_1 (10–5/°C)	k_2 (10–5/°C)	<i>k</i> ₃ (10–5/°C)
1	1	1	-0.382	-0.382	-0.382	6	6	6
2	g	1	r	-0.5	-0.5	0.49	0.49	0.49

Figure 1 shows the variation of \bar{k}_1 and \bar{k}_1 with volume fraction when r = -0.2. The results are presented for g = 1, 10 and 20. g = 1 corresponds to the case where both the phases are isotropic and the example in this special case becomes identical to one considered in Ref.[6]. While \bar{k}_1 is dependent only on thermal expansion coefficients of the phases and their volume fractions, the value of \bar{k}_1 also depends upon elastic properties of the phases. However, if cross coefficients of deformation, i.e. a_{12} , a_{13} , etc. are the same for both



Fig. 1. Linear expansion coefficient vs volume fractions.

the phases, the only elastic constant that affects \bar{k}_1 is the coefficient of deformation in direction 1.

In the example considered, \bar{k}_1 decreases with increase in the value of g or the coefficient of deformation of the second phase in direction 2. The degree with which g (or, in other words a_{22} or a_{33}) affects \bar{k}_1 of course depends on a_{12} or a_{13} . In Fig. 2, the effect of a_{12} on \bar{k}_1 for various values of a_{22} (or, g) is shown. The figure corresponds to a composite containing 10 per cent of phase 2 by volume. The figure indicates that a_{12} has very little effect on \bar{k}_1 for high values of a_{22} . For low values of a_{22} , the effect is considerable.



Fig. 2. $\overline{\overline{K}}_1$ vs r for volume fraction of phase 2 = 0.1.

In the second example, bounds on the effective thermal expansion coefficient are derived for a graphite reinforced composite with the following phase properties (note that the matrix is isotropic):

Fiber Axial Young's modulus $(1/a_{11}) = 60 \times 10^6$ psi transverse Young's modulus $(1/a_{ii}) = 10^6$ psi major Poisson's ratio $(-a_{1i}/a_{11}) = 0.2$ Matrix Young's modulus = 0.54×10^6 psi Poisson's ratio = 0.347thermal expansion coefficient = $60 \times 10^{-6}/^{\circ}C$

Poisson's ratio (transverse plane) $(-a_{23}/a_{ii}) = 0.25$ axial thermal expansion coefficient $(k_1) = -1.1 \times 10^{-6}/^{\circ}C$ transverse thermal expansion coefficient $(k_i) = 11 \times 10^{-6}/^{\circ}C$ (i = 2, 3).

For a fiber content of 50 per cent by volume, the effective elastic modulus of this composite along the fiber axis is approx 30×10^6 psi. From these values the following bounds on the effective thermal expansion coefficient in the direction of the fibers are obtained:

$$-0.91 \times 10^{-6}$$
/°C $\leq K_1 \leq 0.27 \times 10^{-6}$ /°C.

Unfortunately no experimental data on the thermal expansion coefficient for the particular composite is available to confirm the results obtained here. The published data for similar types of graphite reinforced composites indicate that they are around this range. It should be noted that the upper bound and the lower bound obtained in this specific problem are reasonably close. Closer bounds may possibly be found by applying more than one stress component at a time (unlike the present analysis) and running the optimization process with respect to two (or more) arbitrary stresses rather than one (see equations 18–22).

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Абстракт — Путем использования принципов экстремума термоупругости определяются пределы коэффициентов термического расширения для слоистых материалов с анизотропными фазами. Даются численные результаты для двух фазных слоистых материалов, с изотропными и анизотропными фазами.