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Thermal Expansion of Composites[1]

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A theory is developed for the overall thermal expansion of a composite consisting of either spherical or long cylindrical inclusions of one material in a matrix of another. The strain field of a single inclusion consists of a uniform expansion and a short-range strain field. These two components are related by minimizing the elastic strain energy. To account for a dense array of inclusions, average properties of the mixture are used for the long-range field, but those of the matrix alone for the short-range field. The net dilatation is thus found for inclusions of mismatching volume; hence one finds a differential expression for the thermal expansion in terms of the volume fraction of inclusions, the individual thermal expansivities, the bulk moduli of inclusion and matrix, the shear modulus of the matrix, and, in the case of cylinders, the shear modulus of the inclusions. This expression is integrated over temperature; one accounts for plasticity by letting the shear modulus depend on the temperature and on the accumulated shear strain. A representative numerical example is given.

KEY WORDS: composites; dilatation; elasticity; expansion; plasticity; theory.

1. INTRODUCTION

A composite which has inclusions in a matrix with different thermal expansivities develops internal stresses as the temperature is changed. As a result, the overall coefficient of thermal expansion differs from a simple volume average. For small temperature changes these internal stresses remain within the elastic regime, but larger temperature changes give rise to plastic flow and hysteresis.

The problem of an ellipsoidal inclusion inserted with some misfit into an elastic matrix was treated by Eshelby [1]; the special cases of a sphere

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and an infinite cylinder are well known (see, for example, Ref. 2). A random distribution of spherical inclusions was discussed by Eshelby [3] as a model for point defects. Wakashima et al. [4] considered differential thermal expansion for ellipsoidal inclusions, treating the matrix and the inclusions within it as a single effective medium with a uniform strain field. Differential thermal expansions with spherical inclusions had been treated previously by Kerner [5]. All these treatments assumed linear elasticity.

The present treatment is confined to spheres and to infinite cylinders and is thus not novel. It, too, uses the effective medium approximation but expresses the results in a different form by separating the strain field into its dilatational and shear components. In the elastic regime it is equivalent to previous solutions, which are expressed in terms of the Poisson ratio and the Young's modulus, but the present formulation facilitates the extension into the plastic regime.

2. ELASTIC FIELD ABOUT A SPHERICAL INCLUSION

Consider a spherical hole of radius R cut out of the matrix, into which is forced a spherical inclusion, originally of radius $R + \Delta R_2$ so that the surfaces join. The hole expands (or contracts, depending on the sign of ΔR_2) to a radius $R + \Delta R$. The displacement $u(r)$ of a point in the matrix distant r from the center ($r > R$) must be of the form [2]

$$u(r) = Ar + B/r^2 \tag{1}$$

and, in particular, $u(R) = \Delta R$. The spherical inclusion, which changes its radius by $\Delta R - \Delta R_2$, experiences a uniform dilatation. The matrix experiences a uniform dilatation as a result of the term Ar in Eq. (1), while the second term has shear but no dilatation. If there are many inclusions, so that c is the volume fraction of inclusions, we have the following dilatational strain energy:

$$E_{\text{dil}} = E_1 + E_2 \tag{2}$$

where E_1 is the dilatational energy of the inclusions, and E_2 that of the matrix, of fractional volume $(1 - c)$, so that

$$E_1 = (9/2)\, cK_{\text{I}}(\Delta R_2 - \Delta R)^2/R^2 \tag{3}$$

$$E_2 = (9/2)(1 - c)\, K_{\text{M}} A^2 \tag{4}$$

where K_{I} and K_{M} are the bulk moduli of inclusion and matrix material, respectively.

At a point r in the matrix the displacement B/r^2 describes three principal strains, one radially outward, of magnitude $-2B/r^3$, and two normal to the radius vector, each of magnitude B/r^3. The dilatation due to this term in Eq. (1) vanishes, and the strain energy density becomes

$$W_{\text{sh}} = 6\mu B^2/r^6 \tag{5}$$

where μ is the shear modulus of the matrix. The total shear energy around each inclusion is given by

$$E_{\text{sh}} = \int_R^\infty W_{\text{sh}}(r)\, 4\pi r^2\, dr = (4\pi/3)\, R^3 6\mu(B/R^3)^2 \tag{6}$$

ad since $(4\pi/3)\, R^3$ is the volume of each inclusion, the total shear energy, per unit volume of material, becomes

$$E_3 = 6c\mu(B/R^3)^2 \tag{7}$$

The total strain energy per unit volume of material is

$$E = E_1 + E_2 + E_3 \tag{8}$$

Now the parameters A and B are given by the condition that E should be a minimum with respect to variations in A and B. These two conditions suffice to determine these two parameters. Minimizing E is equivalent to balancing the stresses at the interface of inclusion and matrix. The use of the complete solution in Eq. (1) rather than just the term B/r^2 is equivalent to equating to zero the average normal stress at the external surface by introducing an image force. As discussed by Eshelby [3] this changes the net dilatation of the medium; the term Ar in Eq. (1) plays a similar role.

It is convenient to define

$$\beta = B/R^3 \tag{9}$$

and

$$\gamma = \Delta R_2/R \tag{10}$$

The conditions of elastic stability are $\partial E/\partial A = 0$ and $\partial E/\partial \beta = 0$. Note that in E_1

$$(\Delta R_2 - \Delta R)/R = \gamma - A - \beta \tag{11}$$

so that these two conditions become, respectively,

$$9cK_{\text{I}}(\gamma - A - \beta) = 9c(1-c)\, K_{\text{M}} A \tag{12}$$

and

$$9cK_{\mathrm{I}}(\gamma - A - \beta) = 12\mu c\beta \tag{13}$$

By eliminating γ, A, and β in turn from Eqs. (12) and (13),

$$A = \frac{c}{1-c}\,\beta\,\frac{4\mu}{3K_{\mathrm{M}}} \tag{14}$$

$$\beta = \gamma\left[1 + \frac{4\mu}{3K_{\mathrm{I}}} + \frac{4\mu c}{3(1-c)\,K_{\mathrm{M}}}\right]^{-1} \tag{15}$$

$$A = \gamma\,\frac{c}{1-c}\,\frac{4\mu}{3K_{\mathrm{M}}}\left[1 + \frac{4\mu}{3K_{\mathrm{I}}} + \frac{4\mu c}{3(1-c)\,K_{\mathrm{M}}}\right]^{-1} \tag{16}$$

Note that for low concentrations β is proportional to γ but does not depend on c, while A is proportional to c.

3. ELASTIC FIELD ABOUT AN INFINITE CYLINDER

Consider an inclusion which is an infinite cylinder with its axis on the z axis. Choosing cylindrical coordinates (r, θ, z), the displacement field in the matrix is of the form [2]

$$\begin{aligned} u_r &= Ar + B/r \\ u_z &= e_0 z \end{aligned} \tag{17}$$

and the principal strains are

$$e_{zz} = e_0, \qquad e_{rr} = A - B/r^2, \qquad e_{\theta\theta} = A + B/r^2 \tag{18}$$

with dilatation

$$\Delta = 2A + e_0 \tag{19}$$

while the component B/r in u_r is nondilatational.

If there is an assembly of long cylindrical inclusions, randomly oriented, the expansion of the medium must be isotropic; this requires $e_0 = A$.

The principal stresses can be calculated from

$$\sigma_{ii} = 2\mu e_{ii} + \lambda\Delta \tag{20}$$

and the strain energy density $W(r)$ from

$$W(r) = \tfrac{1}{2}\sum \sigma_{ii} e_{ii} \tag{21}$$

where λ is the Lamé constant and $K_M = \lambda + 2\mu/3$ is the bulk modulus of the matrix. Thus, using Eq. (19),

$$\begin{aligned} W(r) &= 3\mu A^2 + 2\mu B^2/r^4 + (9/2)\,\lambda A^2 \\ &= 2\mu B^2/r^4 + \tfrac{1}{2}(3A)^2\,K_M \end{aligned} \tag{22}$$

so that the dilatation and the nondilatational shear components contribute independently to the energy density. The strain energy of the matrix, per unit volume of material, becomes

$$E_M = \tfrac{1}{2}(3A)^2(1-c)\,K_M + c2\mu B^2/R^4 \tag{23}$$

since the B term yields, per unit length of inclusion,

$$E_B = 2\mu B^2 \int_R^\infty 2\pi r r^{-4}\,dr = 2\mu(B^2/R^4)\,\pi R^2 \tag{24}$$

and since one can equate, for an assembly of inclusions, πR^2 with c, the fractional volume of inclusions.

We now assume that the cylindrical inclusions have a dimensional misfit with respect to the matrix which is the same in the plane normal to the z axis as in the z direction itself. This is the misfit between inclusion and matrix which arises from isotropic thermal expansions which differ between inclusion and matrix. Thus let the inclusions have originally radius $R + \Delta R_2$ and fractional length difference $\Delta R_2/R$; the final radius is $R + \Delta R$, and the final longitudinal strain must match the linear strain A of the matrix. The strain within the inclusion is uniform, and the components of principal strain are

$$\begin{aligned} &(\Delta R_2 - \Delta R)/R \qquad \text{(2 transverse components)} \\ &R_2/R - A \qquad \text{(1 longitudinal component)} \end{aligned} \tag{25}$$

Resolving this into a dilatation

$$\begin{aligned} \Delta_I &= 3\Delta R_2/R - 2\Delta R/R - A \\ &= 3\Delta R_2/R - 3A - 2B/R^2 \end{aligned}$$

and three principal strains of zero dilatation and magnitude

$$-2B/R^2, \qquad B/R^2, \qquad B/R^2$$

the strain energy of the inclusions, per unit volume of material, becomes

$$E_I = (9/2)\,cK_I(\gamma - A - 2\beta/3)^2 + 6c\mu_I\beta^2 \tag{26}$$

where K_I and μ_I are the bulk and shear moduli of the inclusion, $\beta = B/R^2$, and $\gamma = \Delta R_2/R$. The total strain energy per unit volume of material is the sum of Eqs. (23) and (26), i.e.,

$$E = E_M + E_I \tag{27}$$

Again, the parameters A and β are given in terms of γ by the condition of stability

$$\partial E/\partial A = 0 \qquad \text{and} \qquad \partial E/\partial \beta = 0 \tag{28}$$

From these, one finds

$$\beta = (3/2)\,\gamma/f_1(\mu) \tag{29}$$

$$A = c(1-c)^{-1}\,\gamma f_2(\mu)/f_1(\mu) \tag{30}$$

where

$$f_1(\mu) = 1 + (\mu_M + 3\mu_I)\left(\frac{1}{K_I} + \frac{c}{(1-c)\,K_M}\right) \tag{31}$$

and where

$$f_2(\mu) = (\mu_M + 3\mu_I)/K_M \tag{32}$$

4. VOLUME CHANGE AND THERMAL EXPANSION

In the case of both spherical and cylindrical inclusions, the volume expansion comes from two sources: the A field of Eq. (1), respectively (17), which is a uniform expansion of the matrix and the included cavities, and the B field in either case, which represents an additional expansion of the cavities containing the inclusions. Since the B field is nondilatational, it transmits the expansion of the cavity

$$\delta V_B = 4\pi r^2 B/r^2 \qquad (\text{or } \delta V_B = 2\pi r B/r),$$

which is independent of r, to the outer boundary. Therefore the overall dilatation becomes

$$\delta V/V = 3A + 3c\beta \text{ (spheres)} \tag{33a}$$

$$\delta V/V = 3A + 2c\beta \text{ (cylinders)} \tag{33b}$$

If the matrix and the inclusions have different coefficients of volumetric thermal expansion, α_M and α_I, respectively, the misfit parameter γ resulting from the differential thermal expansion obeys

$$3d\gamma/dT = \alpha_I - \alpha_M \tag{34}$$

where T is temperature. For an isolated inclusion, Eqs. (33) and (34) determine the overall thermal expansion coefficient α if A and β are expressed in terms of γ. One is, however, interested in the case when c is not small. The following effective medium approximation is made.

For purposes of calculating the misfit between matrix and inclusion, one should replace the thermal expansion of the matrix by the overall thermal expansion of the medium, i.e., Eq. (34) should be replaced by

$$3d\gamma/dT = \alpha_I - \alpha \tag{35}$$

where α, the overall expansion, is given by

$$\alpha = \alpha_M + \frac{d}{dT}\left(\frac{\delta V}{V}\right) \tag{36}$$

and where $\delta V/V$ is given by whichever is the appropriate form of Eq. (33), i.e., dA/dT and $d\beta/dT$ are expressed—either by Eqs. (15) and (16) or by Eqs. (29) and (30)—in terms of $d\gamma/dT$ of Eq. (35).

Also, for purposes of calculating the dilatational strain energy, the relative volume contributions of matrix and inclusions were used, so that this property of the medium was averaged. For purposes of calculating the energy of the shear strain field (B field), it was assumed that this field resides entirely in the matrix, and the shear modulus of the matrix was used. Since the shear strain field is of a short range, this is a good approximation, unless the inclusions touch frequently. Finally, the shear strain energy was calculated for each inclusion individually; this implies that cross-terms in the energy due to neighboring inclusions vanish in the average. This would not be justified if the position of the inclusions have a short-range order: since inclusions cannot overlap, some such error is probably incurred.

In the case of *spherical inclusions* one finds from Eq. (36)

$$\frac{d}{dT}\left(\frac{\delta V}{V}\right) = 3cF(\mu)\frac{d\gamma}{dT} \tag{37}$$

where

$$F(\mu) = \frac{1 + 4\mu/3(1-c)\,K_M}{1 + 4\mu/3K_I + 4c\mu/3(1-c)\,K_M} \tag{38}$$

so that, from Eqs. (36), (37), and (35),

$$\alpha = \alpha_M + cF(\mu)(\alpha_I - \alpha) \tag{39}$$

This leads to the final result

$$(1 + cF)\,\alpha = \alpha_M + cF\alpha_I \tag{40}$$

In the case of *cylindrical inclusions*

$$\frac{d}{dT}\left(\frac{\delta V}{V}\right) = 3cG(\mu)\frac{d\gamma}{dT} \tag{41}$$

where, in terms of f_1 and f_2 of Eqs. (31) and (32),

$$G(\mu) = \left[1 + \frac{f_2}{1-c}\right]\Big/ f_1 \tag{42}$$

and is thus a function of both μ_I and μ_M. Similarly to Eqs. (39) and (40)

$$\alpha = \alpha_M + cG(\alpha_I - \alpha) \tag{43}$$

and

$$(1 + cG)\,\alpha = \alpha_M + cG\alpha_I \tag{44}$$

Equations (40) and (44) give the overall coefficient of thermal expansion in terms of the thermal expansion coefficients of the matrix and the inclusions, the elastic moduli of both components, and the volume fraction of the inclusions. Note that it has the same form as a volume average of matrix and inclusions, except that the volume fraction of inclusions has a modified value of $c/(1+cF)$ or $c/(1+cG)$, respectively.

5. PLASTIC REGIME

Equations (40) and (44) describe the dilatation due to an infinitesimal temperature change and can be integrated over a finite temperature interval even if α_M and α_I are functions of temperature. However, the functions F and G depend on the elastic moduli. Not only are the moduli somewhat temperature dependent, but also the shear moduli are functions of the shear strain. The appropriate shear moduli in F and G are those defined differentially, i.e.,

$$2\mu = d\sigma_{ij}/de_j, \qquad i \neq j \tag{45}$$

in terms of stress and strain components in the contracted notation; in the plastic regime μ depends on the prior shear strain, hence on the net differential expansion.

Now the strain in the matrix is a function of position, so that, strictly speaking, μ becomes a function of r once the plastic regime is reached, and the equations derived for the strain field no longer apply. However, most of the shear strain energy resides at the matrix–inclusion interface $r = R$. Hence one may approximate the shear energy by treating μ as a function of β, the shear strain at the interface.

Using Eqs. (15), (35), and (40) for spherical inclusions and integrating the strain from a temperature T_0 at which the inclusions and matrix are unstrained

$$\beta = \int_{T_0}^{T} (\alpha_{\mathrm{I}} - \alpha_{\mathrm{M}}) \left[1 + \frac{4\mu}{3K_{\mathrm{I}}} + \frac{4c\mu}{(1-c)\,3K_{\mathrm{M}}} \right]^{-1} \frac{1}{3(1+cF)}\, dT \qquad (46)$$

For cylindrical inclusions, using Eqs. (29), (35), and (44),

$$\beta = \int_{T_0}^{T} (\alpha_{\mathrm{I}} - \alpha_{\mathrm{M}})[3f_1(\mu_{\mathrm{M}}, \mu_{\mathrm{I}})(1+cG)]^{-1}\, dT \qquad (47)$$

Thus, to calculate the thermal expansion from Eq. (40) or (44), one must increase the temperature by steps, calculate β, and determine μ, which is a function of β and T. This new value of μ is then used in the next temperature step. In the case of cylinders there are two shear moduli, which are functions of β and T. This procedure cannot be expressed in a closed algebraic form but is suited to numerical integration.

Note that if $\mu = 0$, $F = 1$ and

$$d\beta = (\alpha_{\mathrm{I}} - \alpha_{\mathrm{M}}) \frac{1}{3(1+c)}\, dT \qquad (48)$$

while for cylinders, if $\mu_{\mathrm{I}} = 0$ and $\mu_{\mathrm{M}} = 0$, $f_1 = 1$ and $G = 1$, and the same would hold. Thus in a simple model of plasticity in which μ is constant until it suddenly drops to zero when a yield strain β_{Y} is reached, one can define a yield temperature T_{Y} such that $\beta = \beta_{\mathrm{Y}}$, where β is given by Eq. (46) or (47). Then

$$\Delta = \int_{T_0}^{T} \alpha\, dT = \int_{T_0}^{T_{\mathrm{Y}}} [(1+cF)^{-1}(\alpha_{\mathrm{M}} + cF\alpha_{\mathrm{I}})]\, dT + \int_{T_{\mathrm{Y}}}^{T} (1+c)^{-1}(\alpha_{\mathrm{M}} + c\alpha_{\mathrm{I}})\, dT \qquad (49)$$

for spheres, while a similar expression, with G replacing F, holds for cylinders.

6. NUMERICAL ILLUSTRATION

Consider a matrix and inclusions with the following parameters:

$$\alpha_M = 6 \times 10^{-5}\,\mathrm{K}^{-1} \qquad \alpha_I = 2 \times 10^{-5}\,\mathrm{K}^{-1}$$
$$K_M = 8 \times 10^{10}\,\mathrm{J \cdot m^{-3}} \qquad K_I = 3 \times 10^{11}\,\mathrm{J \cdot m^{-3}}$$
$$\mu_M = 3 \times 10^{10}\,\mathrm{J \cdot m^{-3}} \qquad \mu_I = 1.6 \times 10^{11}\,\mathrm{J \cdot m^{-3}}$$

For volume fractions $c = 0.1$, 0.2, and 0.4; the volume-averaged expansion coefficients would be $\bar{\alpha} = 5.6$, 5.2, and $4.4 \times 10^{-5}\,\mathrm{K}^{-1}$, respectively. For spherical inclusions $F = 1.308$, 1.291, and 1.250, respectively; the overall expansion coefficients are $\alpha_F = 5.54$, 5.18, and $4.67 \times 10^{-5}\,\mathrm{K}^{-1}$. For cylindrical inclusions $G = 2.372$, 2.089, and 1.673, respectively; the overall expansion coefficients are $\alpha_G = 5.23$, 5.02, and $4.40 \times 10^{-5}\,\mathrm{K}^{-1}$. There is a general trend for the expansion to be less than the volume average for low values of c and more than the volume average for higher values of c.

In the case of spheres with $c = 0.2$, if we assume the yield strain of the matrix to be $\beta_Y = 3 \times 10^{-3}$ and independent of T, the plastic regime is reached [see Eq. (46)] if $T - T_0 = 120$ K. In the plastic regime the expansion coefficient becomes the volume average for an effective concentration of $c/(1 + c)$, i.e., for 0.167, which yields $5.33 \times 10^{-5}\,\mathrm{K}^{-1}$, and is thus slightly enhanced. Hysteresis effects should occur over a temperature span of about 240 K with an offset in dilatation of $(120)(0.31 \times 10^{-5}) = 3.7 \times 10^{-4}$.

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