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Theory of Thermal Expansion of Composites[1]

P. G. Klemens[2]

The problem discussed is to find the overall thermal expansion of a composite consisting of inclusions in a matrix of material with different expansion coefficients and elastic moduli. The volume mismatch causes strain fields. The total strain energy must be a minimum. This problem was solved previously for inclusions which are either spheres or randomly oriented long cylinders. In these simple cases the matrix strain field consists of a short-range shear component and a uniform expansion; the inclusion suffers uniform strain. The matrix is replaced by an effective medium having the average properties of the composite. The overall expansion coefficient could be obtained in closed form. This separation of the strain field into short-range shear and long-range uniform dilation is valid, at least to a good approximation, for all inclusion shapes. Simple expressions can thus be obtained in terms of coefficients which, although not calculated exactly, can be deduced approximately or can be determined empirically. Plasticity can be accounted for by allowing the shear modulus tc depend on the temperature and on the maximum shear strain. The size of the inclusions does not enter the theory except through the yield strain, which depends on the extent of the strain field.

KEY WORDS: composites; dilation; elasticity; plasticity; thermal expansion.

1. INTRODUCTION

In the case of a composite material, consisting of two solids with different thermal expansion coefficients, a change of temperature gives rise to elastic strains, and the overall thermal expansion coefficient differs from a simple volume average of the constituents. The problem of calculating this overall expansion is, in general, a difficult one. It has been solved in some simple

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[2] Department of Physics and Institute of Materials Science, University of Connecticut, Storrs, Connecticut 06268, U.S.A.

cases. The present discussion is confined to inclusions of the material in a continuous matrix of another.

A previous paper [1] treated the cases of inclusions which are spheres or long cylinders randomly oriented. In that treatment the total strain energy was minimized, and the effect of other inclusions on the strain field about one given inclusion was treated by replacing the matrix by an effective medium. This requires a knowledge of the strain field for a single inclusion in an infinite matrix, given a volume mismatch between the inclusion and the matrix material which it replaces.

Both for a sphere and for an infinite cylinder the strain field of the matrix is a combination of a uniform dilation and of a short-range strain field of purely shear character. The inclusion is subject to uniform strain. For inclusions of other shapes this is no longer exactly true. Nevertheless, this decomposition into two components—a long-range dilation and a short-range shear—should also hold approximately for other shapes; the actual short-range field would have additional components, some of them dilational, which should increase the strain energy and also modify the connection between the strain of the inclusion and that of the matrix. The method of Ref. 1 is here generalized to other shapes, so that an approximate formula can be obtained for the overall thermal expansion. However, for some of the coefficients in that formula only a lower limit will be obtained. Since these coefficients could be found empirically, the formula thus obtained may be of some practical use.

2. STRAIN ENERGY OF INCLUSIONS

Consider a single inclusion in a matrix, with dimensional mismatch between the inclusion and the cavity with the matrix which accommodates it; let γ be the fractional excess of the linear dimension of the inclusion. There will be a strain field within the inclusion, with strain energy E_1, and there will be a uniform dilation of the matrix (strain energy E_2) as well as a short-range strain field in the matrix surrounding the inclusion (strain energy E_3).

Now the cavity which holds the inclusion will be expanded linearly by a fractional amount $A + \beta$, while the fractional expansion of the matrix far from the inclusion is A, so that β is a measure of the short-range strain at the interface of the inclusion and the matrix. In the case of a sphere or a cylinder that strain will be the same everywhere on the interface [1]. For less regular shapes that strain will vary somewhat over the interface, and β must be understood to be an average.

The linear misfit between the original shape of the inclusion and that of the expanded cavity is $(\gamma - A - \beta)$, so that the strain energy within the inclusion is of the form

$$E_1 = K_1(\gamma - A - \beta)^2 \tag{1}$$

The long-range expansion of the matrix has strain energy of the form

$$E_2 = K_2 A^2 \tag{2}$$

while the strain energy of the short-range strain field has the form

$$E_3 = K_3 \beta^2 \tag{3}$$

The coefficients K_1, K_2, and K_3 depend on the elastic moduli of matrix and inclusion and on the shape of the inclusion.

Strictly speaking, for an infinite matrix surrounding a single inclusion, K_2 should become infinite, being proportional to the volume of the matrix, while A should be inversely proportional to that volume, so that $K_2 A^2$ should be inversely proportional to it and thus tend to zero. The term $K_2 A^2$ of Eq. (2) and the consideration of A in Eq. (1) are important, however, when the inclusion occupies a finite fraction of the total volume and the A field plays a role in the stress-free boundary conditions on external surfaces, as demanded by the treatment of Eshelby [2].

We thus find it more convenient to consider an infinite matrix containing many inclusions, randomly placed, so that c is the fractional volume of the inclusions, and we define E_1, E_2, and E_3 to be the respective strain energies per unit volume of material. The matrix must now be replaced by an effective medium, consisting of matrix (volume fraction $1 - c$) and inclusions (volume fraction c), and the elastic parameters of the effective matrix material must be appropriately adjusted. This affects the coefficients K_2 and K_3 but has the advantage that K_2 becomes large and finite ($K_2 \simeq \frac{1}{2} B_M$, where B_M is the bulk modulus of the medium), while A, K_1, and K_3 become proportional to c for low values of c.

The misfit parameter γ and the volume fraction c of inclusions will be taken as given, while β and A are unknowns to be determined. Since the system adjusts itself so as to minimize the total strain energy

$$E = E_1 + E_2 + E_3 \tag{4}$$

the conditions of stability become

$$\partial E / \partial A = -2K_1(\gamma - A - \beta) + 2K_2 A = 0 \tag{5}$$

$$\partial E / \partial \beta = -2K_1(\gamma - A - \beta) + 2K_3 \beta = 0 \tag{6}$$

These two equations suffice to determine A and β in terms of γ, and one obtains

$$\beta = \gamma K_1 K_2/(K_1 K_2 + K_2 K_3 + K_3 K_1) \tag{7}$$

and

$$A = \beta K_3/K_2 = \gamma K_3 K_1/(K_1 K_2 + K_2 K_3 + K_3 K_1) \tag{8}$$

Note that in the limit of low concentration c, the coefficients K_1 and K_3 are both proportional to c, while K_2, being a property of the matrix, tends to a value independent of c. Thus for low concentrations, $K_1 K_2$ is the dominant term in the denominator of Eqs. (7) and (8). Therefore β becomes independent of c, as one would expect since it is a property of each individual inclusion, while A, the uniform expansion of the matrix, is proportional to the concentration c.

In the spcial case of spherical inclusions [1],

$$\begin{aligned} K_1 &= (9/2)\, cB_i \\ K_2 &= (9/2)(1-c)B_m \\ K_3 &= 6c\mu_m \end{aligned} \tag{9}$$

where B_i and B_m are the bulk moduli of inclusions and matrix, respectively, and μ_m us the shear modulus of the matrix. In this case there is no shear in the inclusions.

For nonspherical inclusions K_1 and K_3 are enhanced, so that β is not changed very much but A becomes somewhat larger.

Plastic deformation tends to reduce μ_m and hence reduces K_3. In the case of nonspherical shapes, when E_1 also contains a shear component, this will also reduce K_1 by a small amount. In the case of extreme plasticity K_3 will tends toward zero, making β approach γ and making A become small.

3. VOLUME CHANGE AND THERMAL EXPANSION

The strain field due to spherical inclusions is composed of two parts: a uniform expansion of the matrix, with fractional volume change $3A$, and a nondilational component which transmits the change in volume of the cavities to the external surfaces. The fractional change in volume of each cavity is 3β, and since c is the fractional volume occupied by cavities, the overall change in volume becomes

$$\delta V/V = 3A + 3c\beta \tag{10}$$

For nonspherical inclusions, this division still holds approximately: although there may be dilations due to the short-range field at some locations near the inclusion, they would be compensated by negative dilations at other places, and Eq. (10) would still hold. The only difference likely to arise is that the effective value of β may change: this is equivalent to a change in K_3. Therefore the fractional change in volume, from Eqs. (10), (7), and (8), is

$$\delta V/V = 3\gamma(c + K_3/K_2)K_1K_2/(K_1K_2 + K_2K_3 + K_3K_1) \tag{11}$$

Note that K_1 and K_3 both vary as c, while $K_2 \propto (1-c)$, so that $c + K_3/K_2$ varies approximately as c, and $\delta V/V$ varies as c for low values of c.

Now γ is a function of temperature if the two materials have different expansion coefficients. When the volume fraction of inclusions is small,

$$3d\gamma/dT = \alpha_\mathrm{i} - \alpha_\mathrm{m} \tag{12}$$

where α_i and α_m are the volume coefficients of thermal expansion of inclusion and matrix material, respectively. The net coefficient of thermal expansion becomes

$$\alpha = \alpha_\mathrm{m} + V^{-1}\, d\delta V/dT \tag{13}$$

where the second term is given by Eqs. (11) and (12), and K_1, K_2, and K_3 are temperature independent.

If the concentration of inclusions is finite, the net expansion of the matrix is no longer α_m but α, replacing the matrix by an effective medium consisting of the matrix and all other inclusions. Thus Eq. (12) should be replaced by

$$3d\gamma/dT = \alpha_\mathrm{i} - \alpha \tag{14}$$

and this should be used in Eq. (11) to obtain the term $V^{-1}d\delta V/dT$ of Eq. (13). Thus

$$\begin{aligned}\alpha &= \alpha_\mathrm{m} + (\alpha_\mathrm{i} - \alpha)(c + K_3/K_2)K_1K_2/(K_1K_2 + K_2K_3 + K_3K_1)\\ &= \alpha_\mathrm{m} + (\alpha_\mathrm{i} - \alpha)\, cF\end{aligned} \tag{15}$$

where

$$F = (1 + K_3/cK_2)K_1K_2/(K_1K_2 + K_2K_3 + K_3K_1) \tag{16}$$

With F thus defined, one obtains from Eq. (15)

$$\alpha = (\alpha_\mathrm{m} + cF\alpha_\mathrm{i})/(1 + cF) \tag{17}$$

4. COMPARISON WITH THE VOLUME MIXING RULE

One can compare the expansion coefficient expressed by Eq. (17) with the simple mixing rule which weighs components by their volume fraction:

$$\bar{\alpha} = c\alpha_i + (1 - c)\alpha_m \tag{18}$$

Equation (17) can be brought into the form of Eq. (18) if the volume fraction c is replaced by an effective concentration

$$c' = cF/(1 + cF) \tag{19}$$

where F, given by Eq. (16), is itself dependent on c.

For low c, $F = (1 + K_3/cK_2)/(1 + K_3/K_1)$, and frequently, but not always, $F > 1$. As c increases, F decreases because the term K_3K_1 gains relative importance. Thus $c' > c$ for low c and $c' < c$ for higher values of c, with a crossover $c' = c$ when $c = (F - 1)/F$. Thus in general Eq. (18) places greater weight on the inclusions than Eq. (18) would when c is small. For large values of c, $F < 1$ and c' will be less than c, so that Eq. (18) overestimates the effect of the inclusions. However the departure from Eq. (18) is usually small.

In the case of spherical inclusions

$$F = (1 + 4\mu_m/3B_m)/(1 + 4\mu_m/3B_i) \tag{20}$$

so that F departs only slightly from unity and departures from Eq. (18) are small.

5. PLASTIC FLOW IN THE MATRIX

For each increment in temperature there is a corresponding increment in the misfit parameter γ and a corresponding increase in β, the maximum strain in the matrix. Since the major contribution to E_3 comes from the region at the interface, where the strain is largest, one can approximately treat the parameter β as a measure of the short-range shear strain.

Now the shear modulus μ_m which enters K_3 must be considered to be an incremental modulus, related to the slope of the stress–strain curve. With increasing shear strain and temperature, this incremental modulus tends to decrease, and correspondingly K_3 will decrease and F will tend toward a value of 1.

The present treatment appears to be independent of the size of the inclusions. This is so in the elastic regime. In the plastic regime, however, it must be remembered that μ_m depends also on the linear extent of the shear strain field. Unless the strain field includes preexisting dislocations, the microscopic yield stress will be much larger than that measured on large samples. Thus the plastic flow in the matrix about an inclusion will be inhibited if the inclusions are less than a micrometer in size, since in soft metals the density of dislocations is no more than $10^8\ \mathrm{cm}^{-2}$.

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