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ON THERMOELASTIC STRESSES IN COMPOSITE MEDIA*

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The thermoelastic stresses are determined in composites that are a homogeneous and isotropic matrix with inclusions of another component of ellipsoidal shape. The thermoelastic stresses within an arbitrary inclusion and in its neighborhood are determined by using one of the modifications of the self-consistent field method /1/ that permits taking account of interaction of the inclusions. An analogous approach was used /2/ to determine the stress concentration factor an ellipsoidal inclusions in an elastic medium. Within the framework of the same scheme, the thermoelastic stresses are found in polycrystal line grains for which the dependence of the thermoelastic stresses on the coordinates is due to the difference in orientations of the crystallographic axes of the individual grains.

1. We examine an ellipsoidal inhomogeneity with elastic modulus tensor $L_1 (M_1 = L_1^{-1})$ and coefficient of thermal expansion α_1 that occupies a domain V in an unlimited medium with the thermoelastic characteristics $L_0 (M_0 = L_0^{-1})$ and α_0. Let the medium be subjected to a uniform change in temperature of Θ degrees. Because of the difference in the thermoelastic constants of the matrix and the inclusions, a stress field $\sigma(x)$, that vanishes at infinity, originates in the medium and satisfies the system of equations

$$\operatorname{div} \sigma(x) = 0, \quad \operatorname{Rot} M(x)\, \sigma(x) = -\operatorname{Rot} \alpha(x)\, \Theta \tag{1.1}$$

If the elastic compliance tensors $M(x)$ and the thermal expansion coefficients $\alpha(x)$ are represented in the form

$$\begin{aligned} M(x) &= M_0 + [M]\, V(x), \quad [M] = M_1 - M_0 \\ \alpha(x) &= \alpha_0 + [\alpha]\, V(x), \quad [\alpha] = \alpha_1 - \alpha_0 \end{aligned} \tag{1.2}$$

where $V(x)$ is the characteristic function of the ellipsoid, then the problem of determining the field $\sigma(x)$ can be reduced to the integral equation

$$\sigma(x) = \int \Gamma_0 (x - y)\, V(y)\, ([M]\, \sigma(y) + [\alpha]\, \Theta)\, dy \tag{1.3}$$

$$\Gamma_0 (x - y) = -L_0 (I \delta (x - y) + G(x - y)\, L_0) \tag{1.4}$$

$$G(x) = (G_{ijkl}(x)) = [U_{ik,\, jl}(x)]_{(ij)(kl)}, \quad I = (I_{ijkl}) = \delta_{i(k}\delta_{l)j}$$

Here $\Gamma_0 (x - y)$ is the Green's tensor for the internal stresses in homogeneous medium with elastic moduli tensor L_0 expressed in terms of the Green's tensor of the Lamé equations $U(x - y)$ (the parentheses denote symmetrization in the corresponding subscripts).

Equation (1.3) can be written in the form of the system

$$\sigma^+ = \Gamma_0^+ ([M]\, \sigma^+ + [\alpha]\, \Theta), \quad \sigma^- = \Gamma_0 ([M]\, \sigma^+ + [\alpha]\, \Theta) \tag{1.5}$$

where Γ_0 is an integral operator with the kernel $\Gamma_0 (x - y)$, and $\Gamma_0^+ = V \Gamma_0 V$ is its contraction in the domain occupied by the ellipsoid. The first equation in (1.5) determines the stress field σ^+ within this domain, while the second is the continuation of the solution outside V. For $\Theta = \text{const}$, the stress field in the inclusions will be homogeneous because of the property of the operator Γ_0 to transform constants into constants /3/, and is determined by the expression

$$\begin{aligned} \sigma^+ &= -Q(\omega)\, B(\omega)\, [\alpha]\, \Theta, \quad Q(\omega) = L_0 (I - P(\omega)\, L_0) \\ B(\omega) &= (I + Q(\omega)\, [M])^{-1} \end{aligned} \tag{1.6}$$

The set of Euler angles giving the orientation of the ellipsoid with respect to the laboratory coordinate system is denoted by ω while $P(\omega)$ is a constant, quadrivalent tensor dependent on the geometric characteristics of the ellipsoid and the elastic moduli of the matrix. For an isotropic matrix with volume k_0 and shear elastic moduli μ_0

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$$P_{ijkl} = S_{ij\alpha\beta} \overset{\circ}{M}_{\alpha\beta kl} = \frac{1}{\mu_0}\left(\delta_{ik}\varphi^+_{,jl} + \frac{3k_0+\mu_0}{3k_0+4\mu_0}\psi^+_{,ijkl}\right)_{(ij)(kl)} \tag{1.7}$$

where φ^+ and ψ^+ are the harmonic and biharmonic potentials of the ellipsoid at an inner point, and S_{ijkl} is the Eshelby tensor (/3/,p.118).

If the point x is fixed outside the inclusion, then we obtain from (1.5)

$$\sigma^-(x) = -L_0 P^-(x) L_0 B(\omega) [\alpha] \Theta \tag{1.8}$$

where $P^-(x)$ is determined by (1.7) in which φ^+ and ψ^+ should be replaced by the potentials φ^- and ψ^- at the exterior point. This expression permits determination of the limit value, from outside, for the stress tensor $\sigma^-(n)$ on the inclusion boundary. Using the relationship for the jumps in derivatives of the potentials when passing through the boundary

$$\varphi^-_{,ij} - \varphi^+_{,ij} = 4\pi n_i n_j, \quad \psi^-_{,ijkl} - \psi^+_{,ijkl} = 8\pi n_i n_j n_k n_l$$

where n_i are components of the unit normal to the surface of the inclusion, we obtain

$$\sigma^-(n) = L_0 (P(\omega) - K(n)) L_0 B(\omega) [\alpha] \Theta \tag{1.9}$$
$$K(n) = (K_{ijkl}(n)) = \frac{1}{\mu_0}\left(\delta_{ik} n_j n_l - \frac{3k_0+\mu_0}{3k_0+4\mu_0} n_i n_j n_k n_l\right)_{(ij)(kl)}$$

2. We now examine a composite material consisting of a homogeneous and isotropic matrix in which ellipsoidal inclusions of another component are distributed. We consider the ellipsoids identical in magnitude but differently oriented in space. We extract the characteristic volume of the composite, i.e., the volume with dimensions substantially exceeding the spacing between inclusions, but within whose limits the change in the temperature field can be neglected. Under these conditions the characteristic volume can be considered unbounded.

We denote the characteristic function of the domain occupied by the inclusions by $V(x) = \bigcup V_i(x)$. Then the integral equation which the stress field $\sigma(x)$ satisfies in the composite will have the same form (1.3). However, this field will now be random because of the randomness of the positions of the centers and the orientations of the ellipsoids. Hence, the exact determination of the stress becomes a complex problem, and an approximate method based on the method of the "effective field" /1/ is used for its solution.

We fix the point x in the domain of an arbitrary inclusion V_k and we rewrite the integral equation to determine the field $\sigma(x)$ as follows:

$$\sigma(x) = -Q(\omega_k)[\alpha]\Theta + \sigma^*(x) + \int \Gamma_0(x-y) V_k(y) [M] \sigma(y)\, dy \tag{2.1}$$
$$\sigma^*(x) = \int \Gamma_0(x-y) V(x;\ y) ([M]\sigma(y) + [\alpha]\Theta)\, dy \tag{2.2}$$
$$V(x;\ y) = \bigcup_{j\neq k} V_j(y), \quad x \in V_k$$

The first term in the right side of (2.1) takes on the role of internal stress sources, and $\sigma^*(x)$ is the effective field which is determined by (2.2) and takes account of the influence of the remaining inclusions in the characteristic volume on the segregated inclusion.

Let us formulate the fundamental hypotheses of the effective field method /1/: 1) the change in the field $\sigma^*(x)$ in domains occupied by the inclusions can be neglected; 2) the field $\sigma^*(x)$ is independent of the geometric characteristics and thermoelastic properties of the segregated inclusion.

The first of these assumptions permits obtaining

$$\sigma(x) = B(x)(\sigma^*(x) - Q(x)[\alpha]\Theta), \quad B(x) = B(\omega_k) \text{ as } x \in V_k \tag{2.3}$$

from (2.1). Substituting (2.3) into the right side of (2.2), we obtain a self-consistent equation to determine the random field

$$\sigma^*(x) = \int \Gamma_0(x-y) V(x;y) B(y) ([M]\sigma^*(y) + [\alpha]\Theta)\, dy \tag{2.4}$$

Denoting the operation of taking the average over the ensemble of realizations of the random field of inclusions for which the domain V contains the fixed point x by symbol $\langle\cdot \mid x\rangle$, by taking the average of both sides of (2.4) we find

$$\langle\sigma^*(x) \mid x\rangle = \int \Gamma_0(x-y) \Psi(x,\ y)([M]\langle\sigma^*(y) \mid x;\ y\rangle + [\alpha]\Theta)\, dy \tag{2.5}$$
$$\Psi(x;y) = \langle V(x;\ y) B(y) \mid x\rangle$$

The mean under the condition that the two points (x and y) are fixed is under the integral sign, and the assumption 2) is used in separating the means. It is logical to consider each inclusion to be in the same effective field σ^* for a homogeneous temperature field and a large quantity of inclusions in the characteristic volume. In this case, the conditional means in

(2.5) are in agreement, as well as with the quantity σ^*. Finally, if the domains V_j in the characteristic volume form a statistically homogeneous and isotropic field, then the function $\Psi(x; y)$ possesses the following properties:

$$\Psi(x; y) = \Psi(|x-y|), \quad \Psi(0) = 0, \quad \Psi(\infty) = c_1\langle B\rangle_\omega$$

where c_1 is the volume concentration of inclusions, and $\langle\cdot\rangle_\omega$ denotes taking the average with respect to the set of ellipsoids orientations. Under these conditions the integral in (2.5) is evaluated /1/, and we consequently will have

$$\sigma^* = c_1 Q_0 \langle B\rangle_\omega D[\alpha]\Theta, \quad D = (I - c_1 Q_0 [M]\langle B\rangle_\omega)^{-1}, \quad Q_0 = \langle Q\rangle_\omega \tag{2.6}$$

Now, substituting the expression for σ^* in (2.3), we find the temperature stress σ^+ within an inclusion with the orientation ω_k

$$\sigma^+(x) = (c_1 Q_0 \langle B\rangle_\omega - Q(\omega_k) B(\omega_k)) D[\alpha]\Theta, \quad x \in V_k \tag{2.7}$$

Therefore, under the assumptions made the field σ^+ turns out to be homogeneous and to depend only on the ellipsoid orientation ω_k. Exactly as in Sect.1, the result obtained permits finding the stress in the matrix directly at the inclusion surface

$$\sigma^-(n) = (c_1 Q_0 \langle B\rangle_\omega + L_0(P(\omega_k) - K(n)) L_0 B(\omega_k)) D[\alpha]\Theta \tag{2.8}$$

Comparing (2.7) and (2.8) with (1.6) and (1.9) shows that the expression for the thermal stresses in one isolated inclusion in the matrix and on its boundary differs from the corresponding stresses in the composite material by the tensor factor D and the term $c_1 Q_0 \langle B\rangle_\omega D[\alpha]\Theta$ which takes account of interaction of the inclusions and the statistical characteristics of their distribution. For low inclusion concentrations, this interaction becomes negligibly small and (2.7) and (2.8) go over into (1.6) and (1.9) as $c_1 \to 0$.

Let the inclusions be spherical in the composite material. In this case the tensors P, Q and B become isotropic, and (2.7) and (2.8) simplify substantially

$$\begin{aligned} &\sigma_{ij}^+ = -c_0 d(\alpha_1 - \alpha_0)\Theta\delta_{ij} \\ &\sigma_{ij}^-(n) = {}^1/_2 d[(1 + 2c_1)\delta_{ij} - 3n_i n_j](\alpha_1 - \alpha_0)\Theta \\ &d = \left(\frac{3}{4\mu_0} + \frac{c_1}{k_0} + \frac{c_0}{k_1}\right)^{-1}, \quad c_0 = 1 - c_1 \end{aligned} \tag{2.9}$$

We note that these formulas agree with the expressions for the thermoelastic stresses in a spherical composite element with ratio $c_1^{1/3}$ between the radii of the inner and outer spheres.

3. The scheme presented can be used also to determine the thermal stresses in single-phase polycrystals. It is impossible to extract the fundamental medium (matrix) in a polycrystal, however, the tensors of the thermoelastic characteristics $M(x)$ and $\alpha(x)$ that are random functions of the coordinates can be written in an analogous form to (1.2)

$$\begin{aligned} &M(x) = \langle M\rangle_\omega + M^*(x), \quad M^*(x) = \sum_r (M(\omega_r) - \langle M\rangle_\omega) V_r \\ &\alpha(x) = \sum_r \alpha(\omega_r) V_r \end{aligned} \tag{3.1}$$

Here V_r is the characteristic function of the r-th crystallite (the summation is over all crystallites in the characteristic volume), while $M(\omega_r)$ and $\alpha(\omega_r)$ are constant values that the quantities $M(x)$ and $\alpha(x)$ take on in a crystallite with orientation ω_r for the principal crystallographic axes. Such a representation permits, in this case also, consideration of each grain as an isolated inhomogeneity in a medium with the elastic compliance tensor $M_0 = \langle M\rangle_\omega$ on which the effective field acts. Considering the grains in the polycrystal to be spherical in shape, for simplicity (the consideration of ellipsoidal grains imposes no difficulties, in principle), we can write under the same hypotheses for the effective field

$$\sigma(x) = B(\omega_k)(-Q_0\alpha(\omega_k) + \sigma^*(x)), \quad B(\omega_k) = (I + Q_0 M^*(\omega_k))^{-1} \tag{3.2}$$

$$\begin{aligned} &\sigma^*(x) = \int \Gamma_0(x-y) B(y)(M^*(y)\sigma^*(y) + \alpha(y)\Theta)\,dy, \\ &x \in V_k, \quad y \in \bigcup_{r\neq k} V_r \end{aligned} \tag{3.3}$$

where $\Gamma_0(x-y)$ is determined by (1.4) for $M_0 = \langle M\rangle_\omega$. Finding the conditional mean of both sises of (3.3), and considering each grain to be in an identical effective field σ^*, we obtain

$$\begin{aligned} &\sigma^* = \int \Gamma_0(x-y)(\Psi(x; y)\sigma^* + \Phi(x; y)\Theta)\,dy, \quad x \in V_k, \\ &y \in \bigcup_{r\neq k} V_r \\ &\Psi(x; y) = \langle B(y) M^*(y) \mid x\rangle, \quad \Phi(x; y) = \langle B(y)\alpha(y) \mid x\rangle \end{aligned} \tag{3.4}$$

The properties of the functions Ψ and Φ for homogeneous and isotropic fields $M(x)$ and $\alpha(x)$ agree with the properties of the function Ψ from composites, i.e., they depend only on $|x-y|$ and

$$\Psi(0) = \Phi(0) = 0, \quad \Psi \to \langle M^*B\rangle_\omega, \ \Phi \to \langle B\alpha\rangle_\omega \ \text{as} \ |x-y| \to \infty$$

Consequently, we obtain after integration

$$\sigma^* = Q_0\bar{\alpha}\Theta, \quad \bar{\alpha} = \langle B\rangle_\omega^{-1}\langle B\alpha\rangle_\omega \tag{3.5}$$

Let us note that the quantity $\bar{\alpha}$ is the effective coefficient of thermal expansion of the polycrystals. It can be derived from the more general results of /4/ obtained by using summation of perturbation theory series and a strong isotropy hypothesis.

Now substituting (3.5) into (3.2), we obtain an expression for the thermal microstresses in an arbitrary polycrystal grain

$$\sigma(x) = Q_0B(\omega_k)(\bar{\alpha} - \alpha(\omega_k)), \quad x \in V_k \tag{3.6}$$

which agrees with that found in /5/ by other means.

As an illustration we compute the thermal stresses originating in hexagonal polycrystal grains for a uniform temperature change. For the crystallite whose principle axes of anisotropy agree with the laboratory coordinate system, (3.6) yields

$$\begin{aligned}
&\sigma_{11} = \sigma_{22} = [(d_{11}+d_{12})(\bar{\alpha}-\alpha_\perp) + d_{13}(\alpha - \alpha_\parallel)]\Theta \\
&\sigma_{33} = [2d_{13}(\bar{\alpha}-\alpha_\perp) + d_{33}(\bar{\alpha}-\alpha_\parallel)]\Theta, \quad \sigma_{12} = \sigma_{13} = \sigma_{23} = 0 \\
&d_{11}+d_{12} = \frac{f_{33}}{f}, \quad d_{13} = -\frac{f_{13}}{f}, \quad d_{33} = \frac{f_{11}+f_{12}}{f} \\
&f = f_{33}(f_{11}+f_{12}) - 2f_{13}^2, \quad f_{11} = p_1 + \frac{4}{3}p_2 + m_{11}, \quad f_{12} = p_1 - \frac{2}{3}p_2 + m_{12} \\
&f_{13} = p_1 - \frac{2}{3}p_2 + m_{13}, \quad f_{33} = p_1 + \frac{4}{3}p_2 + m_{33}, \quad p_1 = 1/12\mu_0 \\
&p_2 = \frac{1}{6}\left(\frac{1}{\mu_0} + \frac{10}{9k_0 + 8\mu_0}\right), \quad k_0 = (2m_{11} + 2m_{12} + 4m_{13} + m_{33})^{-1} \\
&\mu_0 = 7.5\,(7m_{11} + 2m_{33} + 3m_{44} - 5m_{12} - 4m_{13})^{-1}
\end{aligned} \tag{3.7}$$

Here $\alpha_\perp$ and $\alpha_\parallel$ are the principal values of the tensor α_{ij} for hexagonal symmetry, and m_{ij} are the double-subscript components of the crystallite elastic compliance tensor M_{ijkl} in the principal axes of anisotropy. The quantity $\bar{\alpha} = (\bar{\alpha}_{ij})$ is determined by the expression

$$\bar{\alpha}_{ij} = \bar{\alpha}\delta_{ij}, \quad \bar{\alpha} = [2(d_{11}+d_{12}+d_{13})\alpha_\perp + (2d_{13}+d_{33})\alpha_\parallel][2d_{11} + 2d_{12} + 4d_{13} + d_{33}]^{-1}$$

Misprints executed in analogous expressions in /5/ have been corrected in the formulas presented.

One of the representatives of hexagonal polycrystals is zinc for which /6/ $m_{11} = 0.84$, $m_{12} = 0.05$, $m_{13} = -0.73$, $m_{33} = 2.84$, $m_{44} = 2.61 \times 10^{-8}$ m^2/kN, $\alpha_\perp = 12.6$, $\alpha_\parallel = 57.4 \times 10^{-6}$ $^\circ$K^{-1}. Calculations using (3.7) result in the following values for the thermal microstresses for zinc: $\Theta^{-1}\sigma_{11} = \Theta^{-1}\sigma_{22} = 326$ kN/m^2, $\Theta^{-1}\sigma_{33} = -655$ kN/m^2. These values differ substantially from the quantities 563 kN/m^2 and -477 kN/m^2 which are obtained by using a simpler model (one isolated grain in the matrix, possessing the mean elastic properties of the polycrystal, i.e., for $\bar{\alpha} = \langle\alpha\rangle_\omega$ in the notation of this paper).

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