THERMOELASTICITY CONSTANTS OF POLYCRYSTALS

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Exact formulas are derived for the thermoelasticity constants of macroscopically homogeneous polycrystals. A method described earlier [1] is used as the basis. It is assumed that the local parameters form an ergodic homogeneous random field. No restriction is imposed on the degree of anisotropy of the crystals.

1. The field of thermoelastic displacements $u_j(\mathbf{r})$ in an inhomogeneous elastic medium at equilibrium, in the absence of body forces, is determined by the system of equations of thermoelasticity [2]

$$\frac{\partial}{\partial x_k}\left(\lambda_{jklm}\frac{\partial u_l}{\partial x_m}\right)-\frac{\partial}{\partial x_k}(\beta_{jk}\theta)=0\,. \qquad (1.1)$$

Here, $\theta(\mathbf{r})$ is the temperature increment relative to some initial state; $\lambda_{jklm}(\mathbf{r})$ is the elasticity-constant tensor; $\beta_{jk}(\mathbf{r})$ is the thermoelasticity-constant tensor, which is linked to the thermal-expansion coefficient tensor α_{jk} by the relation $\beta_{jk}=\lambda_{jklm}\alpha_{lm}$. The convention of summation over the dummy indices is used in Eq. (1.1) and below; $\mathbf{r}=x_1, x_2, x_3$. In the case of a polycrystal,

$$\lambda_{jklm}=c_{j\alpha}c_{k\beta}c_{l\gamma}c_{m\delta}\mu_{\alpha\beta\gamma\delta}, \quad \beta_{jk}=c_{j\delta}c_{k\varepsilon}\gamma_{\delta\varepsilon}\,, \qquad (1.2)$$

where $\mu_{\alpha\beta\gamma\delta}$ and $\gamma_{\delta\varepsilon}$ are the components of the corresponding tensors in the crystallographic axes and $c_{j\alpha}$ is a matrix for transformation to the laboratory coordinate system. The tensor components, and also the displacements, stresses, etc., undergo discontinuities at the grain boundaries. Below, therefore, we shall treat the parameters that enter Eq. (1.1) and subsequent formulas as generalized functions. The final formulas will not contain operations on generalized functions.

Let the scales of inhomogeneity and correlation be small in comparison with the size of a polycrystal, and let its properties be statistically homogeneous. Then the polycrystal can be considered unbounded, and the elasticity constants $\lambda_{jklm}(\mathbf{r})$ and thermoelasticity constants $\beta_{jk}(\mathbf{r})$ can be considered as forming a homogeneous random field. In a macroscopically homogeneous stressed-strained state, the temperature, stress, and strain fields are also homogeneous (the displacements form a field with homogeneous increments). In this case, stochastic boundary conditions can be brought into agreement with Eq. (1.1) by requiring, for example, that the mathematical expectations of the strains be equal to specified constant values. Let us set up these conditions for the components of the displacement gradient

$$\langle \partial u_j/\partial x_k\rangle = p_{jk} \qquad (1.3)$$

(angular brackets indicate the operation of averaging). The macroscopic elasticity and thermoelasticity constants, which are denoted by λ^*_{jklm} and β^*_{jk}, are found from the condition of equality of the mathematical expectations of the thermoelastic stresses in a polycrystal and an equivalent homogeneous medium:

$$\left\langle\lambda_{jklm}\frac{\partial u_l}{\partial x_m}-\beta_{jk}\theta\right\rangle=\lambda^{*}_{jklm}\left\langle\frac{\partial u_l}{\partial x_m}\right\rangle-\beta^{*}_{jk}\langle\theta\rangle\,. \qquad (1.4)$$

The problem consists in finding a gradient du_j/dx_k that satisfies Eq. (1.1) and additional conditions (1.3) and in calculating the macroscopic constants λ^*_{jklm} and β^*_{jk} from (1.4).

We shall denote the mathematical expectations of the parameters by one prime and their fluctuational components by a double prime. For example,

$$\begin{gathered}\lambda'_{ijlm}=\lambda'_{jklm}+\lambda''_{jklm}, \quad \beta_{jk}=\beta'_{jk}+\beta''_{jk}\,;\\ \lambda'_{jklm}=\langle\lambda_{jklm}\rangle, \quad \beta'_{jk}=\langle\beta_{jk}\rangle\,.\end{gathered} \qquad (1.5)$$

We introduce Green's tensor $G_{jk}(\mathbf{r}, \mathbf{r}_1)$ for a homogeneous elastic medium with constant λ'_{jklm}. This tensor satisfies the equation

$$\lambda'_{jklm}\frac{\partial^2 G_{ln}(\mathbf{r}, \mathbf{r}_1)}{\partial x_k \partial x_m}=-\delta_{jn}\delta(\mathbf{r}-\mathbf{r}_1)\,,$$

where δ_{jn} is the Kronecker symbol and $\delta(\mathbf{r}-\mathbf{r}_1)$ is a three-dimensional delta function. Equation (1.1) and conditions (1.3) correspond to the system of equations

$$\begin{gathered}u_j(\mathbf{r})-\int G_{jl}(\mathbf{r}, \mathbf{r}_1)\frac{\partial}{\partial x_m}\Big[\lambda''_{lmnp}(\mathbf{r}_1)\frac{\partial u_n(\mathbf{r}_1)}{\partial x_p}-\\ -\beta''_{lm}(\mathbf{r}_1)\,\theta(\mathbf{r}_1)\Big]d\mathbf{r}_1=p_{jk}x_k\end{gathered} \qquad (1.6)$$

($d\mathbf{r}_1=dx_1, dx_2, dx_3$; integration is over the entire space). If we differentiate (1.6) term by term and transform the integral using the Gauss theorem, we arrive at a system of linear integral equations in the gradient du_j/dx_k:

$$\begin{gathered}\frac{\partial u_j(\mathbf{r})}{\partial x_k}-\int\frac{\partial^2 G_{jl}(\boldsymbol{\rho})}{\partial\xi_k\partial\xi_m}\Big[\lambda''_{lmnp}(\mathbf{r}+\boldsymbol{\rho})\frac{\partial u_n(\mathbf{r}+\boldsymbol{\rho})}{\partial\xi_p}-\\ -\beta''_{lm}(\mathbf{r}+\boldsymbol{\rho})\,\theta(\mathbf{r}+\boldsymbol{\rho})\Big]d\boldsymbol{\rho}=p_{jk}\\ \boldsymbol{\rho}=\xi_1, \xi_2, \xi_3, \ d\boldsymbol{\rho}=d\xi_1 d\xi_2 d\xi_3\,.\end{gathered} \qquad (1.7)$$

The macroscopic elasticity constants were determined in [1]. Therefore, we shall limit ourselves to determination of the macroscopic thermoelasticity constants, letting all $p_{jk}=0$. System (1.7) is solved by the iteration method:

$$\begin{gathered}\frac{\partial u_j(\mathbf{r})}{\partial x_k}=-\sum_{N=1}^{\infty}\int\cdots\int\frac{\partial^2 G_{jc_1}(\boldsymbol{\rho}_1)}{\partial\xi_k\partial\xi_{d_1}}\cdots\\ \cdots\frac{\partial^2 G_{a_N c_N}(\boldsymbol{\rho}_N)}{\partial\xi_{b_N}\partial\xi_{d_N}}\lambda''_{c_1 d_1 a_2 b_2}(\mathbf{r}+\boldsymbol{\rho}_1)\cdots\end{gathered}$$

$$\ldots \lambda''_{c_{N-1}d_{N-1}a_N b_N}(\mathbf{r} + \boldsymbol{\rho}_1 + \ldots +$$

$$+ \boldsymbol{\rho}_{N-1}) \beta''_{c_N d_N}(\mathbf{r} + \boldsymbol{\rho}_1 + \ldots + \boldsymbol{\rho}_N) \times$$

$$\times \theta(\mathbf{r} + \boldsymbol{\rho}_1 + \ldots + \boldsymbol{\rho}_N) d\boldsymbol{\rho}_1 \ldots d\boldsymbol{\rho}_N.$$

Let us substitute the result into the left side of (1.4):

$$\left\langle \lambda_{jklm} \frac{\partial u_l}{\partial x_m} - \beta_{jk}\theta \right\rangle = -\beta'_{jk}\langle\theta\rangle - \langle\beta''_{jk}\theta''\rangle -$$

$$- \sum_{N=1}^{\infty} \int \ldots \int \frac{\partial^2 G_{a_1 c_1}(\rho_1)}{\partial\xi_{b_1}\partial\xi_{d_1}} \ldots \frac{\partial^2 G_{a_N c_N}(\rho_N)}{\partial\xi_{b_N}\partial\xi_{d_N}} \langle \lambda''_{jka_1b_1}(0) \ldots$$

$$\lambda''_{c_{N-1}d_{N-1}a_N b_N}(\boldsymbol{\rho}_1 + \ldots +$$

$$+ \boldsymbol{\rho}_{N-1}) \beta''_{c_N d_N}(\boldsymbol{\rho}_1 + \ldots + \boldsymbol{\rho}_N) \theta(\boldsymbol{\rho}_1 + \ldots$$

$$\ldots + \boldsymbol{\rho}_N)\rangle d\boldsymbol{\rho}_1 \ldots d\boldsymbol{\rho}_N. \qquad (1.8)$$

The macroscopic thermoelasticity constants β^*_{jk} are equal to the right sides of formulas (1.8) with opposite sign divided by $\langle\theta\rangle$. Hence,

$$\beta_{jk}{}^* = \beta'_{jk} + \frac{1}{\langle\theta\rangle} \sum_{N=1}^{\infty} \int \ldots \int \frac{\partial^2 G_{a_1 c_1}(\rho_1)}{\partial\xi_{b_1}\partial\xi_{d_1}} \ldots \frac{\partial^2 G_{a_N c_N}(\rho_N)}{\partial\xi_{b_N}\partial\xi_{d_N}} \langle \lambda''_{jka_1b_1}(0) \ldots$$

$$\ldots \lambda''_{c_{N-1}d_{N-1}a_N b_N}(\boldsymbol{\rho}_1 + \ldots + \boldsymbol{\rho}_{N-1}) \times$$

$$\times \beta''_{c_N d_N}(\boldsymbol{\rho}_1 + \ldots + \boldsymbol{\rho}_N) \theta(\boldsymbol{\rho}_1 + \ldots$$

$$\ldots + \boldsymbol{\rho}_N)\rangle d\boldsymbol{\rho}_1 \ldots d\boldsymbol{\rho}_N + \frac{\langle\beta''_{jk}\theta''\rangle}{\langle\theta\rangle}. \qquad (1.9)$$

2. Thus, the macroscopic thermoelasticity constants are expressed in terms of the mixed moments of the local elasticity and thermoealsticity constants, and also in terms of the fluctuations of the temperature field (the latter are functions of the fluctuations of the thermal conductivity coefficients). For the state of thermodynamic equilibrium, θ = const. Formula (1.9) can be written as

$$\beta^*_{jk} = \beta'_{jk} + \langle\beta^{**}_{jk}\rangle \qquad (2.1)$$

where $\beta^{**}_{\mathrm{jk}}(\mathbf{r})$ is a solution of the system of linear integral equations

$$\beta^{**}_{jk}(\mathbf{r}) =$$

$$= \lambda''_{jkab}(\mathbf{r}) \int \frac{\partial^2 G_{ac}(\rho)}{\partial\xi_b\partial\xi_d} [\beta_{cd}{}^{**}(\mathbf{r} + \boldsymbol{\rho}) + \beta''_{cd}(\mathbf{r} + \boldsymbol{\rho})] d\boldsymbol{\rho}. \qquad (2.2)$$

Let us find a solution of system (2.2) for strongly isotropic polycrystals (in the sense of the definition introduced in [1]). For this case,

$$\lambda'_{jklm} = \lambda_0\delta_{jk}\delta_{lm} + \mu_0(\delta_{jl}\delta_{km} + \delta_{jm}\delta_{kl}),$$

$$\beta'_{jk} = \beta_0\delta_{jk}. \qquad (2.3)$$

where λ_0 and μ_0 are Lamé coefficients and β_0 is the coefficient of thermal expansion, which are found without allowance for correlation corrections. The expression for Green's tensor has the form

$$G_{jk}(\boldsymbol{\rho}) = \frac{1}{4\pi\mu_0}\left(\frac{\delta_{jk}}{\rho} - \frac{5}{2} g \frac{\partial^2\rho}{\partial\xi_j\partial\xi_k}\right)$$

$$\rho = |\mathbf{r} - \mathbf{r}_1| = (\xi_j\xi_j)^{1/2}, \quad g = \frac{1}{5}\frac{\lambda_0 + \mu_0}{\lambda_0 + 2\mu_0} = \frac{1}{10(1 - \nu_0)}. \qquad (2.4)$$

Here, g is a constant for the material.

The joint correlation functions for the elasticity and thermoelasticity constants, and also of the auxiliary values β^{**}_{jk} of a strongly isotropic medium are functions only of the absolute values of the distances between the points. Let

$$\langle \lambda''_{jka_1b_1}(\mathbf{r}) \ldots \lambda''_{c_{N-1}d_{N-1}a_N b_N}(\mathbf{r}) \beta''_{c_N d_N}(\mathbf{r} + \boldsymbol{\rho})\rangle =$$

$$= \varphi_{jka_1b_1\ldots c_N d_N}(\rho)$$

$$\langle \lambda''_{jka_1b_1}(\mathbf{r}) \ldots \lambda''_{c_{N-1}d_{N-1}a_N b_N}(\mathbf{r}) \beta^{**}_{c_N d_N}(\mathbf{r} + \boldsymbol{\rho})\rangle =$$

$$= \psi_{jka_1b_1\ldots c_N d_N}(\rho). \qquad (2.5)$$

In the new symbols, Eqs. (2.2) after averaging take the form

$$\langle\beta^{**}_{jk}\rangle = \int \frac{\partial^2 G_{ac}(\rho)}{\partial\xi_b\partial\xi_d} [\varphi_{jkabcd}(\rho) + \psi_{jkabcd}(\rho)] d\boldsymbol{\rho}. \qquad (2.6)$$

The method of solving Eqs. (2.2), which is based on recurrence formulas, is described in detail in [1]. The final result has the form

$$\beta_{jk}{}^* = \beta_0\delta_{jk} + \sum_{N=1}^{\infty} I_{jk}^{(N)}. \qquad (2.7)$$

The general term of series (2.7) is expressed in terms of the single-point mixed correlation tensors of the elasticity and thermoelasticity constants as follows:

$$I_{jk}^{(N)} = \left(-\frac{1}{3\mu_0}\right)^N \langle \lambda''_{jka_1b_1}\zeta_{a_1b_1a_2b_2}\lambda_{a_2b_2a_3b_3} \ldots$$

$$\ldots \zeta_{a_{2N-1}b_{2N-1}a_{2N}b_{2N}}\beta''_{a_{2N}b_{2N}}\rangle$$

$$\zeta_{abcd} = (1 - 2g)\delta_{ac}\delta_{bd} - g\delta_{ab}\delta_{cd}. \qquad (2.8)$$

Here, ζ_{abcd} is an isotropic tensor of rank four, which is a function of g, according to formula (2.4).

3. In the case of a strongly isotropic polycrystal, the tensors $\lambda_{\mathrm{jk}l\mathrm{m}}$ and β_{jk} are related to the components $\mu_{\mathrm{jk}l\mathrm{m}}$ and γ_{jk} in crystallographic coordinates by formulas (1.2). We introduce the symbols

$$\mu''_{jklm} = \mu_{jklm} - \lambda'_{jklm}, \qquad \gamma''_{jk} = \gamma_{jk} - \beta'_{jk}. \qquad (3.1)$$

Then, the fluctuational components of tensors $\lambda_{\mathrm{jk}l\mathrm{m}}$ and β_{jk} are determined by formulas similar to (1.2):

$$\lambda''_{jklm} = c_{j\alpha}c_{k\beta}c_{l\gamma}c_{m\delta}\mu''_{\alpha\beta\gamma\delta}, \qquad \beta''_{jk} = c_{j\delta}c_{k\varepsilon}\gamma''_{\delta\varepsilon}. \qquad (3.2)$$

Using expressions (3.2), let us calculate the mixed correlation tensors in formula (2.8):

$$\langle \lambda''_{jka_1b_1}\zeta_{a_1b_1a_2b_2}\lambda''_{a_2b_2a_3b_3} \ldots \zeta_{a_{2N-1}b_{2N-1}a_{2N}b_{2N}}\beta''_{a_{2N}b_{2N}}\rangle =$$

$$= \langle c_{j\alpha_1}c_{k\alpha_2}c_{a_1\alpha_3}c_{b_1\alpha_4}\zeta_{a_1b_1a_2b_2}c_{a_2\alpha_5}c_{b_2\alpha_6}c_{a_3\alpha_7}c_{b_2\alpha_8} \ldots$$

$$\ldots \zeta_{a_{2N-1}b_{2N-1}a_{2N}b_{2N}}c_{a_{2N}\alpha_{4N+1}}c_{b_{2N}\alpha_{4N+2}}\rangle \mu''_{\alpha_1\alpha_2\alpha_3\alpha_4}\mu''_{\alpha_5\alpha_6\alpha_7\alpha_8}$$

$$\ldots \gamma''_{\alpha_{4N+1}\alpha_{4N+2}}.$$

Noting that

$$c_{a_1\alpha_3}c_{b_1\alpha_4}\zeta_{a_1b_1a_2b_2}c_{a_2\alpha_5}c_{b_2\alpha_6} = \zeta_{\alpha_3\alpha_4\alpha_5\alpha_6}, \quad \langle c_{j\alpha_1}c_{k\alpha_2}\rangle = {}^1/{}_3\delta_{jk}\delta_{\alpha_1\alpha_2},$$

we bring formula (2.8) to the form

$$I_{jk}^{(N)} = {}^1/_3\delta_{jk}(-{}^1/_3\mu_0^{-1})^N \mu''_{\alpha_1\alpha_1\alpha_3\alpha_4}\zeta_{\alpha_3\alpha_4\alpha_5\alpha_6}\mu''_{\alpha_5\alpha_6\alpha_7\alpha_8}\cdots$$
$$\cdots\zeta_{\alpha_{4N-1}\alpha_{4N}\alpha_{4N+1}\alpha_{4N+2}}\gamma''_{\alpha_{4N+1}\alpha_{4N+2}}. \qquad (3.3)$$

Substituting formula (3.3) into (2.7), we find that $\beta^*_{jk} = \beta_*\delta_{jk}$. The macroscopic thermoelasticity coefficient β_* is determined by the formula

$$\beta_* = \beta_0 + \frac{1}{3}\sum_{N=1}^{\infty}\left(-\frac{1}{3\mu_0}\right)^N \mu''_{\alpha_1\alpha_1\alpha_3\alpha_4}\zeta_{\alpha_3\alpha_4\alpha_5\alpha_6}\mu''_{\alpha_5\alpha_6\alpha_7\alpha_8}\cdots$$
$$\cdots\zeta_{\alpha_{4N-1}\alpha_{4N}\alpha_{4N+1}\alpha_{4N+2}}\gamma''_{\alpha_{4N+1}\alpha_{4N+2}}. \qquad (3.4)$$

Let us calculate the sum of the series on the right-hand side. For this, we introduce the operator **A**, which converts the tensor of rank two $\mathbf{a} = a_{jk}$ into the tensor $\mathbf{b} = b_{jk}$ such that the equation $\mathbf{b} = \mathbf{Aa}$ is equivalent to the relation

$$b_{jk} = \mu_0^{-1}\mu''_{jkab}\zeta_{abcd}a_{cd}. \qquad (3.5)$$

With the aid of this operator, formula (3.4) can be represented as

$$\beta_* = \beta_0 - {}^1/_3\,\psi_{\alpha\alpha}, \qquad (3.6)$$

where the tensor $\psi = \psi_{\alpha\beta}$ is equal to the sum of the series

$$\psi = \sum_{N=1}^{\infty}\left(-\frac{1}{3}\right)^{N+1}\mathbf{A}^N\boldsymbol{\gamma}'' \qquad (3.7)$$

($\boldsymbol{\gamma}''$ is a tensor with components $\gamma_{\alpha\beta}''$). The right-hand side of formula (3.7) is a solution of the operator equation

$$\psi + {}^1/_3\mathbf{A}\psi = {}^1/_3\mathbf{A}\boldsymbol{\gamma}'' \qquad (3.8)$$

which represents a system of linear algebraic equations in the components $\psi_{\alpha\beta}$. The number of equations depends on the class of the structure (but does not exceed three). In the case of cubic crystals, all $\gamma_{\alpha\beta}'' = 0$, and, therefore, all $\psi_{\alpha\beta} = 0$. In this case, the correlation corrections for the averaged thermoelasticity constants vanish.

REFERENCES

1. V. V. Bolotin and V. N. Moskalenko, "Problem of determining elasticity constants of microheterogeneous media," PMTF [Journal of Applied Mechanics and Technical Physics], no. 1, 1968.

2. B. Boley and J. Weiner, Theory of Temperature Stresses [Russian translation], Izd-vo Mir, 1964.

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