MACROSCOPIC CHARACTERISTICS OF MICROINHOMOGENEOUS SOLIDS

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Abstract

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MACROSCOPIC CHARACTERISTICS OF MICROINHOMOGENEOUS SOLIDS

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In this note formulas are derived for the coefficients of thermal conductivity and diffusion, the elastic constants, and the coefficients of thermal expansion of macroscopically isotropic microinhomogeneous media. The usually imposed ([1–3]) restriction on the smallness of the microinhomogeneity is not made. It is assumed that the local characteristics form a continuous ergodic homogeneous random field. Final formulas are given for the case of strongly isotropic polycrystals. In this case the formulas turn out to be not much more complicated than the corresponding formulas of the Born approximation ([1–4]).

Consider the field of a scalar quantity $\theta(\mathbf{r})$ (temperature, concentration, etc.), which satisfies the equation

$$\frac{\partial}{\partial x_j}\left(\lambda_{jk}\frac{\partial\theta}{\partial x_k}\right)=0, \tag{1}$$

where λ_{jk} is a positive-definite symmetric tensor of the second rank (the tensor of local coefficients of thermal conductivity, diffusion coefficients, etc.). Let $\lambda_{jk}(\mathbf{r})$ form a continuous ergodic homogeneous random field, with

$$\lambda_{jk}=\overset{0}{\lambda}_{jk}+\varepsilon\overset{1}{\lambda}_{jk},$$

where

$$\overset{0}{\lambda}_{jk}=\langle\lambda_{jk}\rangle,$$

and ε is some positive (not necessarily small) number. Angular brackets denote the averaging operation. The solution of equation (1) with stochastic boundary conditions

$$\left\langle\frac{\partial\theta}{\partial x_k}\right\rangle=\overset{0}{p}_k \tag{2}$$

($\overset{0}{p}_k$ is the prescribed macroscopic gradient) is sought in the form of a field with homogeneous ergodic increments,

$$\theta = \overset{0}{p}_k x_k + \varepsilon\tilde{\theta}(\mathbf{r}).$$

The gradient of the random field

$$p_k = \partial\theta/\partial x_k$$

is found by the method of iterations. The macroscopic tensor for the equivalent homogeneous medium is introduced by the relation

$$\langle \lambda_{jk} p_k \rangle = \overset{*}{\lambda}_{jk} \overset{0}{p}_k$$

and is determined as follows:

$$\overset{*}{\lambda}_{jk} = \overset{0}{\lambda}_{jk} + \sum_{N=1}^{\infty} \varepsilon^{N+1} \int \cdots \int \frac{\partial^2 G(\vec{\rho}_1)}{\partial\xi_l^{(1)}\partial\xi_m^{(1)}} \cdots \frac{\partial^2 G(\vec{\rho}_N)}{\partial\xi_s^{(N)}\partial\xi_t^{(N)}} \times$$

$$\times \left\langle \overset{1}{\lambda}_{jl}(\mathbf{r}) \overset{1}{\lambda}_{mn}(\mathbf{r}+\vec{\rho}_1) \cdots \overset{1}{\lambda}_{tk}(\mathbf{r}+\vec{\rho}_1+\cdots+\vec{\rho}_N) \right\rangle d\vec{\rho}_1 \cdots d\vec{\rho}_N. \tag{4}$$

Here $G(\vec{\rho})$ is the Green' s function for a deterministic medium with tensor $\overset{0}{\lambda}_{jk}$, $\vec{\rho} = \mathbf{r}_1 - \mathbf{r}$.

Consider a polycrystal with strong isotropy. In this case

$$\overset{0}{\lambda}_{jk} = \lambda_0 \delta_{jk}, \qquad G(\rho) = (4\pi\lambda_0\rho)^{-1},$$

$$\overset{1}{\lambda}_{jk} = c_{ja} c_{k\beta} \mu_{a\beta}, \qquad \varepsilon\mu_{a\beta} = \mu_{a\beta} - \langle \lambda_{a\beta} \rangle,$$

where $\mu_{\alpha\beta}$ is the tensor of thermal conductivity (diffusion) of the crystallites in crystallographic coordinates, and $c_{j\alpha}$ is the transformation matrix for passing from the crystallographic coordinate system to the laboratory system. Calculations by formula (4) give $\lambda^*_{jk} = \lambda_* \delta_{jk}$, where

$$\lambda_* = \lambda_0 \left(1 - \sum_{\alpha=1}^{3} \frac{\varepsilon^2 \mu_\alpha^{1\,2}/9\lambda_0^2}{1 + \varepsilon\mu_\alpha^1/3\lambda_0} \right) \tag{5}$$

(μ^*_α are the principal values of the tensor $\mu^1_{\alpha\beta}$). The first approximation corresponding to formula (5) was found in paper (2), where the anisotropy of the crystallites was assumed to be very weak, and the parameter ε sufficiently small. In one of the limiting cases of strongly anisotropic crystallites, when $\mu_1 = \mu_2 = \mu_\perp$, $\mu_3 = \mu_\parallel$, $\mu_\perp/\mu_\parallel \to 0$, formula (5) gives $\lambda_* \to {}^2/_{15}\,\mu_\parallel$. At the same time, the first approximation, formally extended to this case, gives $\lambda_* \to {}^1/_9\,\mu_\parallel$.

Let us turn to the more complicated problem of determining the equivalent elastic constants of a microinhomogeneous medium. We solve the system of equations for the displacement vector

$$\frac{\partial}{\partial x_k}\left(\lambda_{jklm}\frac{\partial u_l}{\partial x_m}\right) = 0 \tag{6}$$

under stochastic boundary conditions

$$\langle \partial u_i/\partial x_m\rangle = p_{im}. \tag{7}$$

The macroscopic tensor of elastic constants λ^*_{jklm} for the equivalent homogeneous medium is introduced by means of the relation

$$\langle \lambda_{jklm}\partial u_l/\partial x_m\rangle = \lambda^*_{jklm} p_{lm}. \tag{8}$$

For a polycrystal $\lambda_{jklm} = c_{j\alpha}c_{k\beta}c_{l\gamma}c_{m\delta}\mu_{\alpha\beta\gamma\delta}$, where $\mu_{\alpha\beta\gamma\delta}$ is the tensor of the elastic constants of the crystallite in crystallographic coordinates. In the case of strong isotropy of the polycrystal, the solution of the stochastic problem (6) –(7), after rather laborious calculations, gives the following formulas relating the macroscopic Lamé coefficients λ_* and μ_* to the average Lamé coefficients λ_0 and μ_0:

$$\lambda_* = \lambda_0 - \frac{\varepsilon}{15}(2\chi_{\alpha\alpha\beta\beta} - \chi_{\alpha\beta\alpha\beta}), \qquad \mu_* = \mu_0 - \frac{\varepsilon}{30}(3\chi_{\alpha\beta\alpha\beta} - \chi_{\alpha\alpha\beta\beta}). \tag{9}$$

Here $\vec{\chi} = \chi_{jklm}$ is a tensor whose components are found from the solution of the system of linear algebraic equations

$$\vec{\chi} + {}^1/_\varepsilon\, L\vec{\chi} = {}^1/_\varepsilon\, L\vec{\mu}. \tag{10}$$

By L is denoted a linear operator which transforms a tensor a of rank not lower than two into a tensor a' with components

$$a'_{jk\dots} = \frac{1}{\mu_0}\left[(1-2g)\mu^1_{jkst}a_{st\dots} - g\mu^1_{jkss}a_{tt\dots}\right], \tag{11}$$

$$g = \frac{1}{5}\frac{\lambda_0 + \mu_0}{\lambda_0 + 2\mu_0} = \frac{1}{10(1-\nu_0)}, \qquad \varepsilon\mu^1_{jklm} = \mu_{jklm} - \langle\lambda_{jklm}\rangle$$

(ν_0 is the Poisson coefficient corresponding to the average Lamé coefficients μ_0 and λ_0). The first approximation corresponding to formulas (9)–(11) was computed in papers (1, 3). Macroscopic ···

···the thermoelastic constants $\beta^*_{jk} = \beta_* \delta_{jk}$ (the temperature field is assumed uniform)

$$\beta_* = \beta_0 - \frac{\varepsilon}{3}\psi_{\alpha\alpha}.$$

The components of the tensor $\psi_{\alpha\beta}$ are determined from a system of equations of type (10)

$$\vec{\psi} + \frac{1}{3}\varepsilon \overset{1}{L}\vec{\psi} = \frac{1}{3}\varepsilon \overset{1}{L}\vec{\gamma},$$

where the tensor γ_{jk} is expressed in terms of the tensor of thermoelastic constants in crystallographic coordinates γ_{jk} as follows:

$$\varepsilon\gamma_{jk} = \gamma_{jk} - \langle\gamma_{jk}\rangle.$$

Fig. 1

The proposed method for calculating macroscopic coefficients can be applied to other, more complex media. Of particular interest is the prediction of the macroscopic behavior of elastoplastic polycrystals. Until now, in this field use has mainly been made of an approximate method [5], analogous to the self-consistent-field method in quantum mechanics and consisting in matching the interaction of a single crystallite with an averaged field. The exact formulas obtained here make it possible to estimate the error of the self-consistent-field method (as well as of other approximate methods). We restrict ourselves to the problem of stationary heat conduction in a polycrystalline homogeneous medium polarized in some plane. A comparison of the ratio of the macroscopic coefficient of thermal conductivity to one of the principal values of this coefficient for an individual crystal is carried out in Fig. 1. Curve 1 corresponds to the exact solution, curve 2 to the assumption of constancy of the temperature gradient in the polycrystal (Voigt approximation), and curve 3 to the assumption of constancy of the heat fluxes (Reuss approximation). The first approximation by the small-parameter method (Born approximation) gives curve 4. Finally, curve 5 corresponds to the self-consistent-field method. As should have been expected, the exact solution lies within the "fork" formed by the Voigt and Reuss approximations. The Born approximation and the self-consistent-field method give satisfactory results even for fairly strong anisotropy of the crystallites. The range of applicability of these approximate methods proves to be wider than heuristic considerations would suggest.

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Note: Figure translations are in progress. See original paper for figures.