

THE MACROSCOPIC COEFFICIENTS OF THERMAL CONDUCTIVITY AND DIFFUSION IN MICROINHOMOGENEOUS SOLIDS

V. V. Bolotin and V. N. Moskalenko

Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, Vol. 8, No. 6, pp. 7-13, 1967

A method is given for calculating the macroscopic coefficients of thermal conductivity and diffusion for microinhomogeneous solids whose local coefficients of thermal conductivity (or diffusion) form an ergodic homogeneous stray field. In the case of marked isotropy of the field of the local coefficients, the calculations are taken to a conclusion. The final formulas for the structure are not much more complicated than the corresponding first-approximation formulas. The results of calculations for certain other cases are also given. The effect of anisotropy of the crystallites in polycrystalline material on the coefficients of thermal conductivity and diffusion is discussed.

One of the main problems in the mechanics of microinhomogeneous bodies is the determination of the macroscopic constants from the corresponding microscopic characteristics. The assumption regarding the small inhomogeneity used by a number of authors [1, 2] is not applicable in the case of isotropic polycrystalline aggregates consisting of substantially anisotropic crystallites, stochastic reinforced media, etc. The so-called self-consistent field method [3] opens up some interesting prospects, but this method is an approximate one and its errors have not yet been assessed. Nevertheless, by making certain fairly general assumptions about the correlation properties of the inhomogeneity, it is possible to obtain final accurate formulas for such macroscopic properties of the solids as the coefficients of thermal conductivity, diffusion, elasticity, and thermal expansion. Below we consider some of the simplest problems involved in determining the macroscopic constants which form a second-order tensor and which characterize the distribution of a certain scalar quantity in a microinhomogeneous body.

1. Let the scalar quantity  $\theta(\mathbf{r})$ , where  $\mathbf{r} = (x_1, x_2, x_3)$ , satisfy

$$\frac{\partial}{\partial x_j} \left( \lambda_{jk} \frac{\partial \theta}{\partial x_k} \right) = 0 \tag{1.1}$$

(here and subsequently agreement about summation with respect to "dummy" indices is used.) A certain symmetrical positively defined second-order tensor is determined by the coefficients  $\lambda_{jk}$  at each point in the field. Equation (1.1) can represent the stationary temperature distribution in a solid, the stationary concentration distribution, etc. Correspondingly the tensor field  $\lambda_{jk}(\mathbf{r})$  will represent the distribution of the local coefficients of thermal conductivity, diffusion, etc. In order to be specific, we will treat Eq. (1.1) as the equation of heat conduction in a solid under stationary conditions.

We consider Eq. (1.1) under the assumption that the body has an inhomogeneous microstructure and hence that the thermal-conductivity coefficients  $\lambda_{jk}(\mathbf{r})$  form a stray field. The dimensions of the body are such that, in comparison with the scales of the inhomogeneity and the correlation, it can be regarded as limitless. The field  $\lambda_{jk}(\mathbf{r})$  is assumed homogeneous and ergodic. We consider a medium consisting of crystallites of one kind. Let  $\mu_{jk}$  be the thermal-conductivity tensor for a crystallite referred to the crystallographic axes. This tensor is assumed to be deter-

minate and equal at all points in the field. Transferring to the laboratory coordinate system, we obtain

$$\lambda_{jk} = c_{j\alpha} c_{k\beta} \mu_{\alpha\beta}, \tag{1.2}$$

where  $c_{j\alpha}$  is the transform matrix of the coordinates. We now write  $\lambda_{jk}$  and  $\mu_{jk}$  as

$$\lambda_{jk} = \lambda_{jk}' + \lambda_{jk}'', \quad \mu_{jk} = \mu_{jk}' + \mu_{jk}'', \tag{1.3}$$

where  $\lambda_{jk}' = \mu_{jk}' = \langle \lambda_{jk} \rangle$  are the mathematical expectations of the tensors (here and subsequently the averaging operation will be denoted by angle brackets), and  $\lambda_{jk}''$  and  $\mu_{jk}''$  are the fluctuating components. In [2] it was assumed that  $\lambda_{jk}'' \sim \epsilon \lambda_{jk}'$ , where  $\epsilon$  is a small number. In the present paper no assumption is made regarding the smallness of the fluctuating components.

Let us formulate the boundary conditions corresponding to Eq. (1.1). Since the body is assumed to be unlimited and the field  $\lambda_{jk}(\mathbf{r})$  homogeneous, it is natural to adopt the stochastic boundary conditions, which require that the mathematical expectations of the temperature should be equal to the given values at all points. In the case of a constant temperature gradient throughout the volume, we obtain the condition

$$\langle \partial \theta / \partial x_j \rangle = p_j, \tag{1.4}$$

where  $p_j$  is the given vector. Our problem reduces to find a field  $\theta(\mathbf{r})$  satisfying Eq. (1.1) and conditions (1.4) and to calculate the equivalent thermal-conductivity tensor for a homogeneous body (the macroscopic thermal-conductivity tensor). This tensor is naturally introduced by the condition of equality between the mathematical expectation of the heat flow in a microinhomogeneous body and the heat flow in the equivalent homogeneous body.

$$\langle \lambda_{jk} \partial \theta / \partial x_k \rangle = \lambda_{jk}^* p_k. \tag{1.5}$$

Equation (1.1) and condition (1.4) are equivalent to the integrodifferential equation

$$\theta(\mathbf{r}) - \int G(\mathbf{r}, \mathbf{r}_1) \frac{\partial}{\partial x_j} \left[ \lambda_{ji}(\mathbf{r}_1) \frac{\partial \theta(\mathbf{r}_1)}{\partial x_i} \right] d\mathbf{r}_1 = p_j x_j, \tag{1.6}$$

where  $d\mathbf{r}_1 = dx_1 dx_2 dx_3$ , and  $G(\mathbf{r}, \mathbf{r}_1)$  is the Green's function of the stationary heat conduction equation in a homogeneous medium with the tensor  $\lambda_{jk}'$

$$\lambda_{jk}' \partial^2 G(\mathbf{r}, \mathbf{r}_1) / \partial x_j \partial x_k = -\delta(\mathbf{r} - \mathbf{r}_1). \tag{1.7}$$

If  $\lambda_{jk}''(\mathbf{r})$  is a homogeneous ergodic field,  $\theta(\mathbf{r})$  forms a stray field with uniform ergodic increments. For convenience we transfer from Eq. (1.7) to the equivalent integrodifferential equation for the gradient

$\partial\theta/\partial x_j$ . Differentiating (1.7) term by term, using the fact that  $G(\mathbf{r}, \mathbf{r}_1) = G(\rho)$ , where  $\rho = \mathbf{r}_1 - \mathbf{r}$ , and integrating by parts, we obtain

$$\frac{\partial\theta}{\partial x_j} = \int \frac{\partial^2 G(\rho)}{\partial \xi_j \partial \xi_k} \left[ \lambda_{ki}''(\mathbf{r} + \rho) \frac{\partial\theta(\mathbf{r} + \rho)}{\partial \xi_i} \right] d\rho = p_j. \quad (1.8)$$

Here  $\xi_j = x_{j1} - x_j$ ,  $d\rho = d\xi_1 d\xi_2 d\xi_3$ . Equation (1.8) is solved by iteration

$$\begin{aligned} \frac{\partial\theta(\mathbf{r})}{\partial x_j} &= p_j + p_k \sum_{N=1}^{\infty} \int \dots \int \frac{\partial^2 G(\rho_1)}{\partial \xi_{j1} \partial \xi_{k1}} \dots \\ &\dots \frac{\partial^2 G(\rho_N)}{\partial \xi_{\alpha N} \partial \xi_{\beta N}} \lambda_{\beta_1 \alpha_2}''(\mathbf{r} + \rho_1) \dots \\ &\dots \lambda_{\beta N k}''(\mathbf{r} + \rho_1 + \dots + \rho_N) d\rho_1 \dots d\rho_N. \end{aligned} \quad (1.9)$$

For the mathematical expectations of the heat flows we obtain

$$\begin{aligned} \langle \lambda_{jk} \frac{\partial\theta}{\partial x_k} \rangle &= \lambda_{jk}' p_k + p_l \sum_{N=1}^{\infty} \int \dots \int \frac{\partial^2 G(\rho_1)}{\partial \xi_{\alpha_1} \partial \xi_{\beta_1}} \dots \\ &\dots \frac{\partial^2 G(\rho_N)}{\partial \xi_{\alpha N} \partial \xi_{\beta N}} \langle \lambda_{j\alpha_1}''(0) \lambda_{\beta_1 \alpha_2}''(\rho_1) \dots \\ &\dots \lambda_{\beta N l}''(\rho_1 + \dots + \rho_N) \rangle d\rho_1 \dots d\rho_N. \end{aligned}$$

From this by determining (1.5) we find the tensor of the macroscopic thermal-conductivity coefficients

$$\begin{aligned} \lambda_{jk}^* &= \lambda_{jk}' + \sum_{N=1}^{\infty} \int \dots \int \frac{\partial^2 G(\rho_1)}{\partial \xi_{\alpha_1} \partial \xi_{\beta_1}} \dots \\ &\dots \frac{\partial^2 G(\rho_N)}{\partial \xi_{\alpha N} \partial \xi_{\beta N}} \langle \lambda_{j\alpha_1}''(0) \lambda_{\beta_1 \alpha_2}''(\rho_1) \dots \\ &\dots \lambda_{\beta N k}''(\rho_1 + \dots + \rho_N) \rangle d\rho_1 \dots d\rho_N. \end{aligned} \quad (1.10)$$

Keeping only one term of the series ( $N = 1$ ) in Eq. (1.10) corresponds to the Born approximation [1, 2]. The problem is to calculate the general term of the series (1.10) for the most general properties of the tensors  $\lambda_{jk}'$  and  $\lambda_{jk}''$ , and to carry out the actual summation. Equation (1.10) can also be expressed in the form

$$\lambda_{jk}^* = \lambda_{jk}' + \langle \lambda_{jk}^{**} \rangle. \quad (1.11)$$

The tensor  $\lambda_{jk}^{**}$  is the solution of the integral equation

$$\begin{aligned} \lambda_{jk}^{**}(\mathbf{r}) &= \lambda_{j\alpha}''(\mathbf{r}) \int \frac{\partial^2 G(\rho)}{\partial \xi_{\alpha} \partial \xi_{\beta}} [\lambda_{\beta k}^{**}(\mathbf{r} + \rho) + \\ &+ \lambda_{\beta k}''(\mathbf{r} + \rho)] d\rho. \end{aligned} \quad (1.12)$$

The application of the iteration method of Eq. (1.12) again leads to (1.10).

2. Let the field of the coefficients  $\lambda_{jk}(\mathbf{r})$  be markedly isotropic in the sense that the correlation functions of the tensors  $\lambda_{jk}(\mathbf{r})$  and  $\lambda_{jk}''(\mathbf{r})$  from an isotropic tensor field. This limitation is more rigid than the isotropy requirement for the correlation functions of  $\lambda_{jk}(\mathbf{r})$ . A polycrystalline aggregate whose constants satisfy the condition of marked isotropy will be described as markedly isotropic. For such a polycrystal

line aggregate  $\lambda_{jk}' = \lambda_0 \delta_{jk}$ , where  $\lambda_0$  is the mathematical expectation of the thermal-conductivity coefficient,

$$G(\rho) = (4\pi\lambda_0\rho)^{-1}, \quad \rho = (\xi_j^2)^{1/2}. \quad (2.1)$$

In this case the correlation tensors

$$\begin{aligned} \langle \lambda_{j\alpha_1}''(\mathbf{r}) \dots \lambda_{\beta_{N-1} \alpha_N}''(\mathbf{r}) \lambda_{\beta N k}''(\mathbf{r} + \rho) \rangle &= \Psi_{j\alpha_1 \dots \beta N k} \\ \langle \lambda_{j\alpha_1}''(\mathbf{r}) \dots \lambda_{\beta_{N-1} \alpha_N}''(\mathbf{r}) \lambda_{\beta N k}^{**}(\mathbf{r} + \rho) \rangle &= \Psi_{j\alpha_1 \dots \beta N k} \end{aligned} \quad (2.2)$$

depend only on the distance  $\rho = (\xi_j^2)^{1/2}$  between the points.

The mathematical expectation of the tensor  $\lambda_{jk}^{**}$  is calculated with Eq. (1.12)

$$\langle \lambda_{jk}^{**} \rangle = \int \frac{\partial^2 G(\rho)}{\partial \xi_{\alpha} \partial \xi_{\beta}} [\Psi_{j\alpha\beta k}(\rho) + \Psi_{j\alpha\beta k}(\rho)] d\rho.$$

Noting that

$$\frac{\partial^2 G(\rho)}{\partial \xi_{\alpha} \partial \xi_{\beta}} = -\frac{1}{3\lambda_0} \delta_{\alpha\beta} \delta(\rho) + \frac{1}{4\pi\lambda_0} \left( \frac{3\xi_{\alpha} \xi_{\beta}}{\rho^5} - \frac{\delta_{\alpha\beta}}{\rho^3} \right)$$

and integrating with respect to the spherical coordinates  $\rho$ ,  $\varphi$ ,  $\theta$ , we find

$$\begin{aligned} \langle \lambda_{jk}^{**} \rangle &= -\frac{1}{3\lambda_0} [\Psi_{j\alpha\alpha k}(0) + \Psi_{j\alpha\alpha k}(0)] + \\ &+ \frac{1}{4\pi\lambda_0} \int_0^{\infty} \int_0^{2\pi} \int_0^{\pi} [\Psi_{j\alpha\beta k}(\rho) + \\ &+ \Psi_{j\alpha\beta k}(\rho)] \left( \frac{3\xi_{\alpha} \xi_{\beta}}{\rho^3} - \frac{\delta_{\alpha\beta}}{\rho} \right) \sin\theta d\rho d\varphi d\theta. \end{aligned}$$

Integrating over the sphere  $\rho = \text{const}$ , the integral vanishes. Thus

$$\langle \lambda_{jk}^{**} \rangle = -1/3\lambda_0^{-1} [\Psi_{j\alpha\alpha k}(0) + \Psi_{j\alpha\alpha k}(0)].$$

Repeating the procedure and taking into account Eq. (1.10), we finally obtain

$$\begin{aligned} \lambda_{jk}^* &= \lambda_0 \delta_{jk} + \sum_{N=1}^{\infty} I_{jk}^{(N)}, \\ I_{jk}^{(N)} &= \left( -\frac{1}{3\lambda_0} \right)^N \langle \lambda_{j\alpha_1}'' \lambda_{\alpha_1 \alpha_2}'' \dots \lambda_{\alpha_N k}'' \rangle. \end{aligned} \quad (2.3)$$

We now express (2.3) in terms of  $\mu_{jk}$ . Let  $\mu_{jk}''$  be the fluctuating part of this tensor. Using relationships of the (1.2) type, the single-point correlation tensor in (2.3) becomes

$$\begin{aligned} \langle \lambda_{j\alpha_1}'' \lambda_{\beta_1 \alpha_2}'' \dots \lambda_{\beta_N k}'' \rangle &= \\ &= \langle c_{j\gamma_1} c_{\alpha_1 \gamma_2} \dots c_{\beta_N \gamma_{2N+1}} c_{k \gamma_{2N+2}} \rangle \mu_{\gamma_1 \gamma_2}'' \dots \mu_{\gamma_{2N+1} \gamma_{2N+2}}'' \end{aligned}$$

By contracting the tensor, as indicated in Eq. (2.3), and bearing in mind that

$$c_{\alpha\gamma_1} c_{\alpha\gamma_2} = \delta_{\gamma_1 \gamma_2}, \quad \langle c_{(\alpha) \gamma_1} c_{(\alpha) \gamma_2} \rangle = 1/3 \delta_{\gamma_1 \gamma_2}$$

we obtain

$$\langle \lambda_{j\alpha_1}'' \lambda_{\alpha_1 \alpha_2}'' \dots \lambda_{\alpha_N k}'' \rangle = \frac{1}{3} \delta_{jk} \sum_{\alpha=1}^3 (\mu_{\alpha}'' )^{N+1}. \quad (2.4)$$

Here  $\mu_{\alpha}''$  are the principal values of the tensor  $\mu_{\alpha\beta}''$  (here and subsequently the rule of summation with respect to dummy indices is not extended to the index

a). With (2.3) and (2.4) Eq. (1.10) takes the form  $\lambda_{jk}^* = \lambda_* \delta_{jk}$ , where

$$\frac{\lambda_*}{\lambda_0} = 1 - \sum_{N=2}^{\infty} \sum_{a=1}^3 \left( -\frac{\mu_a''}{3\lambda_0} \right)^N. \quad (2.5)$$

The right-hand side consists of a converging series. It can easily be verified that the sum of the series (2.5) is

$$\frac{\lambda_*}{\lambda_0} = 1 - \sum_{a=1}^3 \left( \frac{\mu_a''}{3\lambda_0} \right)^2 \left( 1 + \frac{\mu_a''}{3\lambda_0} \right)^{-1}. \quad (2.6)$$

3. Equation (2.6) gives an accurate value of the macroscopic thermal-conductivity coefficient for a microinhomogeneous body with marked isotropy, and we use it to evaluate the various approximate methods. If the crystallites are slightly anisotropic, the polycrystalline aggregate will have little inhomogeneity. This case has been discussed in [2]. To obtain a formula corresponding to the assumptions in [2], we replace  $\mu_{\alpha}''$  by  $\varepsilon \mu_{\alpha}'$ , where  $\varepsilon$  is the smallness parameter, and we expand the right-hand side of Eq. (2.6) in a series in powers of  $\varepsilon$ . Retaining terms  $\varepsilon^2$ , we find

$$\frac{\lambda_*}{\lambda_0} \approx 1 - \frac{\varepsilon^2}{9\lambda_0^2} \sum_{a=1}^3 (\mu_a'')^2. \quad (3.1)$$

Let the crystallite have one axis of symmetry, for example. We denote the principal values of the tensor  $\mu_{ijk}$  by  $\mu_1 = \mu_2 = \mu_{\perp}$ ,  $\mu_3 = \mu_{\parallel}$ . Then

$$\begin{aligned} \lambda_0 &= 2/3 \mu_{\perp} + 1/3 \mu_{\parallel}, \quad \mu_1'' = \mu_2'' = -1/3 (\mu_{\parallel} - \mu_{\perp}), \\ \mu_3'' &= 2/3 (\mu_{\parallel} - \mu_{\perp}). \end{aligned} \quad (3.2)$$

The exact formula (2.6) takes the form

$$\frac{\lambda_*}{\lambda_0} = 1 - \frac{4p^2}{3(3+2p)} - \frac{2p^2}{3(3-p)} \quad \left( p = \frac{\mu_{\parallel} - \mu_{\perp}}{\mu_{\parallel} + 2\mu_{\perp}} \right). \quad (3.3)$$

For the case (3.2) Eq. (3.1) has the form (assuming  $\varepsilon = 1$ )

$$\lambda_* / \lambda_0 = 1 - 2/3 p^2. \quad (3.4)$$

For small values of  $p$  (i.e. for  $\mu_{\parallel} \approx \mu_{\perp}$ ) Eqs. (3.3) and (3.4) give similar results. For  $p \rightarrow 1$  (i.e. for  $\mu_{\perp} / \mu_{\parallel} \rightarrow 0$ ), Eq. (3.3) gives  $\lambda_* \rightarrow 2\lambda_0/5$ . Expressions (3.4), formally extended to the case of large inhomogeneities, gives  $\lambda_* \rightarrow \lambda_0/3$ . In the opposite case ( $\mu_{\parallel} / \mu_{\perp} \rightarrow 0$ ),

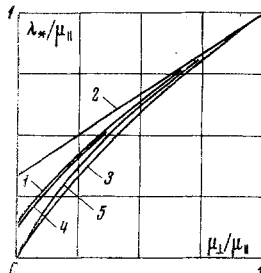


Fig. 1

we have  $p \rightarrow -1/2$ . Then according to Eq. (3.3)  $\lambda_* \rightarrow 11\lambda_0/14$  and according to Eq. (3.4)  $\lambda_* \rightarrow 5\lambda_0/6$ . The graph of the dependence of

$\lambda_*/\mu_{\parallel}$  on  $\mu_{\perp}/\mu_{\parallel}$  is given in Fig. 1, while Fig. 2 shows the dependence of  $\lambda_*/\mu_{\perp}$  on  $\mu_{\parallel}/\mu_{\perp}$ . Curve 1 corresponds to the exact formula (3.3) and curve 4 to formula (3.4). For the sake of completeness we have plotted on the graph curves 2 and 3 corresponding to the approximate values of  $\lambda_*$  obtained by simple averaging of the coefficients of thermal conductivity (curve 2) and thermal resistance (curve 3). As can be seen from the graph, the first (Born) approximation gives satisfactory results in the case of large inhomogeneities too. Let, for example,  $\mu_{\perp} = \mu_{\parallel} / 2$ . Then  $p = 1/4$  and the difference between Eqs. (3.3) and (3.4) is 0.3%.

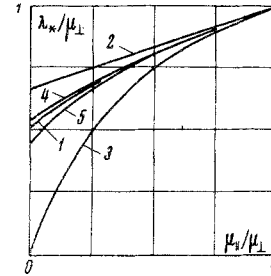


Fig. 2

We will estimate the error of the self-consistent field method for this problem. Following this method, we consider the problem of the stationary heat conduction in an isotropic expanse containing an anisotropic inclusion in the form of a spherical crystallite of radius  $R$ . On the assumption that the tensor of the thermal-conductivity coefficients of the isotropic medium coincides with the tensor of the macroscopic thermal-conductivity coefficients  $\lambda_{jk}^* = \lambda_* \delta_{jk}$ , we obtain it from the condition that the temperature gradient averaged over the volume of the crystallite and the set of realizations coincides with the mathematical expectation of the temperature gradient in the polycrystalline aggregate. Let

$$\begin{aligned} \lambda_{jk} &= \lambda_{jk}^* + \lambda_{jk}^{**}, \\ \lambda_{jk}^* &= \lambda_* \delta_{jk}, \quad \mu_{jk} = \lambda_* \delta_{jk} + \mu_{jk}^{**} \end{aligned}$$

Then to determine the temperature gradient we obtain an integral equation of type (1.8)

$$\frac{\partial \theta(\mathbf{r})}{\partial x_j} - \int \frac{\partial^2 G(\rho - \mathbf{r})}{\partial \xi_j \partial \xi_k} \lambda_{kl}^{**}(\rho) \frac{\partial \theta}{\partial \xi_l} d\rho = p_j. \quad (3.5)$$

Bearing in mind that for the model adopted

$$\begin{aligned} \lambda_{jk}^{**} &\equiv 0 \quad \text{for } |\mathbf{r}| > R \\ \lambda_{jk}^{**}(\mathbf{r}) &= c_{j\alpha} c_{k\beta} \mu_{\alpha\beta}^{**} = \text{const} \quad \text{for } |\mathbf{r}| \leq R \end{aligned}$$

we transform Eq. (3.5) into

$$\frac{\partial \theta(\mathbf{r})}{\partial x_j} - c_{k\alpha} c_{l\beta} \mu_{\alpha\beta}^{**} \int_{|\rho| \leq R} \frac{\partial^2 G(\rho - \mathbf{r})}{\partial \xi_j \partial \xi_k} \frac{\partial \theta(\rho)}{\partial \xi_l} d\rho = p_j. \quad (3.6)$$

Let us average the temperature gradient over the volume of the crystallite. For this purpose we integrate Eq. (3.6) with respect to the volume  $|\mathbf{r}| \leq R$

$$\begin{aligned} p_j^0 &= c_{k\alpha} c_{l\beta} \mu_{\alpha\beta}^{**} \frac{1}{V} \int_{|\mathbf{r}| \leq R} d\mathbf{r} \times \\ &\times \int_{|\rho| \leq R} \frac{\partial^2 G(\rho - \mathbf{r})}{\partial \xi_j \partial \xi_k} \frac{\partial \theta(\rho)}{\partial \xi_l} d\rho = p_j \end{aligned}$$

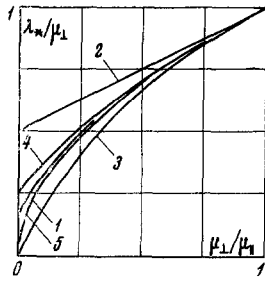


Fig. 3

By altering the order of integration and differentiation, we transform it into

$$p_j^0 = c_{k\alpha} c_{l\beta} \mu_{\alpha\beta}^{**} \frac{1}{V} \int_{|\rho| \leq R} \frac{\partial \theta(\rho)}{\partial \xi_l} \frac{\partial^2}{\partial \xi_j \partial \xi_k} \times \\ \times \left[ \int_{|\mathbf{r}| \leq R} G(\rho - \mathbf{r}) d\mathbf{r} \right] d\rho = p_j.$$

Considering that

$$\int_{|\mathbf{r}| \leq R} G(\rho - \mathbf{r}) d\mathbf{r} = \frac{1}{2\lambda_*} \left( R^2 - \frac{1}{3} \rho^2 \right)$$

and differentiating, we find for the temperature gradient  $p_j^0$  averaged over the volume of the crystallite

$$(2\lambda_*^* \delta_{jk} + c_{j\alpha} c_{k\beta} \mu_{\alpha\beta}) p_k^0 = 3\lambda_* p_j \quad (3.7)$$

The determinant of Eq. (3.7) is independent of the direction cosines and equals

$$D = 8\lambda_*^3 + 4\lambda_* (\mu_1 + \mu_2 + \mu_3) + \\ + 2\lambda_*^2 (\mu_1 \mu_2 + \mu_2 \mu_3 + \mu_3 \mu_1) + \mu_1 \mu_2 \mu_3.$$

From Eq. (3.7) and the condition  $\langle p_i^0 \rangle = p_i$  we obtain an equation for the effective thermal-conductivity coefficient

$$4\lambda_*^2 - \frac{1}{3} \lambda_* [6(\mu_1 \mu_2 + \mu_2 \mu_3 + \mu_3 \mu_1) - \\ - (\mu_1^2 + \mu_2^2 + \mu_3^2)] - \mu_1 \mu_2 \mu_3 = 0. \quad (3.8)$$

For  $\mu_1 \mu_2 \mu_3 \neq 0$ , this equation has only one real positive root. This follows from the fact that the sum of the three roots is zero, while their product is positive. The results of the calculations for the case  $\mu_1 = \mu_2 = \mu_{\perp}$ ,  $\mu_3 = \mu_{\parallel}$  are given in Figs. 1 and 2, curve 5. These graphs show that the self-consistent field method gives good results even with very substantial anisotropy of the crystallites.

4. The calculations can be continued to the end in certain other cases. Let us consider, for example, the field  $\lambda_{jk}(\mathbf{r})$  having the following properties; in the  $x_1, x_2$  plane it is markedly isotropic in the sense of the definition given in section 2, while the  $x_3$ -axis is the principal axis of the tensor  $\lambda_{jk}$  at each point, the component  $\lambda_{33}$  being determined. Certain disordered reinforced glass-like plastics obtained by pressing belong to this type. We will restrict ourselves to the determination of the macroscopic thermal-conductivity coefficients in the  $x_1, x_2$  plane. In this case we arrive at the plane problem

for Eq. (1.1) with conditions (1.4) and the Green's functions

$$G(\rho) = (2\pi\lambda_0)^{-1} \ln \rho, \quad \rho = (\xi_j^2)^{1/2} \quad (j=1, 2). \quad (4.1)$$

Equations (1.11) and (2.2) remain in force. Polar coordinates are used to calculate the tensors  $I_{jk}^{(N)}$ . The calculations lead to a formula similar to (2.3)

$$I_{jk}^{(N)} = \left( -\frac{1}{2\lambda_0} \right)^N \langle \lambda_{j\alpha_1}'' \lambda_{\alpha_1 \alpha_2}'' \dots \lambda_{\alpha_N k}'' \rangle.$$

By using a formula of type (1.2) and bearing in mind that for the plane problem

$$\langle c_{(\alpha)\gamma_1} c_{(\alpha)\gamma_2} \rangle = \frac{1}{2} \delta_{\gamma_1 \gamma_2}$$

(not summing with respect to  $\alpha$ ) we obtain

$$\langle \lambda_{j\alpha_1}'' \lambda_{\alpha_1 \alpha_2}'' \dots \lambda_{\alpha_N k}'' \rangle = \frac{1}{2} \delta_{jk} \sum_{\alpha=1}^2 (\mu_{\alpha}'' )^{N+1}.$$

Whence, after returning to (1.11), we find that  $\lambda_{jk}^* = \lambda_* \delta_{jk}$ , where

$$\frac{\lambda_*}{\lambda_0} = 1 - \sum_{N=2}^{\infty} \left( -\frac{1}{2\lambda_0} \right)^N \sum_{\alpha=1}^2 (\mu_{\alpha}'' )^N. \quad (4.2)$$

The sum in Eq. (4.2) is easily calculated and, since  $\mu_1'' = -\mu_2''$  is

$$\lambda_* / \lambda_0 = 1 - (\mu_1'' / 2\lambda_0)^2 [1 + (\mu_1'' / 2\lambda_0)^2]^{-1}. \quad (4.3)$$

It is not difficult to calculate the corresponding first (Born) approximation

$$\lambda_* / \lambda_0 = 1 - (\mu_1'' / 2\lambda_0)^2. \quad (4.4)$$

Let us denote the principal values of the tensor  $\mu_{jk}$  by  $\mu_1 = \mu_{\perp}$ ,  $\mu_2 = \mu_{\parallel}$ . A graph of the exact dependence of the ratio  $\lambda_*/\mu_{\parallel}$  on the ratio  $\mu_{\perp}/\mu_{\parallel}$  is given in Fig. 3, line 1. Curve 2 corresponds to the averaged thermal conductivity coefficient, curve 3 to the averaged thermal-resistance coefficient, and curve 4 is constructed from the Born approximation Eq. (4.4). In this case the self-consistent field method gives

$$\lambda_* = (\mu_1 \mu_2)^{1/2}$$

from which curve 5 is constructed. As can be seen from the graph, in this problem too the Born approximation and the self-consistent field method have a wider field of application than is to be expected from semiintuitive considerations.

## REFERENCES

1. I. M. Lifshits and L. N. Rozentsveig, "On the theory of the elastic properties of polycrystalline aggregates," *Zh. eksperim. i teor. fiz.*, 16, no. 11, 1946.
2. D. G. Dolgoplov, "The coefficient of diffusion in polycrystalline aggregates," *Fizika metallov i metallovedenie*, 13, no. 2, 1962.
3. R. Hill, "Continuum microelasticity of elastoplastic polycrystals," *J. Mech. Phys. Solids*, vol. 13, no. 1, 1965.