DETERMNATION OF ELASTICITY CONSTANTS FOR MICROHETEROGENEOUS MEDIA

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The foundations of the theory of stochastically heterogeneous solids were laid a long time ago by Voigt [1], who developed a method for determining the macroscopic parameters of polycrystalline materials by averaging the appropriate crystallite parameters with respect to orientations. Lifshits and Rozentzveig [2] showed that it was necessary to consider the correlation properties of the field in computations of macroscopic parameters. They calculated the first corrections for the averaged elastic constants of polycrystallites for the case of cubic and hexagonal crystallites. Assuming a low degree of heterogeneity, these authors used an approximation which corresponds to the Born approximation in the theory of scattering [3]. This method and its modifications were subsequently used by several authors for the computation of macroscopic parameters of polycrystallites [4-6] and of other microheterogeneous materials [8].

Moreover, the assumption of a low degree of heterogeneity of the properties is very restrictive. It precludes use of the method in the case of macroscopically isotropic polycrystallites formed from essentially anisotropic crystallite stochastically glass reinforced plastics, and similar microheterogeneous materials. This rises the problem of developing procedures that could be applied in cases of a high degree of heterogeneity. This problem presents serious analytical difficulties, however. It is sufficient to point out that even computation of the second approximation (i.e., the one following the Born approximation) has not yet been completed. Analogous problems in the classical and quantum theories of scattering are also, as a rule, considered only in the Born approximation. More complicated methods (e.g., Feyman's method) make possible only partial summation of infinite sequences in which the result is obtained. A method analogous to that of a self-consistent field in quantum mechanics [9, 10] is promising; however, this method is approximate and the magnitude of its error has not yet been estimated.

The possibility of accurate determination of mascroscopic parameters for certain classes of microheterogeneous media was demostrated in [11], in which a detailed analysis was presented of parameters forming a second order tensor and characterizing the distribution in the medium of a certain scalar value obeying an equation similar to the steady-state heat-conduction equation. Accurate formulas for macroscopic coefficients of thermal conductivity (diffusion) were derived for the case of a strongly anisotropic medium and for that of a medium with a high degree of transverse isotropy. We made a comparison with various approximate methods and evaluated their degree of error. This article describes an accurate method of computing macroscopic elastic constants for polycrystalline media with a high degree of anisotropy; for the case of polycrystals with a cubic structure [12] the error margin and range of application of approximate methods are estimated.

§1. Consider a heterogeneous elastic medium in a state of equilibrium in the absence of volume forces. The displacement vector $u_j(r)$, where $r = (x_1, x_2,$ and $x_3)$, satisfies equations

$$\frac{\partial}{\partial x_k}\left(\lambda_{jklm}\frac{\partial u_l}{\partial x_m}\right) = 0 \qquad (1.1)$$

(here and henceforth a convention about summation in respect to "dummy" subscripts is used). The coefficients λ_{jklm} define at each point of the field a certain fourth-order tensor, i.e., a tensor of elastic constants. If it is assumed that the solid has a random microstructure, the coefficients $\lambda_{jklm}(r)$ form a random tensor field. The dimensions of the solid are assumed to be large enough (in comparison with the scales of heterogeneity and correlation) to rate as infinite. At the same time the field $\lambda_{jklm}(r)$ is assumed to be homogeneous and ergodic. Let us represent the field $\lambda_{jklm}(r)$ in the form

$$\lambda_{jklm} = \lambda'_{jklm} + \lambda''_{jklm} \qquad (1.2)$$

where $\lambda_{jklm} = \langle\lambda_{jklm}\rangle$ denotes the mathematical expectation of the tensor; (the angular brackets denote an operation of averaging in respect to a set of parameters which in this case coincides with the operation of averaging in respect to space). In [2, 5] the fluctuation components λ''_{jklm} was introduced only with a small parameter. In [6, 8], where a correlation method was used, only pair interactions were taken into account. In the final analysis, this is equivalent to assuming a small magnitude of fluctuation components. No such limitation is introduced in our work.

Let us formulate supplementary stochastic conditions corresponding to Eq. (1.1). Let the solid be in a macroscopically homogeneous stress–strain state. We can stipulate that either the mathematical expectations of the stresses or the mathematical expectations of the strains must be equal to prescribed values. Let us choose the latter method for setting the supplementary conditions. For certain reasons it is preferable to define the mathematical expectations p_{jk} of the displacement gradient

$$\langle \partial u_j/\partial x_k\rangle = p_{jk}\,.$$

The problem is to find the probability characteristics of the field $u_j(r)$ which satisfies Eq. (1.1) and conditions (1.3), and to compute the tensor of elastic constants λ^*_{jklm} for an equivalent quasihomogeneous medium. This tensor can be determined from the condition of equality of the mathematical expectations of the stresses in a microheterogeneous medium and from the corresponding stresses in the equivalent medium

$$\langle\lambda_{jklm}\,\partial u_l/\partial x_m\rangle = \lambda^*_{jklm}\,p_{lm}\,. \qquad (1.4)$$

Let us introduce the Green's tensor $G_{jk}(r, r_1)$ for a homogeneous medium with the elasticity constants λ'_{jklm} as the solution of a tensor equation

$$\lambda'_{iklm}\,\partial^2 G_{ln}(\mathbf{r},\ \mathbf{r}_1)/\partial x_k \partial x_m = -\,\delta_{jn}\delta(\mathbf{r}-\mathbf{r}_1)\,. \qquad (1.5)$$

With the aid of this tensor it is easy to write a tensor integral equation equivalent to (1.1) and (1.3):

$$\frac{\partial u_j(\mathbf{r})}{\partial x_k} - \int \frac{\partial^2 G_{jl}(\rho)}{\partial \xi_k \partial \xi_m}\,\lambda''_{lmnp}(\mathbf{r}+\rho)\,\frac{\partial u_n(\mathbf{r}+\rho)}{\partial \xi_p}\,d\rho = p_{jk}\,,$$

$$\rho = (\xi_1,\ \xi_2,\ \xi_3), \qquad d\rho = d\xi_1 d\xi_2 d\xi_3 \qquad (1.6)$$

The solution of Eq. (1.6) is obtained by iteration:

$$\frac{\partial u_j(\mathbf{r})}{\partial x_k} = p_{jk} + p_{lm}\sum_{N=1}^{\infty}\int\ldots\int \frac{\partial^2 G_{j\gamma_1}(\rho_1)}{\partial\xi_k\partial\xi_{\delta_1}}\ldots$$

$$\ldots\frac{\partial^2 G_{\alpha_N\gamma_N}(\rho_N)}{\partial\xi_{\beta_N}\partial\xi_{\delta_N}}\lambda''_{\gamma_1\delta_1\alpha_2\beta_2}(\mathbf{r}+\boldsymbol{\rho}_1)\ldots$$

$$\ldots\lambda''_{\gamma_N\delta_N lm}(\mathbf{r}+\boldsymbol{\rho}_1+\ldots+\boldsymbol{\rho}_N)\,d\boldsymbol{\rho}_1\ldots d\boldsymbol{\rho}_N. \qquad (1.7)$$

With formula (1.7) we formulate expressions for the mathematical expectations of the stresses:

$$\left\langle\lambda_{jklm}\frac{\partial u_l}{\partial x_m}\right\rangle = \lambda'_{jklm}p_{lm} + p_{st}\sum_{N=1}^{\infty}\int\ldots\int\frac{\partial^2 G_{\alpha_1\gamma_1}(\rho_1)}{\partial\xi_{\beta_1}\partial\xi_{\delta_1}}\ldots$$

$$\ldots\frac{\partial^2 G_{\alpha_N\gamma_N}(\boldsymbol{\varrho}_N)}{\partial\xi_{\beta_N}\partial\xi_{\delta_N}}\langle\lambda''_{jk\alpha_1\beta_1}(0)\,\lambda''_{\gamma_1\delta_1\alpha_2\beta_2}(\boldsymbol{\rho}_1)\ldots$$

$$\ldots\lambda''_{\gamma_N\delta_N st}(\boldsymbol{\rho}_1+\ldots+\boldsymbol{\rho}_N)\rangle\,d\boldsymbol{\rho}_1\ldots d\boldsymbol{\rho}_N. \qquad (1.8)$$

Hence, in accordance with (1.4), we find the tensor of macroscopic elasticity constants

$$\lambda^*_{jklm} = \lambda_{jklm} + \sum_{N=1}^{\infty}\int\ldots\int\frac{\partial^2 G_{\alpha_1\gamma_1}(\rho_1)}{\partial\xi_{\beta_1}\partial\xi_{\delta_1}}\ldots$$

$$\ldots\frac{\partial^2 G_{\alpha_N\gamma_N}(\rho_N)}{\partial\xi_{\beta_N}\partial\xi_{\delta_N}}\langle\lambda''_{jk\alpha_1\beta_1}(0)\,\lambda''_{\gamma_1\delta_1\alpha_2\beta_2}(\boldsymbol{\rho}_1)\ldots$$

$$\ldots\lambda''_{\gamma_N\delta_N lm}(\boldsymbol{\rho}_1+\ldots+\boldsymbol{\rho}_N)\rangle\,d\boldsymbol{\rho}_1\ldots d\boldsymbol{\rho}_N. \qquad (1.9)$$

Subsequently (1.9) will be written as:

$$\lambda^*_{jklm} = \lambda'_{jklm} + \langle\lambda^{**}_{jklm}\rangle, \qquad (1.10)$$

where λ^{**}_{jklm} is a solution of a tensor integral equation

$$\lambda^{**}_{jklm}(\mathbf{r}) = \qquad (1.11)$$

$$= \lambda''_{jk\alpha\beta}(\mathbf{r})\int\frac{\partial^2 G_{\alpha\gamma}(\rho)}{\partial\xi_\beta\partial\xi_\delta}[\lambda^{**}_{\gamma\delta lm}(\mathbf{r}+\boldsymbol{\rho}) + \lambda''_{\gamma\delta lm}(\mathbf{r}+\boldsymbol{\rho})]\,d\boldsymbol{\rho}.$$

In fact, solving Eq. (1.11) by the iteration method and using the operation of mathematical expectation, we obtain a series which appears in the right-hand side of (1.9).

§2. If in the right-hand side of (1.9) only one term (N = 1) is retained, we obtain a formula for the Born approximation [2]. The problem is to compute the general term of series (1.9) and to perform factual summation. In the general case this problem is apprently insoluble. Let us therefore narrow the class of random fields and consider only the highly isotropic fields determined in [1]. A random field of constants $\lambda_{jklm}(\mathbf{r})$ will be termed highly isotropic if the correlation functions of the tensor $\lambda^{**}_{jklm}(\mathbf{r})$, which corresponds to this field, form an isotropic field. There are grounds to expect that a medium with a high degree of isotropic of elastic properties is a satisfactory model for describing elastic strains in real isotropic polycrystallites.

In the case of an isotropic field

$$\lambda'_{jklm} = \lambda_0\delta_{jk}\delta_{lm} + \mu_0(\delta_{jl}\delta_{km} + \delta_{jm}\delta_{kl}). \qquad (2.1)$$

where λ_0 and μ_0 are the appropriate Lamé coefficients; The Green's tensor $G_{jk}(\mathbf{r}, \mathbf{r}_1)$ is a function of the modulus of the distance between the points $\rho = |\mathbf{r}-\mathbf{r}_1|$; in addition

$$G_{jk}(\boldsymbol{\rho}) = \frac{1}{4\pi\mu_0}\left(\frac{\delta_{jk}}{\rho} - \frac{5}{2}g\frac{\partial^2\rho}{\partial\xi_j\partial\xi_k}\right), \qquad (2.2)$$

$$g = \frac{1}{5}\frac{\lambda_0+\mu_0}{\lambda_0+2\mu_0} = \frac{1}{10(1-\nu_0)}. \qquad (2.3)$$

Here ν_0 is the Poisson ratio corresponding to the tensor λ'_{jklm}.

In the case of a strongly isotropic polycrystals the correlation tensor for λ''_{jklm} also depend only on the moduli of the distances between points. In particular,

$$\langle\lambda''_{jk\alpha_1\beta_1}(\mathbf{r})\ldots\lambda''_{\gamma_{N-1}\delta_{N-1}\alpha_N\beta_N}(\mathbf{r})\,\lambda''_{\gamma_N\delta_N lm}(\mathbf{r}+\boldsymbol{\rho})\rangle =$$

$$= \varphi_{jk\alpha_1\beta_1\ldots\gamma_N\delta_N lm}(\rho). \qquad (2.4)$$

The tensor λ^{**}_{jklm} has an analogous property. To facilitate subsequent calculations we introduce the notation

$$\langle\lambda''_{jk\alpha_1\beta_1}(\mathbf{r})\ldots\lambda''_{\gamma_{N-1}\delta_{N-1}\alpha_N\beta_N}(\mathbf{r})\,\lambda^{**}_{\gamma_N\delta_N lm}(\mathbf{r}+\boldsymbol{\rho})\rangle =$$

$$= \psi_{jk\alpha_1\beta_1\ldots\gamma_N\delta_N lm}(\rho). \qquad (2.5)$$

With (1.10) and Eq. (1.11) we find macroscopic elastic constants. Averaging Eq. (1.11) and taking into account notation (2.4) and (2.5), we obtain an equation for the correlation correction of the averaged tensor λ_{jklm}:

$$\langle\lambda^{**}_{jklm}\rangle =$$

$$= \int\frac{\partial^2 G_{\alpha\gamma}(\rho)}{\partial\xi_\beta\partial\xi_\delta}[\varphi_{jk\alpha\beta\gamma\delta lm}(\rho) + \psi_{jk\alpha\beta\gamma\delta lm}(\rho)]\,d\rho. \qquad (2.6)$$

We substitute (2.2) into (2.6). Noting that

$$\frac{\partial^2 G_{\alpha\gamma}(\rho)}{\partial\xi_\beta\partial\xi_\delta} = -\frac{1}{3\mu_0}[(1-2g)\,\delta_{\alpha\gamma}\delta_{\beta\delta} - g\delta_{\alpha\beta}\delta_{\gamma\delta}]\,\delta(\boldsymbol{\rho}) +$$

$$+\frac{1}{4\pi\mu_0}\left\{\delta_{\alpha\gamma}\left(\frac{3\xi_\beta\xi_\delta}{\rho^5} - \frac{\delta_{\beta\delta}}{\rho^3}\right) -\right.$$

$$-\frac{5}{2}g\left[-\frac{1}{\rho^3}(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} +\right.$$

$$+\delta_{\alpha\delta}\delta_{\beta\gamma}) + \frac{3}{\rho^5}(\delta_{\alpha\beta}\xi_\gamma\xi_\delta + \delta_{\alpha\gamma}\xi_\beta\xi_\delta + \delta_{\alpha\delta}\xi_\beta\xi_\gamma +$$

$$\left.\left.+\delta_{\beta\gamma}\xi_\alpha\xi_\delta + \delta_{\beta\delta}\xi_\alpha\xi_\gamma + \delta_{\gamma\delta}\xi_\alpha\xi_\beta) - \frac{15}{\rho^7}\xi_\alpha\xi_\beta\xi_\gamma\xi_\delta\right]\right\},$$

and integrating by parts, we obtain

$$\langle\lambda^{**}_{jklm}\rangle =$$

$$= -\frac{1}{3\mu_0}\{(1-2g)[\varphi_{jk\alpha\beta\alpha\beta lm}(0) + \psi_{jk\alpha\beta\alpha\beta lm}(0)] -$$

$$-g[\varphi_{jk\alpha\alpha\beta\beta lm}(0) + \psi_{jk\alpha\alpha\beta\beta lm}(0)]\} +$$

$$+\frac{1}{4\pi\mu_0}\int_0^\infty\int_0^{2\pi}\int_0^\pi[\varphi_{jk\alpha\beta\gamma\delta lm}(\rho) +$$

$$+\psi_{jk\alpha\beta\gamma\delta lm}(\rho)]\left\{\delta_{\alpha\gamma}\left(\frac{3\xi_\beta\xi_\delta}{\rho^5} -\right.\right.$$

$$\left.-\frac{\delta_{\beta\delta}}{\rho^3}\right) - \frac{5}{2}g\left[-\frac{1}{\rho^3}(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) +\right.$$

$$+\frac{3}{\rho^5}(\delta_{\alpha\beta}\xi_\gamma\xi_\delta + \delta_{\alpha\gamma}\xi_\beta\xi_\delta + \delta_{\alpha\delta}\xi_\beta\xi_\gamma + \delta_{\beta\gamma}\xi_\alpha\xi_\delta +$$

$$+ \delta_{\beta\delta}\xi_\alpha\xi_\gamma + \delta_{\gamma\delta}\xi_\alpha\xi_\beta) - \frac{15}{\rho^7}\xi_\alpha\xi_\beta\xi_\gamma\xi_\delta\Big]\Big\}\rho^2 d\rho \sin\theta\, d\varphi d\theta.$$

Direct calculations show that the triple integral vanishes.
Hence

$$\langle\lambda^{**}_{jklm}\rangle = -{}^1/_3\,\mu_0^{-1}\{(1-2g)[\varphi_{jk\alpha\beta\alpha\beta lm}(0) + \psi_{jk\alpha\beta\alpha\beta lm}(0)] - g[\varphi_{jk\alpha\alpha\beta\beta lm}(0) + \psi_{jk\alpha\alpha\beta\beta lm}(0)]\}. \quad (2.7)$$

On the right-hand side of (2.7) there appears a mixed correlation tensor of type (2.5). To determine this tensor we again use Eq. (1.11). Repeating the calculations described above, we obtain the final formula

$$\lambda^*_{jklm} = \lambda_0\delta_{jk}\delta_{lm} + \mu_0(\delta_{jl}\delta_{km} + \delta_{jm}\delta_{kl}) + \sum_{N=1}^{\infty} I^{(N)}_{jklm}, \quad (2.8)$$

in which the general term of the series $I^{(N)}_{jklm}$ is expressed as follows:

$$I^{(N)}_{jklm} = ({}^1/_3\mu_0^{-1})^N\langle\lambda''_{jk\alpha_1\beta_1}\zeta_{\alpha_1\beta_1\gamma_1\delta_1}\lambda''_{\gamma_1\delta_1\alpha_2\beta_2}\zeta_{\alpha_2\beta_2\gamma_2\delta_2}\ldots\lambda''_{\gamma_N\delta_N lm}\rangle. \quad (2.9)$$

Here $\zeta_{\alpha\beta\gamma\delta}$ denotes an isotropic tensor:

$$\zeta_{\alpha\beta\gamma\delta} = (1-2g)\,\delta_{\alpha\gamma}\delta_{\beta\delta} - g\delta_{\alpha\beta}\delta_{\gamma\delta}. \quad (2.10)$$

§3. Let us apply formulas (2.8) and (2.9) to a strongly isotropic polycrystal. Its local elasticity constants are given by a formula

$$\lambda_{jklm} = c_{j\alpha}c_{k\beta}c_{l\gamma}c_{m\delta}\mu_{\alpha\beta\gamma\delta}, \quad (3.1)$$

where μ_{jklm} is the tensor of elasticity constants of a crystallite, referred to the crystallographic axes, and $c_{j\alpha}$ denotes the conversion matrix for changing over from the crystallographic axes to a laboratory system of coordinates. The components λ_{jklm} lose discontinuities at grain boundaries. As a result, elasticity constants, displacements, stresses, etc. in Eq. (1.1) and subsequent quent formulas must be treated as generalized functions. However, the final formulas (2.8) and (2.9) express the macroscopic elastic constants through single-point correlation tensors and do not contain operations over generalized functions.

We introduce the notation $\mu''_{jklm} = \mu_{jklm} - \gamma'_{jklm}$. Then, by analogy witn (3.1),

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

We substitute formula (3.2) into the right-hand side of (2.9). Noting that

$$\langle\lambda''_{jk\alpha_1\beta_1}\zeta_{\alpha_1\beta_1\gamma_1\delta_1}\lambda''_{\gamma_1\delta_1\alpha_2\beta_2}\zeta_{\alpha_2\beta_2\gamma_2\delta_2}\ldots\lambda''_{\gamma_N\delta_N lm}\rangle = \langle c_{j\nu_1}c_{k\nu_2}c_{\alpha_1\nu_3}c_{\beta_1\nu_4}\zeta_{\alpha_1\beta_1\gamma_1\delta_1}c_{\gamma_1\nu_5}c_{\delta_1\nu_6}c_{\alpha_2\nu_7}\ldots c_{m\nu_{4N+4}}\rangle\mu''_{\nu_1\nu_2\nu_3\nu_4}\ldots\mu''_{\nu_{4N+1}\nu_{4N+2}\nu_{4N+3}\nu_{4N+4}}$$

$$c_{\alpha_1\nu_3}c_{\beta_1\nu_4}\zeta_{\alpha_1\beta_1\gamma_1\delta_1}c_{\gamma_1\nu_5}c_{\delta_1\nu_6} = \zeta_{\nu_3\nu_4\nu_5\nu_6},$$

we transform formula (2.9) to

$$I^{(N)}_{jklm} = (-{}^1/_3\mu_0^{-1})^N\langle c_{j\nu_1}c_{k\nu_2}c_{l\nu_{4N+3}}c_{m\nu_{4N+4}}\rangle\mu''_{\nu_1\nu_2\nu_3\nu_4}\zeta_{\nu_3\nu_4\nu_5\nu_6}\ldots\mu''_{\nu_{4N+1}\nu_{4N+2}\nu_{4N+3}\nu_{4N+4}}. \quad (3.3)$$

We calculate fourth-order moments from elements of the conversion matrix $c_{j\alpha}$. In the case of equally probable crystallite orientations we have

$$\langle c_{a\alpha}c_{a\beta}c_{a\gamma}c_{a\delta}\rangle = {}^1/_{15}(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}),$$

$$\langle c_{a\alpha}c_{a\beta}c_{b\gamma}c_{b\delta}\rangle = {}^2/_{15}\delta_{\alpha\beta}\delta_{\gamma\delta} - {}^1/_{30}(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})$$

(here $a \neq b$; no summation is done in respect to the subscripts a and b). Formula (2.8) for macroscopic elastic constants is reduced to the form

$$\lambda^*_{jklm} = \lambda_*\delta_{jk}\delta_{lm} + \mu_*(\delta_{jl}\delta_{km} + \delta_{jm}\delta_{kl}),$$

where λ_* and μ_* are microscopic Lamè coefficients;

$$\lambda_* = \lambda_0 + \frac{1}{30}\sum_{N=1}^{\infty}\left(-\frac{1}{3\mu_0}\right)^N[4\delta_{\nu_1\nu_2}\delta_{\nu_{4N+3}\nu_{4N+4}} - (\delta_{\nu_1\nu_{4N+3}}\delta_{\nu_2\nu_{4N+4}} + \delta_{\nu_1\nu_{4N+4}}\delta_{\nu_2\nu_{4N+3}})]\,\mu''_{\nu_1\nu_2\nu_3\nu_4}\zeta_{\nu_3\nu_4\nu_5\nu_6}\ldots\mu''_{\nu_{4N+1}\nu_{4N+2}\nu_{4N+3}\nu_{4N+4}}$$

$$\mu_* = \mu_0 + \frac{1}{60}\sum_{N=1}^{\infty}\left(-\frac{1}{3\mu_0}\right)^N[-2\delta_{\nu_1\nu_2}\delta_{\nu_{4N+3}\nu_{4N+4}} + 3(\delta_{\nu_1\nu_{4N+3}}\delta_{\nu_2\nu_{4N+4}} + \delta_{\nu_1\nu_{4N+4}}\delta_{\nu_2\nu_{4N+3}})]\,\mu''_{\nu_1\nu_2\nu_3\nu_4}\zeta_{\nu_3\nu_4\nu_5\nu_6}\ldots\mu''_{\nu_{4N+1}\nu_{4N+2}\nu_{4N+3}\nu_{4N+4}}. \quad (3.4)$$

Formulas (3.4) can be rewritten in a more compact form

$$\lambda_* = \lambda_0 - {}^1/_{15}(2\chi_{\alpha\alpha\beta\beta} - \chi_{\alpha\beta\alpha\beta}),$$

$$\mu_* = \mu_0 - {}^1/_{30}(3\chi_{\alpha\beta\alpha\beta} - \chi_{\alpha\alpha\beta\beta}). \quad (3.5)$$

Here $\chi = \chi_{jklm}$ is a fourth-order tensor associated with the tensor $\mu'' = \mu''_{jklm}$ by the formula

$$\chi = -\sum_{N=1}^{\infty}\left(-\frac{1}{3}\right)^N A^N\mu''. \quad (3.6)$$

In ths case A is a linear operator over fourth-order tensors which is defined as follows: $a = Ab$, if

$$a_{jklm} = \mu_0^{-1}\mu''_{jk\alpha\beta}\zeta_{\alpha\beta\gamma\delta}b_{\gamma\delta lm}. \quad (3.7)$$

It is easy to see that there is a solution of an operator equation in the right-hand side of (3.6):

$$\chi + {}^1/_3 A\chi = {}^1/_3 A\mu'' \quad (3.8)$$

Equation (3.8) represents a system of linear algebraic equations relative to the elements of the tensor $\chi = \chi_{jklm}$. The number of equations forming this system depends on the crystallographic class of a

	Elastic constants of crystallites			Shear modulus of a polycrystal			
	c_{11}	c_{12}	c_{44}	(1)	(2)	(3)	(4)
Ag	12.40	9.34	4.61	3.02	3.38	3.07	2.55
Al	10.82	6.13	2.85	2.63	2.64	2.63	2.62
Au	18.60	15.70	4.20	2.81	3.10	2.84	2.41
Cu	16.84	12.14	7.54	4.83	5.47	4.91	4.00
Pb	4.66	3.92	1.44	0.87	1.01	0.89	0.67

(1) exact solution, (2) Voigt averaging (3) Born approximation, and (4) Reiss averaging.

given crystallite. This number is equal to three in the case of a cubic structure, to six in the case of a hexagonal structure, etc. Formulas (3.5) and (3.8) give an exact solution of the problem. We obtain approximate solution corresponding to the Born approximation by retaining in (3.6) the first term of the series or, and this the same, by replacing Eq. (3.8) with an approximation relation $\chi \approx 1/3\ A\mu$". It will be seen that the final exact formulas are not very much more complex than the approximate formulas.

§4. As a most simple example let us consider a polycrystal with a cubic structure. Changing over, as is usual, to matrix notation, we reduce subscripts: $11 \to 1$, $22 \to 2, 33 \to 3, 12 \to 4$, $23 \to 5$, and and $31 \to 6$. The matrix of elastic constants for the crystallite contains three different elements which are not equal to zero:

$$\mu = \left\| \begin{matrix} M_{11} & M_{12} & M_{12} & 0 & 0 & 0 \\ & M_{11} & M_{12} & 0 & 0 & 0 \\ & & M_{11} & 0 & 0 & 0 \\ & & & M_{44} & 0 & 0 \\ & & & & M_{44} & 0 \\ & & & & & M_{44} \end{matrix} \right\| \tag{4.1}$$

Lamé coefficients averaged by the Voigt method are given by

$$\lambda_0 = {}^1/_5\ (M_{11} + 4M_{12} - 2M_{44}),$$

$$\mu_0 = {}^1/_5\ (M_{11} - M_{12} + 3M_{44}). \tag{4.2}$$

Formulas (3.5) become

$$\lambda_* = \lambda_0 - {}^1/_5\ (\chi_{11} + 4\chi_{12} - 2\chi_{44}),$$

$$\mu_* = \mu_0 - {}^1/_5\ (\chi_{11} - \chi_{12} + 3\chi_{44}). \tag{4.3}$$

The solution of Eqs. (3.8) for the case of matric (4.1) of elastic constants will be

$$\chi_{11} = \frac{6\chi_0\gamma}{1+3\gamma}, \quad \chi_{12} = -\frac{3\chi_0\gamma}{1+3\gamma}, \quad \chi_{44} = \frac{2\chi_0\gamma}{1-2\gamma},$$

$$\chi_0 = {}^1/_5\ (M_{11} - M_{12} - 2M_{44}),\ \gamma = {}^1/_3\ \chi_0\mu_0^{-1}\ (1 - 2g), \tag{4.4}$$

where g is determined from (2.3). The Born approximation formula, first derived in [2], has the same form (4.3); however, $\chi_{11} = 6\chi_0\gamma$, $\chi_{12} = 3\chi_0\gamma$ and $\chi_{44} = 2\chi_0\gamma$.

To compare the results yielded by different methods, tne values of elastic constants (4.2) from [2] are cited in the first three columns of a table; the next columns shows values of the macroscopic shear modulus calculated from exact formulas (4.e) and (4.4) from the Voigt method, from the Born approximation formulas, and from the Reiss method which yields a lower limit for the elasticity constants. To express the elasticity constants in newtons/m^2 the values cited in the table should be multiplied by 10^{10}. In the example considered the degree of crystallite anisotropy is not excessive; consequently, the Born approximation gives quite accurate results. In the case of a cubic structure the macroscopic volume modulus coincides exactly with vlaues averaged by the Voigt or Reiss methods as a result, another Lame elastic constant $\gamma = K - (2/3)\mu$ is less affected by the method of calculation than the shear modulus.

REFERENCES

1. W. Voigt, Lehrbuch der Kristallphysik, Teubner-Verlag, 1910.
2. I. M. Lifshits and L. N. Rozentsveig, "Theory of elastic properties of polycrystals," Zh. eksperim. i. teor. fiz., vol. 16, no. 11, 1946.
3. F. M. Morse and G. Feshach, Methods of Theoretical Physics, Vol. 2 [Russian translation], Izd. inostr. lit., 1960.
4. D. G. Dolgopolov, "Coefficients of diffusion in polycrystals", Fizika metallov i metallovedenie, vol. 13, no. 2, 1962.
5. V. A. Lomakin, "Deformation of microheterogeneous elastic solids," PMM, vol. 29, no. 5, 1965.
6. B. M. Darinskii and T. D. Shermergor, "Elastic moduli of cubic polycrystals," PMTF [Journal of Applied Mechanics and Technical Physics], no. 4, 1965.
7. V. V. Bolotin, "Layered elastic and viscoelastic media with small initial irregularities," Mekhanika tverdogo tela [Mechanics of Solids], no. 3, 1966.
8. G. N. Savin and L. P. Khoroshun, "Statistically isotropic deformation of composite materials," Dokl. An UkrSSR, ser. A, no. 9. 1967.
9. E. Kroner, "Berechnung der elastischen Konstanten des Vielkristalls aus den Konstanten des Einkristalls," Z. Physik, vol. 151, no. 4, 1958.
10. R. Hill, "Continuum micro-mechanics of elastoplastic polycrystals," J. Mech. Phys. Solids, vol. 13, no. 1, 1965.
11. V. V. Bolotin and V. N. Moskalenko, "Macroscopic coefficients of thermal conductivity and diffusion in microheterogeneous solids,"PMTF [Journal of Applied Mechanics and Technical Physics] no. 6, 1967.
12. H. Huntington, "Elastic constants of crystals," [Russian translation] Uspekhi fiz. nauk, vol. 74, nos. 2, 3, 1961.

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