A METHOD FOR CALCULATING THE PHYSICAL CONSTANTS OF POLYCRYSTALLINE MATERIALS

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Abstract

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A METHOD FOR CALCULATING THE PHYSICAL CONSTANTS OF POLYCRYSTALLINE MATERIALS

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Numerous works have been devoted to the development of methods for calculating the properties of polycrystalline materials with allowance for the composition of the material, the physical properties, and the preferred orientation of the crystallites entering into the material ([1–9]). A description and analysis of all known averaging methods, without analyzing them in detail, may be found in ([3,4,7]); we shall dwell only on those methods that pertain to the calculation of physical properties described by symmetric tensors of even rank ([10]). Among these properties are the dielectric, electrical, magnetic, and elastic properties of polycrystals, textures, and mixtures.

Let, in a single crystal, the property of interest to us be described by a tensor $[R]$. To the tensor $[R]$ one may associate an inverse tensor $[Q]$ (for example, resistance and conductivity, elastic stiffness c_{iklm} and compliance s_{iklm}, etc.). The constants of the matrix $\|Q\|$ can be obtained from $\|R\|$ by known methods ([10]). The problem consists in calculating the quantities $\bar{R}$ (or $\bar{Q}$) that would characterize the given property in a polycrystalline material.

The principal difficulty in calculating the quantities $\bar{R}$ is that, with a large number of crystallites, their random mutual orientations, and a significant anisotropy of the property under investigation in each of the crystallites, a rigorous allowance for the boundary conditions is practically impossible, and one has to abandon a general solution of the problem. Historically, the first and simplest methods for calculating the quantities $\bar{R}$ and $\bar{Q}$ were calculations of the arithmetic mean for the quantities $\|R\|$ or $\|Q\|$ ([1,8,19]), or, equivalently, direct averaging of the quantities R_i' written for an arbitrary direction in a single crystal:

$$R_i' = \sum_j \Phi_{ij} R_j; \qquad Q_i' = \sum_j \Phi_{ij} Q_j; \tag{1}$$

$$\bar{R}_i^a = \sum_j p_{ij} R_j; \qquad \bar{Q}_i^a = \sum_j r_{ij} Q_j, \tag{2}$$

where R_j and Q_j are the eigenvalues of the matrices $\|R\|$ and $\|Q\|$, and p_{ij} and r_{ij} are the mean values of the orientation functions Φ_{ij} in (1), calculated by formula (3) for $f \equiv 1$:

$$p_{ij} = \frac{1}{8\pi^2} \iiint f(\theta, \varphi, \psi) \Phi_{ij}(\theta, \varphi, \psi) \sin\theta \, d\theta \, d\varphi \, d\psi. \tag{3}$$

Allowance for the influence of texture on the properties of an aggregate was reduced to changing the weighting factors $p_{ij}(r_{ij})$ in accordance with the distribution function (f) of the crystallite orientations.

Until now, this method has been the principal method for taking into account the influence of texture on the physical properties of a polycrystal ([2,11,12]). Later it was shown ([3,4]) that the calculations of the arithmetic means $\bar{R}^a$ and $\bar{Q}^a$ correspond to boundary conditions that are certainly not fulfilled. It is also known that $R^a \neq (\bar{a}^a)^{-1}$, and the difference between them increases with increasing anisotropy.

the property under study in a single crystal. To improve agreement with experiment, it was proposed to seek the quantity $\bar{R}$ as the half-sum of these means, i.e. $2\bar{R} = \bar{R}^a + (\bar{Q}^a)^{-1}$ [13]. It turned out that the values of $\bar{R}$ obtained in this way satisfy the experimental data rather well [14,15].

More rigorous attempts were made to take boundary conditions into account. Thus, in calculating the elastic constants of isotropic polycrystals, variational methods [6], the Green' s-function method [2], methods of the continuum theory of dislocations [3], etc., were used. These methods give more accurate values of $\bar{R}$, but the restrictions underlying the calculation (small anisotropy of the crystal or small misorientation of grains in [2], spherical grains in [3,6]), and very complicated calculations, make it difficult to use these methods in computing the elastic properties even of isotropic single-phase materials composed of low-symmetry crystals.

In the present work an attempt is made to bypass the mathematical difficulties of taking boundary conditions into account and to find a general method for calculating the quantities $\bar{R}$, applicable to isotropic materials, textures, and mixtures.

Let the property under study in a material constituting an aggregate be described by constants $R_j > 0$. By the quantities R_j we may understand either the eigenvalues of the matrix $\|R\|$ of a single crystal, or the values of the constant R for the j-th phase of a multicomponent mixture. Consider such a matrix $\|Q\|$ that its eigenvalues are $Q_j = R_j^{-1}$. In a polycrystalline material (isotropic body,

texture, mixture) the property under study is described by the matrices $\|\bar{Q}\|$ and $\|\bar{R}\|$, and for their eigenvalues the relations $\bar{Q}_i = \bar{R}_i^{-1}$ again hold.

We shall consider the mean value $\mathfrak{M}_\varphi(R_j)$ with an arbitrary averaging function $\varphi(R_j)$, where $\varphi(R_j)$ is continuous and strictly monotone, and φ^{-1} is its inverse function:

$$\bar{R}_i = \mathfrak{M}_\varphi(R_j) = \varphi^{-1}\left\{\sum_{j=1}^{n} p_{ij}\varphi(R_j)\right\}, \tag{4}$$

where $p_{ij} \geq 0,\ \sum_j p_{ij} = 1, \quad i, j = 1, 2, \ldots, n.$

It is assumed that the sought values $\bar{Q}_i$ and $\bar{R}_i$ are the mathematical means $\mathfrak{M}_\varphi(Q_j)$ and $\mathfrak{M}_\varphi(R_j)$. This assumption, laid as the basis for the subsequent solution, seems physically obvious, but has not been proved. In favor of its correctness is the fact that all mathematical means known to us (including those used in physics) are special cases of expression (4). The sought mean value must satisfy two conditions:

1. The averaging function φ must be such that

$$\bar{Q}_i = \mathfrak{M}_\varphi(Q_j) = \left[\mathfrak{M}_\varphi(R_j)\right]^{-1} = \bar{R}_i^{-1}, \tag{I}$$

i.e. the result of averaging must not depend on which of the quantities R_j or Q_j are averaged with the aid of (4).

2. The sought mean must be a homogeneous mean

$$\mathfrak{M}_\varphi(kR_j) = k\mathfrak{M}_\varphi(R_j), \tag{II}$$

which physically means the independence of the result of averaging from scale (the chosen system of units).

From condition (II) it follows (see [16], pp. 88, 86) that $\varphi(R) = aR^k + \beta,\ k \neq 0$, or $\varphi(R) = a\ln R + \beta$, where α and β are constants, $\alpha \neq 0$.

Put $\psi(R) = \varphi(1/R)$; then $\psi^{-1} = 1/\varphi^{-1}$, and from condition (I) we obtain $\mathfrak{M}_\varphi(R) = \mathfrak{M}_\psi(R)$; therefore (see [16], p. 86) $\psi(R) = \alpha_1\varphi(R) + \beta_1$, i.e. $\varphi(1/R) = \alpha_1\varphi(R) + \beta_1,\ \alpha_1 \neq 0$. It is easy to see that the function $\varphi(R) = aR^k + \beta$ does not satisfy the condition found. Thus, the only averaging function possessing all the required properties,

has the form $\varphi(R) = \alpha\ln R + \beta$. The only mean value obtained from (4) with the aid of this function for arbitrary $\alpha \neq 0$ and β,

$$\overline{R}_i = \mathfrak{M}_{\alpha\ln R+\beta}(R_j) = \mathfrak{M}_{\ln R}(R_j) = \exp\left[\sum_{j=1}^{n} p_{ij}\ln R_j\right] = \prod_j R_j^{p_{ij}} \tag{5}$$

does indeed satisfy conditions (I) and (II).

Thus, if the sought values $\overline{R}_i$ are only some mathematical means of R_j, then

$$\ln \overline{R}_i = \sum_j p_{ij} \ln R_j; \qquad \sum_j p_{ij} = 1. \tag{5a}$$

Expressions (5) and (5a) do not yet solve the problem posed, since it is still unknown how the weight factors p_{ij} are determined. However, from (5), even without strictly determining p_{ij}, it is possible to obtain valuable results. Thus, for an isotropic polycrystalline aggregate, at first sight there are no apparent reasons for a difference between p_{ij} for different R_j, i.e., there is no predominant contribution of one of the R_j to $\overline{R}_i$. If $R_j > 0$ have the meaning of eigenvalues of a 3×3 matrix, for example the dielectric constants ε_j of a single crystal, then for an isotropic polycrystal one may put $p_{ij} = 1/3$ and

$$\overline{\varepsilon} = (\varepsilon_1 \varepsilon_2 \varepsilon_3), \tag{6}$$

i.e., we arrive at the same result as in work (17), where it was obtained from the condition of equality of the higher invariants of the matrices $\|\overline{R}\|$ and $\|R\|$. Calculations show that the mean value (6) differs from the experimental one by no more than a few percent, so long as the quantities R_j differ from one another by no more than one order of magnitude. For the same anisotropy values, the arithmetic means (2) differ from the mean (6) and from one another by several times.

Let us consider the dielectric properties of a macroscopically isotropic mixture of n isotropic phases. The properties of each phase are determined by the quantity ε_j, and again, so long as the differences between ε_j do not exceed one order of magnitude, it may be assumed that p_{ij} in (5) is determined only by the volume concentration of the phases, i.e., $p_{ij} = v_j \left(\sum_j v_j = 1\right)$. Then from (5) we obtain the expression

$$\ln \overline{\varepsilon} = \sum_{j=1}^{n} v_j \ln \varepsilon_j, \tag{7}$$

known in the physics of dielectrics as Lichtenecker' s formula for the dielectric properties of mixtures (18).

In order to describe the elastic properties of polycrystals by means of (5) and (5a), it is necessary to define the quantities R_j so that $R_j = Q_j^{-1}$. It is clear that the components of the matrices c_{ij} and s_{ij} themselves do not satisfy this condition. However, calculating by known methods the eigenvalues of the matrices $\|c_{ij}\|$ and $\|s_{ij}\|$, we find that this condition is satisfied for them. Thus, for a cubic crystal we have

$$R_1 = c_{11} + 2c_{12}, \qquad R_{2,3} = c_{11} - c_{12}, \qquad R_{4,5,6} = 2c_{44}. \tag{8}$$

The first of expressions (8) is an invariant for a cubic crystal and, consequently, $\overline{R}_1 = R_1$, $\overline{K} = K$, where K is the bulk-compression modulus. For the shear modulus (G) of a polycrystal, again assuming that R_j ($j = 2, \ldots, 6$) make equal contributions to $\overline{R}_i = 2G$, we have $p_{ij} = 1/5$ and

$$G = c_{44} a^{2/5}, \tag{9}$$

where $a = (c_{11} - c_{12})/2c_{44}$ is the anisotropy of the elastic constants.

Calculations carried out earlier show that, for all values $0.1 < a < 5$ so far encountered in cubic crystals, expression (9) gives a value of G very close to the experimental one (17).

Finally, for the elastic constants $\overline{K}$ and $\overline{G}$ of a homogeneous isotropic mixture of n isotropic phases, each of which is defined by two independent constants K_j and G_j, we obtain

$$\ln \overline{K} = \sum_{j=1}^{n} v_j \ln K_j, \qquad \ln \overline{G} = \sum_{j=1}^{n} v_j \ln G_j. \tag{10}$$

The latter expressions, similar in form to Lichteneker' s formulas (7), give values of $\overline{K}$ and $\overline{G}$ that lie not only between the rough (arithmetic-mean) bounds for the properties of the mixture ([19]), but also between the narrower bounds obtained in ([20]).

It has been noted above more than once that expressions (6)–(10), found from (5) under the assumption that the quantities p_{ij} are independent of the anisotropy of the crystal (of the difference between R_j in the mixture), are approximate. However, the range of anisotropy values for which (6)–(10) give values in good agreement with experiment is considerably wider than for (2) and, at any rate, no worse than for other methods of averaging ([3,6,7]).

The quantities p_{ij} in (5) probably depend only weakly on anisotropy, and therefore formulas (7) and (10) prove unsuitable for limiting cases of strong anisotropy (for example, in estimating the influence of porosity on the elastic properties of a mixture).

With the aid of expressions (5), it is also possible to calculate the constants of a polycrystalline aggregate possessing texture. In this case it can be shown that, in the presence of a preferred orientation and with not very strong anisotropy, the indices p_{ij} in (5) are described by expressions (3). In particular, it has been shown that the quantities Φ_{ij} in (3) for a tensor of the second rank have the same form as in the calculation of arithmetic means.

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