MEAN VALUES OF TENSOR QUANTITIES

1965

SovietRxiv

Abstract

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CRYSTALLOGRAPHY

K. S. ALEKSANDROV

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(Presented by Academician A. V. Shubnikov, February 26, 1965)

The physical properties of anisotropic media are described by tensors of various ranks. Thus, dielectric and optical properties, electrical conductivity, thermal expansion, etc., are described by a symmetric polar tensor of the second rank. The elastic properties of a crystal are described by a polar tensor of the fourth rank ([1,2]).

The problem of calculating mean values of physical constants from the values of the corresponding constants of a single crystal has long attracted the attention of researchers, both for describing the properties of a polycrystalline aggregate or texture and for solving a number of problems in solid-state physics ([1,3–9]). One such problem is that of calculating the mean value of the velocities of elastic waves in a crystal when computing the Debye characteristic temperature from the values of the elastic constants of the crystal ([10,11]).

In earlier works devoted to the so-called averaging methods, the calculation of the mean value T of a certain tensor quantity $[t]$ is carried out by averaging the quantity t', written for an arbitrary direction, i.e.

$$T = \frac{1}{4\pi} \int t'(\Omega)\, d\Omega, \tag{1}$$

where $d\Omega$ is an element of solid angle.

In many cases the tensor $[t]$ corresponds to the inverse tensor $[q] \equiv [t^{-1}]$ (for example, resistance and conductivity, the constants of elastic stiffness c_{iklm} and compliance s_{iklm}). Application of averaging (1) to the quantities q' gives a mean value $Q \neq T^{-1}$.

For all these averaging methods two features are characteristic. First, the mean quantities obtained from (1) agree satisfactorily with experimental data only when the anisotropy of the property under study in the single crystal is small. Second, the discrepancy with experimental data and the difference between the mean values obtained from $[t]$ and from $[q]$, i.e., the difference between T and Q^{-1}, increase with increasing anisotropy. Experimental data for an isotropic polycrystal practically always lie between the quantities T and Q^{-1} ([12]).

Thus, the averages (1) are approximate. To improve the averaging methods it was proposed to calculate the mean value of the quantity $[t]$ as the half-sum of the quantities T and Q^{-1} (^{12}), but no basis for such a secondary averaging has so far been found. Recently, statistical methods for calculating mean values have been developed (^{4,5}), methods have been devised for taking account of the interaction of grains in a polycrystalline material (^{3,6}), and, for particular models of a polycrystalline aggregate, data have been obtained that agree well with experiment ($^{3-5,13}$).

The purpose of the present work is to propose a method for calculating mean values by means of the invariants of the corresponding tensors and to show, using tensors of even rank as an example, that many of the existing averaging methods are the first or second approximation to the mean values obtained from invariants.

Let us consider, for definiteness, the tensor of the dielectric properties of a crystal $[\varepsilon_{ik}]$. A tensor of the second rank is always reducible to diagonal form and in the principal coordinate system contains three constants $\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}$ (1). Suppose we have to compute the quantity $\bar{\varepsilon}$, describing the dielectric properties of a polycrystalline aggregate with a chaotic (equally probable) distribution of crystallite orientations.

It is well known that a tensor of the second rank has three invariants of rotation (^{1,14,15})

$$\begin{aligned} I_1 &= \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}, & I_1^0 &= 3\varepsilon, \\ I_2 &= \varepsilon_{11}\varepsilon_{33} + \varepsilon_{33}\varepsilon_{22} + \varepsilon_{11}\varepsilon_{22}, & I_2^0 &= 3\varepsilon^2, \\ I_3 &= \varepsilon_{11}\varepsilon_{22}\varepsilon_{33} & I_3^0 &= \varepsilon^3, \end{aligned} \tag{2}$$

where I_i^0 are the invariants of the matrix $[\bar{\varepsilon}]$ for an isotropic body.

It is much less widely known that simple methods of averaging can be obtained without the cumbersome integration (1), directly from the conditions of equality of invariants. Imposing the condition

$$I_1 = I_1^0, \tag{3}$$

we immediately obtain

$$\bar{\varepsilon} = \frac{1}{3}(\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}), \tag{4a}$$

or

$$\bar{\eta} = \frac{1}{3}(\eta_{11} + \eta_{22} + \eta_{33}) \tag{4b}$$

for the reciprocal quantities

$$\eta_{ii} = \varepsilon_{ii}^{-1}. \tag{5}$$

As in (1), $\bar{\varepsilon} \neq \bar{\eta}^{-1}$. Equating $I_2 = I_2^0$, one can obtain corrections to (4a) and (4b), and in this case the difference between $\bar{\varepsilon}$ and $\bar{\eta}^{-1}$ decreases. The optimal method of averaging the tensor quantity $[\varepsilon]$ is the requirement of equality of the higher invariants of the tensor $[\varepsilon]$, i.e., $I_3 = I_3^0$. In this case

$$\bar{\varepsilon} = (\varepsilon_{11}\varepsilon_{22}\varepsilon_{33})^{1/3}, \qquad \bar{\eta} = (\eta_{11}\eta_{22}\eta_{33})^{1/3} \tag{6}$$

and, what is especially important,

$$\bar{\varepsilon} = \bar{\eta}^{-1}.$$

Thus, the proposed method of calculating mean values of a tensor of the second rank gives one and the same value for the direct and reciprocal quantities. Using the example of a uniaxial crystal ($\varepsilon_{11} = \varepsilon_{22}$), it is easy to show that expressions (4) are the first approximation to (6) for small values of the anisotropy of the dielectric properties of the crystal, $a = \varepsilon_{33}/\varepsilon_{11}$. Indeed, expression (6) can be expanded in a series

$$\bar{\varepsilon} = \varepsilon_{11} a^{1/3} = \left[1 + \frac{1}{3}(a-1) - \frac{1}{9}(a-1)^2 + \ldots\right]\varepsilon_{11}, \tag{7}$$

and the first two terms of the series correspond to (4). The values of $\bar{\varepsilon}$ from (4) and (6) are close to one another for $a \simeq 1$.

Let us now consider a tensor of the 4th rank describing the elastic properties of a crystal. There are known (^{16,17}) two invariants of the tensor $[c_{iklm}]$, linear in c_{iklm}:

$$I_1 = \sum_{i,k=1}^{3} c_{iikk} = 9K, \qquad I_2 = \sum_{i=1}^{3} c_{iiii} + 2\sum_{i,k=1}^{3} c_{ikik}, \tag{8}$$

where K is the bulk-compression modulus.

The elastic properties of an isotropic body are described by two constants (we shall choose K^0 and G^0), and expressions (8) then have the form:

$$I_1^0 = 9K^0; \qquad I_2^0 = 3K^0 + 10G^0. \tag{9}$$

Leibfried noted (^{17}) that averaging by Voigt' s method (^{8}) for a crystal of any symmetry can be obtained not only from expressions of the type (1), but also from the condition of equality of the invariants (8) and (9), i.e., from

$$I_1 = I_1^0, \qquad I_2 = I_2^0.$$

Let us show, using the example of a cubic crystal, that the use of a higher invariant $[c_{iklm}]$—the determinant of the matrix of elastic constants $\|c_{rs}\|$, $r, s = 1, 2, \dots, 6$—leads to mean values K^0 and G^0 that agree well with experimental data.

Computing the determinant $\|c_{rs}\|$, we obtain for a cubic crystal

$$I_6 = 12Ka^2c_{44}^5 \tag{10}$$

and for an isotropic body

$$I_6^0 = 12K^0(G^0)^5, \tag{11}$$

where $a = (c_{11} - c_{12})/2c_{44}$ is the anisotropy constant of the elastic properties of the crystal. Equating (10) and (11) and using $I_1 = I_1^0$, we have

$$G^0 = c_{44}a^{2/5}, \qquad K = K^0, \tag{12}$$

or, for the compliances $[s_{iklm}]$,

$$\frac{1}{G^0} = s_{44}a^{-2/5}. \tag{13}$$

It follows from (12) and (13) that averaging the direct (c_{iklm}) and inverse (s_{iklm}) quantities again gives identical results.

The right-hand side of expression (12) can be expanded in a series

$$G^0 = c_{44}\left[1 + \frac{2}{5}(a-1) - \frac{3}{25}(a-1)^2 + \dots\right], \tag{14}$$

and the first two terms of the series (14) represent Voigt averaging, while the third term of the series is, in form, analogous to the correction to Voigt averaging calculated by Lifshitz and Rosenzweig (^{6}), but has a larger numerical coefficient.

Table 1

Crystal	c_{11}	c_{12}	c_{44}	G_V	G_R	$\frac{1}{2}(G_V + G_R)$	G^0	G_{KR}	$K = K_0$	a
Au	19,234	16,314	4,195	3,101	2,398	2,749	2,750	2,811	17,287	0,348
Ag	12,399	9,367	4,612	3,374	2,358	2,956	2,955	3,011	10,378	0,329
V	22,8	11,9	4,26	4,736	4,668	4,702	4,701	4,704	15,533	1,279
Nb	24,6	13,4	2,87	3,962	3,565	3,763	3,750	3,786	17,133	1,951
Ta	26,7	16,1	8,25	7,070	6,748	6,909	6,912	6,926	19,633	0,642
Pb	4,953	4,229	1,490	1,033	0,663	0,848	0,846	0,87	4,470	0,243

It is of interest to compare the averaging results from (12) with the data of Kröner and Kneer ([3], [13]). The results of the calculations are presented in Table 1. It is seen from the table that the proposed method of averaging gives values close to the values of the half-sum of the Voigt and Reuss averages ([9]), denoted by $\frac{1}{2}(G_V + G_R)$. The data in the works ([3], [13]), G_{KR}, are systematically higher than G^0 and $\frac{1}{2}(G_V + G_R)$. Judging from the data of Anderson' s work ([11]), who used the average $\frac{1}{2}(G_V + G_R)$ to calculate the characteristic Debye temperatures θ_D for a number of crystals, one may suppose that the proposed method of averaging with the aid of invariants will give better agreement with calorimetric measurements of θ_D for crystals of any symmetry.

In conclusion, we note that if the equality of the lower invariants (see expressions (3), (8), (9)) corresponds to averaging quantities by formulas (1), then, by equating the higher invariants of the tensor $[t]$, we change the method of calculating the mean values and, what is especially interesting, can calculate these mean values without carrying out an integration still more complicated than in (1). In the author' s opinion, this method of averaging may be applied also to many other tensor quantities. A mathematical justification of the proposed method for computing mean values can probably be obtained in a general form.

Institute of Physics, Siberian Branch
Academy of Sciences of the USSR

Received
25 II 1965

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

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