ON THE CALCULATION OF ELASTIC CONSTANTS OF QUASI-ISOTROPIC POLYCRYSTALLINE MATERIALS

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Abstract

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ON THE CALCULATION OF ELASTIC CONSTANTS OF QUASI-ISOTROPIC POLYCRYSTALLINE MATERIALS

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The purpose of the present communication is to prove that various statistical methods for calculating the elastic constants of an isotropic polycrystalline aggregate ($^{1-5}$) are interrelated and constitute different degrees of approximation to Kröner’ s “self-consistent” solution (in Hill’ s terminology (^{6})) (^{5}).

The variational method of Hashin–Shtrikman (^{1,2}), for the case of crystallites of the cubic system (when the bulk-compression moduli K of the polycrystal and the single crystal are equal to each other), leads to the following expression for the limiting values of the shear modulus of the polycrystal G (see (3.23) in (^{2})):

$$G^* \gtreqless G_0 + B_2(1 + 2\beta B_2)^{-1}, \tag{1}$$

where

$$5B_2 = \left[\frac{1}{2(G_1 - G_0)} - \beta\right]^{-1} + 3\left[\frac{1}{G_2 - G_0} - 2\beta\right]^{-1}, \tag{2}$$

$$\beta = -\frac{3}{5G_0}\frac{K + 2G_0}{3K + 4G_0}. \tag{3}$$

In the second term on the right-hand side of equation (2), the term 2β has been introduced instead of β (Shtrikman, private communication).

The quantities G_0 are chosen by the authors from condition (A), which requires that the matrix $R_{ijkl} = C_{ijkl} - C^0_{ijkl}$ be positive definite in one case (^{1}). Then from (1) the quantities G_1^* and G_2^* can be obtained, which bound the true value of the shear modulus of the polycrystal G. Hashin and Shtrikman chose as the quantities G_0 the quantities $G_1 = \frac{1}{2}(C_{11} - C_{12})$ and $G_2 = C_{44}$, which certainly satisfy condition A, and obtained for G_1^* and G_2^* the expressions:

$$
\begin{aligned}
G_1^* &= G_1 + 3\left(\frac{5}{G_2 - G_1} - 4\beta_1\right)^{-1}, \\
G_2^* &= G_2 + 2\left(\frac{5}{G_1 - G_2} - 6\beta_2\right)^{-1},
\end{aligned}
\tag{4}
$$

where β_1 and β_2 are determined from (3) by replacing in it the quantity G_0 by G_1 and G_2, respectively.

Analysis of expressions (4) shows that the quantities G_1^* and G_2^* give considerably narrower bounds for G than the known Voigt average (G_V) and Reuss average (G_R), i.e., the inequality holds

$$
\begin{aligned}
&G_2 > G_V > G_2^* > G > G_1^* > G_R > G_1 \quad (G_2 > G_1), \\
&G_1 > G_V > G_1^* > G > G_2^* > G_R > G_2 \quad (G_1 > G_2).
\end{aligned}
\tag{5}
$$

It is not difficult to show that the expressions (4) themselves are only the first approximation in the solution of the variational problem of finding G, determined by expression (1). Indeed, the choice as G_0 of the quantities G_1 and G_2, which are far from G for large anisotropy $a = G_1/G_2$ of the elastic properties of the single crystal, seems very crude. Condition A can also be satisfied by the quantities G_V and G_R from (5), which are certainly greater and less than G.

In other words, equation (1) makes it possible to solve the problem by the method of successive approximations. Thus, choosing G_0 to be the value $G_0 = G_V$, we have, in the second approximation:

$$
\begin{aligned}
G_2^{(2)} &= G_V + \frac{2\beta_V(G_1 - G_V)(G_2 - G_V)}{2\beta_V(G_1 + G_2 - 2G_V) - 1} \simeq \\
&\simeq G_V - \frac{12}{125}\frac{(G_1 - G_2)^2}{G_V}\left[1 + \left(\frac{3K}{2G_V} + 2\right)^{-1}\right],
\end{aligned}
\tag{6}
$$

where the index V on β_V corresponds to replacing G_0 by $G_V = G_2[1 + {}^2/{}_5(a-1)]$ in (3).

It is interesting to note that expression (6) coincides with the result of Lifshitz and Rosenzweig (^{3})—the first of the works in this series, and later undeservedly criticized in the works of Eshelby (^{7}). It is now becoming clear that the result of Lifshitz and Rosenzweig is, for $a < 1$, the upper (for $a > 1$, the lower) limiting value for G in the second approximation, i.e., for the case $a < 1$:

$$
G_2 > G_V > G_2^* > G_2^{(2)} > G > G_1^{(2)} > G_1^* > G_R > G_1.
$$

The quantity $G_1^{(2)}$—the lower bound in the second approximation—can be found by replacing $G_0 = G_R = G_2[1 + {}^2/_5(a^{-1} - 1)]^{-1}$ in expressions (1)–(3).

Recently a paper by Darinskii and Shemergor (^{4}) was published; its authors used essentially the same method as in (^{3}), but dealt with the quantities S_{ijkl}, inverse (in matrix form) to C_{ijkl}. Analysis of their result for a cubic crystal shows that, under the same conditions $a < 1$, the authors obtained an upper limiting value for G, also in the second approximation of the Hashin–Shtrikman variational problem, formulated for quantities inverse to C_{ijkl} in work (^{1}). The conclusion of the authors of (^{4}) that the true value of G lies between the values obtained by them and in the work of Lifshitz and Rosenzweig (see equation (6)) is apparently incorrect, since both of these results are upper ($a < 1$) or lower ($a > 1$) limiting values for G, obtained in one approximation, but for different formulations of the variational problem.

The process of successive approximation could be continued further, but more attractive is the possibility of a self-consistent solution of the variational problem. Indeed, returning to equation (1), one can see that, instead of determining G_0 by successive approximations, one may require the second term in equation (1) to be equal to zero, i.e., set equal to zero the left-hand side of equation (2). Thus, the quantity G_0 is determined from the equation:

$$\frac{1}{G_2 - G_0} + \frac{3}{G_1 - G_0} + \frac{3k + 6G_0}{G_0(3k + 4G_0)} = 0, \tag{7}$$

which is a cubic equation with respect to G_0, and after transformations is reduced to the form:

$$G_0^3 + {}^1/_8(9k + 4\nu)G_0^2 - {}^3/_8(k + 4\nu)\mu G_0 - {}^3/_4 k\mu\nu = 0, \tag{8}$$

where the notation $G_1 = \nu,\ G_2 = \mu$ has been used.

The equation (8) obtained in this way is equivalent to the "self-consistent" solution of the problem under consideration in Kröner's work (^{5}) and, apparently, requires no further comment, since the results of Kröner' s work have already been discussed in detail ($^{8—10}$).

Thus it has been shown that the results of the work of Hashin and Shtrikman (^{2}) (see equation (4)) and of works (^{3},^{4}) are, respectively, the first and second approximations in the solution of the problem of the elastic properties

of a cubic polycrystal by the variational method. It is also shown that the equation (1) obtained by this method makes it possible to bring together the limiting values for G by the method of successive approximations and to obtain the exact solution (8), called by Hill (^{6}) Kröner' s (^{5}) self-consistent solution.

On the other hand, obtaining the self-consistent solution (8) from the results of (^{2}) proves the validity of such a refinement of the solution of the variational problem, and this device can also be used in other cases. Recently a paper ([11]) appeared in the literature in which all the necessary data are given for obtaining the self-consistent solution in computing the elastic properties of a polycrystal composed of crystallites of the hexagonal and trigonal systems. In addition, the literature ([12,13]) also contains a solution of the problem of the elastic properties of multiphase mixtures, obtained by the same variational method. In the case of two-phase mixtures, the self-consistent solution of this problem leads to a fourth-degree equation describing the concentration dependence of the shear modulus G, and to a fractional-linear function G for the bulk-compression modulus. A detailed analysis of these results will be carried out in another paper.

In conclusion it is necessary to note that in all the cited works the elastic properties were considered of a polycrystal (heterogeneous mixture) consisting of grains of spherical shape. The proposed method for obtaining the self-consistent solution from the solution of the variational problem may prove useful for finding the solution of an analogous problem for an arbitrary shape of the regions of inhomogeneity. In one of the papers in the collection ([7]) the case of an ellipsoidal inhomogeneity is considered, and these data in principle make it possible to find the solution of the problem of the elastic properties of a polycrystal for any grain shape.

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CITED LITERATURE

[1] Z. Hashin, S. Shtrikman, J. Mech. Phys. Solids, **10**, 335 (1962).
[2] Z. Hashin, S. Shtrikman, J. Mech. Phys. Solids, **10**, 343 (1962).
[3] I. M. Lifshits, L. I. Rozentsveig, ZhETF, **16**, 967 (1946).
[4] B. M. Darinskii, T. D. Shermergor, Zhurn. prikl. mekh. i tekhn. fiz., **4**, 121 (1965).
[5] E. Kröner, Zs. Phys., **151**, 504 (1958).
[6] R. Hill, J. Mech. Phys. Solids, **13**, 89 (1965).
[7] J. Eshelby, *Continuum Theory of Dislocations*, IL, 1963, p. 68.
[8] G. Kneer, Phys. Status Solidi, **3**, 331 (1963).
[9] K. S. Aleksandrov, DAN, **164**, 800 (1965).
[10] E. Kröner, B. Datta, D. Kessel, J. Mech. Phys. Solids, **14**, 21 (1966).
[11] L. Peselnick, R. Meister, J. Appl. Phys., **36**, 2879 (1965).
[12] Z. Hashin, S. Shtrikman, J. Franklin Inst., **271**, 336 (1961).
[13] Z. Hashin, S. Shtrikman, J. Mech. Phys. Solids, **11**, 127 (1963).