

THE CALCULATION OF THE ELASTIC MODULI OF POLYCRYSTALLINE AGGREGATES

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The elastic moduli of polycrystalline aggregates can be calculated by various methods from the known elastic constants of single crystals. Direct averaging, based on the hypotheses of uniform deformation (Voigt's method [1]) or of uniform stress (Reuss's method [2]), gives a pair of values for the elastic moduli, between which the true value lies. The difference in the values of the elastic moduli averaged by the Voigt and the Reuss methods results from ignoring the correlations between the crystals in the aggregate. The discrepancy can be reduced for example, by means of the so-called self-consistent method [3, 4] which has been applied to polycrystalline aggregates by Kröner [5] and Kneer [6, 7]. A drawback to this method is the necessity of introducing model concepts.

A more general approach, based on the use of the theory of random functions, has been developed by I. M. Lifshits and his co-workers [8, 9]. This method is based on the calculation of the correlation corrections to the tensor of the elastic moduli λ_{iklm} . There is another possible method of approach, based on calculating the correlation corrections to the tensor of elastic compliance $s_{iklm} = \lambda_{iklm}^{-1}$. This method has been developed for polycrystalline aggregates of cubic structure in [10], and below it is extended to polycrystalline aggregates with structures of lower symmetry. Since the method of calculating the correlation corrections to the tensor of the elastic moduli is somewhat different from that adopted in [8], for ease of comparison of the methods the calculation of the corrections to the moduli of compliance s_{iklm} given below is accompanied by the corresponding calculation for the elastic moduli λ_{iklm} .

By taking account only of the pair correlations, we obtain the following equilibrium and incompatibility equations [10, 11]:

$$\begin{aligned} (L_{il} - \langle R_{im} g_{mn} * R_{nl} \rangle) \langle u_l \rangle &= -f_i, \\ (L_{iklm} - \langle R_{ikpq} g_{pqrs} * R_{rstm} \rangle) \langle \sigma_{lm} \rangle &= -\eta_{ik}. \end{aligned} \quad (1)$$

Here u_l is the displacement vector, σ_{lm} is the stress tensor, and L and R are, respectively, the regular and random components of the operator Q

$$Q_{il} = \nabla_k \lambda_{iklm} \nabla_m, \quad Q_{iklm} = \varepsilon_{irp} \varepsilon_{ksq} \nabla_p \nabla_q s_{rstm}. \quad (2)$$

The unit antisymmetric tensor is denoted ε_{irp} and the tensor Green function of the operators L is denoted g. The latter are determined by the equations

$$L_{il} g_{ln} = \delta(r) \delta_{in}, \quad L_{pqik} g_{iklm} = \delta(r) \delta_{m(p} \delta_{q)n}, \quad (3)$$

symmetrization being carried out with respect to the indices given in parentheses.

The Fourier transforms of the Green functions are

$$\begin{aligned} k^2 G_{jn} &= -\frac{1}{c_2} \left(\delta_{jn} - \frac{c_1 + c_2}{c_1 + 2c_2} n_j n_n \right), \\ k^2 G_{pqmn} &= \frac{1}{2s_2} \delta_{m(p} \delta_{q)n} - \frac{s_1 + 2s_2}{4s_2 (s_1 + s_2)} \delta_{mn} (\delta_{pq} - n_p n_q). \end{aligned} \quad (4)$$

Here $n_p = k_p/k$, and the coefficients c_i and s_i determine the elastic constants averaged without taking into account the correlations in the Voigt and Reuss methods, respectively

$$\begin{aligned} \langle \lambda_{iklm} \rangle &= c_1 \delta_{ik} \delta_{lm} + c_2 (\delta_{il} \delta_{km} + \delta_{im} \delta_{kl}), \\ \langle s_{iklm} \rangle &= s_1 \delta_{ik} \delta_{lm} + s_2 (\delta_{il} \delta_{km} + \delta_{im} \delta_{kl}). \end{aligned} \quad (5)$$

From Eqs. (1) and (3) the following expressions are obtained for the effective tensors Λ_{iklm} and S_{iklm} :

$$\begin{aligned} \Lambda_{iklm} &= \langle \lambda_{iklm} \rangle - \int g_{jn} \varepsilon_p^{ikjs} a_{nplm}^2 dV, \\ S_{rsik} &= \langle s_{rsik} \rangle - \varepsilon_{aju} \varepsilon_{blv} \int g_{mnab, uv} b_{jlik}^{rsmn} dV. \end{aligned} \quad (6)$$

Here a_{nplm}^{ikjs} and b_{jlik}^{rsmn} are the binary correlation tensor functions

$$\begin{aligned} a_{nplm}^{ikjs}(\mathbf{r} - \mathbf{Q}) &= \langle \lambda'_{ikjs}(\mathbf{r}) \lambda'_{nplm}(\mathbf{Q}) \rangle, \\ b_{jlik}^{rsmn}(\mathbf{r} - \mathbf{Q}) &= \langle s'_{rsmn}(\mathbf{r}) s'_{jlik}(\mathbf{Q}) \rangle. \end{aligned} \quad (7)$$

In the case of an untextured medium

$$a_{nplm}^{ikjs}(\mathbf{r}) = \alpha_{nplm}^{ikjs} \varphi(\mathbf{r}), \quad b_{jlik}^{rsmn}(\mathbf{r}) = \beta_{jlik}^{rsmn} \varphi(\mathbf{r}), \quad (8)$$

with $\varphi(0) = 1$.

Let us first consider polycrystalline aggregates of the tetragonal system. Then for classes of symmetry with six independent elastic constants, the tensors of the elastic moduli and compliances of a crystallite in the crystallographic system of coordinates may be represented in the form

$$\begin{aligned} \lambda_{iklm}^o &= c_1^o \delta_{ik} \delta_{lm} + c_2^o (\delta_{il} \delta_{km} + \delta_{im} \delta_{kl}) + c_3^o \delta_{i3} \delta_{k3} \delta_{l3} \delta_{m3} + \\ &+ c_4^o (\delta_{ik} \delta_{l3} \delta_{m3} + \delta_{i3} \delta_{k3} \delta_{lm}) + c_5^o (\delta_{il} \delta_{k3} \delta_{m3} + \\ &+ \delta_{i3} \delta_{l3} \delta_{km} + \delta_{im} \delta_{k3} \delta_{l3} + \delta_{i3} \delta_{m3} \delta_{kl}) + c_6^o \sum_n \delta_{in} \delta_{kn} \delta_{ln} \delta_{mn}, \\ s_{iklm}^o &= s_1^o \delta_{ik} \delta_{lm} + s_2^o (\delta_{il} \delta_{km} + \delta_{im} \delta_{kl}) + s_3^o \delta_{i3} \delta_{k3} \delta_{l3} \delta_{m3} + \\ &+ s_4^o (\delta_{ik} \delta_{l3} \delta_{m3} + \delta_{i3} \delta_{k3} \delta_{lm}) + s_5^o (\delta_{il} \delta_{k3} \delta_{m3} + \delta_{i3} \delta_{l3} \delta_{km} + \\ &+ \delta_{im} \delta_{k3} \delta_{l3} + \delta_{i3} \delta_{m3} \delta_{kl}) + s_6^o \sum_n \delta_{in} \delta_{kn} \delta_{ln} \delta_{mn}, \end{aligned} \quad (9)$$

the constants c_i and s_i being related to the two-index elastic constants c_{ij} and s_{ij} by the equations

$$\begin{aligned} c_1 &= c_1^o + 1/15 c_3 + 2/3 c_4 + 1/5 c_6, \\ c_2 &= c_2^o + 1/15 c_3 + 2/3 c_5 + 1/5 c_6, \quad c_1^o = c_{12}, \quad c_2^o = c_{66}, \\ c_3 &= c_{33} - c_{11} + 2c_{12} - 2c_{13} - 4c_{44} + 4c_{66}, \\ c_4 &= c_{13} - c_{12}, \quad c_5 = c_{44} - c_{66}, \quad c_6 = c_{11} - c_{12} - 2c_{66}, \\ s_1 &= s_1^o + 1/15 s_3 + 2/3 s_4 + 1/5 s_6, \\ s_2 &= s_2^o + 1/15 s_3 + 2/3 s_5 + 1/5 s_6, \quad s_1^o = s_{12}, \quad 4s_2 = s_{66}, \\ s_3 &= s_{33} - s_{11} - 2s_{13} + 2s_{12} - s_{44} + s_{66}, \\ s_4 &= s_{13} - s_{12}, \quad 4s_5 = s_{44} - s_{66}, \quad s_6 = s_{11} - s_{12} - 1/2 s_{66}. \end{aligned} \quad (10)$$

By means of Eqs. (7)-(9) we can find the total contractions of the autocorrelation tensors

$$\begin{aligned} \alpha_{ijqq}^{ijpp} &= 2/3 (c_3 + 3c_4 + 4c_6)^2, \\ \alpha_{ijpq}^{ijpq} &= 2/3 \alpha_{ijqq}^{ijpp} + 2/9 (1.6c_3^2 + 8c_3c_5 + 28c_5^2) + 2/3 c_6 (2c_3 + 3c_6), \\ \beta_{ijqq}^{ijpp} &= 2/3 (s_3 + 3s_4 + 4s_6)^2, \\ \beta_{ijpq}^{ijpq} &= 2/3 \beta_{ijqq}^{ijpp} + 2/9 (1.6s_3^2 + 8s_3s_5 + 28s_5^2) + \\ &+ 2/3 s_6 (2s_3 + 3s_6), \end{aligned} \quad (11)$$

by which the partial contractions are expressed

$$\begin{aligned} \alpha_{ilmq}^{ilpq} &= 1/9 \alpha_{sspq}^{rrpq} \delta_{ik} \delta_{lm} + 1/10 (\alpha_{rspp}^{rspp} - 1/3 \alpha_{sspq}^{rspp}) D_{iilm}, \\ \alpha_{ilmq}^{ikpp} &= 1/10 \alpha_{rsqq}^{rspp} D_{iklm}, \\ D_{iklm} &\equiv \delta_{il} \delta_{km} + \delta_{im} \delta_{kl} - 2/3 \delta_{il} \delta_{lm}. \end{aligned} \quad (12)$$

There are similar relationships for β_{jlik}^{rsmn} .

Converting to integration in transform space in (6) by means of the Parseval theorem and taking into account Eqs. (8)-(12), we obtain

$$\Lambda_{iklm} - \langle \lambda_{iklm} \rangle = \Delta K_V \delta_{ik} \delta_{lm} + \Delta \mu_V D_{iklm}, \quad (13)$$

Table 1
Cubic System

	Ag	Al	Au	K	Li	Na
μ_V	3.38	3.22	3.11	0.1747	0.694	0.380
μ_V^*	3.07	2.94	2.86	0.1428	0.539	0.296
μ_R^*	3.06	2.93	2.85	0.1373	0.495	0.274
μ_R	2.55	2.49	2.41	0.0346	0.248	0.152
Δ_V^h	0.377	0.379	0.363	0.353	0.348	0.335
Δ_R^h	0.609	0.608	0.632	0.586	0.553	0.537

	Ni	Pb	Cu	Ge	Th	Pa
μ_V	9.47	1.012	5.46	5.64	3.40	5.32
μ_V^*	8.78	0.890	4.91	5.49	2.98	4.89
μ_R^*	8.75	0.883	4.88	5.48	2.95	4.88
μ_R	7.77	0.638	4.00	5.30	2.33	4.16
Δ_V^h	0.406	0.354	0.380	0.452	0.389	0.375
Δ_R^h	0.579	0.625	0.600	0.541	0.578	0.615

$$S_{iklm} - \langle s_{iklm} \rangle = 1/9 \Delta K_R^{-1} \delta_{ik} \delta_{lm} + 1/4 \Delta \mu_R^{-1} D_{iklm}, \quad (13)$$

(Cont'd)

$$c_7 (\delta_{i_1} \delta_{j_1} - \delta_{i_2} \delta_{j_2}) (\delta_{k_3} \delta_{l_3} + \delta_{k_3} \delta_{l_2}) + (\delta_{i_3} \delta_{j_3} + \delta_{i_3} \delta_{j_2}) \times \\ \times (\delta_{k_1} \delta_{l_1} - \delta_{k_2} \delta_{l_2}) + (\delta_{i_1} \delta_{j_3} + \delta_{i_3} \delta_{j_1}) (\delta_{k_1} \delta_{l_2} + \delta_{k_2} \delta_{l_1}) + \\ + (\delta_{i_1} \delta_{j_2} + \delta_{i_2} \delta_{j_1}) (\delta_{k_1} \delta_{l_3} + \delta_{k_3} \delta_{l_1}), \quad (18)$$

where

$$\Delta K_V = -\alpha_1 \frac{3c_1 + 8c_2}{135c_2(c_1 + 2c_2)}, \\ \Delta \mu_V = -\frac{5c_2\alpha_1 + (3c_1 + 8c_2)\alpha_2}{450c_2(c_1 + 2c_2)}, \\ \Delta \frac{1}{K_R} = -\beta_1 \frac{6s_1 + 7s_2}{30s_2(s_1 + s_2)}, \\ \Delta \frac{1}{\mu_R} = -\frac{10s_2\beta_1 + (6s_1 + 7s_2)\beta_2}{225s_2(s_1 + s_2)}, \quad (14)$$

$$\alpha_1 \equiv \alpha_{ijmm}^{ijmm}, \quad \alpha_2 \equiv 3\alpha_{ijmn}^{ijmn} - 2\alpha_1, \\ \beta_1 \equiv \beta_{ijnn}^{ijnn}, \quad \beta_2 \equiv 3\beta_{ijmn}^{ijmn} - 2\beta_1, \quad (15)$$

with the values of the elastic moduli averaged without taking the correlations into account equal to

$$K_V = c_1 + 2/3 c_2, \quad \mu_V = c_2, \quad K_R^{-1} = 9s_1 + 6s_2, \quad \mu_R^{-1} = 4s_2. \quad (16)$$

Expressions (14) are applicable to polycrystalline aggregates of random crystallographic symmetry. In the case of tetragonal symmetry the tensor contractions α_{ijkl}^{ijkl} and β_{pqrs}^{ijhl} , which determine the coefficients α and β that appear in (14) are given by relationships (11) and (12). For higher symmetry—hexagonal and cubic—expressions (11) are simplified. In the first case it is necessary to put $c_6 = s_6 = 0$ and in the second to put $c_3 = c_4 = c_5 = s_3 = s_4 = s_5 = 0$. It is not difficult to show that when the effective moduli of shear and hydrostatic compression for a cubic system coincide with the values previously obtained in [10] and those for a hexagonal system with the values obtained from (14), they lead to the correlation corrections that were derived in a different way by Lifshits and Rozentsveig [8].

Similar calculations for polycrystalline aggregates of classes 32 3m and 3m of the trigonal system lead to elastic moduli which are determined as usual by means of formulas (11)–(15). However, we shall now have the contractions

$$\alpha_{ijpq}^{ijpq} = 2/3 \alpha_{ijpq}^{ijpp} + 2/9 (1.6c_8^2 + 8c_3c_5 + 28c_6^2) + 16c_7^2, \\ \beta_{ijpq}^{ijpq} = 2/3 \beta_{ijpq}^{ijpp} + 2/9 (1.6s_8^2 + 8s_3s_5 + 28s_6^2) - 16s_7^2. \quad (17)$$

The elastic moduli λ_{ijkl}^{ijkl} and s_{ijkl}^{ijkl} for the trigonal crystals differ from the expressions in (9) because the terms which include the factors c_6 and s_6 (which indicate the transition to hexagonal symmetry) vanish and the following addition is made:

to λ_{ijkl}^{ijkl} and a similar term to s_{ijkl}^{ijkl} . The relationship between the one-index and two-index elastic constants is described by expressions (10), in which we have to put $c_6 = s_6 = 0$, $c_7 = c_{14}$, and $s_7 = s_{14}/2$.

The mean and effective values of the elastic moduli for metals of the cubic system are given in Table 1 and those for polycrystalline aggregates of lower symmetry in Table 2. Some of the elements of the cubic system were calculated less accurately in [10]. The two-index elastic constants were taken for Zr, Ti, and Be from [12], for Zn from [7], and for the remainder from [13]. If several values of the elastic constants were reported in [13], the first were always taken.

In the last two lines of the tables, after the values of μ and K , the relative values of the ranges

$$\Delta V^h = (\mu_V - \mu_V^*) / (\mu_V - \mu_R), \\ \Delta R^h = (\mu_R^* - \mu_R) / (\mu_V - \mu_R)$$

are given, and similarly for the modulus of hydrostatic compression. Each of the relative ranges characterizes the magnitude of the inter-val to which the subject method leads.

The data given by Huntington [13] for the inverse matrices of the elastic constants contain a considerable number of errors; hence, the experimental data were taken as the basic material, the inverse matrices (c_{ij} and s_{ij}) being checked on a "Nairi" computer. Bearing in mind that in certain cases the correlation corrections are small, we carried out the calculations formally with an accuracy up to nine significant figures. The final results for the absolute values of the elastic moduli and the differences between them, given in the tables, were rounded off to three significant figures, which corresponds to the accuracy of the experimental data. It can be seen from the tables that, although in the majority of cases the extent of the range in the Reuss method is greater than that in the Voigt method, both methods give similar values for the effective elastic moduli if the anisotropy of the material is not too great.

To illustrate the effect of the anisotropy on the magnitude of the correlation correction, Fig. 1 gives curves showing the extent of the deviation h from the arithmetic mean value in the two methods as a function of the anisotropy parameter $A_1 = c_{13}/c_{12}$, the elastic constants being chosen as follows: $c_{11} = c_{33} = 3c_{12} = 3c_{44} = 3$. The deviation h is associated with the correlation corrections by the relationships $h_V^K = 0.5 - \Delta_V^K$, $h_R^K = -0.5 + \Delta_R^K$. The value $h = 0$ corresponds

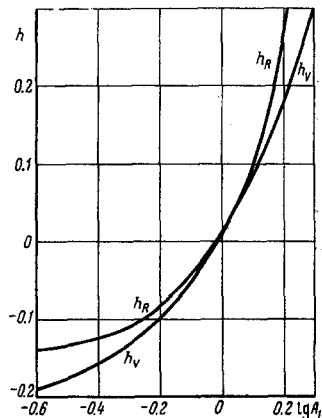
Table 2
Hexagonal System

	Cd	Co	Zn	Zr	Ti	Be
K_V	6.28	19.05	7.30	9.54	10.73	11.45
K_V^*	5.91	19.04	7.05	9.53	10.73	11.44
K_R	6.08	19.04	7.35	9.53	10.73	11.44
K_R^*	5.03	19.04	6.20	9.52	10.73	11.43
Δ_V^K	0.295	0.729	0.228	0.609	0.607	0.550
Δ_R^K	0.837	0.326	1.046	0.401	0.400	0.450
μ_V	2.51	8.44	4.56	3.64	4.41	14.93
μ_V^*	2.31	8.15	4.25	3.60	4.34	14.86
μ_R^*	2.31	8.17	4.41	3.60	4.33	14.86
μ_R	2.06	8.01	3.64	3.56	4.26	14.80
Δ_V^μ	0.449	0.660	0.343	0.562	0.469	0.507
Δ_R^μ	0.562	0.369	0.838	0.444	0.505	0.490

Tetragonal Trigonal System

	Sn	In	Sb	Bi	Hg	Te
K_V	5.27	4.16	3.94	3.60	3.35	3.36
K_V^*	5.26	4.16	3.86	3.46	3.30	3.08
K_R	5.26	4.16	3.94	3.57	3.49	3.69
K_R^*	5.26	4.16	3.62	3.37	3.23	2.49
Δ_V^K	0.865	0.132	0.277	0.593	0.415	0.324
Δ_R^K	0.230	0.198	0.989	0.843	2.09	1.372
μ_V	1.914	0.592	2.51	1.326	0.806	2.34
μ_V^*	1.711	0.491	2.26	1.243	0.606	1.301
μ_R^*	1.777	0.502	2.26	1.242	0.573	0.943
μ_R	1.497	0.372	2.04	1.145	0.326	0.366
Δ_V^μ	0.487	0.458	0.527	0.460	0.417	0.526
Δ_R^μ	0.671	0.592	0.465	0.537	0.514	0.293

to the arithmetic mean of the moduli averaged by the Voigt and Reuss methods without taking account of the correlations, while $h_V^K = 0.5$ and $h_R^K = -0.5$ determine the limits of the range $K_V - K_R$ which is taken as unity for any value of A_1 .



It can be seen from Fig. 1 that h_V^K and $h_R^K > 0$ if $A_1 > 1$. For $A_1 < 1$, the two curves intersect the abscissa and lie in the negative region. Thus, when $A_1 > 1$ the extent of the range in the Voigt method is greater than in the Reuss method, while when $A_1 < 1$ the reverse is true. As was to be expected, as $A_1 \rightarrow 1$, when the contribution of the higher-order correlations is negligibly small, the two methods of calculation give identical values. It should be noted that in the limit $A_1 \rightarrow 1$ the effective value of the modulus K^* differs somewhat from the arithmetic mean $(K_V + K_R)/2$. Similar results are also obtained for h_V^μ and h_R^μ as a function of A_1 , and also in the change of the other anisotropy constants $A_2 = c_{33}/c_{11}$ and $A_3 = 2c_{44}/(c_{11} - c_{12})$.

In the limiting transition to the isotropic point $A_2 = A_3 = 1$, $A_1 \rightarrow 1$, we find $h_V^K = h_R^K = 1/90$. At the same values of the parameters we obtain for shear deformations $h_V^\mu = h_R^\mu = 1/139$. A similar calculation in the case $A_1 = A_3 = 1$, $A_2 \rightarrow 1$ gives $h_V = h_R = 1/90$ and $h_V^\mu = h_R^\mu = -1/490$. If $A_1 = A_2 = 1$, and $A_3 \neq 1$, hexagonal material degenerates into cubic. Hence, for $A_3 \rightarrow 1$ we obtain $h_V^K = h_R^K = 0$ and $h_V^\mu = h_R^\mu = 1/90$.

Obviously, if the other isotropic point is chosen, the limiting transitions $A \rightarrow 1$ lead to other numerical values of h_V and h_R . However, in terms of the order of magnitude, the departure of the true elastic modulus from the arithmetic mean will not be great. Since, as $A \rightarrow 1$, the correlation functions higher than the second order may be omitted, the numerical values given show that the true values of the elastic moduli agree within about 1% with the arithmetic mean

of the moduli found by averaging by the Voigt and Reuss methods without taking the correlations into account.

With increase in the anisotropy parameter the values of h_V and h_R also increase, indicating that higher-order correlations must be taken into account. In those cases where the effective value of the elastic modulus exceeds the limits of the range $\mu_V - \mu_R$ or $K_V - K_R$, the anisotropy of the material is so great that limiting the correlations to those of the second order only is no longer admissible.

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