

ELASTIC MODULI OF CUBIC POLYCRYSTALS

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The averaged elastic constants of polycrystals can be found by averaging the stresses (Voigt method [1]) or the strains (Reuss method [2]). Comparison of the elastic moduli, averaged according to Voigt and Reuss, with the experimental values shows that in the first case averaging gives values that are too high, and in the second values that are too low [3]. The reason for this is that direct averaging of the moduli with respect to arbitrary orientations of the crystallites does not take account of correlation effects. There are two ways of allowing for such correlations between polycrystal grains.

1. In the Voigt scheme the stresses are averaged. Therefore to calculate the correlation effects we use the equilibrium equation

$$\sigma_{ik,k} + f_i \equiv 0, \quad \sigma_{ik,k} \equiv \nabla_k \sigma_{ik} \equiv \partial \sigma_{ik} / \partial x_k. \quad (1.1)$$

Here the repeated subscript summation convention is used. Using Hooke's law

$$\sigma_{ik} = \lambda_{iklm} e_{lm}, \quad (1.2)$$

we can write the equilibrium equations in the form

$$\nabla_k \lambda_{iklm} u_{l,m} + f_i = 0, \quad e_{lm} = 1/2 (u_{l,m} + u_{m,l}), \quad (1.3)$$

where  $e_{lm}$  is the strain tensor,  $u_l$  is the displacement vector, and  $\lambda_{iklm} = \lambda_{ikml} = \lambda_{lmik}$  is the elastic constant tensor.

Thus, in the Voigt scheme the problem reduces to averaging and calculating the correlation increments to the elastic constant tensor. For Reuss averaging it is necessary to write the differential equation for the strain tensor. Such an equation is the definition [4] of the incompatibility tensor  $\eta_{pq}$

$$\epsilon_{prm} \epsilon_{qsn} e_{rs,mn} + \eta_{pq} = 0. \quad (1.4)$$

Here  $\epsilon_{prm}$  is the unit skew-symmetric tensor. For an ideal medium in which there are no sources of internal stresses  $\eta_{pq} = 0$  and (1.4) degenerates into the compatibility condition.

Using Hooke's law

$$e_{rs} = s_{rsik} \sigma_{ik} \quad (1.5)$$

we can rewrite Eq. (1.4) in the form

$$\epsilon_{prm} \epsilon_{qsn} \nabla_m \nabla_n s_{rsik} \sigma_{ik} + \eta_{pq} = 0. \quad (1.6)$$

Thus, in the Reuss scheme the problem reduces to averaging and calculating the correlation increments to the elastic compliance tensor  $s_{rsik}$ .

The elastic moduli of a polycrystal of cubic structure were calculated in [5] according to the Voigt scheme with account for pair correlations between crystallites. Subsequent approximations must take into account correlations of higher order—ternary, quaternary, etc. However, this involves very laborious calculations and is complicated by the lack of sufficient experimental data for choosing the ternary and quaternary correlation functions.

Clearly, it is better to follow the other path, that is, to approach the Voigt- and Reuss-averaged values of the elastic moduli by taking into account the correlation effects in both calculating schemes. Since the first steps of the approximation are the easiest, this approach enables one to reduce by countersteps the interval of values of the elastic moduli of the polycrystal calculated by the different methods.

2. Below we calculate the effect of pair correlations between the grains of a polycrystal of cubic structure using the Reuss scheme. We start from Eq. (1.6).

For a medium with cubic structure the elastic compliance tensor has the form

$$s_{rsik} = s_1 \delta_{rs} \delta_{ik} + s_2 (\delta_{ri} \delta_{sk} + \delta_{rk} \delta_{si}) + s_3 \sum_i \delta_{rj} \delta_{sj} \delta_{ij} \delta_{ki}. \quad (2.1)$$

We represent the tensor  $s_{rsik}$  in the form of a value  $\langle s_{rsik} \rangle$  averaged over the polycrystal and a fluctuation component  $\delta s_{rsik}(r)$ . Then, assuming that there is no texture, we get

$$\langle s_{rsik} \rangle = s_1 \delta_{rs} \delta_{ik} + s_2 (\delta_{ri} \delta_{sk} + \delta_{sk} \delta_{si}), \quad (2.2)$$

$$\delta s_{rsik} = s_3 \sum_j \alpha_{rj} \alpha_{sj} \alpha_{ij} \alpha_{kj} - \frac{1}{5} s_3 (\delta_{rs} \delta_{ik} + \delta_{ri} \delta_{sk} + \delta_{rk} \delta_{si}), \quad (2.3)$$

where  $\alpha_{ij}$  are the direction cosines between the crystallographic axes and the coordinate axes. The constants  $s_1, s_1^0$  and the two-index constants  $s_{ij}$  are related as follows:

$$s_1 = s_1^0 + 1/5 s_3, \quad s_2 = s_2^0 + 1/5 s_3, \quad (2.4)$$

$$s_{11} = s_1^0 + 2s_2^0 + s_3, \quad s_{12} = s_1^0, \quad s_{44} = 4s_2^0. \quad (2.5)$$

We substitute values of the tensor  $s_{rsik}$  in (1.6). This gives

$$s_1 \epsilon_{prm} \epsilon_{qsn} \sigma_{ii,mn} + 2s_2 \epsilon_{prm} \epsilon_{qsn} \sigma_{rs,mn} = f_{pq}, \quad (2.6)$$

$$f_{pq} \equiv -\eta_{pq} - \epsilon_{prm} \epsilon_{qsn} \nabla_m \nabla_n \delta s_{rsik} \sigma_{ik}. \quad (2.7)$$

We substitute in (2.6) the relation

$$\epsilon_{prm} \epsilon_{qsn} = \begin{vmatrix} \delta_{pq} & \delta_{ps} & \delta_{pn} \\ \delta_{rq} & \delta_{rs} & \delta_{rn} \\ \delta_{mq} & \delta_{ms} & \delta_{mn} \end{vmatrix} \quad (2.8)$$

and use the equation of motion (1.1). We then get

$$-(s_1 + 2s_2) \sigma_{ii,pq} - 2s_2 \sigma_{pq,nn} + (s_1 + 2s_2) \delta_{pq} \sigma_{ii,nn} = \varphi_{pq}; \quad (2.9)$$

$$\varphi_{pq} \equiv f_{pq} - 2s_2 \delta_{pq} f_{i,i}.$$

It is easy to see that when  $\varphi \equiv 0$  Eq. (2.9) is a homogeneous Beltrami equation. In fact, setting, for example,  $p = q = 1$  and keeping in mind that

$$2s_2 / (s_1 + 2s_2) = 1 + \nu, \quad (2.10)$$

where  $\nu$  is Poisson's ratio, we find

$$(1 + \nu) \frac{\partial^2 \sigma}{\partial x^2} + \Delta \sigma_x + \Delta \sigma = 0 \quad (\sigma \equiv \sigma_{ii}, \quad \sigma_x \equiv \sigma_{xx}). \quad (2.11)$$

The remaining Beltrami equations are similarly obtained. Summing them, we see that  $\Delta \sigma = 0$  and may be omitted, which leads to the general form of the Beltrami equations.

We now determine the regular  $L_{pqik}$  and random  $R_{pqik}$  operators from the equations

$$L_{pqik} = (s_1 + 2s_2) \delta_{ik} (\nabla^2 \delta_{pq} - \nabla_p \nabla_q) - 2s_2 \nabla^2 \delta_{ip} \delta_{kq}, \quad (2.12)$$

$$R_{pqik} = -\epsilon_{prm} \epsilon_{qsn} \nabla_m \nabla_n \delta s_{rsik}. \quad (2.13)$$

Then Eq. (2.9) may be written in the form

$$L_{pqik} \sigma_{ik} = -\chi_{pq} + R_{pqik} \sigma_{ik}. \quad (2.14)$$

The function  $\chi_{pq}$  is the external source of the field and is related to  $\eta_{pq}$  and  $f_i$  as follows:

$$\chi_{pq} = \eta_{pq} + 2s_2 \delta_{pq} f_{i,i}. \quad (2.15)$$

3. To calculate the correlation increment to the tensor  $\langle s_{pqrs} \rangle$

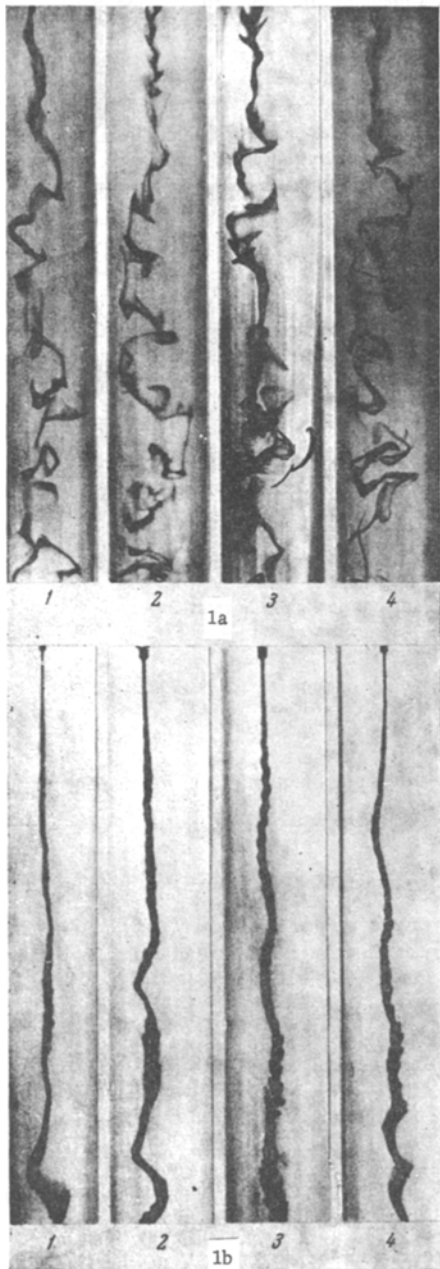


Fig. 1

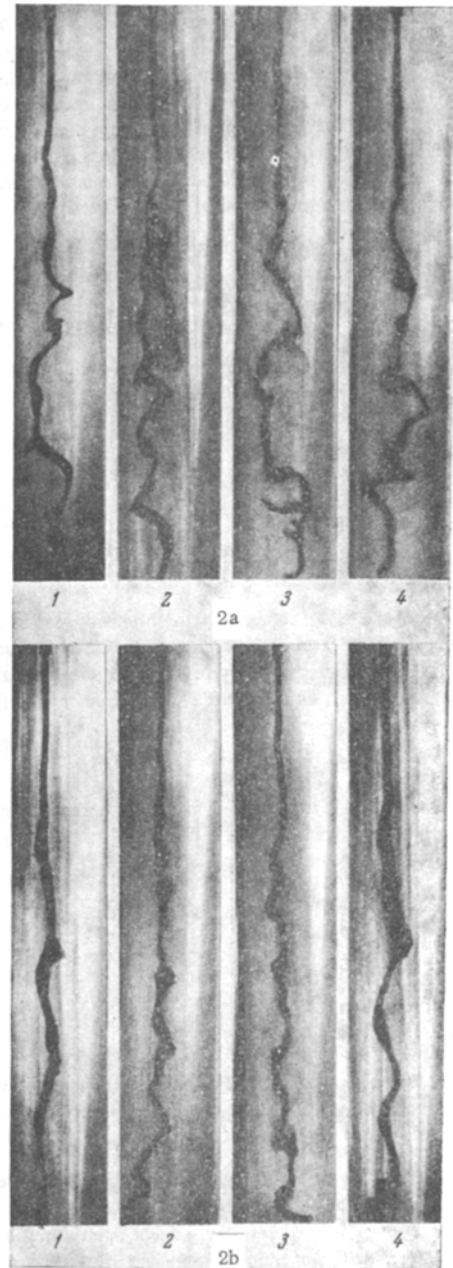


Fig. 2

it is first necessary to calculate the Green's tensor  $g_{iklm}$  of the operator  $L_{pqik}$ . This is found from the equation

$$L_{pqik}g_{iklm} = \delta_{pi}\delta_{qm}\delta(r). \quad (3.1)$$

The Green's tensor thus introduced enables us to write the solution of the inhomogeneous Beltrami equation

$$L_{pqik}\sigma_{ik} = \varphi_{pq} \quad (3.2)$$

in the form of a convolution

$$\sigma_{ik} = g_{iklm} * \varphi_{lm}. \quad (3.3)$$

We can convince ourselves of the validity of this by considering the chain of equalities

$$L_{pqik}\sigma_{ik} = L_{pqik}g_{iklm} * \varphi_{lm} = \delta_{pq}\delta_{lm}\delta(r) * \varphi_{lm} = \varphi_{pq}. \quad (3.4)$$

where we have used the property of the  $\delta$ -function:  $\delta * f = f$ .

To compute  $g_{iklm}$  we use the Fourier integral transform

$$G(k) = \int g(r) e^{ikr} dV, \quad (3.5)$$

$$g(r) = \frac{1}{8\pi^3} \int G(k) e^{-ikr} dV_k. \quad (3.6)$$

Then, substituting in (3.1) the explicit value of the operator  $L_{pqik}$ , in accordance with (2.12), we get

$$(s_1 + 2s_2)(k_p k_q - k^2 \delta_{pq}) G_{ilmn} + 2s_2 k^2 G_{pqmn} = \delta_{mp} \delta_{nq}. \quad (3.7)$$

Multiplying both sides by  $\delta_{pq}$ , we find

$$G_{ilmn} = -\frac{1}{k^2} \frac{\delta_{mn}}{2(s_1 + s_2)}, \quad (3.8)$$

which, after substitution in (3.7), gives

$$G_{pqmn} = \frac{1}{2s_2 k^2} \delta_{mp} \delta_{nq} - \frac{s_1 + 2s_2}{4s_2(s_1 + s_2)} \frac{\delta_{mn}}{k^2} (\delta_{pq} - n_p n_q) \quad (3.9)$$

$$\left( n_p \equiv \frac{k_p}{k} \right).$$

We can pass from the transform back to the original using (3.6) and the integral

$$\frac{1}{\pi^2} \int k^{-4} k_p k_q e^{ikr} dV_k = r_{,pq}. \quad (3.10)$$

This gives

$$8\pi g_{pqmn} = \frac{1}{2s_2} \delta_{mp} \delta_{nq} r_{,ii} - \frac{s_1 + 2s_2}{4s_2(s_1 + s_2)} \delta_{mn} (r_{,ii} \delta_{pq} - r_{,pq}). \quad (3.11)$$

Hence, it is clear that the Green's function, as required, tends to zero at infinity.

4. Representing the stress  $\sigma_{ik}$  in the polycrystal in the form of a regular value  $\langle \sigma_{ik} \rangle$  and a fluctuation component  $\delta\sigma_{ik}$ , we can show that, in the approximation in which only pair correlations between crystallites are taken into account, from the inhomogeneous equation (2.14) there follows the following equation for the regular part of the stress tensor [6]

$$[L_{pqik} - \langle R_{pqrs} M_{rsuv} R_{uvik} \rangle] \langle \sigma_{ik} \rangle = -\chi_{pq}. \quad (4.1)$$

Here  $M_{rsuv}$  denotes the integral Green's operator, which is related to the Green's function by the expression

$$M_{rsuv}\sigma_{uv} = g_{rsuv} * \sigma_{uv}. \quad (4.2)$$

The first term on the left side of (4.1) gives the usual Reuss averaging, whereas the second takes into account the correlation effects.

Using (2.15), we pass from the operator  $L_{pqik}$  back to the initial operator  $\epsilon_{prmn}\epsilon_{qsn}\nabla_m\nabla_n$ . Moreover, we shall assume that the regular

part of  $\sigma_{ik}$  varies only slightly at distances for which correlation effects still occur. This enables us to write (4.1) in the form

$$\epsilon_{prmn}\epsilon_{qsn}\nabla_m\nabla_n S_{rsik} \langle \sigma_{ik} \rangle = -\eta_{pq}, \quad (4.3)$$

where the effective elastic compliance tensor

$$S_{rsik} = \langle s_{rsik} \rangle - \langle \delta s_{rsmn} g_{mnab} * \epsilon_{aju} \epsilon_{blv} \nabla_u \nabla_v \delta s_{jik} \rangle. \quad (4.4)$$

We determine the binary correlation function from the equation

$$b_{jik}^{rsmn}(r-r') = \langle \delta s_{rsmn}(r) \delta s_{jik}(r') \rangle. \quad (4.5)$$

Then the correlation increment may be written in the form

$$S_{rsik} - \langle s_{rsik} \rangle = - \int g_{mnab,uv}(r-r') b_{jik}^{rsmn}(r-r') dV' \epsilon_{aju} \epsilon_{blv} = - \frac{1}{8\pi^3} \epsilon_{aju} \epsilon_{blv} \int G_{mnab}(k) k_u k_v B_{jik}^{rsmn}(k) dV_k. \quad (4.6)$$

Here we substitute the explicit value of the Fourier transform of the tensor Green's function (3.9) and take into account that for cubic symmetry

$$b_{jik}^{rsmn} \delta_{mn} = 0.$$

We get

$$S_{rsik} = \langle s_{rsik} \rangle - \frac{1}{6s_2} \left[ 1 + \frac{4}{5} \frac{2s_{12} + 3s_{11} + s_{44}}{12s_{12} + 8s_{11} + s_{44}} \right] A_{rsik}. \quad (4.7)$$

Here  $A_{rsik}$  denotes the autocorrelation tensor

$$A_{rsik} = b_{mnik}^{rsmn}(0) = s_{25} s_2^2 D_{rsik}, \quad (4.8)$$

$$D_{rsik} \equiv \delta_{ri} \delta_{sk} + \delta_{rk} \delta_{si} - \frac{2}{3} \delta_{rs} \delta_{ik}.$$

Hence it follows that the correlation increment to the compression modulus  $K$  is zero. For the effective shear modulus  $\mu^*$  we get the following expression

$$\frac{1}{\mu_R^*} = \frac{1}{\mu_R} \left\{ 1 - \frac{8}{25} \mu_R^2 \left( s_{11} - s_{12} - \frac{1}{2} s_{44} \right)^2 \times \right. \quad (4.9)$$

$$\left. \times \left[ 1 + \frac{4}{5} \frac{2s_{12} + 3s_{11} + s_{44}}{12s_{12} + 8s_{11} + s_{44}} \right] \right\},$$

where  $1/\mu_R$  is the value of the Reuss-averaged reciprocal shear modulus without account for correlation effects:

$$1/\mu_R = 1/5 [4(s_{11} - s_{12}) + 3s_{44}]. \quad (4.10)$$

For comparison we present the results of a calculation of the correlation increment using the Voigt scheme [5]:

$$\mu_V^* = \mu_V \left\{ 1 - \frac{(c_{11} - c_{12} - 2c_{44})^2}{25\mu_V^2} \left[ 1 - \frac{2}{5} \frac{3c_{12} + 2c_{11} + c_{44}}{3c_{11} + 2c_{12} + 4c_{44}} \right] \right\}. \quad (4.11)$$

Here the value of the averaged modulus without allowance for correlations

$$\mu_V = 1/5 (c_{11} - c_{12} + 3c_{44}). \quad (4.12)$$

As an example we give numerical data on the averaged shear moduli with and without allowance for the correlation increments

Metal	$\mu_V$	$\mu_V^*$	$\mu_R^*$	$\mu_R$ , 10 <sup>11</sup> dyne/cm <sup>2</sup>	$\Delta\mu_V/2\mu_V$	%	$\mu$ (exp.)
Cu	5.46	4.91	4.80	4.0	10	10	4.83
Ag	3.38	3.06	3.04	2.55	9.5	9.0	3.03
Au	3.10	2.84	2.83	2.41	8.4	8.7	2.78
Pb	1.01	0.89	0.83	0.67	12	12	0.56
K	0.174	0.14	0.14	0.085	20	18	—

As the table shows, the correlation increments are approximately the same for both schemes. Taking them into account substantially reduces the interval between averaged values of the shear modulus within which lies the exact value of  $\mu$ .

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