THE BOUNDARIES OF THE EFFECTIVE ELASTIC MODULI FOR INHOMOGENEOUS SOLIDS

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The calculation of the effective elastic moduli of inhomogeneous solids, which connect the stresses and strains averaged for the material, is accompanied by certain mathematical difficulties owing to correlation relationships of arbitrary orders. Neglect of correlation relationships leads to average elastic moduli, where averaging according to Voigt and Reuss establishes boundaries containing the effective elastic moduli [1]. Approximate values of the latter can be found by taking into account the correlation relationships of the second order in both calculation schemes [2, 3]. Another method of evaluating the true moduli consists of narrowing the boundaries of Voigt and Reuss on the basis of model representations [4-6]. The approximate effective elastic moduli for a series of polycrystals with various common-angle values are presented in [7]. An analysis of the effect of the correlation relationships between the grains of a mechanical mixture of isotropic components on the effective elastic moduli is carried out in [8], although in all the papers just mentioned the use of correlative corrections to narrow the range of elastic moduli is not investigated.* Below it is shown that the calculation of the correlation corrections in the second approximation allows the range for the effective moduli to be narrowed.

1. We consider an inhomogeneous solid which can be either a polycrystal or a solid mechanical mixture of isotropic components. We assume that the boundaries separating the components exclude the sliding of the grains relative to one another. Then the elastic field of the deformed material can be described by a system of equations, including the equations of equilibrium, compatibility, and Hooke's law. The explicit form of these equations, in the presence of internal and external stresses, is given, for example, in [9]. Below, the unified matrix form is used for equations of equilibrium and compatibility

$$LZ + F = 0, \qquad (1.1)$$

where the operator and the function in the equations of equilibrium have the form

$$L_{il} = \nabla_k \lambda_{iklm} \nabla_m, \quad Z_i = u_i, \quad F_i = f_i. \qquad (1.2)$$

*In [3] it was proposed that the scheme of Reuss be used for the calculation of the correlative corrections. Although the formulas introduced in this investigation are correct, the statement that the second approximation of the schemes of Voigt and Reuss (consideration of binary correlations) provides the upper and lower limits is incorrect. In reality the upper and lower limits are provided by the first and, as is shown below, the third approximations of the method, while the effective moduli calculated in the second approximation of the schemes of Voigt and Reuss lie on the same side of their true values.

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In the equations of compatibility, respectively, we have

$$L_{iklm} = e_{ipq}e_{krs}\nabla_p\nabla_r s_{qslm}, \quad Z_{lm} = \sigma_{lm}, \quad F_{ik} = \eta_{ik}. \tag{1.3}$$

Here $\lambda_{ikl m}$ and s_{sqlm} are, respectively, the tensors of the elastic moduli and flexibilities; u_i and f_i are the vectors of displacements and density of the body forces; σ_{lm} and η_{ik} are the tensors of the stresses and displacements; e_{ipq} is the antisymmetric unit tensor.

By dividing the operators and functions into regular and random components and from Eq. (1.1), we find that

$$\langle L\rangle\langle Z\rangle + \langle L'Z'\rangle + F = 0, \tag{1.4}$$

where the angular brackets are used to denote averaging. The averaging is carried out over a region of dimensions small in comparison to the distance over which the regular part of the functions varies significantly, but large in comparison to the space scale of correlation. Expressing the random component Z' in terms of the regular component $\langle Z \rangle$ by means of a certain integral operator Q'

$$Z' = Q' \langle Z\rangle \tag{1.5}$$

we rewrite Eq. (1.4) in the form

$$L^* \langle Z\rangle + F = 0, \quad L^* = \langle L\rangle + \langle L' Q'\rangle. \tag{1.6}$$

The explicit expression of the operator Q' has the form [10]

$$Q' = X + (X^2 - \langle X^2\rangle) + (X^3 - X\langle X^2\rangle - \langle X^3\rangle) + \\ + (X^4 - X^2\langle X^2\rangle - X\langle X^3\rangle - \langle X^4\rangle + \langle X^2\rangle^2) + \ldots, \tag{1.7}$$

Here X is used to denote the operator M*L', where M* is given by the equation

$$\langle L\rangle M^* + I = 0. \tag{1.8}$$

Here the unit matrix I in the second order has the components δ_{ij}, while in the fourth order it has the components $\delta_{i(p}\delta_{q)j}$, where symmetrication is carried out with respect to the subscripts enclosed by the round brackets. The kernel of the integral operator M* is the Green function G of the operator $\langle L \rangle$:

$$M^*\delta(\mathbf{r}) = G(\mathbf{r}). \tag{1.9}$$

The explicit form of the Green functions for the equations of equilibrium and compatibility is given by the expressions [11, 12]

$$G_{ij}(\mathbf{r}) = \frac{1}{8\pi\mu}(\delta_{ij}r_{,pp} - \varkappa r_{,ij}), \quad \varkappa \equiv \frac{\lambda+\mu}{\lambda+2\mu}, \tag{1.10}$$

$$G_{iklm}(\mathbf{r}) = \frac{1}{32\pi q}\left\{\left[-\frac{s}{s+q}(\delta_{ik}\delta_{lm}\nabla^2 - \delta_{ik}\nabla_l\nabla_m - \delta_{lm}\nabla_i\nabla_k) + \right.\right. \\ \left.\left. + 2e_{lp(i}e_{k)mq}\nabla_p\nabla_q\right] r - \frac{s}{12(s+q)}\nabla_i\nabla_k\nabla_l\nabla_m r^3\right\}, \tag{1.11}$$

where λ, μ, s, and q are used to denote the elastic constants averaged over the aggregate

$$\langle\lambda_{iklm}\rangle = \lambda\delta_{ik}\delta_{lm} + 2\mu\delta_{i(l}\delta_{m)k}, \tag{1.12}$$

$$\langle s_{iklm}\rangle = s\delta_{ik}\delta_{lm} + 2q\delta_{i(l}\delta_{m)k}. \tag{1.13}$$

The operator L^* determines the renormalized equations of equilibrium and compatibility. Substituting into (1.6) the definitions of the original operator L, we find

$$L_{il}^* = \nabla_k \lambda_{iklm}^* \nabla_m, \qquad L_{iklm}^* = e_{ipq} e_{krs} \nabla_p \nabla_r s_{qslm}^*, \tag{1.14}$$

where λ_{iklm}^* and s_{qslm}^* are the effective tensors of the elastic constants and flexibilities, giving the relationship between the average tensors of stresses and strains according to Hooke's law

$$\langle \sigma_{ik} \rangle = \lambda_{iklm}^* \langle \varepsilon_{lm} \rangle, \qquad \langle \varepsilon_{ik} \rangle = s_{iklm}^* \langle \sigma_{lm} \rangle. \tag{1.15}$$

In [7] the effective tensors of the elastic moduli and flexibilities were calculated in the second approximation obtained from (1.6), (1.7), and (1.14) with the condition that $Q' = X$

$$\lambda_{iklm}^* \approx \langle \lambda_{iklm} \rangle + \langle \lambda_{ikpq}' M_{pr,\, qs}^* \lambda_{rslm}' \rangle, \tag{1.16}$$

$$s_{iklm}^* \approx \langle s_{iklm} \rangle + \langle s_{ikpq}' e_{vur} e_{njs} M_{pqvn,\, uj}^* s_{rslm}' \rangle. \tag{1.17}$$

2. We show that (1.16) and (1.17) do not give a range containing the exact value of the effective elastic moduli or flexibilities. For this we consider the model of an inhomogeneous medium formed from a mixture of isotropic components for which the shear moduli coincide. For such a medium the series (1.7) can be summed [8], giving

$$K^* = \langle K \rangle - \frac{D_K}{c_1 K_2 + c_2 K_1 + {}^4/_3 \mu}, \qquad \mu^* = \mu, \qquad D_K \equiv \langle K'^2 \rangle. \tag{2.1}$$

Equations (2.1) are obtained by using either the scheme of Voigt or the scheme of Reuss. The coincidence of the results is a consequence of the fact that both schemes lead to the exact value of the effective elastic moduli.

To establish the relations between the exact values of the effective elastic moduli and their approximate values, in the schemes of Voigt and Reuss we draw attention to the fact that one of the expansion series for the effective elastic moduli or the flexibilities is of constant sign, while the other is of alternating sign. Indeed, for the model of an inhomogeneous medium under consideration, the operator Q' can be represented in the schemes of Voigt and Reuss, respectively, by the following expressions:

$$Q_{ij}' = \frac{1}{4\pi} \nabla_i \frac{1}{r} * \alpha' \nabla_j, \qquad \alpha' \equiv x' \sum_0^\infty \xi^n; \tag{2.2}$$

$$Q_{ijkl}' = \frac{1}{2} \left(\delta_{ij} + \frac{1}{4\pi} \nabla_i \nabla_j \frac{1}{r} * \right) \beta' \delta_{kl}, \qquad \beta' \equiv - y' \sum_0^\infty \eta^n; \tag{2.3}$$

$$x \equiv \frac{K}{\langle K + {}^4/_3 \mu \rangle}, \qquad y \equiv \frac{1}{K} \left\langle \frac{1}{K} + \frac{3}{4\mu} \right\rangle^{-1},$$

$$\xi \equiv (c_1 - c_2)(x_1 - x_2), \qquad \eta \equiv (c_1 - c_2)(y_1 - y_2). \tag{2.4}$$

Here the asterisk sign denotes operation of integral convolution, while the subscripts in (2.4) indicate the component number of the mixture. Since ξ and η have different signs, one of series (2.2) or (2.3) is of constant sign, while the other is of alternating sign. Therefore, we denote the effective moduli of all-sided compression, calculated in the n-th approximation in the schemes of Voigt and Reuss, by $K_V^{(n)}$ and $K_R^{(n)}$ and we find that

$$K^* = K_V^{(n)} + \Delta K_V^{(n)} = K_R^{(n)} + \Delta K_R^{(n)}, \tag{2.5}$$

$$K_V^{(n)} = \langle K \rangle - \frac{D_K}{\langle K + {}^4/_3 \mu \rangle} \sum_0^{n-2} \xi^k, \tag{2.6}$$

$$\frac{1}{K_R^{(n)}} = \left\langle \frac{1}{K} \right\rangle - D_{1/K} \left\langle \frac{1}{K} + \frac{3}{4\mu} \right\rangle^{-1} \sum_0^{n-2} \eta^k. \quad (2.7)$$

By comparing (2.1) with Eq. (2.6) and (2.7), we obtain

$$\Delta K_V^{(n)} = -\frac{D_K}{\langle K + {}^4/_3\mu \rangle} \frac{\xi^{n-1}}{1-\xi}, \quad (2.8)$$

$$\Delta K_R^{(n)} = K_R^{(n)} K^* D_{1/K} \left\langle \frac{1}{K} + \frac{3}{4\mu} \right\rangle^{-1} \frac{\eta^{n-1}}{1-\eta}. \quad (2.9)$$

Hence we see that for even n the corrections $\Delta K_V^{(n)}$ and $\Delta K_R^{(n)}$ have the same sign, while for odd n their signs are opposite. Thus, even approximations for $K_V^{(n)}$ and $K_R^{(n)}$ give values that lie on one side of K*. Contrarily, odd approximations form a range containing the exact value of the effective modulus K*.

3. We now consider the more common case of a mixture of two isotropic components which differ from one another not only by the volume modulus but also by the shear modulus. Here it is not possible to find the exact values of the effective elastic moduli. The following results are obtained in the second approximation:

$$K_V^{(2)} = \langle K \rangle - \frac{D_K}{\langle K + {}^4/_3\mu \rangle}, \qquad \mu_V^{(2)} = \langle \mu \rangle - \frac{2D_\mu \langle K + 2\mu \rangle}{5\langle \mu \rangle \langle K + {}^4/_3\mu \rangle}; \quad (3.1)$$

$$\frac{1}{K_R^{(2)}} = \left\langle \frac{1}{K} \right\rangle - D_{1/K} \left\langle \frac{1}{K} + \frac{3}{4\mu} \right\rangle^{-1},$$

$$\frac{1}{\mu_R^{(2)}} = \left\langle \frac{1}{\mu} \right\rangle - \frac{2}{5} D_{1/\mu} \left\langle \frac{1}{K} + \frac{9}{8\mu} \right\rangle \left[\left\langle \frac{1}{\mu} \right\rangle \left\langle \frac{1}{K} + \frac{3}{4\mu} \right\rangle \right]^{-1}. \quad (3.2)$$

In the third approximation of Voigt's scheme the effective tensor of elastic moduli is given by

$$\lambda_{iklm}^{(3)} = \lambda_{iklm}^{(2)} + \langle \lambda'_{ikpq} G_{pr,\,qs} * \lambda'_{rstv} G_{tj,\,vn} * \lambda'_{jnlm} \rangle. \quad (3.3)$$

Hence

$$K_V^{(3)} = K_V^{(2)} + [D_K^{(3)} \delta_{pq} \delta_{rs} + \langle K'^2 \mu' \rangle D_{pqrs}] I_{krls}^{ipjq} \delta_{ij} \delta_{kl},$$
$$\mu_V^{(3)} = \mu_V^{(2)} + {}^1/_5 [\langle K' \mu'^2 \rangle \delta_{pq} \delta_{rs} + D_\mu^{(3)} D_{pqrs}] I_{krls}^{ipjq} D_{ijkl}; \quad (3.4)$$

where

$$I_{krls}^{ipjq} \equiv \frac{1}{(8\pi^3)^3} \int \overline{G}_{ip,\,jq}(\mathbf{k}_1) \overline{G}_{kr,\,ls}(\mathbf{k}_2) \overline{\varphi}(\mathbf{k}, |\mathbf{k}-\mathbf{k}_1|, |\mathbf{k}-\mathbf{k}_2|);$$
$$d\mathbf{k} d\mathbf{k}_1 d\mathbf{k}_2, \qquad D_K^{(3)} \equiv \langle K'^3 \rangle, \qquad D_\mu^{(3)} \equiv \langle \mu'^3 \rangle. \quad (3.5)$$

Here a bar is used to denote the Fourier integral transformation and Φ denotes the function describing the coordinate dependence of the trinary correlation function of the tensor of elastic moduli

$$\langle \lambda'_{ijkl}(\mathbf{r}) \lambda'_{pqrs}(\mathbf{r}_1) \lambda'_{nmuv}(\mathbf{r}_2) \rangle = \langle \lambda'_{ijkl}(\mathbf{r}),$$
$$\lambda'_{pqrs}(\mathbf{r}) \lambda'_{nmuv}(\mathbf{r}) \rangle \varphi(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2). \quad (3.6)$$

In (3.5) we have taken into account the quasi homogeneity and isotropy of the space the relation

$$\varphi(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2) = \varphi(|\mathbf{r}-\mathbf{r}_1|, |\mathbf{r}_1-\mathbf{r}_2|, |\mathbf{r}_2-\mathbf{r}|)$$

holds.

To determine the sign for the correlative correction of the third order we consider, for the sake of being definite, the total deviatoric integral convolutions (3.5). The deviatoric contractions of the Fourier transformed Green functions derivatives give

$$D_{pqrs}D_{ijkl}\overline{G}_{ip,\,jq}\overline{G}_{kr,\,ls} = \frac{16}{9}(1-\varkappa)^2 + 2t^2 + \\ + \frac{1}{3}(1-t^2)(8\varkappa - 1 - 4\varkappa^2 - 12\varkappa^2 t^2), \tag{3.7}$$

where $t \equiv k_1k_2/k_1k_2$, the Fourier transform of the function φ ($\mathbf{r}$, $\mathbf{r}_1$, $\mathbf{r}_2$) for an isotropic medium with deterministic boundaries, between parts of inhomogeneities, can be represented in the form [8]

$$\overline{\varphi}(\mathbf{k}', \mathbf{k}'', \mathbf{k}''') = \overline{\varphi}_0(\mathbf{k}')\,\overline{\varphi}_0(\mathbf{k}'')\,\overline{\varphi}_0(\mathbf{k}'''),\ \overline{\varphi}_0(\mathbf{k}) = \frac{8\pi}{(1+k^2)^2}. \tag{3.8}$$

Hence we see that the integrand of the quantity $D_{pqrs}D_{ijkl}\,I^{ipjq}_{krls}$ is a positive definite function of its arguments. At the same time it is shown that the constant $D_{pqrs}\,D_{ijkl}\,I^{ipjq}_{krls} > 0$. Analogously we can show that the tensorial contractions $\delta_{pq}\ \delta_{rs}\ D_{ijkl}\ I^{ipjq}_{krls}$ and $\delta_{pq}\ \delta_{rs}\ \delta_{ij}\ \delta_{kl}\ I^{ipjq}_{krls}$ are positive. Thus, the sign of correlative correction for the third approximation is determined by the sign of the central moments of the third order for the elastic moduli K and μ.

Let now the inequalities $(c_1-c_2)\ (K_1-K_2) > 0$ and $(c_1-c_2)\ (\mu_1-\mu_2) > 0$ be satisfied simultaneously. Then, taking the central moments of the third order in the form

$$< K'^2\ \mu' > = c_1c_2\,(c_2-c_1)\,(K_1-K_2)^2\ (\mu_1-\mu_2), \tag{3.9}$$

we find that the correlative additions of the third order to the average moduli K and μ are negative; i.e., the signs of the correlative corrections in the second and third approximations coincide. Analogously, we can consider higher approximations of the method, and it can show that the correlative corrections in the case $(c_1-c_2)(K_1-K_2) > 0$ and $(c_1-c_2)(\mu_1-\mu_2) > 0$ are negative.

By the same method we can show that, for the above relations between the concentrations and the elastic moduli, the expansions of K^* and μ^*, with respect to the correlation function in the scheme of Reuss, are given by series of alternating signs.

Another approach to determine the range containing the true value of the elastic moduli is based on variational principles [4]. Such an approach enabled Hashin to establish the following boundaries for mechanical mixtures:

$$K_+ = \langle K\rangle - \frac{D_K}{c_1K_2 + c_2K_1 + {}^4/_3\mu_1}, \quad K_- = \langle K\rangle - \frac{D_K}{c_1K_2 + c_2K_1 + {}^4/_3\mu_2}, \\ \mu_+ = \langle \mu\rangle - \frac{D_\mu}{c_1\mu_2 + c_2\mu_1 + b_1\mu_1}, \quad \mu_- = \langle \mu\rangle - \frac{D_\mu}{c_1\mu_2 + c_2\mu_1 + b_2\mu_2}, \\ b_i \equiv \frac{9K_i + 8\mu_i}{6(K_i + 2\mu_i)}, \quad K_1 > K_2, \quad \mu_1 > \mu_2. \tag{3.10}$$

Here, the plus and minus signs denote respectively the upper and lower boundaries of the elastic moduli. Comparing (3.1) and (3.2) with the boundaries (3.10) of Hashin, we find that for $c_1 > c_2$ the values of $K_V^{(2)}$ and $\mu_V^{(2)}$ are located within the range of Hashin for the concentration of the first component $c_1 = 1 - c_V$, while $K_R^{(2)}$ and $\mu_R^{(2)}$ lie within it for $c_1 < 1 - c_R$. Here c_V and c_R are given by

$$c_V = \frac{1}{2(1+y_V)}, \quad c_R = \frac{1}{2(1+y_R)}, \\ y_V = \frac{2}{3}\,\frac{\mu_1-\mu_2}{K_1-K_2}, \quad y_R = y_V\,\frac{9}{16}\,\frac{K_1K_2}{\mu_1\mu_2}. \tag{3.11}$$

Since in the case under consideration $K_1 > K_2$, $\mu_1 > \mu_2$, and $c_1 > c_2$, averaging in the second approximation of random-function theory gives $K_V^{(2)} > K^*$ and $K_R^{(2)} > K^*$, and analogously for μ, the elastic moduli $K^{(2)}$ and $\mu^{(2)}$ are located on the right of the exact value of K^* and μ^*. Therefore, if $K_-^{(2)} < K_-$, then the right boundary of the range can be replaced by its value, where $K_-^{(2)}$ is the smaller one of the value of $K_V^{(2)}$ and $K_R^{(2)}$. For $c_1 < 1 - c_+$ both values of $K_V^{(2)}$ and $K_R^{(2)}$ lie within the range of Hashin, while for $c_1 < 1 - c_-$ only $K_-^{(2)}$ lies within this range. Here c_+ and c_- are respectively the larger and smaller values of the quantities c_V and c_R. Analogous conclusions hold also for the shear modulus, where the concentrations c_V and c_R are determined as before by (3.11).

If $K_1 > K_2$ and $\mu_1 > \mu_2$, while $c_1 < c_2$, then the quantities $K^{(2)}$ and $\mu^{(2)}$ lie on the left of the exact values for the effective elastic moduli K^* and μ^*. This allows us to improve the left boundary of Hashin. In this case, for $c_1 > c_+$, both $K_V^{(2)}$ and $K_R^{(2)}$ lie within the range of Hashin, while for $c_1 > c_-$ only the larger of them, $K_+^{(2)}$, lies within the range.

As an illustration we consider $K = {}^4/_3\,\mu$, $K_1 = 2$, $K_2 = 1$ and $c_1 = 0.6$. Then $c_+ = c_- = {}^1/_3$. Hence we find that $K_V = 1.6$; the range without the correlations taken into account is $K_V - K_R = 0.171$; the range of Hashin is $K_+ - K_- = 0.029$, and the improved range, with the second approximation of the random-function theory taken into account, is $K_-^{(2)} - K_- = 0.022$.

4. We now proceed to consider the elastic moduli of polycrystals. We confine ourselves to the consideration of a cubic system. Then the tensors of elastic moduli and flexibilities of the crystallite in a crystallographic coordinate system can be written in the form

$$\lambda_{iklm} = \lambda_1^\circ \delta_{ik}\delta_{lm} + 2\lambda_2^\circ \delta_{i(l}\delta_{m)k} + \lambda_3 \Sigma \delta_{in}\delta_{kn}\delta_{ln}\delta_{mn}, \tag{4.1}$$

$$s_{iklm} = s_1^\circ \delta_{ik}\delta_{lm} + 2s_2^\circ \delta_{i(l}\delta_{m)k} + s_3 \Sigma \delta_{in}\delta_{kn}\delta_{ln}\delta_{mn}. \tag{4.2}$$

Here the elastic constants with a single subscript are connected with those having two subscripts by the relations

$$\lambda_1^0 = c_{12}, \quad \lambda_2^0 = c_{44}, \quad \lambda_3 = c_{11} - c_{12} - 2\,c_{44},$$
$$s_1^0 = s_{12}, \qquad 4s_2^0 = s_{44}, \qquad s_3 = s_{11} - s_{12} - {}^1/_2 s_{44}. \tag{4.3}$$

The second approximation of random-function theory leads to the following expressions for the effective moduli of all-sided compression and shear [2, 3, 7]:

$$\lambda_{iklm}^{(2)} = \lambda_1 \delta_{ik}\delta_{lm} + 2\lambda_2 \delta_{i(l}\delta_{m)k} - \frac{(3\lambda_1 + 8\lambda_2)\lambda_3^2}{125\lambda_2(\lambda_1 + 2\lambda_2)} D_{iklm}; \tag{4.4}$$

$$s_{iklm}^{(2)} = s_1 \delta_{ik}\delta_{lm} + 2s_2 \delta_{i(l}\delta_{m)k} - \frac{(6s_1 + 7s_2)s_3^2}{250 s_2 (s_1 + s_2)} D_{iklm}$$
$$(\lambda_1 = \lambda_1^\circ + {}^1/_5\lambda_3,\ \lambda_2 = \lambda_2^\circ + {}^1/_5\lambda_3,\ s_1 = s_1^\circ + {}^1/_5 s_3,\ s_2 = s_2^\circ + {}^1/_5 s_3). \tag{4.5}$$

From (4.4) and (4.5) it is seen that

$$\mu_V^{(2)} = \lambda_2 - \frac{(3\lambda_1 + 8\lambda_2)\lambda_3^2}{125\lambda_2(\lambda_1 + 2\lambda_2)}, \qquad \frac{1}{\mu_R^{(2)}} = 4s_2 - \frac{2(6s_1 + 7s_2)s_3^2}{125 s_2 (s_1 + s_2)}, \tag{4.6}$$

while the effective volume modulus coincides with the average modulus [13]. In the third approximation, for Voigt's scheme and from (3.3), we find that

$$\mu_V^{(3)} = \mu_V^{(2)} + {}^1/_{50}\lambda_3 A_{pqkl}^{ijrs} I_{krls}^{ipjq}. \tag{4.7}$$

Here the auto-correlation tensor is given by [14]

$$A_{pqkl}^{ijrs} = \frac{\lambda_3^2}{60 \cdot 7!!}\left(35\delta_{pqkl}^{ijrs} + 63\delta_{ijrs}\delta_{pqkl} - 45\beta_{pqkl}^{ijrs}\right), \tag{4.8}$$

where $\delta_{ij\ldots l}$ is the sum of products of the Kronecker δ symbols with all possible permutations of any 2n subscripts. The number of terms of such a sum equals $(2n-1)!!$. By β_{pqkl}^{ijrs} in (4.8) we have denoted

$$\beta_{pqkl}^{ijrs} \equiv \delta_{ij}\delta_{rspqkl} + \delta_{ir}\delta_{jspqkl} + \delta_{is}\delta_{jrpqkl} + \delta_{jr}\delta_{ispqkl} + \delta_{js}\delta_{irpqkl} + \delta_{rs}\delta_{ijpqkl}. \tag{4.9}$$

To determine the correlative addition sign in (4.7) we consider auto-correlation tensor contractions with the Fourier transforms of Green function derivatives. Carrying out the calculations, analogously to that of deriving (3.7), we obtain

$$A_{pqkl}^{ijrs}\overline{G}_{ip,\,jq}\overline{G}_{rk,\,sl} = \frac{1}{5!!\,7!!}\frac{\lambda_3^2}{\lambda_2^2}\,[(190-155\varkappa+12\varkappa^2)+ + (1-t^2)(72\varkappa-1-24\varkappa^2)+3(1-t^2)^2\varkappa^2]. \tag{4.10}$$

Since $1/4<\varkappa\leq 1$, (4.10) is positive definite. Hence it follows that the quantity $A_{pqkl}^{ijrs}\,I_{rksl}^{ipjq}>0$. Thus, the sign of the correlative addition in Voigt's scheme is determined by the sign of the elastic constant λ_3.

From (4.3) it follows that $\lambda_3 s_3 < 0$. Therefore, the signs of the correlative increments to the moduli of elasticity and flexibility in the third approximation are opposing one another; i.e. the shear moduli, with the third order correlation taken into account, form a range containing the exact value of the effective shear modulus, just as in a mechanical mixture.

From the above analysis it follows that if $\lambda_3<0$ the effective shear moduli in the second approximation, $\mu_V^{(2)}$ and $\mu_R^{(2)}$, are larger than the exact value μ^*, while in the case $\lambda_3>0$ both values $\mu_V^{(2)}$ and $\mu_R^{(2)}$ are less than μ^*.

The results obtained here can be used to establish the boundaries containing the exact value of the effective shear modulus. For the sake of being definite, let us confine ourselves to $\lambda_3<0$. We then have the following inequalities:

$$\mu_R<\mu^*<\mu^{(2)}<\mu_V, \qquad \mu_R=\frac{1}{4s_2}, \qquad \mu_V=\lambda_2. \tag{4.11}$$

Since $\lambda_3<0$, the inequality $\mu_R^{(2)}<\mu_V^{(2)}$ holds, and the right boundary of μ_V can be replaced by $\mu_R^{(2)}$.

Another method of narrowing the range was worked out by Hashin [5] who obtained the following inequalities:

$$\mu_R<G_1^*<\mu^*<G_2^*<\mu_V. \tag{4.12}$$

Here the following notations have been used:

$$G_1^* = G_1+3\left(\frac{5}{G_2-G_1}-4\beta_1\right)^{-1}; \qquad G_2^* = G_2-2\left(\frac{5}{G_2-G_1}+6\beta_2\right)^{-1};$$
$$\beta_i = -\frac{3(K+2G_i)}{5G_i(3K+4G_i)}; \qquad G_1=\frac{1}{2}(c_{11}-c_{12});$$
$$G_2=c_{44},\ K=c_{11}+2c_{12}. \tag{4.13}$$

By a direct calculation we can show that the following inequalities hold: $\mu_R^{(2)}<\mu_V^{(2)}\,G_2^*$. Therefore in the role of the right boundary we must take the value $\mu_R^{(2)}$, while G_1^* can be taken as the left boundary

$$G_1^*<\mu^*<\mu_R^{(2)}. \tag{4.14}$$

Equation (4.14) determines the improved range for the effective shear modulus of polycrystals of cubic structure. In a contrary case of $\lambda_3>0$, instead of (4.14) we have

$$\mu_V^{(2)}<\mu^*<G_1. \tag{4.15}$$

For illustration purposes, values of the shear moduli of cubic polycrystals are given in the table. In the table the values of the elastic constants are taken with accuracy up to three significant digits. The

	Ag	Au	Cu	K	Li	Mo
c_{11}	12.40	18.63	16.84	0.458	1.480	45.5
c_{12}	9.34	15.68	12.14	0.374	1.250	17.57
c_{44}	4.61	4.20	7.54	0.263	1.080	10.99
μ_R	2.5537	2.4131	4.0034	0.0846	0.2479	12.0135
G_1^*	2.9017	2.7206	4.5964	0.1119	0.3614	12.0954
$\mu_R^{(2)}$	3.0558	2.8534	4.8792	0.1373	0.4945	12.0963
$\mu_V^{(2)}$	3.0676	2.8573	4.9086	0.1428	0.5387	12.0970
G_2^*	3.0886	2.8780	4.9445	0.1453	0.5820	12.1034
μ_V	3.3780	3.1101	5.4640	0.1747	0.6940	12.1300
z	21	18	23	32	66	25

values of average and effective elastic moduli are given with accuracy to five significant digits, three of which correspond to the initial accuracy of the experimental data, while the subsequent two allow us to calculate, with accuracy up to two significant digits, the absolute values of the differences in the moduli. In the case $\lambda_3 < 0$ the difference $G^*_2 - G^*_1$ gives the range of Hashin, while $\mu_R^{(2)} - G_1^*$ gives the improved range. In the last row of the table the quantity z is given, characterizing the narrowing of the range of Hashin due to the substitution $G_2^* \to \mu_R^{(2)}$. The quantity z is given by

$$z = \left(\frac{G_2^* - G_1^*}{\mu_R^{(2)} - G_1^*} - 1\right) 100\%, \quad z = \left(\frac{G_1^* - G_2^*}{\mu_V^{(2)} - G_2^*} - 1\right) 100\%, \tag{4.16}$$

the first of which refers to the condition $\lambda_3 < 0$, while the second refers to $\lambda_3 > 0$. In all cases, with the exception of molybdenum $\lambda_3 < 0$ and therefore $G_2^* > G_1^*$. For molybdenum $G^*_2 < G^*_1$, but for the sake of convenience the values G^*_1 and G^*_2 are written in the table as before in rising order. From the table it is seen that the method considered here allows us to narrow the Hashin boundaries by several tens of per cent.

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