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# Upper and Lower Bounds of Average Elastic Constants of an Anisotropic Polycrystalline Medium: Calculations and *A Priori* Estimates

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**Abstract**—A general procedure is suggested for calculating the upper (Voigt) and lower (Reuss) bounds of the average elastic constants of an anisotropic medium from crystallographic directions. The elastic tensors of Hooke's law can be expanded into irreducible representations of the rotation group. The Voigt/Reuss-averaged elastic constants depend on the second and fourth moments of the distribution function rather than on the entire function used for the averaging. In this case, the distribution function depends on one angle, while the elastic constants depend on two variables. The limitations imposed by the probability theory on the moment values are investigated and used to derive general constraints on the Voigt (Reuss) bounds of elastic constants.

*Keywords:* seismic anisotropy, microheterogeneous media, averaging, Hooke's law, stiffness tensor, Voigt bound, distribution function, inequality for function moment

## INTRODUCTION

Seismology commonly deals with complex media that are microheterogeneous on the scale of seismic wavelengths, with poorly constrained orientations of crystal lattice planes and stronger anisotropy in minerals than in large-scale rock volumes. Olivine, one of most widespread mantle minerals, has strongly anisotropic elastic properties, with a 25% difference of *P*-wave velocities along fast and slow directions, but the mantle is generally isotropic (anisotropy within 5%). The elastic constants of rocks and minerals are calculated as averages over some distribution function chosen for lattice orientations.

The averaging of elastic constants of microheterogeneous media has a very long history dating back to the works of Voigt (1889) and Reuss (1929) who suggested to average the elastic tensors of Hooke's law: stiffness tensor and compliance tensor (its inverse), respectively. Later it was shown that the two average tensors are, respectively, the upper and lower bounds of the volume average tensor. Originally it was assumed that all lattice plane orientations were equally probable and that the average medium was isotropic, though some cases of preferred orientation were mentioned in the review of Shermergor (1977). Nontrivial distribution functions of crystal plane orientations were discussed in some publications (Roe, 1965; Morris, 1969; Sayers, 1994, 2005, 2013; Zuo et al., 1989; Jacobsen et al., 2003). However, the results were obtained for specific cases and presented in the tabular form, which failed to provide a clear picture, apparently, because of poorly suitable formalism. The averaging was applied directly to the components of three-dimensional tensors, which were transformed using a matrix of 3D rotations, and the matrix elements were expressed via Euler angles; the procedure also included integration of numerous dot products of sines and cosines.

The key idea of this study consists in preliminary use of some linear combinations of tensor components which corresponds to expansion of the tensor into irreducible rotation group representations, in the same way as the distribution function in the cited publications was expanded into generalized spherical functions. Thus the averaging becomes trivial and can be performed in the most general case for any symmetry and distribution function of lattice plane orientations.

With this approach, quite different distribution functions turn out to be equivalent, i.e., may lead to the same average elastic constants. Or, more precisely, the bounds of elastic constants depend on second or fourth moments of the distribution function rather than on the entire function, altogether on 106 variables. Any two distribution functions that have identical sets of moments will lead to the same bounds of the average elastic constants. In mathematical notations, all distribution functions are divided into classes of equivalent functions. The classes can be enumerated by defining the second and fourth moments of the distribution function, while the bounds of elastic constants turn out to be the linear functions of the moments rather than the functionals of the distribution function. Some of these properties were noted in previous studies but their origin is explicable uniquely using the expansion of elastic tensors. This fact allows simplification for further analysis.

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Note that the above case is the simplest one, with triclinic symmetry in both the whole medium and in its constituents, while the symmetry patterns in practical seismology are much more complicated. Macroscopic anisotropy is commonly interpreted in terms of transverse isotropy, and the microscopic medium constituents are either transversely isotropic as well or have orthorhombic symmetry (like many minerals). Eventually, the scaring number 106 reduces to only two variables for the distribution function of a transversely isotropic medium consisting of transversely isotropic elements and to five variables for that consisting of orthorhombic elements.

Note especially that the consideration below, although addressing Voigt averaging (upper bounds of elastic constants), actually is based on the transformation properties of the stiffness tensor associated with rotation of coordinates and on its symmetry. This approach is also valid for Reuss averaging (lower bound of elastic constants). Furthermore, since the compliance tensor $s_{ijkl}$ is inverse to the stiffness tensor $c_{ijkl}$, the two have the same symmetry (transverse isotropy). Thus, the general equation, as well as those for specific cases, hold also for the components of $s_{ijkl}$ corresponding to those of $c_{ijkl}$. All conclusions likewise apply to any tensor that characterizes any property of the medium (not only elasticity) and has the same symmetry as the elastic tensors. The approach can be obviously extended to other tensor types related to anisotropy (e.g., dielectric permittivity).

The Voigt and Reuss bounds are either close to or far from the average elastic tensors depending on microstructure, which is evident when the tensor can be calculated precisely. For instance, Schoenberg and Muir (1989) suggested a calculus for a finely layered anisotropic medium assuming constant strain within each layer, constant stress normal to the layer boundaries, and constant strain tensor in the layer planes over the whole medium.

The medium modeled in this study consists of alternating layers of two types and equal thicknesses composed of the same transversely isotropic material with the stiffness tensor

$$c=\begin{pmatrix} 50.0000 & 34.0000 & 19.3666 & 0 & 0 & 0 \\ . & 50.0000 & 19.3666 & 0 & 0 & 0 \\ . & . & 25.0000 & 0 & 0 & 0 \\ . & \text{SYM} & . & 4.0000 & 0 & 0 \\ . & . & . & . & 4.0000 & 0 \\ . & . & . & . & . & 8.0000 \end{pmatrix},$$

and the symmetry axis normal to the layer boundaries in the first layer and the crystallographic directions rotated through the orthogonal matrix in the second layer

$$u_1=\begin{pmatrix} 0.3330 & 0.5768 & -0.7459 \\ -0.7381 & 0.6518 & 0.1745 \\ 0.5868 & 0.4924 & 0.6428 \end{pmatrix}.$$

Then, the Voigt average stiffness tensor corresponds to orthorhombic symmetry:

$$c^a=\begin{pmatrix} 43.4076 & 30.5525 & 22.5825 & -1.2113 & -2.9524 & -2.2617 \\ . & 45.1080 & 22.9014 & -2.8042 & -1.8331 & -2.5601 \\ . & . & 29.8784 & -2.2567 & -2.6894 & -0.9044 \\ . & \text{SYM} & . & 5.7039 & 0.6319 & 0.1724 \\ . & . & . & . & 5.9267 & 0.4715 \\ . & . & . & . & . & 7.6724 \end{pmatrix},$$

while the exact volume average stiffness tensor corresponds to monoclinic symmetry:

$$c^e=\begin{pmatrix} 41.7069 & 29.1243 & 20.7635 & -0.5581 & -1.8317 & -1.9712 \\ . & 43.2189 & 20.9677 & -1.7618 & -0.9331 & -2.3162 \\ . & . & 27.6542 & -1.2496 & -1.4892 & -0.5790 \\ . & \text{SYM} & . & 5.0915 & 0.2194 & 0.0543 \\ . & . & . & . & 5.1689 & 0.2704 \\ . & . & . & . & . & 7.6173 \end{pmatrix}.$$

The quantitative difference between the two tensors can be expressed as a norm ratio of the difference $c^a - c^e$ to $c^e$; the norm square is assumed to be the tensor self convolution along all components: $\|c^2\| = c_{ijkl}\,c_{ijkl}$. Then $\|c^a - c^e\| / \|c^e\| = 0.085$.

The matrix $u_1$ corresponds to the rotation of the symmetry axis of the transversely isotropic medium through the angle 50°. At the 10° rotation about the $x$ axis

$$u_2=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0.9848 & -0.1736 \\ 0 & -0.1736 & 0.9848 \end{pmatrix},$$

the Voigt average tensor becomes

$$c^a=\begin{pmatrix} 50.0000 & 33.7794 & 19.5872 & 1.2512 & 0 & 0 \\ . & 49.3267 & 19.6629 & 1.8830 & 0 & 0 \\ . & . & 25.0806 & 0.2546 & 0 & 0 \\ . & \text{SYM} & . & 4.2963 & 0 & 0 \\ . & . & . & . & 4.0603 & 0.3420 \\ . & . & . & . & . & 7.9397 \end{pmatrix},$$

while the exact volume average tensor is

$$c^e=\begin{pmatrix} 49.6347 & 33.2299 & 19.5127 & 1.1635 & 0 & 0 \\ . & 48.5001 & 19.5509 & 1.7514 & 0 & 0 \\ . & . & 25.0653 & 0.2364 & 0 & 0 \\ . & \text{SYM} & . & 4.2737 & 0 & 0 \\ . & . & . & . & 4.0594 & 0.3369 \\ . & . & . & . & . & 7.9109 \end{pmatrix}.$$

In this case, $\|c^a - c^e\| / \|c^e\| = 0.013$.

Another result of this study arises from the reasonable intention to analyze the general dependence of Voigt average elastic constants on the distribution function of crystallographic orientations (orientation distribution), which is reduced to a linear function of few parameters. The only assumption for the distribution function itself is that it exists. This assumption, along with the generalized assumptions on the symmetry of single crystals and the average polycrystalline medium, is sufficient to arrive at interesting conclusions. For instance, the Voigt average elastic constants are linear functions of two variables if both the polycrystalline material and the constituent crystals are transversely isotropic, while the variables are the second and fourth moments of the distribution function (variance and kurtosis, respectively) which obey the probability inequalities that bracket the range of their permitted values. Therefore, the upper and lower bounds of five elastic constants of a transversely isotropic medium correlate with one another and their ranges are quite rigorously constrained. The constraints show whether the anisotropy bounds fit specific medium models.

The mathematical problems relevant to this consideration are of two types related to the theories of (1) group representation and (2) probability. The problems of type 1 concern the groups of three-dimensional Euclidean space rotations and use the concepts of irreducible tensor, quantum mechanic angular momentum, spinor, expansion into irreducible representations, and generalization of spherical functions. The type 2 probability problems include the restricted moment problem: whether a distribution function with specified values of several lower moments can exist and, if yes, how does this function (the simplest function of this kind) may look. The problems were solved in 1D in the 19th century by Chebyshev and Markov (Krein and Nudelman, 1973), and the results are directly applicable to analysis of transversely isotropic polycrystalline materials composed of transversely isotropic crystals, which is the subject of this study. However, the case of a transversely isotropic medium with orthorhombic constituents requires a 2D solution for moments. The latter problem can have independent applications and will be a subject of a separate study.

## PROBLEM FORMULATION

The problem is formulated for a microheterogeneous medium with invariable symmetry and elastic constants, i.e., with the specified stiffness tensor $c_{ijkl}$ and the crystallographic directions distributed according to the function $f(\psi, \theta, \phi)$, where $\psi$, $\theta$, and $\phi$ are the Euler angles of the lattice planes rotated with respect to the laboratory coordinates (Fig. 1).

Two problems are solved, for (1) Voigt average stiffness tensor in laboratory coordinates and (2) its correlation and boundary values.

Problem (1) consists in calculating the average

$$c^a_{ijkl} = c_{pqrs} \int u_{ip} u_{jq} u_{kr} u_{ls} f \, du, \tag{1}$$

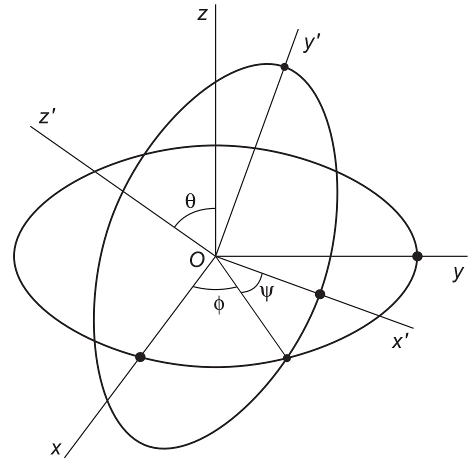


**Fig. 1.** Euler angles.

where $u_{ik}$ are the orthogonal matrices of three-dimensional rotations, and the integration along the rotation group is

$$\int f \, du = \frac{1}{8\pi^2} \int_0^{2\pi} d\psi \int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\phi \left(\psi, \theta, \phi\right). \tag{2}$$

In problem (2), correlation of the Voigt average stiffness tensor means linear dependence of the $c^a$ components when the distribution function moments are fewer than the tensor components. The problem is solved in this study for a transversely isotropic polycrystalline material consisting of transversely isotropic single crystals.

## EXPANSION INTO IRREDUCIBLE REPRESENTATIONS

Problem 1 can be solved in the group representation theory by expansion of variables into irreducible representations of the rotation group. The tensor $c_{ijkl}$ is a reducible representation, while irreducible tensors are those that are fully symmetrical and convolve to zero along any two components. The stiffness tensor is symmetrical (allowing the permutation of subscripts):

$$c_{ijlk} = c_{klij} = c_{jikl} = c_{ijlk} \tag{3}$$

and can form two nonzero convolutions

$$a_{ij} = c_{ijkk}, \quad b_{ik} = c_{ijkj}, \tag{4}$$

known as the bulk modulus and Voigt stiffness tensor (Helbig, 1994). These tensors, in their turn, are symmetrical and expandable into a unit tensor and a traceless part

$$a_{ij} = \bar{a}_{ij} + \frac{1}{3}\delta_{ij} a, \;\; b_{ij} = \bar{b}_{ij} + \frac{1}{3}\delta_{ij} b, \tag{5}$$

where

$$a = a_{ii}, \;\; b = b_{ii}. \tag{6}$$

Thus, the irreducible tensor $\bar{c}_{ijkl}$ (symmetrical along all components and convolving to zero) can be obtained by adding the combined tensor $\bar{a}_{ij}$, $\bar{b}_{ij}$ and the unit tensor to the stiffness tensor. This combination obviously satisfies the same symmetry properties as the stiffness tensor. There are eight possible combinations, and

$$\begin{aligned} c_{ijkl} &= \bar{c}_{ijkl} + \alpha\left(\bar{a}_{ij}\delta_{kl} + \bar{a}_{kl}\delta_{ij}\right) + \\ &\beta\left(\bar{a}_{ik}\delta_{jl} + \bar{a}_{jl}\delta_{ik} + \bar{a}_{il}\delta_{jk} + \bar{a}_{jk}\delta_{il}\right) + \\ &+\gamma a\delta_{ij}\delta_{kl} + \delta a\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + \varepsilon\left(\bar{b}_{ij}\delta_{kl} + \bar{b}_{kl}\delta_{ij}\right) + \\ &+\zeta\left(\bar{b}_{ik}\delta_{jl} + \bar{b}_{jl}\delta_{ik} + \bar{b}_{il}\delta_{jk} + \bar{b}_{jk}\delta_{il}\right) \\ &+\eta b\delta_{ij}\delta_{kl} + \xi b\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right). \end{aligned} \tag{7}$$

The coefficients are found assuming that the convolution of the left-hand side along *kl* and *jl* gives the tensors $a_{ij}$ and $b_{ik}$, respectively:

$$\begin{aligned} &\alpha = 5/7,\ \ \beta = -2/7,\ \ \gamma = 2/15,\ \ \delta = -1/30, \\ &\varepsilon = -4/7,\ \ \zeta = 3/7,\ \ \eta = -1/15,\ \ \xi = 1/10. \end{aligned} \tag{8}$$

The stiffness tensor has 21 independent components in the general case, and can be reconstructed according to irreducible tensors: $\bar{c}_{ijkl}$ (9 independent components), $\bar{a}_{ij}$ and $\bar{b}_{ij}$ (5 components each), the scalars *a* and *b* (1 component each), which makes altogether 9 + 5 + 5 + 1 + 1 = 21 components.

To change from the tensor notation $t_{i_1 \ldots i_l}$ to that of moments $t_m^{(l)}$, where $m = -l, \ldots, l$ denote independent components (altogether $2l + 1$ components for the irreducible tensor of $l$ components), one has first to use the spinor representation, i.e., find the irreducible spinor $t_{\mu_1\nu_1\ldots\mu_l\nu_l}$ corresponding to the irreducible tensor $t_{i_1 \ldots i_l}$. The spinor is likewise symmetrical on all subscripts and zeroes upon convolution, but the subscripts take the values 1 and 2 (section 57 in (Landau and Lifshitz, 1991)):

$$t_{\mu_1\nu_1\ldots\mu_l\nu_l} = \left(-\frac{i}{\sqrt{2}}\right)^l \left(g\sigma_{i_1}\right)_{\mu_1\nu_1} \ldots \left(g\sigma_{i_l}\right)_{\mu_l\nu_l} t_{i_1\ldots i_l}. \tag{9}$$

The equation includes the metric *g* in the spinor representation and the Pauli matrices

$$\begin{aligned} &g = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ &\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \tag{10}$$

Inverse transformation of (9) gives

$$t_{i_1\ldots i_l} = \left(-\frac{i}{\sqrt{2}}\right)^l \left(\sigma_{i_1} g\right)^{\mu_1\nu_1} \ldots \left(\sigma_{i_l} g\right)^{\mu_l\nu_l} t_{\mu_1\nu_1\ldots\mu_l\nu_l}. \tag{11}$$

The moment notation

$$t_m^{(l)} = \sqrt{\frac{(2l)!}{(l+m)!(l-m)!}}\ t_{\underbrace{1\ldots1}_{l+m}\underbrace{2\ldots2}_{l-m}}. \tag{12}$$

corresponds to the spinor representation. After all transformations, the stiffness tensor becomes represented by $\bar{c}_m^{(4)}$, $\bar{a}_m^{(2)}$, $\bar{b}_m^{(2)}$, *a* and *b*. The explicit equations (with two subscripts $c_{ijkl} \to c_{(i,j)(k,l)}$ in the right-hand side, where $(i,i) = i$, $(1,2) = 6$, $(2,3) = 4$, $(3,1) = 5$) are

$$\begin{aligned} &\bar{c}_0^{(4)} = \frac{1}{2\sqrt{70}}\left(3c_{11} + 3c_{22} + 8c_{33} + 2c_{12} - 8c_{13} - \right. \\ &\left. 8c_{23} - 16c_{44} - 16c_{55} + 4c_{66}\right), \\ &\bar{c}_{\pm1}^{(4)} = \frac{1}{\sqrt{14}}\left(\pm\left(3c_{15} + c_{25} - 4c_{35} + 2c_{46}\right) + \right. \\ &\left. i\left(c_{14} + 3c_{24} - 4c_{34} + 2c_{56}\right)\right), \\ &\bar{c}_{\pm2}^{(4)} = \frac{1}{2\sqrt{7}}\left(-c_{11} + c_{22} + 2c_{13} - 2c_{23} - \right. \\ &\left. 4c_{44} + 4c_{55} \mp 2i\left(c_{16} + c_{26} - 2c_{36} - 4c_{45}\right)\right), \\ &\bar{c}_{\pm3}^{(4)} = \frac{1}{\sqrt{2}}\left(\mp\left(c_{15} - c_{25} - 2c_{46}\right) - i\left(c_{14} - c_{24} + 2c_{56}\right)\right), \\ &\bar{c}_{\pm4}^{(4)} = \frac{1}{4}\left(c_{11} + c_{22} - 2c_{12} - 4c_{66}\right) \pm i\left(c_{16} - c_{26}\right), \\ &\bar{a}_0^{(2)} = \frac{1}{\sqrt{6}}\left(c_{11} + c_{22} - 2c_{33} + 2c_{12} - c_{13} - c_{23}\right), \\ &\bar{a}_{\pm1}^{(2)} = \pm\left(c_{15} + c_{25} + c_{35}\right) + i\left(c_{14} + c_{24} + c_{34}\right), \\ &\bar{a}_{\pm2}^{(2)} = -\frac{1}{2}\left(c_{11} - c_{22} + c_{13} - c_{23}\right) \mp i\left(c_{16} + c_{26} + c_{36}\right), \\ &\bar{b}_0^{(2)} = \frac{1}{\sqrt{6}}\left(c_{11} + c_{22} - 2c_{33} - c_{44} - c_{55} + 2c_{66}\right), \\ &\bar{b}_{\pm1}^{(2)} = \pm\left(c_{15} + c_{35} + c_{46}\right) + i\left(c_{24} + c_{34} + c_{56}\right), \\ &\bar{b}_{\pm2}^{(2)} = -\frac{1}{2}\left(c_{11} - c_{22} - c_{44} + c_{55}\right) \mp i\left(c_{16} + c_{26} + c_{45}\right), \\ &a = c_{11} + c_{22} + c_{33} + 2c_{12} + 2c_{13} + 2c_{23}, \\ &b = c_{11} + c_{22} + c_{33} + 2c_{44} + 2c_{55} + 2c_{66}. \end{aligned} \tag{13}$$

The expression $c = \left(\bar{c}_m^{(4)}, \bar{a}_m^{(2)}, \bar{b}_m^{(2)}, a, b\right)$ means that the set of variables $\bar{c}_m^{(4)}$, $\bar{a}_m^{(2)}$, $\bar{b}_m^{(2)}$, $a, b$ is equivalent to the tensor $c_{ijkl}$.

The new notation highlights the independent components explicitly, but it is the way of their transformation during the rotation of coordinates that is especially important. If the initial tensor components are transformed as

$$c'_{ijkl} = u_{ip}u_{jq}u_{kr}u_{ls}c_{pqrs}, \tag{14}$$

where the 3×3 orthogonal rotation matrices $u$ are expressed via the Euler angles $\phi$, $\theta$, $\psi$, the new components $t_m^{(l)}$ are transformed as (Vilenkin, 1991)

$$t_m^{(l)'} = D_{mn}^{(l)}\left(\psi, \theta, \phi\right) t_n^{(l)}, \tag{15}$$

where $D$ are the generalized spherical functions

$$D_{mn}^{(l)}\left(\psi,\theta,\phi\right) = e^{-i(m\psi+n\phi)} P_{mn}^{l}\left(\cos\theta\right), \tag{16}$$

and $P_{mn}^{l}\left(z\right)$ are the Legendre functions (in the specific case, $m = 0$ and $n = 0$ are the Legendre polynomials; $m = 0$ and $n \neq 0$ are the associated Legendre functions).
The $D$ functions have two important properties. First, $D_{mn}^{(l)}$ at constant $l$ is a unitary matrix:

$$D_{mn}^{(l)}\left(u\right) D_{mk}^{(l)}\left(u\right) = \delta_{nk}, \tag{17}$$

and the transformation inverse to (15), which expresses the tensor in fixed laboratory coordinates through that in the rotated crystallographic directions, is

$$t_m^{(l)} = D_{nm}^{(l)}\left(\psi, \theta, \phi\right) t_n^{(l)'}. \tag{18}$$

Second, the $D$ functions form a complete orthogonal system of rotation group functions

$$\int D_{mn}^{(l)}\left(u\right) D_{m'n'}^{(l')}\left(u\right)\ du = \frac{1}{2l+1}\delta_{ll'}\delta_{mm'}\delta_{nn'}. \tag{19}$$

For the Voigt average, it only remains to expand the distribution function $f$ into the $D$ functions

$$f\left(\psi,\theta,\phi\right) = 1 + \sum_{l=1}^{\infty}\ \sum_{m,n=-l}^{l} \left(2l+1\right) f_{nm}^{(l)} D_{mn}^{(l)}\left(\psi,\theta,\phi\right) \tag{20}$$

(first term is 1 by the norm conditions for the distribution function $f$), where

$$f_{nm}^{(l)} = \int D_{mn}^{(l)}\left(u\right) f\left(u\right) du, \tag{21}$$

and to take into account the orthogonality of the $D$ functions. This leads to

$$c = \left(\overline{c}_m^{(4)}, \overline{a}_m^{(2)}, \overline{b}_m^{(2)}, a, b\right) \tag{22}$$

which is averaged to

$$c^a = \left(f_{mn}^{(4)}\overline{c}_n^{(4)}, f_{mn}^{(2)}\overline{a}_n^{(2)}, f_{mn}^{(2)}\overline{b}_n^{(2)}, a, b\right). \tag{23}$$

To calculate the average elastic constants, one has to (a) transform crystallographic components to the notation of equations (13), (b) find average values with equations (23), and (c) recalculate back to crystallographic components using equations (13).

Thus, the components of the average stiffness tensor depend on 81 variables $f_{mn}^{(4)}$, $m$, $n$ = 0, ±1, ±2, ±3, ±4 and 25 variables $f_{mn}^{(2)}$, $m$, $n$ = 0, ±1, ±2, altogether 81 + 25 = 106 variables, while the other parameters of the distribution function are insignificant for the averaging.

Note that the expansion of the distribution function along the complete orthogonal set of functions was used previously as well, but the suggested expansion of the stiffness tensor is novel.

## SIMPLIFICATIONS FOR ISOTROPIC, TRANSVERSELY ISOTROPIC, AND ORTHORHOMBIC CASES

Equations (13) can be simplified for specific cases of orthorhombic, transversely isotropic, and isotropic media. In the orthorhombic case, odd components disappear while even ones become real:

$$\begin{aligned}
&\overline{c}_0^{(4)} = \frac{1}{2\sqrt{70}}\left(3c_{11} + 3c_{22} + 8c_{33} + 2c_{12} - 8c_{13} - \right.\\
&\left. 8c_{23} - 16c_{44} - 16c_{55} + 4c_{66}\right),\\
&\overline{c}_{\pm1}^{(4)} = 0,\\
&\overline{c}_{\pm2}^{(4)} = \frac{1}{2\sqrt{7}}\left(-c_{11} + c_{22} + 2c_{13} - 2c_{23} - 4c_{44} + 4c_{55}\right),\\
&\overline{c}_{\pm3}^{(4)} = 0,\ \ \overline{c}_{\pm4}^{(4)} = \frac{1}{4}\left(c_{11} + c_{22} - 2c_{12} - 4c_{66}\right),\\
&\overline{a}_0^{(2)} = \frac{1}{\sqrt{6}}\left(c_{11} + c_{22} - 2c_{33} + 2c_{12} - c_{13} - c_{23}\right),\\
&\overline{a}_{\pm1}^{(2)} = 0,\ \ \overline{a}_{\pm2}^{(2)} = -\frac{1}{2}\left(c_{11} - c_{22} + c_{13} - c_{23}\right),\\
&\overline{b}_0^{(2)} = \frac{1}{\sqrt{6}}\left(c_{11} + c_{22} - 2c_{33} - c_{44} - c_{55} + 2c_{66}\right),\\
&\overline{b}_{\pm1}^{(2)} = 0,\ \ \overline{b}_{\pm2}^{(2)} = -\frac{1}{2}\left(c_{11} - c_{22} - c_{44} + c_{55}\right),\\
&a = c_{11} + c_{22} + c_{33} + 2c_{12} + 2c_{13} + 2c_{23},\\
&b = c_{11} + c_{22} + c_{33} + 2c_{44} + 2c_{55} + 2c_{66}.
\end{aligned} \tag{24}$$

In the transversely isotropic case, only the components with $m = 0$ hold and do not change when rotated about the axis $z$

$$\begin{aligned}
&\overline{c}_0^{(4)} = \frac{4}{\sqrt{70}}\left(c_{11} + c_{33} - 2c_{13} - 4c_{44}\right),\\
&\overline{a}_0^{(2)} = \frac{2}{\sqrt{6}}\left(c_{11} - c_{33} + c_{12} - c_{13}\right),\\
&\overline{b}_0^{(2)} = \frac{1}{\sqrt{6}}\left(3c_{11} - 2c_{33} - c_{12} - 2c_{44}\right),\\
&a = 2c_{11} + c_{33} + 2c_{12} + 4c_{13},\\
&b = 3c_{11} + c_{33} - c_{12} + 4c_{44}.
\end{aligned} \tag{25}$$

In the isotropic case, only scalar components hold:

$$a = 3c_{11} + 6c_{12},\ \ b = 6c_{11} - 3c_{12}. \tag{26}$$

The inverse equations for the isotropic and transversely isotropic cases are

$$\lambda = c_{12} = \frac{2}{15}a - \frac{1}{15}b,$$
$$\mu = \frac{1}{2}\left(c_{11} - c_{12}\right) = -\frac{1}{30}a + \frac{1}{10}b, \quad (27)$$
$$\lambda + 2\mu = c_{11} = \frac{1}{15}a + \frac{2}{15}b$$

and

$$c_{11} = \frac{1}{15}a + \frac{2}{15}b + \frac{\sqrt{6}}{21}\left(\bar{a}_0^{(2)} + 2\bar{b}_0^{(2)}\right) + \frac{3}{2\sqrt{70}}\bar{c}_0^{(4)},$$
$$c_{33} = \frac{1}{15}a + \frac{2}{15}b - \frac{2\sqrt{6}}{21}\left(\bar{a}_0^{(2)} + 2\bar{b}_0^{(2)}\right) + \frac{4}{\sqrt{70}}\bar{c}_0^{(4)},$$
$$c_{12} = \frac{2}{15}a - \frac{1}{15}b + \frac{\sqrt{6}}{21}\left(5\bar{a}_0^{(2)} - 4\bar{b}_0^{(2)}\right) + \frac{1}{2\sqrt{70}}\bar{c}_0^{(4)}, \quad (28)$$
$$c_{13} = \frac{2}{15}a - \frac{1}{15}b - \frac{\sqrt{6}}{42}\left(5\bar{a}_0^{(2)} - 4\bar{b}_0^{(2)}\right) - \frac{2}{\sqrt{70}}\bar{c}_0^{(4)},$$
$$c_{44} = -\frac{1}{30}a + \frac{1}{10}b + \frac{\sqrt{6}}{42}\left(2\bar{a}_0^{(2)} - 3\bar{b}_0^{(2)}\right) - \frac{2}{\sqrt{70}}\bar{c}_0^{(4)}.$$

In the simplest Voigt averaging, the medium is isotropic or transversely isotropic. If the orientation distribution does not depend on angles, only the component $f_{00}^{(0)} = 1$ is nonzero. With only $a$ and $b$ surviving in the Voigt average tensor, the medium is isotropic. The Voigt average elastic constants are expressed by equations coinciding with (1.3)–(1.6) from Chapter 3 in the book of Shermergor (1977).

If the distribution function does not depend on the angle $\phi$, only the components $f_{0n}^{(l)}$ and, correspondingly, the $m = 0$ components of the average stiffness tensor are nonzero. The tensor does not change upon rotation about the axis $z$, and the Voigt average medium is transversely isotropic.

In the transversely isotropic case, the most general distribution function depends only on the angle $\theta$ and the Voigt average tensor depends on two coefficients $f_{00}^{(2)}$ and $f_{00}^{(4)}$, denoted hereafter as $f_2$ and $f_4$ for simplicity. Of course, the distribution function which depends only on $\theta$ applies to an arbitrary initial medium, and the Voigt average elastic components will still depend on two variables.

In the orthorhombic case, the dependence of the distribution function on $\theta$ and $\psi$ is essential. The medium parameters depend on five variables $f_{00}^{(4)}$, $f_{02}^{(4)} + f_{0,-2}^{(4)}$, $f_{04}^{(4)} + f_{0,-4}^{(4)}$, $f_{00}^{(2)}$, $f_{02}^{(2)} + f_{0,-2}^{(2)}$, because the tensor components are real and equal $\bar{c}_m^{(4)} = \bar{c}_{-m}^{(4)}$, $\bar{a}_m^{(2)} = \bar{a}_{-m}^{(2)}$, $\bar{b}_m^{(2)} = \bar{b}_{-m}^{(2)}$.

The averaging equations (23) for these specific cases are simplified as

$$\left(\bar{c}^a\right)_0^{(4)} = f_4\bar{c}_0^{(4)}, \ \left(\bar{a}^a\right)_0^{(2)} = f_2\bar{a}_0^{(2)},$$
$$\left(\bar{b}^a\right)_0^{(2)} = f_2\bar{b}_0^{(2)}. \quad (29)$$

for a transversely isotropic case and as

$$\left(\bar{c}^a\right)_0^{(4)} = f_{00}^{(4)}\bar{c}_0^{(4)} + \left(f_{02}^{(4)} + f_{0,-2}^{(4)}\right)\bar{c}_2^{(4)} + \left(f_{04}^{(4)} + f_{0,-4}^{(4)}\right)\bar{c}_4^{(4)},$$
$$\left(\bar{a}^a\right)_0^{(2)} = f_{00}^{(2)}\bar{a}_0^{(2)} + \left(f_{02}^{(2)} + f_{0,-2}^{(2)}\right)\bar{a}_2^{(2)}, \quad (30)$$
$$\left(\bar{b}^a\right)_0^{(2)} = f_{00}^{(2)}\bar{b}_0^{(2)} + \left(f_{02}^{(2)} + f_{0,-2}^{(2)}\right)\bar{b}_2^{(2)}$$

for the orthorhombic case.

## *A PRIORI* ESTIMATES OF VOIGT AVERAGE ELASTIC CONSTANTS

*A priori* estimates of Voigt average elastic constants are of special interest because the probability orientation distribution is poorly constrained. The *a priori* estimation is done assuming only the very existence of the distribution function, which in this study depends on $\theta$ only:

$$f(\theta) = 1 + \sum_{l=1}^{\infty}(2l+1)f_{00}^{(l)}P_l(\cos\theta), \quad (31)$$

where $P_l(x)$ are the Legendre polynomials; the group averaging is

$$\int g\,du = \frac{1}{2}\int_0^{\pi} g(\theta)\sin\theta\,d\theta. \quad (32)$$

The second and fourth Legendre polynomials are

$$P_2(x) = \frac{1}{2}\left(3x^2 - 1\right),$$
$$P_4(x) = \frac{1}{8}\left(35x^4 - 30x^2 + 3\right), \quad (33)$$

and the substitution $\cos\theta = x$ leads to the distribution function and the averaging

$$f(x) = 1 + \sum_{l=1}^{\infty}(2l+1)\,f_{00}^{(l)}P_l(x),$$
$$\int g\,du = \frac{1}{2}\int_{-1}^{1} g(x)\,dx. \quad (34)$$

The coefficients $f_{2,4}$ of our interest are expressed via the second and fourth moments of the distribution function

$$f_2 = \frac{1}{2}\int_{-1}^{1} f(x)P_2(x)\,dx = \frac{1}{2}\left(3\overline{x^2} - 1\right),$$
$$f_4 = \frac{1}{2}\int_{-1}^{1} f(x)P_4(x)\,dx = \frac{1}{8}\left(35\overline{x^4} - 30\overline{x^2} + 3\right). \quad (35)$$

Therefore, the calculation of the permitted values of $f_2$ and $f_4$ is a reduced problem of moments which checks the

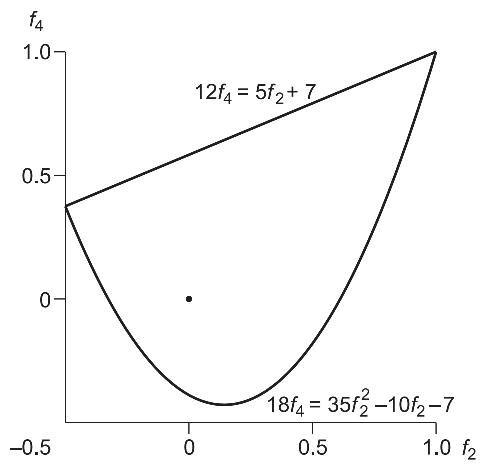


**Fig. 2.** Domain of permitted ($f_2$, $f_4$) variations. Bold point marks the distribution (0,0) equivalent to the isotropic case.

existence of a distribution function in the range $-1 < x < 1$, with the second and fourth moments $M_2$ and $M_4$.

If such function exists,

$$M_2^2 < M_4 < M_2 < 1 \tag{36}$$

and, vice versa, the distribution function exists if the inequalities fulfill. This can be proven with an example (Krein and Nudelman, 1973):

$$\frac{1}{2} f(x) = \left(1 - \frac{M_2^2}{M_4}\right)\delta(x) + \frac{M_2^2}{M_4}\delta\left(x - \sqrt{\frac{M_4}{M_2}}\right). \tag{37}$$

Note that (37) is not the only possible orientation function but is rather the simplest representative of equivalent functions.

In terms of $f_{2,4}$, the inequalities (36) arrive at

$$12 f_4 \langle 5 f_2 + 7, 18 f_4 \rangle 35 f_2^2 - 10 f_2 - 7\,. \tag{38}$$

They have simple geometrical meaning: the domain of permitted values in the plane $(f_2, f_4)$ is confined between a parabola below and a straight line above (Fig. 2). Each point of this parabolic segment has its corresponding distribution function (or rather a class of equivalent functions).

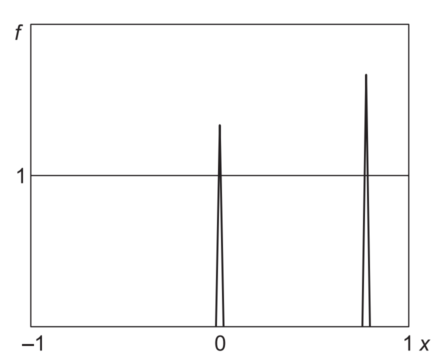


**Fig. 3.** Any distribution function is equivalent to a sum of two delta functions.

The distribution functions on the parabola correspond to the equation $M_2^2 = M_4$ and can be called variance-free because they are expressed via a single delta function:

$$\frac{1}{2} f(x) = \delta\left(x - \sqrt{M_2}\right). \tag{39}$$

Note that the distribution functions of this kind were suggested previously (e.g., equations (2.32) and the following derivation in Chesnokov, 1977), but without understanding of their role as a bound of possible distributions; neither there was understanding that adding another delta function may lead to all possible distribution functions (representatives of the respective classes of equivalent functions).

The distribution functions on the straight line correspond to $M_2 = M_4$ and have the greatest variance as they are expressed via the most distant delta functions

$$\frac{1}{2} f(x) = (1 - M_2)\delta(x) + M_2\delta(x - 1). \tag{40}$$

The isotropic distribution (point in Fig. 2) is given by

$$\frac{1}{2} f(x) = \frac{4}{9}\delta(x) + \frac{5}{9}\delta\left(x - \sqrt{3/5}\right). \tag{41}$$

Although looking different, this function is equivalent to $f(x) = 1$ which is commonly associated with isotropic distribution, as it leads to the same values of Voigt average elastic constants (Fig. 3).

The *a priori* bounds of the Voigt average elastic constants can be obtained knowing the permissible range of $f_{2,4}$ variations.

## VOIGT AVERAGE ELASTIC CONSTANTS OF A MIXTURE OF OLIVINE WITH AN ISOTROPIC MATERIAL: CALCULATION EXAMPLE

To illustrate the above derivations, different possibilities of Voigt averaging are considered below for a mixture of olivine (20%) with an isotropic material, with the following assumptions (Vinnik et al., 2014): the stiffness tensor components ($10^{11}$ Pa) of olivine are according to Clark (1966)

$$\begin{aligned} &\rho = 3.324, \quad c_{11} = 3.24, \quad c_{22} = 1.98, \\ &c_{33} = 2.49, \quad c_{44} = 0.667, \\ &c_{55} = 0.810, \quad c_{66} = 0.793, \\ &c_{12} = 0.59, \quad c_{13} = 0.79, \quad c_{23} = 0.78, \end{aligned} \tag{42}$$

the isotropic material has the same density as olivine, and the $P$ and $S$ velocities are 8.1 and 4.5 km/s. The stiffness tensor of the mixture is expressed via the respective tensors of the constituents:

$$c^{\text{mix}} = (1 - \alpha)c^{\text{isotropic}} + \alpha c^{\text{olivine}}, \tag{43}$$

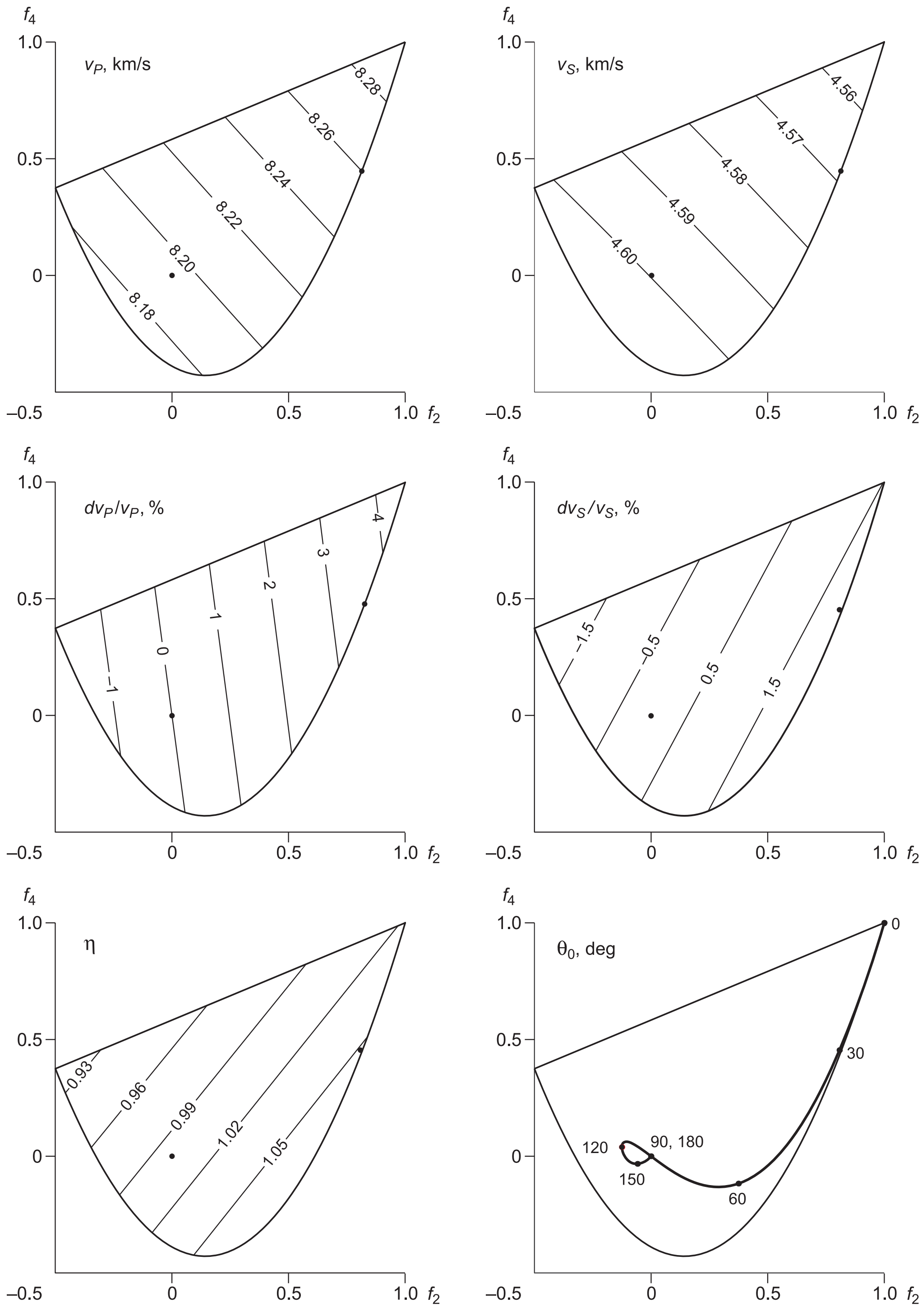


**Fig. 4.** Variations of $v_P$, $v_S$, $dv_P/v_P$, $dv_S/v_S$. Bold points mark isotorpic averaging (0,0) and averaging (0.81, 0.45) used by Vinnik et al. (2014). The pattern in the bottom right panel shows a set of averaging versions described by (44).

where α = 0.2. If the distribution function does not depend on angles, the *P* and *S* velocities are 8.56 and 4.98 km/s in olivine and 8.19 and 4.60 km/s in the mixture, respectively.

Vinnik et al. (2014) considered a distribution function depending on θ between the symmetry axis of the average medium and lattice plane 1:

$$\frac{1}{2} f(\theta) = \frac{\Theta(\theta_0 - \theta)}{1 - \cos\theta_0}, \tag{44}$$

where θ = 30° and Θ($x$) is the Heaviside step function, i.e., orientation 1 is assumed to be evenly distributed over a 30° cone, with the distribution parameters $f_2 = 0.81$ and $f_4 = 0.45$.

For clarity, seismology commonly deals with some combinations of the stiffness tensor components of transversely isotropic media, rather than with the components themselves. These combinations may be average velocities of quasi-compressional and quasi-shear waves, their variations (in percent), and the parameter η that refers to the shape of the velocity indicatrix

$$
\begin{aligned}
v_P &= \frac{1}{2}\left(\sqrt{c_{33}/\rho} + \sqrt{c_{11}/\rho}\right),\\
v_S &= \frac{1}{2}\left(\sqrt{c_{44}/\rho} + \sqrt{c_{66}/\rho}\right),\\
dv_P &= \sqrt{c_{33}/\rho} - \sqrt{c_{11}/\rho},\\
dv_S &= \sqrt{c_{44}/\rho} - \sqrt{c_{66}/\rho},\\
\eta &= \frac{c_{13}}{c_{11} - 2c_{44}},
\end{aligned}
\tag{45}
$$

where $c_{66} = \frac{1}{2}\left(c_{11} - c_{12}\right)$. In the study of Vinnik et al. (2014), they were $v_P$ = 8.26 km/s, $v_S$ = 4.57 km/s, $dv_P/v_P$ = 3.5%, $dv_S/v_S$ = 1.8%, and η = 10.5.

The patterns of Figure 4 show the behavior of these parameters in the same model at an arbitrary distribution function depending on one angle. The $v_p$ and $v_s$ curves fit well the relationship $v_P + 2.085\, v_S - 17.784 = 0$. The $dv_P/v_P$, $dv_S/v_S$ and η curves are straight lines, which is evident directly from (45) for η; for the velocity variations, it follows from

$$
\frac{dv_{P,S}}{2v_{P,S}} = \frac{1-\sqrt{c_{11,66}/c_{33,44}}}{1-\sqrt{c_{11,66}/c_{33,44}}}
\tag{46}
$$

and from the linear dependence of $c_{11,33,44,66}$ on $f_2$ and $f_4$.

## CONCLUSIONS

Voigt averaging, with an unknown distribution function, was previously assumed to provide much flexibility in manipulations with the parameters of the average medium. However, this is not the case actually. The averaging uses only a few lower moments of the distribution function instead of the function as a whole, which are significant for the medium parameters described by finite-rank tensors. The small number of these moments in physically interesting cases offers a basically new opportunity of fitting all possible patterns of the orientation distribution instead of guessing how it might be.

The lower moments of the distribution function satisfy the probability inequalities and can vary within a limited domain, with its bounds constrained by Voigt average parameters.

If the Voigt average elastic constants are controlled by few moments (as in the case of a transversely isotropic medium with transversely isotropic constituents), the values of each constant are bracketed within a certain range, and not all combinations are permitted. The Voigt average parameters are interrelated: if some of them are locked, the others are predetermined.

Thus, the reported results place more rigorous constraints on the distribution of the components of a microheterogeneous medium according to crystallographic directions.

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## REFERENCES

Chesnokov, E.M., 1977. Seismic Anisotropy of the Upper Mantle [in Russian]. Nauka, Moscow.

Clark, S.P. (Ed.), 1966. Handbook of Physical Constants. Geol. Soc. Am., Mem. 97, New York.

Helbig, K., 1994. Foundations of Anisotropy for Exploration Seismics. Elsevier Sci. Ltd, Oxford.

Jakobsen, M., Hudson, J.A., Johansen, T.A., 2003. *T*-matrix approach to shale acoustics. Geophys. J. Int. 154 (2), 533–558.

Krein, M.G., Nudelman, A.A., 1973. Markov Moment Problem [in Russian]. Nauka, Moscow.

Landau, L.D., Lifshitz, E.M., 1991. Quantum Mechanics. Non-relativistic Theory. Elsevier.

Morris, P.R., 1969. Averaging fourth-rank tensors with weight functions. J. Appl. Phys. 40 (2), 447–448.

Reuss, A., 1929. Berechnung der Fließ grenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle. Z. angew. Math. Mech. 9, 49–58.

Roe, R.J.,1965. Description of crystallite orientation in polycrystalline materials. III. General solution to pole figure inversion. J. Appl. Phys. 36 (6), 2024–2031.

Sayers, C.M., 1994. The elastic anisotrophy of shales. J. Geophys. Res. 99 (B1), 767–774.

Sayers, C.M., 2005. Seismic anisotropy of shales. Geophys. Prosp. 53 (5), 667–676.

Sayers, C.M., 2013. The effect of anisotropy on the Young's moduli and Poisson's ratios of shales. Geophys. Prosp. 61 (2), 416–426.

Schoenberg, M., Muir, F., 1989. A calculus for finely layered anisotropic media. Geophysics 54 (5), 581–589.

Shermergor, T.D., 1977. Elasticity Theory for Microheterogeneous Media [in Russian]. Nauka, Moscow.

Vilenkin, N.Ya., 1991. Special Functions and Group Representation Theory [in Russian]. Nauka, Moscow.

Vinnik, L., Oreshin, S., Makeyeva, L., Peregoudov, D., Kozlovskaya, E., POLENET/LAPNET Working Group, 2014. Anisotropic lithosphere under the Fennoscandian shield from P receiver functions and SKS waveforms of the POLENET/LAPNET array. Tectonophysics 628, 45–54.

Voigt, W., 1889. Über die Beziehung zwischen den beiden Elasticitätsconstanten isotroper. Körper Ann. Phys. 274, 573–587.

Zuo, L., Xu, J., Liang, Z., 1989. Averaging fourth-rank elastic tensors for textured polycrystalline aggregates without physical symmetry. J. Appl. Phys. 66 (6), 2338–2341.

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