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REVIEW OF DETERMINISTIC METHODS OF CALCULATION OF POLYCRYSTAL ELASTIC CONSTANTS

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The paper is a critical review of non-stochastic (referred here as deterministic) methods of calculation of effective elastic constants of single phase statistically homogeneous polycrystals. The methods are briefly described. They are compared and grouped according to their basic assumptions. Their degree of generality is discussed. The analysis of their compliance with formal requirements is provided. Moreover, the possible but unknown completions and generalizations of some methods are considered. For most methods, example calculations are carried out for a special case of quasi-isotropic aggregate with cubic crystal symmetry. To make the paper self-contained, well-known essentials of the problem of effective constants are included.

KEY WORDS: Polycrystals, elastic constants, effective properties, texture, averaging methods.

1. INTRODUCTION

The essence of the problem of the effective elastic properties is to calculate the elastic constants of a composite basing on the known properties of its components and on the structure of the material. For polycrystal – the special case of the composite – the constituents are crystallites with elastic properties determined by their orientations and single crystal data.

Diverse methods of solving the problem have been proposed. They can be roughly divided into stochastic methods and other, non-stochastic or deterministic ones.

The deterministic methods are characterized by simple assumptions, relatively simple calculations and unique results. The involved information about the structure of the material is reduced to orientation distribution. At the same time, they lack strict theoretical basis. Such basis is a feature of the stochastic methods which use more sophisticated statistical information (many-point probability functions) about composition of material. Moreover, for real polycrystal, the available information cannot be exhaustive, thus, instead of a unique result, only bounds for effective constants can be obtained. In fact, the problem is, to find optimal (i.e., narrowest) bounds for a given portion of statistical information.

One can argue that according to the above distinction, also the self-consistent method (Hershey, 1954; Marutake, 1956; Kröner, 1958) or the singular approximation method (e.g., Fokin, 1972; Kuzmenko, Korneev and Shermergor, 1983) have deterministic character. Because of their close relation to the stochastic methods they will not be discussed here.

Basic Assumptions

First, for completeness, some standard assumptions will be repeated. The existing deterministic methods deal only with local theory. The static case, without body forces will be considered here. Therefore, divergence of the stress tensor σ is assumed to vanish and σ is assumed to be symmetric, i.e., in an established cartesian coordinate system

$$\partial_j \sigma_{ij} = 0 \ , \ \sigma_{ij} = \sigma_{ji} \quad . \tag{1.1}$$

(The set of second rank symmetric tensors will be denoted by $\mathbb{T}^2$; hence, $\sigma \in \mathbb{T}^2$.) Furthermore, only small deformations will be taken into account. They will be described by the strain tensor $\varepsilon \in \mathbb{T}^2$ defined as symmetrized gradient of the displacement vector field $\mathbf{u}$

$$\varepsilon_{ij} = \partial_{(i} u_{j)} \quad . \tag{1.2}$$

For a given (twice differentiable) tensor field $\varepsilon \in \mathbb{T}^2$, the existence of a displacement $\mathbf{u}$ satisfying (1.2) is guaranteed, if the compatibility conditions are fulfilled

$$e_{ijk} e_{lmn} \partial_j \partial_m \varepsilon_{kn} = 0 \quad . \tag{1.3}$$

The e_{ijk} denotes the symbol of Levi-Civita.

Although there exist some deterministic solutions for the effective constants of the third order, only those concerning the linear theory (second order elastic constants) will be analyzed here. Hence, the elastic energy U is assumed to be a quadratic function of the components of strain tensor

$$2U = \varepsilon \ \mathbf{c} \ \varepsilon \tag{1.4}$$

and the stress and strain tensors are related through Hooke's law

$$\sigma = \mathbf{c} \ \varepsilon \ , \ (\mathbf{c} \ \varepsilon)_{ij} = c_{ijkl} \varepsilon_{kl} \ . \tag{1.5}$$

Following definition (1.4), tensor $\mathbf{c}$ satisfies the symmetry conditions

$$c_{ijkl} = c_{jikl} = c_{ijlk} \tag{1.6}$$

and

$$c_{ijkl} = c_{klij} \quad . \tag{1.7}$$

The set of fourth rank tensors with symmetry given by both, (1.6) and (1.7), conditions will be denoted by $\mathbb{T}^4$; hence, $\mathbf{c} \in \mathbb{T}^4$. Moreover, let $\overline{\mathbb{T}}^4$ be the algebra of tensors satisfying at least (1.6) with the multiplication rule

$$(\mathbf{t}^1 \mathbf{t}^2)_{ijkl} = t^1{}_{ijmn} \ t^2{}_{mnkl} \ , \quad \mathbf{t}^1, \mathbf{t}^2 \in \overline{\mathbb{T}}^4 \tag{1.8}$$

and the unit tensor $\mathbf{I}$ defined by

$$I_{ijkl} = \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \ . \tag{1.9}$$

It is shown in the Appendix A that vectors and symmetric matrices, respectively, can be assigned to tensors of $\mathbb{T}^2$ and $\mathbb{T}^4$. Because the elastic energy is positive for any non-zero deformation, the matrix corresponding to $\mathbf{c}$ is positive definite. Hence, it is not singular and, subsequently, there exists the inverse matrix and the corresponding tensor $\mathbf{s}\in\mathbb{T}^4$

$$\mathbf{cs} = \mathbf{sc} = \mathbf{I} \ . \tag{1.10}$$

The tensor $\mathbf{s}$ can be used to write down the energy ($U=\sigma\mathbf{s}\sigma/2$) and Hooke's law ($\varepsilon=\mathbf{s}\sigma$).

Below, to express the positive definiteness of $\mathbf{t}\in\mathbb{T}^4$ the symbol $\mathbf{t}>0$ will be used. Moreover, for $\mathbf{t}_1,\mathbf{t}_2\in\mathbb{T}^4$, $\mathbf{t}_1>\mathbf{t}_2$ ($\mathbf{t}_1\geq\mathbf{t}_2$) denotes that $\mathbf{t}_1-\mathbf{t}_2$ is positive (semi-) definite. (See also Appendix B.)

Volume Average and Statistical Homogeneity

The average of a quantity $\mathbf{q}$ over a volume V (large in comparison with the inhomogeneities – grains) is defined by

$$\langle\mathbf{q}\rangle := \frac{1}{V}\int_V \mathbf{q}(\mathbf{x})d_3\mathbf{x} \quad . \tag{1.11}$$

The notion of statistical homogeneity can be precisely defined using the ensemble average. However, the idea is intuitively obvious and can be also clearly explained basing on the volume average: Let the sample be large compared to V. The sample is considered to be statistically homogeneous (regarding a given quantity $\mathbf{q}$) if the average $\langle\mathbf{q}\rangle$ does not depend on the location of V. This means that $\mathbf{q}$ is stationary on the sample and its value fluctuates around that constant average value.

Orientation Average

Further, it is assumed that the material properties (and hence the tensor field $\mathbf{q}$ ($=\mathbf{c}$ or $\mathbf{s}$)) at a given point $\mathbf{x}\in$ V are determined by the orientation $g\in SO(3)$ of the crystallite containing this point. That is, in fact, the field is determined on the orientation space and indirectly at points of the sample. Let $\vartheta:\mathbf{x}\mapsto g$ be the mapping, which to the point $\mathbf{x}$, assigns the orientation $g=\vartheta(\mathbf{x})$ of the crystallite containing the point. Hence, writing in a compact, although not completely precise way, $\mathbf{q}(\mathbf{x})=\mathbf{q}(\vartheta(\mathbf{x}))$. Moreover, $\mathbf{q}(\mathbf{x})$ can be given in the form

$$\mathbf{q}(\mathbf{x}) = \int_{SO(3)} \mathbf{q}(g)\ \delta(\vartheta(\mathbf{x}),g)\ dg \ . \tag{1.12}$$

The volume average can be replaced by the orientation average

$$\langle\mathbf{q}\rangle = \frac{1}{V}\int_V \mathbf{q}(\mathbf{x})d_3\mathbf{x} = \int_{SO(3)}\mathbf{q}(g)f(g)dg =: M^f(\mathbf{q}) \tag{1.13}$$

where $f:SO(3) \longrightarrow \mathbb{R}_+$ given by

$$f(g):=\frac{1}{V}\int_V \delta(\vartheta(x),g)d_3x \tag{1.14}$$

denotes the texture function (Morawiec, Pospiech, 1992) and M^f is the operator of orientation averaging with f as weight function.

Definition of Effective Elastic Constants

From the macroscopic viewpoint, the statistically homogeneous material appears as homogeneous. Thus, one expects the existence of a constant effective tensor $\mathbf{c}^*$ which describes the overall elastic properties. Due to the assumed linearity, the elastic energy should be expressible as the quadratic function of a macro-strain and, moreover, the macro-strain should be related to a macro-stress through macroscopic Hooke's law. In both cases, tensor $\mathbf{c}^*$ should supply appropriate coefficients.

The question is, how to express the macro-variables through local variables. In the considered case, it can be done relatively easily. Because of statistical homogeneity, the macro-variables are constant, provided the boundary conditions are homogeneous. Therefore, the standard procedure of defining the effective tensors uses such boundary conditions. Let they be given by

$$u_i\big|_{\partial V} = \bar{\varepsilon}_{ij}\, x_j \tag{1.15}$$

or

$$\sigma_{ij}\big|_{\partial V}\, n_j = \bar{\sigma}_{ij} n_j \ , \tag{1.16}$$

where $\bar{\varepsilon}$ and $\bar{\sigma}$ are constant tensors. The most natural form of a macro-variable is the average of the corresponding local field. The volume averages $\langle\varepsilon\rangle$ and $\langle\sigma\rangle$ are equal to $\bar{\varepsilon}$ and $\bar{\sigma}$, respectively. This follows from

$$\langle\varepsilon\rangle_{ij}=\frac{1}{V}\int_V \partial_{(i}u_{j)}d_3\,\mathbf{x} = \frac{1}{V}\int_{\partial V} u_{(i}n_{j)}d_2\,\mathbf{x} = \bar{\varepsilon}_{k(i}\frac{1}{V}\int_{\partial V} n_{j)}x_k\, d_2\,\mathbf{x} = \bar{\varepsilon}_{ij} \tag{1.17}$$

and

$$\langle\sigma\rangle_{ij}=\frac{1}{V}\int_V \sigma_{ij}d_3\mathbf{x}=\frac{1}{V}\int_V \partial_k(\sigma_{ik}x_j)-\partial_k\sigma_{ik}x_j)d_3\mathbf{x} = \frac{1}{V}\int_{\partial V}\sigma_{ik}x_j n_k d_2\mathbf{x} = \bar{\sigma}_{ij} \tag{1.18}$$

where Gauss theorem and the equilibrium conditions (1.1) were used. Let $\langle\varepsilon\rangle=\bar{\varepsilon}$, $\langle\sigma\rangle=\bar{\sigma}$ be the sought strain and stress macro-variables, and let the average $\langle U\rangle$ of the local elastic energy be considered as the macro-variable of energy. This means that

$$\langle\sigma\rangle = \mathbf{c}^*\langle\varepsilon\rangle, \tag{1.19}$$

and

$$2\langle U\rangle = \langle\varepsilon\rangle\mathbf{c}^*\langle\varepsilon\rangle. \tag{1.20}$$

The last two relations and the whole picture will be consistent provided the Hill's condition

$$<\varepsilon\sigma> = <\varepsilon><\sigma> \tag{1.21}$$

is fulfilled. This requirement follows from the sequence $<\varepsilon\sigma> = <\varepsilon c\varepsilon> = 2<U> = <\varepsilon>\mathbf{c}^*<\varepsilon> = <\varepsilon><\sigma>$.

To show that the relation $<\varepsilon\sigma> = <\varepsilon><\sigma>$ really occurs for homogeneous boundary conditions (1.15–16), one has to use again the Gauss theorem and the conditions of local equilibrium

$$<\varepsilon\sigma> = \frac{1}{V}\int_V \sigma_{ij}\partial_j u_i \, d_3\,\mathbf{x} = \frac{1}{V}\int_{\partial V} \sigma_{ij}u_i n_j \, d_2\,\mathbf{x} = \tag{1.22}$$

$$= \left\{ \begin{array}{ll} \bar{\varepsilon}_{ik}\dfrac{1}{V}\displaystyle\int_{\partial V}\sigma_{ij}x_k n_j \, d_2\,\mathbf{x} & = \bar{\varepsilon}_{ij}\dfrac{1}{V}\displaystyle\int_V \sigma_{ij}\, d_3\,\mathbf{x} \\ \bar{\sigma}_{ij}\dfrac{1}{V}\displaystyle\int_{\partial V} u_i n_j \, d_2\,\mathbf{x} & = \bar{\sigma}_{ij}\dfrac{1}{V}\displaystyle\int_V \varepsilon_{ij}\, d_3\,\mathbf{x} \end{array} \right\} = <\varepsilon><\sigma>$$

(Bishop & Hill, 1951). Now both relations (1.19) and (1.20) can serve as equivalent definitions of the effective properties. The first (standard) one, takes the form

$$\mathbf{c}^*<\varepsilon> = <c\varepsilon>, \tag{1.23}$$

and the second (Hill's) definition, can be written as

$$<\varepsilon>\mathbf{c}^*<\varepsilon> = <\varepsilon\ \mathbf{c}\ \varepsilon>. \tag{1.24}$$

Using $\mathbf{s}^* := (\mathbf{c}^*)^{-1}$ they can be transformed into

$$\mathbf{s}^*<\sigma> = <s\sigma>\ ,\ <\sigma>\mathbf{s}^*<\sigma> = <\sigma\ \mathbf{s}\ \sigma>\ . \tag{1.25}$$

Such equivalent forms are related to the requirement called here the reciprocity condition.

Reciprocity Condition

This is the demand to obtain the same result from a procedure of effective constants calculation, regardless of the fact which of equivalent equations are the basis of calculation. For simple tensor averaging, it means that a method satisfies the condition, if, when applied to mutually reciprocal tensors, it gives the mutually reciprocal results; shortly, if the operation of averaging commutes with the matrix inversion.

2. VOIGT AND REUSS AVERAGES

The methods proposed by Voigt (1889, 1928) and Reuss (1929) were chronologically the first ways to determine the effective elastic constants. Moreover, for other reasons explained below, the averages are important for the whole problem.

The Voigt method consists in recognizing the average of the stiffness tensor as the tensor describing effective properties

$$\mathbf{c}^* = \langle \mathbf{c} \rangle =: \mathbf{c}^V. \tag{2.1}$$

The above average is related to the assumption that any deformation is homogeneous throughout the material. From $\varepsilon(\mathbf{x})=\text{const}=\langle\varepsilon\rangle$ and $\mathbf{c}^*\langle\varepsilon\rangle=\langle\mathbf{c}\varepsilon\rangle$ (or $\langle\varepsilon\mathbf{c}^*\langle\varepsilon\rangle=\langle\varepsilon\mathbf{c}\varepsilon\rangle$) one has $\mathbf{c}^*\langle\varepsilon\rangle=\langle\mathbf{c}\rangle\langle\varepsilon\rangle$ ($\langle\varepsilon\rangle\mathbf{c}^*\langle\varepsilon\rangle=\langle\varepsilon\rangle\langle\mathbf{c}\rangle\langle\varepsilon\rangle$; because $\langle\varepsilon\rangle$ is arbitrary, then $\mathbf{c}^*=\mathbf{c}^V$.

The Reuss average is dual to the Voigt average: the inverse of the effective stiffness tensor is taken to be the average of $\mathbf{c}^{-1}(=:\mathbf{s})$, i.e.,

$$\mathbf{c}^* = \langle \mathbf{c}^{-1} \rangle^{-1} =: \mathbf{c}^R \text{ or equivalently } \mathbf{s}^* = \langle \mathbf{s} \rangle. \tag{2.2}$$

The existence of mutually dual relations causes some analogies; the corresponding formulae can be obtained by replacing symbols $\mathbf{c}^*$, $\mathbf{c}$ and ε by $\mathbf{s}^*$, $\mathbf{s}$ and σ, respectively. E.g., assuming that all stresses are homogeneous ($\sigma(\mathbf{x})=\text{const}$) one gets Reuss average from the definition of effective constants.

The results of Voigt and Reuss averages are generally different, i.e., $\mathbf{c}^V \neq \mathbf{c}^R$. (This is related to the simple statement that, in general, arithmetic and harmonic means are different.) In a sense, the tensors $\mathbf{c}^V$ and $\mathbf{c}^R$ bound the proper result. To show this, the simplified version (homogeneous boundary conditions) of the well known classical variational principles of elasticity will be shortly considered.

Variational Principles

According to the first variational principle for the first boundary problem, among all differentiable displacements which fulfill the given boundary conditions, those satisfying the equilibrium equations lead to minimum of potential energy. More precisely: Let the differentiable displacements $\mathbf{u}$ and $\mathbf{u}^*$ be given on V. Moreover, let $\varepsilon_{ij}=\partial_{(i}u_{j)}$, $\varepsilon^*_{ij}=\partial_{(i}u^*_{j)}$ and let both, $\mathbf{u}$ and $\mathbf{u}^*$, satisfy the homogeneous boundary conditions $u^*_{i\partial V}=\langle\varepsilon\rangle_{ij}x_j=u_{i\partial V}$. If $\mathbf{c}\varepsilon$ satisfies the equilibrium relations (i.e., $\partial_j(c_{ijkl}\varepsilon_{kl})=0$), then

$$\langle \varepsilon \mathbf{c} \varepsilon \rangle \leq \langle \varepsilon^* \mathbf{c} \varepsilon^* \rangle. \tag{2.3}$$

On the other hand, if σ and σ^* satisfy the equilibrium relations and, moreover, $\mathbf{s}\sigma$ satisfies the compatibility conditions, then

$$< 2\sigma\langle\varepsilon\rangle - \sigma\mathbf{s}\sigma > \geq < 2\sigma^*\langle\varepsilon\rangle - \sigma^*\mathbf{s}\sigma^* >. \tag{2.4}$$

Similarly, for the second boundary problem, let ε, ε^* satisfy the compatibility conditions and σ, σ^* satisfy the equilibrium relations on V. Moreover, let $\sigma^*_{ij}n_{j\partial V} = \langle\sigma\rangle_{ij}n_{j\partial V}=\sigma_{ij}n_{j\partial V}$ with $\langle\sigma\rangle$ being constant. If $\mathbf{s}\sigma$ satisfies the compatibility conditions, then

$$< \sigma\mathbf{s}\sigma > \leq \langle \sigma^*\mathbf{s}\sigma^* \rangle \quad . \tag{2.5}$$

If $\mathbf{c}\varepsilon$ satisfies the equilibrium relations, then

$$< 2\varepsilon\langle\sigma\rangle - \varepsilon\mathbf{c}\varepsilon > \geq < 2\varepsilon^*\langle\sigma\rangle - \varepsilon^*\mathbf{c}\varepsilon^* >. \tag{2.6}$$

Now one can easily get the mentioned bounds.

Voigt-Reuss Bounds

The inequality (2.3) and the substitution $\varepsilon^*=\langle\varepsilon\rangle$ lead to

$$\langle\varepsilon c\varepsilon\rangle = \langle\varepsilon\rangle c^*\langle\varepsilon\rangle \leq \langle\varepsilon\rangle\langle c\rangle\langle\varepsilon\rangle \tag{2.7}$$

or shortly, to $c^* \leq \langle c\rangle = c^V$. On the other hand, Eq. (2.4) and $\sigma^*=\langle\sigma\rangle$ give

$$\langle\sigma s\sigma\rangle = \langle\sigma\rangle s^*\langle\sigma\rangle \leq \langle\sigma\rangle\langle s\rangle\langle\sigma\rangle \tag{2.8}$$

or $s^* \leq \langle s\rangle$. From the statement proved in Appendix B this is equivalent to the inequality $c^* \geq \langle c^{-1}\rangle^{-1} = c^R$. Putting both results together, one finally has

$$c^R \leq c^* \leq c^V. \tag{2.9}$$

The relations (2.5–6) based on the second boundary problem give the same inequalities. Summarizing, Voigt and Reuss averages are upper and lower bounds for the tensor of effective constants (Hill, 1952).

Orientation Average of c and s

Let the properties (i.e., the stiffness tensor $c(x)$) at a given point of the polycrystal be determined by the orientation of the crystallite containing this point. Let $\underline{c}_{ijkl}$ be components of the stiffness tensor in a coordinate system related to the crystal lattice of the crystallite and g_{ij} be components of the orthogonal matrix corresponding to orientation g. The components of $c(g)$ in the laboratory (sample) coordinate system are given by

$$(c(g))_{ijkl} = g_{si}g_{tj}g_{uk}g_{wl}\underline{c}_{stuw}. \tag{2.10}$$

The position of subscripts follows the convention used in texture analysis. According to Eqs (1.12–14), the volume average can be expressed as the orientation average with texture function as a weight function

$$c^V = \frac{1}{V}\int_V c(x)d_3x = \frac{1}{V}\int_V c(\vartheta(x))d_3x = \int_{SO(3)} c(g)f(g)dg = M^f(c). \tag{2.11}$$

Analogously, for Reuss average, it occurs

$$c^R = \left(\int_{SO(3)} c^{-1}(g)f(g)dg\right)^{-1} = (M^f(c^{-1}))^{-1} \tag{2.12}$$

In general, the problem of the determination of Voigt and Reuss averages, due to Eqs (2.10–12), is reduced to the calculation of the integrals

$$M^f_{ijklstuw} := \int_{SO(3)} g_{is}g_{jt}g_{ku}g_{lw}f(g)dg \ . \tag{2.13}$$

See (Ganster & Geiss, 1985) for the comprehensive description of a method allowing to get those coefficients.

Example: When the orientation distribution is uniform (f(g)=1 for all g∈SO(3), formulae (2.11–13) lead to isotropic forms of the tensors $\mathbf{c}^V$ and $\mathbf{c}^R$. In such case, $c^V_{ijkl}=M_{ijklstuw}\underline{c}_{stuw}$, where the M operator ($M:=M^{f=1}$) is given by

$$M_{ijklstuw} = \frac{1}{6}(\delta_{ij}\delta_{kl}\delta_{st}\delta_{uw} + \delta_{ik}\delta_{jl}\delta_{su}\delta_{tw} + \delta_{il}\delta_{jk}\delta_{sw}\delta_{tu}) - \\ - \frac{1}{30}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\,(\delta_{st}\delta_{uw} + \delta_{su}\delta_{tw} + \delta_{sw}\delta_{tu}) \tag{2.14}$$

(Morawiec, 1989).

The effective tensor can also be calculated using the rotation invariants of tensors (Leibfried, 1953). There are two independent linear invariants

$$(\mathbf{c}(g))_{iijj}=\underline{c}_{iijj}=:\mathrm{tr}_1(\mathbf{c}), \\ (\mathbf{c}(g))_{ijij}=\underline{c}_{ijij}=:\mathrm{tr}_2(\mathbf{c}). \tag{2.15}$$

Due to linearity, the operators tr_p (p=1,2) commute with integration in Eqs (2.11–12) and hence

$$\mathrm{tr}_p(\mathbf{c}^V)=\mathrm{tr}_p(\mathbf{c}) \quad , \\ \mathrm{tr}_p((\mathbf{c}^R)^{-1})=\mathrm{tr}_p(\mathbf{c}^{-1}) \quad . \qquad p=1,2 \tag{2.16}$$

The invariants determine the isotropic tensors because such tensors depend only on two parameters. Let, for isotropic $\mathbf{c}^V$, these parameters be κ^V (=3K) and γ^V (=2G); below, the notation $\mathbf{c}^V=\mathbf{iso}(\kappa^V,\gamma^V)$ will be used (see Appendix C). According to (C.9) one gets

$$\mathrm{tr}_1(\mathbf{iso}(\kappa^V,\gamma^V))=3\kappa^V, \\ \mathrm{tr}_2(\mathbf{iso}(\kappa^V,\gamma^V))=\kappa^V+5\gamma^V, \tag{2.17}$$

and hence

$$\mathbf{c}^V = M(\mathbf{c}) = \mathbf{iso}\left(\frac{1}{3}\,\mathrm{tr}_1(\mathbf{c}),\frac{1}{15}\,(3\mathrm{tr}_2(\mathbf{c}) - \mathrm{tr}_1(\mathbf{c}))\right) \tag{2.18}$$

Similarly for isotropic Reuss average, it occurs

$$\mathbf{c}^R=\mathbf{iso}\left((\frac{1}{3}\mathrm{tr}_1(\mathbf{c}^{-1}))^{-1},\ (\frac{1}{15}\,(3\mathrm{tr}_2(\mathbf{c}^{-1})-\mathrm{tr}_1(\mathbf{c}^{-1})))^{-1}\right) \tag{2.19}$$

For cubic symmetry, tensor $\mathbf{c}$ describing crystal properties can be expressed by three parameters. Let them be κ, ρ and γ, and let $\mathbf{c}$ be denoted by $\mathbf{c}=\mathbf{cub}(\kappa, \rho, \gamma)$; see Appendix C. Basing on (C.9), the relations (2.18–19) can be written using moduli κ, ρ and γ

$$\mathbf{c}^V=\mathbf{iso}(\kappa,\frac{2\rho + 3\gamma}{5}), \\ \mathbf{c}^R=\mathbf{iso}(\kappa,\frac{5\rho\gamma}{3\rho + 2\gamma}). \tag{2.20}$$

The first modulus is the same in both relations. This is a special case of a more general feature: for cubic symmetry the bulk modulus is invariant of a very general averaging procedure (given by $\mathbf{c}^*=\langle\mathbf{cA}\rangle$ with $\langle\mathbf{A}\rangle=\mathbf{I}$, see Appendix D).

Geometrical Sense of Isotropic Voigt and Reuss Averages

The Voigt and Reuss averages have an interesting geometric property which will be shortly explained. Let '$\circ$' denote the scalar product in $\mathbb{T}^4$

$$\mathbf{t}_1\circ\mathbf{t}_2:=\ \mathrm{tr}_2(\mathbf{t}_1\mathbf{t}_2),\ \ \mathbf{t}_1,\mathbf{t}_2\in\mathbb{T}^4. \tag{2.21}$$

The norm $|\bullet|$ and the distance d can be defined in the standard way

$$|\mathbf{t}|:=\sqrt{(\mathbf{t}\circ\mathbf{t})},\quad \mathbf{t}\in\mathbb{T}^4,\quad d(\mathbf{t}_1,\ \mathbf{t}_2):=\ |\mathbf{t}_1-\mathbf{t}_2|,\ \ \mathbf{t}_1,\mathbf{t}_2\in\mathbb{T}^4 \tag{2.22}$$

(Rychlewski, 1984; Krause, Kuska & Wedell, 1989). From the definition, the isotropic tensors preserve their form when rotated, i.e., $t_{ijkl}=g_{si}g_{tj}g_{uk}g_{wl}t_{stuw}$ for isotropic $\mathbf{t}$. Thus, the linear space of isotropic tensors is the subspace of $\mathbb{T}^4$, which is invariant under rotations, and $\mathbb{T}^4$ is the direct sum of the subspace of isotropic tensors and its orthogonal complement. In other words, any $\mathbf{t}\in\mathbb{T}^4$ can be uniquely decomposed into $\mathbf{t}=\mathbf{t}^i+\mathbf{t}^a$, where $\mathbf{t}^i$ is the isotropic part of $\mathbf{t}$ and $\mathbf{t}^a$ satisfies the orthogonality relation $\mathbf{t}^i\circ\mathbf{t}^a=0$. Moreover, the distance $d(\mathbf{t},\mathbf{x}^i)$ as the function of isotropic tensor $\mathbf{x}^i\in\mathbb{T}^4$ takes the absolute minimum for $\mathbf{x}^i=\mathbf{t}^i$.

The clue of the above remarks is that for the uniform orientation distribution, the average $\mathrm{M}(\mathbf{t})$ is the isotropic part of $\mathbf{t}$, i.e, $\mathbf{t}^i=\mathrm{M}(\mathbf{t})$. Moreover, $\mathrm{M}(\mathbf{t})$ is the isotropic tensor closest to tensor $\mathbf{t}$ in the sense of the distance d. One can check it applying the standard procedure of calculation of extrema for the function given by $d(\mathbf{c},\mathbf{iso}(\kappa_x,\gamma_x))$ (with two variables κ_x,γ_x).

Going back to effective properties, Voigt average $\mathrm{M}(\mathbf{c})$ is equal to the isotropic part of the stiffness tensor $\mathbf{c}$. Analogously, Reuss average $\mathrm{M}(\mathbf{s})$ is the isotropic part of tensor $\mathbf{s}$.

Averaging Procedure by Laurent and Eudier

Laurent and Eudier (1950) proposed an averaging method concerning quasi-isotropic materials with cubic crystal symmetry (see also Wawra & Subrahmanyam, 1968). Taking into account the equality of the single crystal and the effective bulk moduli, Ledbetter (1974) showed that it is equivalent to the special case of Voigt average.

3. HILL METHOD

Hill method (1952) in its traditional form concerns quasi-isotropic materials and is a conclusion from the inequalities $\mathbf{c}^R\le\mathbf{c}^*\le\mathbf{c}^V$ applied to this specific case. It should be noticed that $\mathbf{iso}(\kappa,\gamma)\ge 0$ is equivalent to $\kappa\ge 0$ and $\gamma\ge 0$. Let the appropriate moduli be defined by $\mathbf{iso}(\kappa^*,\gamma^*):=\mathbf{c}^*$ and $\mathbf{iso}(\kappa^V,\gamma^V):=\mathbf{c}^V$. Hence, one has

$$\mathbf{iso}(\kappa^V-\kappa^*,\gamma^V-\gamma^*)=\mathbf{iso}(\kappa^V,\gamma^V)-\mathbf{iso}(\kappa^*,\gamma^*)=\langle\mathbf{c}\rangle-\mathbf{c}^*\ge 0 \tag{3.1}$$

or

$$\kappa^* \leq \kappa^V \quad \text{and} \quad \gamma^* \leq \gamma^V \ . \tag{3.2}$$

Analogously

$$\kappa^* \geq \kappa^R \quad \text{and} \quad \gamma^* \geq \gamma^R \ , \tag{3.3}$$

where $\mathbf{iso}(\kappa^R,\gamma^R):=\mathbf{c}^R$ defines κ^R and γ^R (Hill, 1952).

These results are the basis for defining Hill average. To satisfy the above inequalities it is usually taken to be the common arithmetic or geometric mean of bounds for the bulk and shear moduli, i.e.,

$$\kappa^* = (\kappa^R + \kappa^V)/2 \ , \quad \gamma^* = (\gamma^R + \gamma^V)/2 \ (=:\gamma^H) \tag{3.4}$$

or

$$\kappa^* = (\kappa^R\kappa^V)^{1/2} \ , \quad \gamma^* = (\gamma^R\gamma^V)^{1/2} \tag{3.5}$$

(Hill, 1952). Along with (2.18–19) these are the most commonly used formulae for polycrystal elastic constants calculation. The example results are shown in Figure 1.

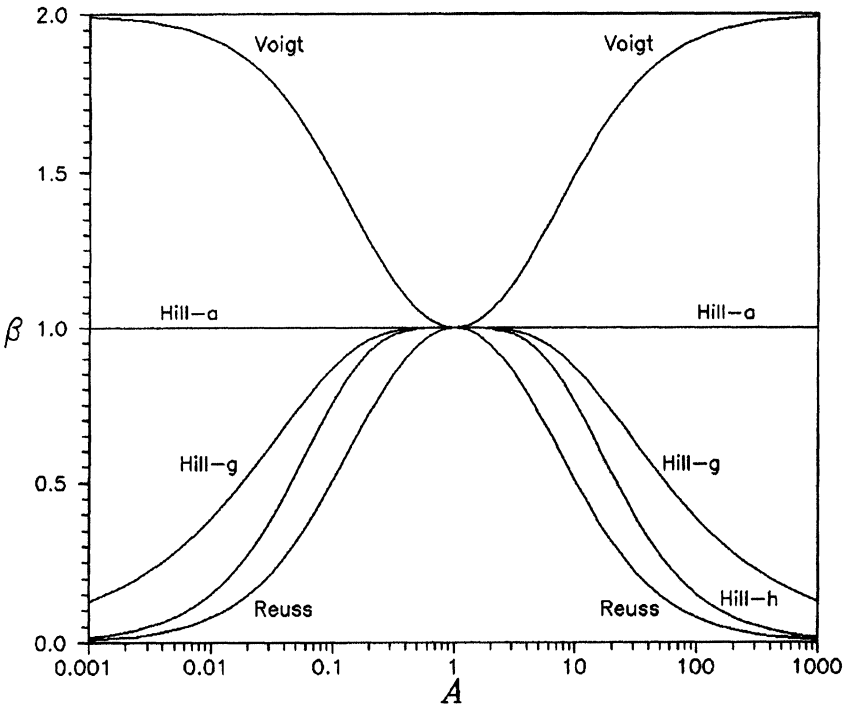

Figure 1 The figure (and also Figures 2,3,5 and 7) displays how the effective bulk modulus of the quasi-isotropic polycrystal depends on the cubic crystal aniostropy. The Zener anisotropy coefficient $A:=\gamma/\rho$ is marked on the abscissa. The ordinate represents the ratio β of the effective modulus γ^* and the modulus γ^H obtained from arithmetic Hill procedure Eq.(3.4), i.e., $\beta:=\gamma^*/\gamma^H$. The third parameter (κ) of $\mathbf{cub}(\kappa,\rho,\gamma)$ is eliminated by accepting Cauchy condition which, in this case, reduces to $\kappa=\rho+3\gamma/2$. Symbols *a*, *g* and *h* denote Hill's arithmetic, geometric and harmonic means, respectively.

Shukla-Padial and Verma-Aggarwal Suggestions

There exist some other but very similar concepts: Shukla and Padial (1973) proposed γ^* to be equal to the harmonic averages of bounds $(1/\gamma^R+1/\gamma^V)^{-1}$, whereas Verma and Aggarwal (1975) suggested to use the formula $\gamma^*=(2\gamma^R+\gamma^V)/3$. Both ideas are based on the comparison of Debye temperatures calculated from γ^* with temperatures considered to be correct.

Generalized Hill Average

The arithmetic Hill average can be easily generalized to the anisotropic case. The inequality $\mathbf{c}^R \leq \mathbf{c}^* \leq \mathbf{c}^V$ is fulfilled by the arithmetic average of the tensors $\mathbf{c}^V$ and $\mathbf{c}^R$

$$\mathbf{c}^* = (\mathbf{c}^V + \mathbf{c}^R)/2. \tag{3.6}$$

On the other hand, one can follow the concept of Shukla and Padial assuming dual relations

$$(\mathbf{c}^*)^{-1}=((\mathbf{c}^V)^{-1}+(\mathbf{c}^R)^{-1})/2, \tag{3.7}$$

i.e., the harmonic average of bounds. The formulae (3.6) and (3.7) give different results, thus the reciprocity condition is not satisfied. To achieve this objective, let's consider a new solution in the form of the series

$$\mathbf{c}^{n+1}:=\frac{1}{2}(\mathbf{c}^n+\mathbf{c}_n)\ , \qquad \mathbf{c}_{n+1}^{-1}:=\frac{1}{2}((\mathbf{c}^n)^{-1}+(\mathbf{c}_n)^{-1})\ , \tag{3.8}$$

where

$$\mathbf{c}^0:=\mathbf{c}^V \quad \text{and} \quad \mathbf{c}_0:=\mathbf{c}^R. \tag{3.9}$$

When the series are convergent to the same limit, one can accept this limit to be the effective tensor

$$\lim_{n\to\infty} \mathbf{c}_n = \lim_{n\to\infty} \mathbf{c}^n = \mathbf{c}^*. \tag{3.10}$$

The Hill average modified in this way satisfies the reciprocity condition.

Example: Below, the formulae (3.8–10) will be applied to the uniform texture. Tensors $\mathbf{c}_0$ and $\mathbf{c}^0$, and hence, tensors $\mathbf{c}_n$ and $\mathbf{c}^n$ are isotropic

$$\mathbf{c}_n = \mathbf{iso}(\kappa_n,\gamma_n)\ , \quad \mathbf{c}^n = \mathbf{iso}(\kappa^n,\gamma^n)\ , \quad n=0,1,2,\ldots\ . \tag{3.11}$$

Let us concentrate on the second modulus. From (3.8) one has

$$1-\frac{1}{2}\left|\gamma^{n+1}(\gamma_{n+1})^{-1}+\gamma_{n+1}(\gamma^{n+1})^{-1}\right| =\frac{1}{2}\left(1-\frac{1}{2}\left|\gamma^n(\gamma_n)^{-1}+\gamma_n(\gamma^n)^{-1}\right|\right). \tag{3.12}$$

Hence $\lim_{n\to\infty} \gamma^n(\gamma_n)^{-1}=1$ and this subsequently leads to the relation

$$\lim_{n\to\infty} \gamma_n = \lim_{n\to\infty} \gamma^n \tag{3.13}$$

proving that the reciprocity condition is fulfilled here. To calculate the common limit of the series, it is enough to notice that

$$\gamma^{n+1}\gamma_{n+1} = \gamma^{n}\gamma_{n}. \tag{3.14}$$

From (3.13) one has $\lim_{n\to\infty} \gamma^{n}\gamma_{n}=(\gamma^{*})^{2}$ and, on the other hand, from Eq (3.14) $\lim_{n\to\infty} \gamma^{n}\gamma_{n}=\gamma^{0}\gamma_{0}=\gamma^{V}\gamma^{R}$. Hence, finally

$$\gamma^{*}= \sqrt{(\gamma^{V}\gamma^{R})}. \tag{3.15}$$

Analogous calculations can be performed for bulk modulus; therefore

$$\kappa^{*}= \sqrt{(\kappa^{V}\kappa^{R})}. \tag{3.16}$$

These are the same results as (3.5). Hence, the above procedure is a generalization of the traditional geometric Hill average.

4. OTHER METHODS CONSTRUCTED TO SATISFY THE RECIPROCITY CONDITION

Aleksandrov Method

As was mentioned before, to tensor $\mathbf{t}\in\overline{\mathbb{II}}^{4}$ there corresponds a unique 6x6 matrix. The det(**t**) will be considered to be the determinant of this matrix.

Aleksandrov (1965) and Aleksandrov & Aizenberg (1966) proposed the method of the moduli determination based on the assumption that the determinants corresponding to the effective stiffness tensor and to the stiffness tensor of the single crystal are equal

$$\det(\mathbf{c}^{*}) = \det(\mathbf{c}). \tag{4.1}$$

The bulk modulus of polycrystals with cubic crystal symmetry is given by $\kappa^{*}=\kappa$, and only the shear modulus is to be determined. The single equation (4.1) is enough in this case. Because the determinant of the cubic tensor has the form

$$\det(\mathbf{cub}(\kappa,\rho,\gamma)) = \kappa\rho^{2}\gamma^{3} \tag{4.2}$$

and, moreover,

$$\det(\mathbf{iso}(\kappa^{*}, \gamma^{*})) = \kappa^{*}\gamma^{*5}, \tag{4.3}$$

one gets

$$\gamma^{*} = (\rho^{2}\gamma^{3})^{1/5}. \tag{4.4}$$

This is the Aleksandrov's result expressed by the ρ and γ moduli. (See Figure 2.)

Peresada's Suggestion

Peresada (1971) (independently) proposed a scheme analogous to Aleksandrov procedure but for general symmetries. Because, in such a case, an additional relation is necessary, Peresada assumed that $\kappa^{*}=(\kappa^{V}\kappa^{R})^{1/2}$; hence

$$\gamma^{*} = (\det(\mathbf{c}))^{1/5} / (\kappa^{V}\kappa^{R})^{1/10} \tag{4.5}$$

The formulae for particular symmetries can be found in (Peresada, 1971).

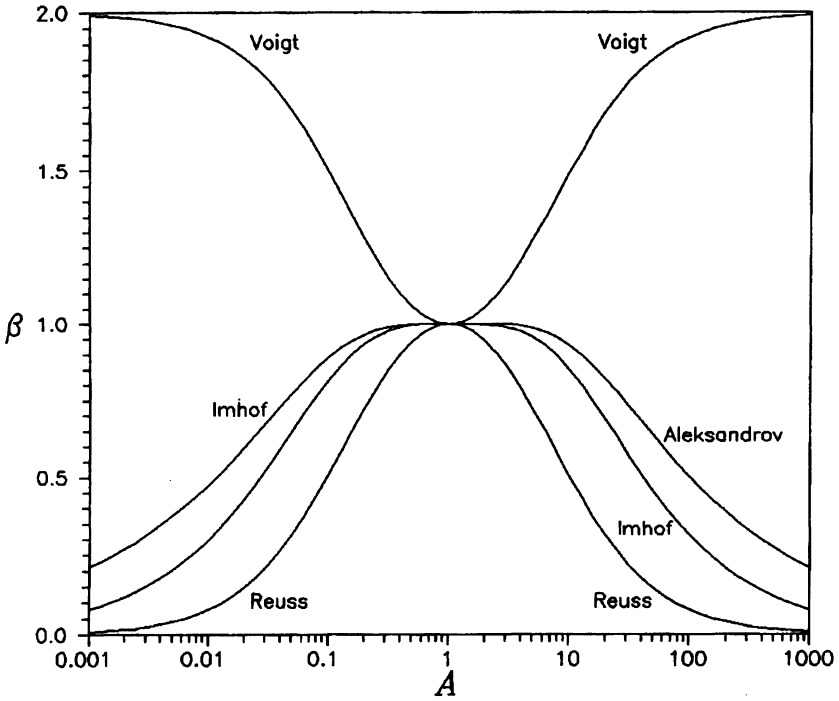

Figure 2 The shear modulus obtained from Aleksandrov and Imhof methods versus anisotropy of cubic crystal. See caption of Figure 1 for more detailed explanation.

Generalized Aleksandrov Procedure

To define the generalized Aleksandrov method, one has to determine two mappings of $\mathbb{T}^4$ into $\mathbb{T}^4$. Let the exponential mapping be given by

$$\mathbf{exp}: \mathbb{T}^4 \ni \mathbf{t} \longmapsto -\sum_{n=0}^{\infty} \frac{\mathbf{t}^n}{n!} \in \mathbb{T}^4 \ . \tag{4.6}$$

If two elements $\mathbf{t}_1, \mathbf{t}_2$ of $\mathbb{T}^4$ commute, there occurs $\mathbf{exp}(\mathbf{t}_1+\mathbf{t}_2)=\mathbf{exp}(\mathbf{t}_1)\mathbf{exp}(\mathbf{t}_2)$, and hence $\mathbf{exp}(-\mathbf{t}) = (\mathbf{exp}(-\mathbf{t}))^{-1}$.

Let the norm in $\mathbb{T}^2$ be given by $\| \xi \| = (\xi_{ij}\xi_{ij})^{1/2}$, $\xi \in \mathbb{T}^2$. One can define the norm in $\mathbb{T}^4$ as $\| \mathbf{t} \| := \sup_{\| \xi \| \le 1} \| \mathbf{t}\xi \|$. There exists the neighborhood $\mathbb{V} \subset \mathbb{T}^4$ of the unit element $\mathbf{I}$ where the mapping

$$\mathbf{log}: \quad \mathbb{V} \ni \mathbf{t} \longmapsto -\sum_{n=1}^{\infty} \frac{(\mathbf{I}-\mathbf{t})^n}{n} \in \mathbb{T}^4 \tag{4.7}$$

satisfying the condition $(\mathbf{exp}_{|\log(\mathbb{V})})^{-1}=\mathbf{log}$ is correctly defined. The neighborhood $\mathbb{V}$ is described by $\mathbb{V}=\{\mathbf{t} \in \mathbb{T}^4: \ \| \mathbf{I}-\mathbf{t} \| < 1\}$. For $\mathbf{t}_1, \mathbf{t}_2 \in \mathbb{V}$ such that $\mathbf{t}_1\mathbf{t}_2 \in \mathbb{V}$ and $\mathbf{t}_1\mathbf{t}_2=\mathbf{t}_2\mathbf{t}_1$, there occurs $\mathbf{log}(\mathbf{t}_1\mathbf{t}_2)= \mathbf{log}(\mathbf{t}_1)+\mathbf{log}(\mathbf{t}_2)$.

Let us define the average of a tensor $\mathbf{t}\in\mathbb{V}$ by $\mathbf{exp}\langle\mathbf{log(t)}\rangle$. Such operation is homogeneous (i.e., $\mathbf{exp}\langle\mathbf{log}(\alpha\mathbf{t})\rangle = \alpha\,\mathbf{exp}\langle\mathbf{log(t)}\rangle$, $\alpha\in\mathbb{R}_+$) and, moreover, it commutes with the operator of tensor inversion

$$\mathbf{exp}\langle\mathbf{log}(\mathbf{t}^{-1})\rangle = (\mathbf{exp}\langle\mathbf{log(t)}\rangle)^{-1}\,. \tag{4.8}$$

Assuming that the effective tensor $\mathbf{c}^*$ is given by the average of $\mathbf{c}$

$$\mathbf{c}^* = \mathbf{exp}\langle\mathbf{log(c)}\rangle, \tag{4.9}$$

the reciprocity condition is satisfied automatically (Morawiec, 1989).

The condition that the argument of the **log** mapping has to belong to $\mathbb{V}$ is not a strong limitation; due to the homogeneity of the operation one can reduce the stiffness tensor to $\mathbb{V}$ by multiplying it by a non-negative number. In the general case, determination of $\mathbb{V}$ is rather complicated. In the special case of cubic symmetry, it is described by the inequalities $0<\alpha\kappa$, $\alpha\rho$, $\alpha\gamma<2$. Thus the average (4.9) can be calculated for any positive definite tensor of cubic symmetry.

Replacing the volume average by the orientation average, the expression for the effective tensor takes the form

$$\mathbf{c}^* = \mathbf{exp}(\mathbf{M}^f(\mathbf{log(c)})). \tag{4.10}$$

In practice, to apply this formula, it is necessary to use definitions (4.6) and (4.7), and take the same average as in Voigt method but of $\mathbf{log}(\mathbf{c})$ instead of $\mathbf{c}$.

To the invariants tr_p (p=1,2) of the $\mathbf{M}^f$ operation there correspond the invariants $\mathrm{Tr}_p(\mathbf{t}):=\exp(\mathrm{tr}_p(\mathbf{log(t)}))$ of the operation determined by Eq (4.10), i.e., for $\mathbf{t}\in\mathbb{V}$, there occurs $\mathrm{Tr}_p(\mathbf{t})=\mathrm{Tr}_p(\mathbf{exp}(\mathbf{M}^f(\mathbf{log(t)})))$. One can show that $\mathrm{Tr}_2(\mathbf{t})=\det(\mathbf{t})$. It means that the described average is a generalization of Aleksandrov procedure.

Example: One can check that the actions of **exp** and **log** on a cubic tensor give

$$\mathbf{exp}(\mathbf{cub}(\kappa,\rho,\gamma)) = \mathbf{cub}(e^{\kappa},e^{\rho},e^{\gamma}), \tag{4.11}$$

$$\mathbf{log}(\mathbf{cub}(\kappa,\rho,\gamma)) = \mathbf{cub}(\ln(\kappa),\ \ln(\rho),\ \ln(\gamma)) \text{ for } \kappa,\rho,\gamma > 0, \tag{4.12}$$

respectively. Thus, for the quasi-isotropic material and cubic crystal summetry one has

$$\mathbf{c}^* = \mathbf{exp}(\mathbf{M}^{f=1}(\mathbf{cub}(\kappa,\rho,\gamma))) = \mathbf{iso}(\kappa,\ (\rho^2\gamma^3)^{1/5}). \tag{4.13}$$

This special result is the same as one obtained from Aleksandrov method. In the same case, it is possible to show that the result is bounded by Voigt and Reuss averages. There should occur $\gamma^R\le\gamma^{geom}\le\gamma^V$ or in full

$$\left(\frac{1}{5}\left(\frac{2}{\rho}+\frac{3}{\gamma}\right)\right)^{-1} \le (\rho^2\gamma^3)^{1/5} \le \frac{2\rho+3\gamma}{5} \tag{4.14}$$

For positive ρ and γ both conditions can be reduced to the same form

$$(2x+3y)^5-5^5x^2y^3 = (32x^3+304x^2y+1296xy^2+243y^3)(x-y)^2 \ge 0, \tag{4.15}$$

where (x=γ , y=ρ) corresponds to the first, and (x=ρ, y=γ) to the second of the inequalities (4.14). It is enough to notice that Eq (4.15) is true for all non-negative x,y.

Imhof Method

Looking for a method satisfying the reciprocity condition, Imhof (1989) proposed an iterative averaging procedure. It is based on two series

$$\mathbf{c}^{n+1} = M^f\{[\mathbf{s}_n+\mathbf{s}(g)]^{-1}\ \mathbf{s}(g)\ [\mathbf{c}(g)+\mathbf{c}^n]\} \tag{4.16}$$

and

$$\mathbf{s}_{n+1} = M^f\{[\mathbf{c}^n+\mathbf{c}(g)]^{-1}\ \mathbf{c}(g)\ [\mathbf{s}(g) + \mathbf{s}_n]\}, \tag{4.17}$$

with $\mathbf{s}^n=(\mathbf{c}^n)^{-1}$ and $\mathbf{s}_n=\mathbf{c}_n^{-1}$. The starting tensors $\mathbf{c}^0$ and $\mathbf{c}_0$ are given by $\mathbf{c}^0:=\mathbf{c}^V$ i $\mathbf{c}_0:=\mathbf{c}^R$. It is assumed that

$$\mathbf{c}^* = \lim_{n\to\infty} \mathbf{c}_n = \lim_{n\to\infty} \mathbf{c}^n \tag{4.18}$$

Even in the simplest case of cubic symmetry and uniform orientation distribution, numerical calculations are necessary to obtain the effective tensor (Figure 2).

In his paper Imhof (1989) stresses the fact of the fast convergence of the series (4.16) and (4.17) and stops iteration after two steps. Calculations for concrete examples show that it is really true, provided the orientation distribution is not 'far' from uniform. The number of iterations necessary to obtain similarly close $\mathbf{c}_n$ and $\mathbf{c}^n$ increases with growing sharpness of texture. Even more important is that in some cases the result

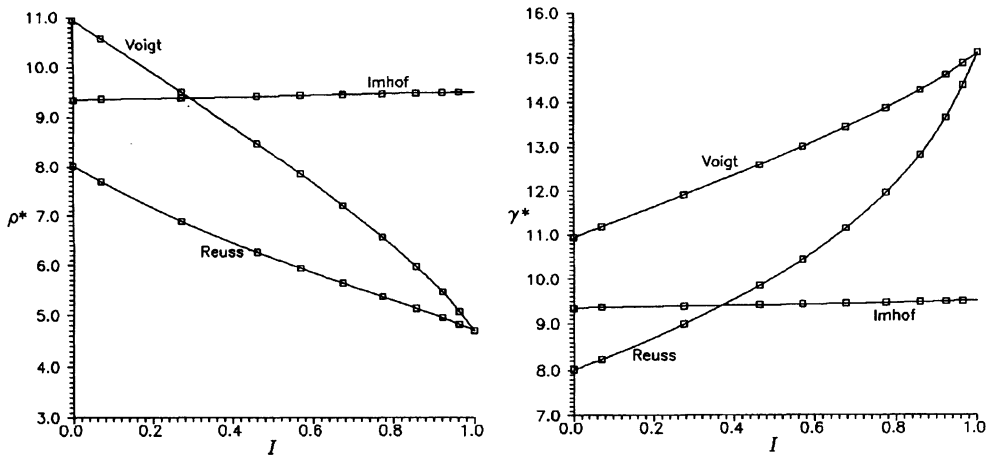

Figure 3 The result of Imhof method for non-uniform orientaiton distributions. The textures here are assumed to consist only of the cubic component with changing sharpness. In such a case, the statistical sample symmetry is cubic and the effective tensors have the forms $\mathbf{c}^*=\mathbf{cub}(\kappa^*, \rho^*, \gamma^*)$. The parameters ρ* (Figure a) and γ* (Figure b) are shown versus the texture index $I:=\int_{SO(3)} |f(g)-1|dg$ describing the texture sharpness. The inequalitits $\mathbf{c}^R \le \mathbf{c}^* \le \mathbf{c}^V$ would be satisfied if the curves of ρ* and γ* were located between those corresponding to Voigt and Reuss averages.

(i.e., the effective tensor) is outside Voigt-Reuss bounds (see Figure 3) and, moreover, it always has isotropic form except the case of monocrystal ($f(g)= \delta(g_0)$) when $\mathbf{c}^*=\mathbf{c}$. Thus, in spite of the author's claims (Imhof, 1989), applicability of the method to the textured material is doubtful.

5. BRUGGEMAN METHOD

The method given by Bruggeman (1930, 1934) has specific features characteristic for more contemporary concepts about the effective properties. Bruggeman admitted not only texture but also grain shapes to influence these properties.

It is assumed that grains have lamella-like shapes and thus some components of strain as well as some components of stress tensors are constant throughout the material. More precisely, for the direction normal to the lamellae being parallel to 'x_3' axis, the components ε_{11}, ε_{22}, σ_{33}, σ_{23}, σ_{31}, ε_{12} are assumed to be constant. To explain the main idea of the method, let each of these components be denoted by ζ with proper subscripts. Using Hooke's law, the elastic energy density U can be expressed as

$$2U = c_{ijkl}\varepsilon_{ij}\varepsilon_{kl} = X(\mathbf{c})_{ijkl}\ \zeta_{ij}\ \zeta_{kl} \tag{5.1}$$

where X is a (not-tensor) function of c_{ijkl}. On the other hand, using Hill's definition, one has

$$\langle 2U\rangle = c^*_{ijkl}\langle\varepsilon\rangle_{ij}\langle\varepsilon\rangle_{kl}=X(\mathbf{c}^*)_{ijkl}\ \zeta_{ij}\ \zeta_{kl}. \tag{5.2}$$

Averaging (5.1) over all orientations and comparing to the last formula, one obtains the expression for $X(\mathbf{c}^*)$

$$X(\mathbf{c}^*) = \int_{SO(3)} X(\mathbf{c}(g))\ f\ (g)\ dg, \tag{5.3}$$

where $\mathbf{c}(g)$ is determined by the crystal properties and crystallite's orientation. It remains to solve the above equation with respect to the components of the tensor $\mathbf{c}^*$. But it involves only 12 from among the 21 components of $\mathbf{c}^*$; for the axial symmetry of $\mathbf{c}^*$ – 4 out of 5 independent constants. To avoid this problem, instead of U, Bruggeman (1930) used a slightly different function φ given by

$$2\varphi = (-1)^{\delta_{(i)3}}c_{ijkl}\varepsilon_{ij}\varepsilon_{kl}. \tag{5.4}$$

The calculations were carried for the cubic and hexagonal crystal symmetries and orthorhombic and axial sample symmetries.

The dual equations can be obtained by replacing $\mathbf{c}$ and $\mathbf{c}^*$ in the starting equations (5.1–4) by $\mathbf{s}$ and $\mathbf{s}^*$, respectively. In the original work, such mutually dual relations are used by turns, according to which is more convenient. Moreover, in case of this method, one can proceed in another way, not noticed by Bruggeman: Replacing $\mathbf{c}$ and $\mathbf{c}^*$ by $\mathbf{s}$ and $\mathbf{s}^*$ in final equations, one gets the result corresponding to the exchanged roles of σ and ε, with the components σ_{11}, σ_{22}, ε_{33}, ε_{23}, ε_{31} and σ_{12} being constant. The appropriate material is composed of needles parallel to the 'x_3' direction.

Besides the (primary) aggregate described above, Bruggeman considered a 'secondary

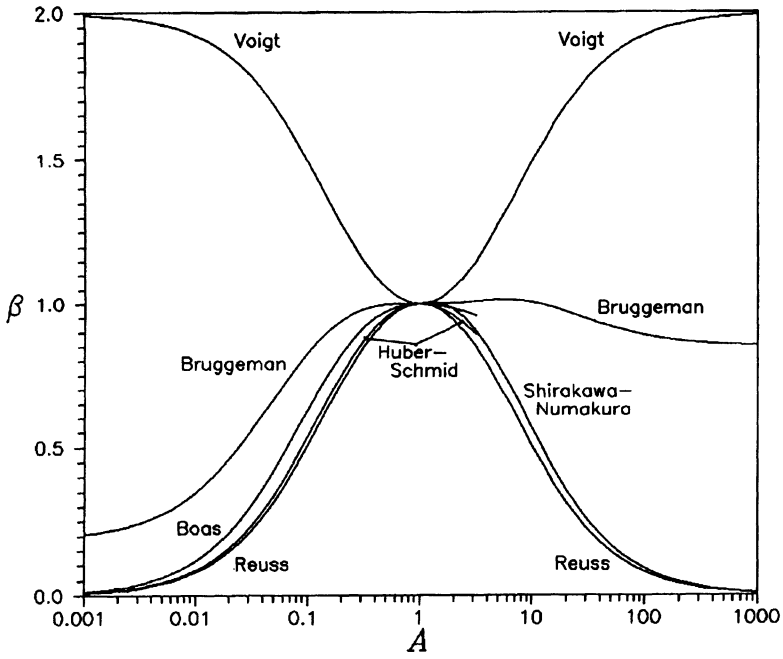

Figure 4 The results of Bruggeman, Huber-Schmid and Boas methods for the quasi-isotropic polycrystal and cubic crystal symmetry. Data outside Voigt-Reuss bounds are discarded. (See also caption to Figure 1).

aggregate' being a random composition of blocks of primary aggregates. To obtain the secondary effective constants, the Voigt procedure was applied to the primary ones. The curve in Figure 4 was calculated in that way.

6. AVERAGING OF YOUNG AND SHEAR MODULI

Huber-Schmid and Boas Methods

The method of Huber and Schmid (1934) concerns only quasi-isotropic material. The effective Young (E*) and shear (G*) moduli are calculated by averaging

$$(s_{3333}(g))^{-1} \quad \text{and} \quad (2(s_{2323}(g)+s_{1313}(g)))^{-1}, \tag{6.1}$$

respectively, over all orientations g.

One should mention here, that calculation of two moduli in the quasi-isotropic case of cubic crystal symmetry is in contradiction to the fact that one of the two moduli describing the effective properties is established ($\kappa^*=\kappa$), and only one remains to be determined.

The procedure led to relatively complicated integrals. Huber and Schmid (1934) gave the solutions for cubic and hexagonal symmetries, whereas Boas (1934) solved the

problem for tetragonal symmetry. Furthermore, Boas (1935) changed the expression for shear modulus, slightly correcting the results. The second formula of (6.1) was replaced by

$$\left(2[s_{2323}\ (g)+s_{1313}(g)] - \frac{2[s_{3323}(g)+s_{3313}(g)]}{s_{3333}(g)} \right)^{-1} \tag{6.2}$$

Again, the averaging gave complex integrals but their form was close to those used by Bruggeman (1930), and this allowed to apply the already existing solutions.

The final results of Huber-Schmid and Boas methods (as well as the Bruggeman method) are relatively intricate and, therefore, the example will be omitted here. The curves for shear modulus are given in Figure 4. Only their displayed parts lie between Voigt-Reuss bounds.

Method of Shirakawa and Numakura

Shirakawa and Numakura (1958) proposed to average the inverse of Young modulus over all crystallographic directions. In practical calculations they bounded themselves to the established directions ([100], [110], [111]) in crystals of cubic symmetry. Their formula

$$\frac{1}{E^*} = \frac{1}{13} \left(3\ \frac{1}{E_{[100]}} + 6\ \frac{1}{E_{[110]}} + 4\ \frac{1}{E_{[111]}} \right) \tag{6.3}$$

transformed to parameters used here, with $\kappa^*=\kappa$ taken into account, has the form

$$\gamma^* = \frac{26\rho\gamma}{17\rho + 9\gamma} \tag{6.4}$$

If $\gamma \geq \rho$, the result is contained between Voigt-Reuss bounds. Otherwise, it is smaller than Reuss average.

7. BUNGE METHOD

The method was originally presented in Fourier series formalism of texture analysis (Bunge, 1974). Here, it will be described in notation used for other methods.

Let " ' " (prime) denote a deviation from the average. Because $\langle\varepsilon'\rangle=0=\langle\mathbf{c}'\rangle$, the elastic energy density $U=\langle\varepsilon\mathbf{c}\varepsilon\rangle/2=\langle(\langle\varepsilon\rangle+\varepsilon')(\langle\mathbf{c}\rangle+\mathbf{c}')(\langle\varepsilon\rangle+\varepsilon')\rangle/2$ can be written as

$$2U = \langle \langle\varepsilon\rangle\mathbf{c}\langle\varepsilon\rangle+\varepsilon'\langle\mathbf{c}\rangle\varepsilon'+2\langle\varepsilon\rangle\mathbf{c}'\varepsilon'+\varepsilon'\mathbf{c}'\varepsilon' \rangle . \tag{7.1}$$

Assuming that $\langle\varepsilon'\mathbf{c}'\varepsilon'\rangle$ is small in comparison to other components and omitting it, one finds that the variation of U with regard to ε' leads to the following stationarity condition

$$\langle\mathbf{c}\rangle\varepsilon' + \mathbf{c}'\langle\varepsilon\rangle = 0. \tag{7.2}$$

Hence, one has

$$\varepsilon' = -\langle c\rangle^{-1}\, c' \,\langle\varepsilon\rangle \tag{7.3}$$

Using the last expression to substitute ε' in $\langle\sigma\rangle=\langle c\varepsilon\rangle=\langle c(\langle\varepsilon\rangle+\varepsilon')\rangle$ and taking into account the definition $\langle\sigma\rangle = c^*\langle\varepsilon\rangle$ one gets

$$c^* = \langle c\rangle - \langle c\langle c\rangle^{-1}c'\rangle = \langle c\rangle - \langle c'\langle c\rangle^{-1}c'\rangle. \tag{7.4}$$

This result is equivalent to that obtained by Bunge (1974).

Example: For uniform orientation distribution and cubic symmetry of crystal lattice with properties described by $c=\mathbf{cub}(\kappa,\rho,\gamma)$, formula (7.4) leads to

$$c^* = \mathbf{iso}\left(\kappa\,,\ \frac{2\rho+3\gamma}{5}\ \left(1-6\left(\frac{\rho-\gamma}{2\rho+3\gamma}\right)^2\right)\right). \tag{7.5}$$

The corresponding graph is displayed in Figure 5.

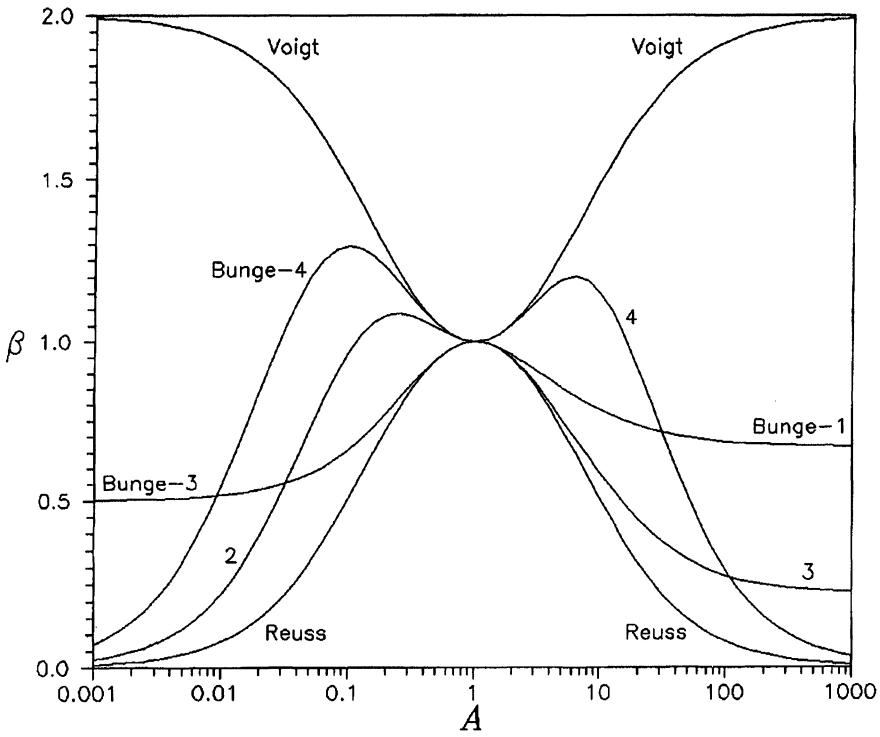

Figure 5 Quasi-isotropic result of Bunge method. Bunge-1 denotes the curve obtained from original Bunge procedure – Eq. (7.5). Symbol 2 marks the dual result – Eq. (7.7). Parts of curves falling outside Voigt-Reuss bounds are discarded. Bunge-3 and -4 are calculated from Hill's definition and written as Eqs (7.9) and (7.11), respectively.

Dual Solution

One can consider analogous dual calculations for energy density expressed by $U = \langle \sigma s \sigma \rangle /2 = \langle (\langle \sigma \rangle + \sigma')(\langle s \rangle + s')(\langle \sigma \rangle + \sigma') \rangle /2$. The assumption $\langle \sigma' s' \sigma' \rangle = 0$ and variation of U with regard to σ' give

$$\mathbf{c}^* = (\langle \mathbf{s} \rangle - \langle \mathbf{s}' \langle \mathbf{s} \rangle^{-1} \mathbf{s}' \rangle)^{-1}, \quad \mathbf{s}' := \mathbf{s} - \langle \mathbf{s} \rangle. \tag{7.6}$$

In the special case of uniform orientation distribution and cubic symmetry, the effective tensor takes the form

$$\mathbf{c}^* = \mathbf{iso}\left(\kappa \,, \frac{5\rho\gamma}{2\gamma + 3\rho} \left(1 - 6 \left(\frac{\gamma - \rho}{2\gamma + 3\rho} \right)^2 \right)^{-1} \right) . \tag{7.7}$$

Comparing Eq (7.7) and Eq (7.5) one notices that the method does not fulfill the reciprocity condition.

Short calculation shows that the result (7.5) is above Reuss limit, provided $\rho - \gamma < 0$. On the other hand, (7.7) is below Voigt limit, only if $\rho - \gamma > 0$. Therefore, for materials with anisotropy coefficient $A := \gamma / \rho$ less than 1, Eq (7.7) would be the proper formula, whereas for A greater than 1, relation (7.5) would be correct.

The problem is more complicated; for a given material with the result corresponding to uniform texture being inside Voigt-Reuss bounds, the results corresponding to other orientation distributions may be outside these bounds (see Figure 6). This makes the application of the method to textured materials questionable. (See, e.g., Sakata, Daniel & Jonas 1989 for an attempt to use the original Bunge method as the basis for texture estimation from ultrasonic measurements of single crystal and effective elastic constants.)

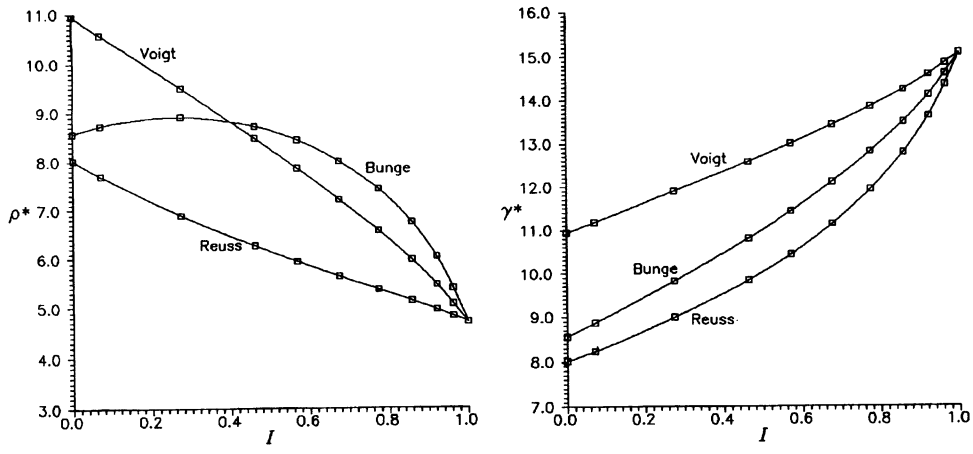

Figure 6 The result of Bunge procedure for non-uniform texture. The symbols used here are explained in the caption to Figure 3.

The Result Based on Hill's Definition

Using Hill's definition of effective constants ($\langle\varepsilon\rangle\mathbf{c}^*\langle\varepsilon\rangle=\langle\varepsilon\mathbf{c}\varepsilon\rangle$) and relations (7.3) one obtains the subsequent formulae. Instead of Eqs (7.4) and (7.5) the results are

$$\mathbf{c}^* = \langle\mathbf{c}\rangle - \langle\mathbf{c}'\langle\mathbf{c}\rangle^{-1}\mathbf{c}'\rangle + \langle\mathbf{c}'\langle\mathbf{c}\rangle^{-1}\mathbf{c}'\langle\mathbf{c}\rangle^{-1}\mathbf{c}'\rangle \tag{7.8}$$

and

$$\mathbf{c}^* = \mathbf{iso}\left(\kappa, \frac{2\rho+3\gamma}{5}\,(1-6\,(\frac{\rho-\gamma}{2\rho+3\gamma})^2 + 6(\frac{\rho-\gamma}{2\rho+3\gamma})^3)\right). \tag{7.9}$$

Similarly, Eqs (7.6) and (7.7) correspond to

$$\mathbf{c}^* = (\langle\mathbf{s}\rangle - \langle\mathbf{s}'\langle\mathbf{s}\rangle^{-1}\mathbf{s}'\rangle + \langle\mathbf{s}'\langle\mathbf{s}\rangle^{-1}\mathbf{s}'\langle\mathbf{s}\rangle^{-1}\mathbf{s}'\rangle)^{-1} \tag{7.10}$$

and

$$\mathbf{c}^* = \mathbf{iso}\left(\kappa, \frac{5\rho\gamma}{2\gamma+3\rho}\left((1-6\,(\frac{\gamma-\rho}{2\gamma+3\rho})^2 + 6(\frac{\gamma-\rho}{2\gamma+3\rho})^3)\right)^{-1}\right). \tag{7.11}$$

Although the results (7.9) and (7.11) are contained within Voigt-Reuss bounds, this is not true for more general cases of non-trivial textures.

8. METHODS BASED ON AVERAGING OF THE VELOCITY OF ELASTIC WAVES

Assuming a given one-to-one relation between elastic constants and the velocity of elastic waves, one can calculate the effective properties according to the following scheme: crystal elastic constants → velocity in crystal → velocity in polycrystal → effective elastic constants. The constants considered here are adiabatic, contrary to the previous methods concerning the isothermic constants. The velocities v_i of the longitudinal (i=1) and two transverse (i=2,3) modes of elastic monochromatic planar wave can be obtained from the roots of Christoffel equation

$$\det(c_{ijkl}n_jn_l - qv^2\delta_{ik}) = 0, \tag{8.1}$$

where q denotes density and the integration is over all possible directions of $\mathbf{n}$. Methods considered below assume analogous relation to occur for polycrystalline aggregate

$$\det(c^*_{ijkl}n_jn_l - q\bar{v}^2\delta_{ik}) = 0. \tag{8.2}$$

with $\bar{v}_i$ being the velocities of wave propagation in the aggregate.

Substituting $\mathbf{c}^*$ in the equation

$$c^*_{ijkl}n_jn_l\psi_k = q\bar{v}^2\psi_i \tag{8.3}$$

by the isotropic tensor

$$c^*_{ijkl} = \gamma^* I_{ijkl} + \frac{1}{3}(\kappa^* - \gamma^*)\delta_{ij}\,\delta_{kl} \quad , \tag{8.4}$$

one gets

$$\frac{1}{2}\left(\gamma^*\delta_{ik} + \frac{1}{3}(2\kappa^* + \gamma^*)\, n_i n_k\right)\psi_k = q\bar{v}^2\psi_i \quad . \tag{8.5}$$

It is easy to check that the eigenvectors are $\psi_i = n_i$ and $\psi_i = e_{ijk}n_j m_k$ (degenerated, **m**-any non-zero vector, not collinear with **n**). The corresponding eigenvalues are

$$q\bar{v}_1^{-2} = \frac{1}{3}(\kappa^* + 2\gamma^*) \quad , \quad q\bar{v}_2^{-2} = q\bar{v}_3^{-2} = \frac{1}{2}\gamma^* \tag{8.6}$$

Hence, one gets effective moduli, provided the velocities in the aggregate ($\bar{v}_i$) are known.

Method of Ledbetter and Naimon

The method of Ledbetter and Naimon (1974) is based on the assumption that Debye temperatures of the poly- and the single crystal are equal. Analogously to the crystal case, the Debye temperature θ of the polycrystal is considered to be proportional to the average phase velocity $\{v\}$

$$\theta = K\,\{v\} \quad , \tag{8.7}$$

which is given by

$$\{v\} = \left(\frac{1}{4\pi}\int_{\Omega_n}\frac{1}{3}\sum_{i=1}^{3}(\bar{v}_i(\mathbf{n}))^{-3}d_2\mathbf{n}\right)^{-1/3} \tag{8.8}$$

where **n** is the unit vector with the direction of the wave propagation vector and the integration is performed over all directions of **n**. After substituting $\bar{v}_i$ (i=1,2,3) from (8.6), the integral can be easily calculated because $\bar{v}_i$ does not depend on **n**. As the result one gets

$$3\left(\frac{K}{\theta\sqrt{q}}\right)^3 = 3\sqrt{3}\,(\kappa^* + 2\gamma^*)^{-3/2} + 4\sqrt{2}\,(\gamma^*)^{-3/2} \tag{8.9}$$

With the left hand-side known (the same as for the single crystal) and $\kappa^*=\kappa$ (cubic symmetry) one obtains the equation for the effective shear modulus γ^*.

Markham Method

It is worth mentioning that the Ledbetter and Naimon assumption of the equality of Debye temperatures is secondary in relation to the assumption of equality of the average phase velocities $\{v\}$ for single- and polycrystal. In fact, a similar idea is the base of a method proposed by Markham (1962) and later by Middya, Paul and Basu (1985). The average velocities for longitudinal and transverse modes are assumed to be given

by the harmonic averages of the corresponding crystal velocities

$$\bar{v}_1^{-1} = \frac{1}{4\pi} \int_{\Omega_n} (v_1\ (\mathbf{n}))^{-1} d_2\mathbf{n} \quad , \tag{8.10}$$

and

$$\bar{v}_2^{-1} = \bar{v}_3^{-1} = \frac{1}{2} \sum_{i=2}^{3} \frac{1}{4\pi} \int_{\Omega_n} (v_i\ (n))^{-1} d_2\mathbf{n} \quad , \tag{8.11}$$

respectively.

The following arguments led the authors to the formulae: In a polycrystalline material, where velocity in a given direction is $\bar{v}$, the time of passing the distance L is equal to the sum of intervals necessary for passing subsequent grains on the wave's path. I.e., $L/\bar{v}=\sum_p l_p/v^p$, where l_p and v^p are the distance and the velocity in p-th grain, respectively. Assuming uniform orientation distribution and such a grain shape that no crystallographic direction is preferred, one gets $\bar{v}$ as harmonic average of the velocities in all possible crystallographic directions.

Having Eqs (8.10–11) and using Eq (8.6) one can calculate the effective shear and bulk moduli.

Gold Method

Gold (1950), while estimating the elastic constants of beryllium, used an analogous method for calculation of the effective constants of the quasi-isotropic polycrystal. The assumption there is that the squares of longitudinal and transverse wave velocities in the polycrystal ($\bar{v}_i^2$) are equal to arithmetic averages (over all crystallographic directions) of squares of velocities in the crystal ($(v_i(\mathbf{n}))^2$). Formally, this corresponds to the modified relations (8.10–11).

In the original paper Gold assumed weak anisotropy and equality of the mean velocities $\bar{v}_2$ and $\bar{v}_3$ of transverse modes. To obtain the curve shown in Figure 7 the harmonic average of $\bar{v}_2^2$ and $\bar{v}_3^2$ was used in Eq (8.6).

9. CONCLUDING REMARKS

The degree of generality of the particular methods is different. The original Aleksandrov procedure or the Ledbetter and Naimon method can be applied only to quasi-isotropic materials with cubic crystal symmetry. Besides in those, quasi-isotropy is the immanent assumption of the methods by Huber-Schmid-Boas, Shirakawa-Numakura, Verma-Aggarwal and Imhof. The Markham and Gold methods, originally proposed for the quasi-isotropic case, can be generalized to include non-trivial textures or grain shapes but, to the author's knowledge, this has not been attempted up to now.

The group of procedures considered to be general without restrictions, i.e., applicable to all symmetries and arbitrary textures, is not numerous. It contains the Voigt and Reuss averages, the Bunge method and the generalized Hill and Aleksandrov procedures.

Among the diverse statements and assumptions about the effective constants, there are some of unquestionable validity: The effective tensor should be positive definite

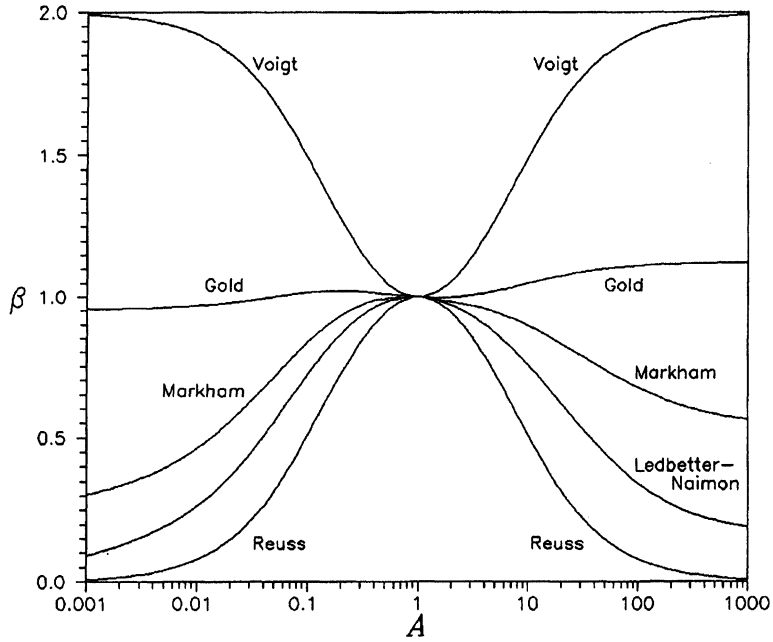

Figure 7 β vs. A for Ledbetter-Naimon, Markham and Gold procedures. See Figure 1 for explanation.

and contained within Voigt-Reuss bounds. The reciprocity condition should be fulfilled. The procedure following from the definition of the effective stiffness tensor, should give equivalent results for both (Hill's and standard) definitions. Moreover, the method should agree with the strict solution for bulk modulus of the cubic material. For results obeying Voigt-Reuss bounds, the last condition is the consequence of that property.

The fulfillment of Voigt-Reuss bounds and of the reciprocity condition was considered in the main body of the paper. As to the exact solution for bulk modulus of cubic materials, only early papers on the subject (e.g., Huber & Schmid 1934) took no account of it. The situation is specific for the procedures based on averaging of the velocity of elastic waves. In fact, the adiabatic constants are considered there, but the authors assume them to be equal to the isothermic ones. The equality of single- and polycrystal bulk moduli does not occur for those methods.

Procedures using the definition of the effective stiffness tensor are based on the following scheme. First, the strain tensor is expressed as $\varepsilon=\mathbf{A}\langle\varepsilon\rangle$. Substituting it in the standard definition, due to arbitrariness of $\langle\varepsilon\rangle$, one gets $\mathbf{c}^*=\langle\mathbf{cA}\rangle$. Analogously, Hill's definition gives $\mathbf{c}^*=\langle\mathbf{A}^T\mathbf{cA}\rangle$, with 'T' denoting matrix transposition. Among the considered methods only three (Voigt, Reuss and Bunge procedures) can be easily reduced to the scheme. In case of Voigt method $\mathbf{A}=\mathbf{I}$ and both definitions give the same effective tensor. For Reuss average, $\mathbf{A}=\mathbf{sc}^*$ and the formula $\mathbf{c}^*=\langle\mathbf{s}\rangle^{-1}$ follows from Hill's definition, whereas the standard definition reduces to identity. The example of $\mathbf{A}$ for Bunge method can be easily read from Eq (7.3) ($\mathbf{A}=\mathbf{I}-\langle\mathbf{c}\rangle^{-1}\mathbf{c}'$). As was stated before, in this case, the standard and Hill's definitions give different results.

The Bruggeman method has to be treated separately. It is an early attempt to take into account the texture as well as the shape of grains. This is close to the essence

of statistical methods. On the other hand, it deals with a material of a very special internal structure. A generalization to other structures and symmetries, although possible, would require extensive transformations. Moreover, some arbitrary assumptions are included (e.g., there is no firm justification of the form of the potential φ). Generally the procedure is very cumbersome; calculations are carried out not in the compact tensor form, but using directly separate tensor components. It is difficult to check if the formal requirements listed above are satisfied. In particular, it concerns obeying the Voigt-Reuss bounds. As to the effective bulk modulus of the cubic material, it is equal to the single crystal bulk modulus due to the extra condition imposed in this case.

The generalizations of Hill method and methods described in part 4 are constructed *ad hoc*, to satisfy some of the formal requirements for effective constants. Besides those conditions, they are arbitrary and physically groundless. Similarly, there is no firm justification of averaging separately Young or shear moduli.

The methods based on velocity averaging use assumptions of a somehow external nature. There are no arguments in support of the Gold procedure. The assumption of Ledbetter and Naimon (equality of Debye temperatures) is doubtful. It would be more reasonable, to go in opposite direction, i.e., to consider the differences between Debye temperatures basing on the known effective properties as was done by, e.g., Anderson (1965) or Ledbetter himself (1973). Among those methods, the most clear is Markham's justification. One has to remember, however, that it is an extreme simplification of the phenomenon of wave propagation in the heterogeneous medium of the polycrystal. In other words, simplistic assumptions of the static problem are replaced by a trivial dynamic model.

The approximation used in the elegant Bunge method appears to be too crude and, in effect, the result falls outside Voigt-Reuss bounds.

Summarizing, none of the reviewed methods can be considered as firmly justified and, as giving satisfactory results, at the same time. Each of them includes some arbitrary assumptions. In fact, this is the way to evade the lack of complete statistical information about the composition of the material. Unfortunately, none of such substitutes is satisfactory and application of more complete statistical information seems to be inevitable, especially for crystals with strong anisotropy.

APPENDIX A: *Matrices corresponding to tensors of* $\overline{\mathbb{T}}^4$

Due to the symmetries (1.6) calculations involving tensors of $\overline{\mathbb{T}}^4$ can be carried out equivalently using (6x6) matrices. It is not convenient to use traditional Voigt assignment because it is not the same for all tensors. The other ascription used, e.g., by Wooster (1949) requires a special kind of 'matrix' multiplication (Morawiec, 1989). The best way to describe the correspondence is the following one (see, e.g., Gubernatis & Krumhansl, 1975):

a) pairs of tensor subscripts 11, 22, 33, 23, 13 and 12 correspond traditionally to matrix subscripts 1, 2, 3, 4, 5 and 6, respectively,
b) if one of the matrix subscripts, either of column or of row, is greater than 3, then to obtain the matrix element, one has to multiply the corresponding tensor element by $\sqrt{2}$.
c) if subscripts of both, column and row, are greater than 3, then to obtain the matrix element, the corresponding tensor element should be multiplied by 2.

Elements of the set $\mathbb{T}^4$ correspond to symmetric matrices. Using rules a) and b) elements of $\mathbb{T}^2$ can be prescribed to column matrices 6x1 (vectors) and the Hooke's law will also have the form of matrix multiplication.

APPENDIX B: *Inequalities*

Let for $\mathbf{t}\in\mathbb{T}^4$ the symbol $\mathbf{t}>0$ denote that the matrix corresponding to $\mathbf{t}$ is positive definite, i.e., if $\mathbf{t}>0$, then for any $\xi\neq 0$ ($\xi\in\mathbb{T}^2$) $\xi\mathbf{t}\xi>0$.

The notation $\mathbf{t}\geq 0$ will denote that $\mathbf{t}$ is positive semi-definite. Moreover, for $\mathbf{t}_1,\mathbf{t}_2\in\mathbb{T}^4$ the inequality $\mathbf{t}_1>\mathbf{t}_2$ ($\mathbf{t}_1\geq\mathbf{t}_2$) will be equivalent to $\mathbf{t}_1-\mathbf{t}_2>0$ ($\mathbf{t}_1-\mathbf{t}_2\geq 0$).

It is well known from linear algebra that symmetric positive definite (semi-definite) matrices can be diagonalized with positive (non-negative) eigenvalues on the diagonal.

For $\mathbf{t},\mathbf{t}_1,\mathbf{t}_2\in\mathbb{T}^4$, if $\mathbf{t}_1$, $\mathbf{t}_2>0$ then $\mathbf{t}_1+\mathbf{t}_2>0$, and if $\mathbf{t}>0$ then $\mathbf{t}^{-1}>0$. Moreover, it is easy to show that the inequality $\mathbf{t}_1>\mathbf{t}_2$ is equivalent to $\mathbf{t}_1+\mathbf{t}>\mathbf{t}_2+\mathbf{t}$. Analogously, $\mathbf{t}_1\geq\mathbf{t}_2$ iff $\mathbf{t}_1+\mathbf{t}\geq\mathbf{t}_2+\mathbf{t}$.

The main aim here is to prove that for $\mathbf{t}_1,\mathbf{t}_2>0$, from the inequality $\mathbf{t}_1>\mathbf{t}_2$ follows $\mathbf{t}_2^{-1}>\mathbf{t}_1^{-1}$. Having this proven, one can easily show that $\mathbf{t}_1>\mathbf{t}_2$ and $\mathbf{t}_2^{-1}>\mathbf{t}_1^{-1}$ are equivalent. The same is true for $\mathbf{t}_1\geq\mathbf{t}_2$ and $\mathbf{t}_2^{-1}\geq\mathbf{t}_1^{-1}$.

Now, let's prove $\mathbf{t}_1>\mathbf{t}_2\Rightarrow\mathbf{t}_2^{-1}>\mathbf{t}_1^{-1}$. Because $\mathbf{t}_i>0$ (i=1,2), then there exists the orthogonal matrix $\mathbf{u}_i\in\mathbb{T}^4$, such that $\mathbf{t}_i=\mathbf{u}_i\mathbf{t}_i^d\mathbf{u}_i^{-1}$, where $\mathbf{t}_i^d$ is diagonal matrix with positive diagonal elements. Let $\mathbf{y}_i^d$ be the diagonal matrix with elements being square roots of diagonal elements of $\mathbf{t}_i^d$, i.e., $\mathbf{y}_i^d\mathbf{y}_i^d=\mathbf{t}_i^d$, $\mathbf{y}_i^d>0$. Defining $\mathbf{y}_i:=\mathbf{u}_i\mathbf{y}_i^d\mathbf{u}_i^{-1}$ one has $\mathbf{y}_i\mathbf{y}_i=\mathbf{t}_i$ along with $\mathbf{y}_i>0$. Let $\mathbf{z}:=\mathbf{y}_1^{-1}\mathbf{y}_2\mathbf{y}_2\mathbf{y}_1^{-1}$, thus $\mathbf{z}>0$. Inequality $\mathbf{t}_1-\mathbf{t}_2>0$ is equivalent to $\mathbf{y}_1^{-1}(\mathbf{t}_1-\mathbf{t}_2)\mathbf{y}_1^{-1}=\mathbf{I}-\mathbf{z}>0$. On the other hand, $\mathbf{t}_2^{-1}-\mathbf{t}_1^{-1}>0$ corresponds to $\mathbf{z}^{-1}-\mathbf{I}>0$. It is enough to show that $\mathbf{I}-\mathbf{z}>0$ leads to $\mathbf{z}^{-1}-\mathbf{I}>0$. Because $\mathbf{z}>0$, there exists an orthogonal matrix $\mathbf{u}_z$, such that $\mathbf{z}^d$ given by $\mathbf{z}^d=\mathbf{u}_z^{-1}\mathbf{z}\mathbf{u}_z$ is diagonal. $\mathbf{I}-\mathbf{z}>0$ leads to $\mathbf{I}-\mathbf{z}^d=\mathbf{u}_z^{-1}(\mathbf{I}-\mathbf{z})\mathbf{u}_z>0$, i.e., each of the diagonal elements of $\mathbf{z}^d$ is greater than zero and less than one. Thus $(\mathbf{z}^d)^{-1}-\mathbf{I}>0$ and $\mathbf{z}^{-1}-\mathbf{I}=\mathbf{u}_z[(\mathbf{z}^d)^{-1}-\mathbf{I}]\mathbf{u}_z^{-1}>0$ which ends the proof of the statement.

APPENDIX C: *Cubic and isotropic tensors of* $\mathbb{T}^4$

The tensors of $\mathbb{T}^4$ corresponding to the material with cubic crystal symmetry (T,T_h,T_d,O,O_h) are described by three independent parameters. Let for $\mathbf{t}$ these parameters be

$$\begin{aligned}\kappa: &= \underline{t}_{1111} + 2\underline{t}_{1122} &,\\ \rho: &= \underline{t}_{1111} - \underline{t}_{1122} &,\\ \gamma: &= 2\underline{t}_{1212} &,\end{aligned} \tag{C.1}$$

Where $\underline{t}_{ijkl}$ are tensor components in the cartesian coordinate system referred to the lattice of the cubic crystal. The tensor can be written in the form

$$\mathbf{t} = \kappa\mathbf{E}^1 + \rho\mathbf{E}^2 + \gamma\,\mathbf{E}^3 =: \mathbf{cub}(\kappa,\rho,\gamma), \tag{C.2}$$

where

$$\mathbf{E}^1_{ijkl} := \frac{1}{3}\,\delta_{ij}\delta_{kl}$$

$$E^2_{ijkl} := \sum_{m=1}^{3} \delta_{i(m)}\delta_{j(m)}\delta_{k(m)}\delta_{l(m)} - \frac{1}{3}\delta_{ij}\delta_{kl} \quad , \tag{C.3}$$

$$E^3_{ijkl} := I_{ijkl} - \sum_{m=1}^{3} \delta_{i(m)}\delta_{j(m)}\delta_{k(m)}\delta_{l(m)} \quad .$$

The above tensors $\mathbf{E}^1$, $\mathbf{E}^2$, $\mathbf{E}^3 \in \mathbb{T}^4$ satisfy the relations

$$\mathbf{E}^i\mathbf{E}^j = \delta_{ij}\,\mathbf{E}^{(i)} \tag{C.4}$$

Therefore, there occurs the simple multiplication rule

$$\mathbf{cub}(\kappa_1,\rho_1,\gamma_1)\ \mathbf{cub}(\kappa_2,\rho_2,\gamma_2) = \mathbf{cub}(\kappa_1\kappa_1,\rho_1\rho_2,\gamma_1\gamma_2). \tag{C.5}$$

Moreover, because $\mathbf{I}=\mathbf{cub}(1,1,1)$, then

$$(\mathbf{cub}(\kappa,\rho,\gamma))^{-1} = \mathrm{cub}(\kappa^{-1},\rho^{-1},\gamma^{-1}) \tag{C.6}$$

The algebra is completed by the relations

$$\mathbf{cub}(\kappa_1,\rho_1,\gamma_1) + \mathbf{cub}(\kappa_2,\rho_2,\gamma_2) = \mathbf{cub}\ (\kappa_1+\kappa_2,\ \rho_1+\rho_2,\ \gamma_1+\gamma_2) \tag{C.7}$$

$$\alpha\ \mathbf{cub}(\kappa,\rho,\gamma) = \mathbf{cub}(\alpha\kappa,\ \alpha\rho,\ \alpha\gamma)\ ,\quad \alpha \in \mathbb{R} \quad . \tag{C.8}$$

One can easily check the validity of

$$\begin{aligned} \mathrm{tr}_1(\mathbf{cub}(\kappa,\rho,\gamma)) &= 3\kappa \\ \mathrm{tr}_2(\mathbf{cub}(\kappa,\rho,\gamma)) &= \kappa + 2\rho + 3\gamma \quad . \end{aligned} \tag{C.9}$$

It is worth mentioning, that the parameters κ, ρ and γ are eigenvalues of the matrix corresponding to $\mathbf{cub}(\kappa,\rho,\gamma)$.

The isotropy of tensor $\mathbf{t}=\mathbf{cub}(\kappa,\rho,\gamma))$ is equivalent to $\gamma=\rho$. Let the case be denoted by $\mathbf{iso}(\bullet,\bullet)$ which is defined by

$$\mathbf{iso}(\kappa,\gamma) := \mathbf{cub}(\kappa,\gamma,\gamma) \quad . \tag{C.10}$$

From (C.3) one has $\mathbf{iso}(\kappa,\gamma)=\kappa\mathbf{E}^1+\gamma(\mathbf{E}^2+\mathbf{E}^3)=\gamma\mathbf{I}+(\kappa-\gamma)\mathbf{E}^1$. Relations (C.6–9) hold also in the special case, when the second parameter of **cub** is equal to the third one. Thus analogous relations are true for isotropic (**iso**) tensors.

Parameters κ and γ of the isotropic stiffness tensor $\mathbf{c}=\mathbf{iso}(\kappa,\gamma)$ are related to the bulk (K) and shear (G) moduli by $\kappa=3K$ and $\gamma=2G$, respectively. They are called by the same names. (Other relations are given in Table 1.)

The following formula is also useful

$$\mathbf{M}^{f=1}(\mathbf{cub}(\kappa,\rho,\gamma)) = \mathbf{iso}(\kappa, \frac{2\rho+3\gamma}{5}) \quad . \tag{C.11}$$

It can be obtained from Eqs (2.11), (C.9) and the first set of (2.16).

Table 1 Relations between the moduli κ, γ and other elastic moduli of the isotropic material. (λ, μ) – Lamé moduli, K – bulk modiulus, G – shear modulus, E – Young modulus, υ – Poisson modulus.

	(κ,γ)	(λ,μ)	(K,G)	(E,υ)
κ		$3\lambda+3\mu$	3K	$\frac{E}{1-2\upsilon}$
γ		2μ	2G	$\frac{E}{1+\upsilon}$
λ	$\frac{\kappa-\gamma}{3}$			
μ=G	$\frac{\kappa}{2}$			
K	$\frac{\kappa}{3}$			
E	$\frac{3\kappa\gamma}{2\kappa+\gamma}$			
υ	$\frac{\kappa-\gamma}{2\kappa+\gamma}$			

APPENDIX D: *Invariance of κ with respect to averaging procedure*

For a given $\mathbf{t}\in\overline{\mathbb{T}}^4$, let's consider the operation $\mathbf{t}\mapsto\mathbf{E}^1\mathbf{t}$. Tensor $\mathbf{E}^1\mathbf{t}$ has the symmetry (1.6), i.e., $\mathbf{E}^1\mathbf{t}\in\overline{\mathbb{T}}^4$. By direct verification one checks that (for any crystal symmetry) the bulk modulus $\kappa:=c_{iijj}/3(=3K)$ can be expressed as $\frac{1}{3}\mathrm{tr}_2(\mathbf{E}^1\mathbf{c})$. Let $\mathbf{c}=\mathbf{cub}(\kappa,\rho,\gamma)$; in such a case

$$\mathbf{E}^1\mathbf{c} = \mathbf{cub}(1,0,0)\ \mathbf{cub}(\kappa,\rho,\gamma) = \mathbf{cub}(\kappa,0,0) = \kappa\mathbf{E}^1 \qquad \text{(D.1)}$$

and this is consistent with the above definition.

Let's consider the effective properties. If $\varepsilon=\mathbf{A}\langle\varepsilon\rangle$ for arbitrary ε, then $\langle\mathbf{A}\rangle=\mathbf{I}$, and from the definition $\mathbf{c}^*\langle\varepsilon\rangle=\langle\mathbf{c}\varepsilon\rangle$, the formula for the effective tensor is $\mathbf{c}^*=\langle\mathbf{cA}\rangle$. This is the form of exact stochastic solutions of the problem.

In the special case of cubic symmetry of $\mathbf{c}$, tensor $\mathbf{E}^1\mathbf{c}^*$ is given by

$$\mathbf{E}^1\mathbf{c}^* = \mathbf{E}^1\langle\mathbf{cA}\rangle = \langle\mathbf{E}^1\mathbf{cA}\rangle = \langle\kappa\mathbf{E}^1\mathbf{A}\rangle = \kappa\mathbf{E}^1\langle\mathbf{A}\rangle = \kappa\mathbf{E}^1 \qquad \text{(D.2)}$$

and hence, $\kappa^*=\frac{1}{3}\mathrm{tr}_2(\mathbf{E}^1\mathbf{c}^*)=\kappa$. One concludes that, provided the crystal symmetry is cubic, in all procedures based on $\mathbf{c}^*=\langle\mathbf{cA}\rangle$, the bulk modulus is preserved (Walpole, 1985; see also Chandrasekar & Santhanam, 1989).

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