

# METHODS OF CALCULATING PETROPHYSICAL PROPERTIES FROM LATTICE PREFERRED ORIENTATION DATA

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**Abstract.** We consider the theoretical problems of calculating the physical properties of an aggregate from the constituent crystal properties and the lattice preferred orientation. The notion of a macroscopically homogeneous sample with an internally varying distribution of stress and strain fields is introduced to explain why further efforts have to be made to improve on the physically based Voigt and Reuss bounds. It is shown that the Voigt and Reuss bounds become increasingly separated with increasing anisotropy, emphasising the need for better methods. The problem of highly anisotropic minerals is illustrated with polycrystals of plagioclase feldspar and biotite. Biotite is used to illustrate the mean velocity, the geometric mean and the self-consistent methods. The self-consistent method, which is generally accepted to give the best estimate, is almost identical to geometric mean recently introduced by Matthies and Humbert (1993) and similar to the arithmetic mean of the Voigt and Reuss bounds (Hill, 1952). The geometric mean has the powerful physical condition that the aggregate mean is equal to the mean of the inverse property (e.g. mean elastic stiffness and compliance). Despite its lack of theoretical justification the Hill average remains a useful estimate.

**Key words:** Physical properties, lattice preferred orientation, averaging methods, elasticity, seismic velocity

## 1. Introduction

The estimation of physical properties of crystalline aggregates from the properties of the component crystals has been the subject of an extensive literature since the classical work of Voigt (1928) and Reuss (1929). Such an approach is only feasible if the bulk properties of the crystals dominate the physical property of the aggregate and the effects of grain boundary interfaces can be ignored. For example, the methods discussed here cannot be applied to the electrical properties of water saturated rock, where the role of interfacial conduction is likely to be important. Many properties of geophysical interest can be evaluated, for example thermal conductivity, thermal expansion, diamagnetism, elasticity and seismic velocities.

The majority of rock forming minerals have strongly anisotropic physical properties and many rocks also have strong lattice preferred orientations (LPO's, or textures as they are called in Materials Science). The combination of strong LPOs and anisotropic single crystal properties results in a three dimensional variation in rock properties which is difficult, or too time consuming, to evaluate by direction laboratory measurement in every orientation. Petrophysical mea-

measurements are usually made under hydrostatic pressure, and often at elevated temperature to simulate conditions in the Earth where presumably the fractures present at ambient conditions are closed. The necessity to work at high pressure and temperature conditions limits the number of orientations that are measured. Typically, three orthogonal directions are measured parallel to structural features, such as the lineation and foliation normal defined by grain shape. The evaluation of physical properties from LPO allows the determination of properties over the complete sphere. As most geophysical properties are centrosymmetric (e.g. thermal conductivity, magnetic susceptibility and seismic velocity), only a part of the texture information, the even function (e.g. Humbert and Diz, 1991), is required for their determination by averaging methods. The even texture function is determined from volume-true texture measurement by X-ray or neutron diffraction. Such techniques are well adapted for monomineralic aggregates (e.g. quartzites, calcite marbles), however most rocks are polyphase, therefore individual measurement techniques are more appropriate for routine analysis.

## 2. Methods of Calculation

Ideally we would like to have a general description of the stress and strain fields at every point ( $\mathbf{r}$ ) in a linear elastic polycrystal which are completely determined by Hooke's law as follows

$$\sigma_{ij}(\mathbf{r}) = C_{ijkl}(\mathbf{r})\varepsilon_{kl}(\mathbf{r})$$

where  $\sigma_{ij}(\mathbf{r})$  is the stress tensor,  $C_{ijkl}(\mathbf{r})$  is the elastic stiffness tensor and  $\varepsilon_{kl}(\mathbf{r})$  the strain tensor at point  $\mathbf{r}$ . The evaluation of the effective constants of a polycrystal would be the summation all components as a function of position if we know the spacial functions of stress and strain.

However, if we only need to characterize the macroscopic (i.e. limited by the specimen boundary conditions) elastic behaviour, then we only need to evaluate the effective properties, which are generally representative of the experimental measurements.

The sample may be microscopically heterogeneous due to grain size, shape, orientation or phase distribution, but will be considered macroscopically uniform. The complete structural details of the sample are in general never known, but a "statistically uniform" sample contains many regions which are compositionally and structurally similar, each fairly representative of the entire sample. If this is so then the average stress  $\langle\sigma\rangle$  and strain  $\langle\varepsilon\rangle$  of a statistically uniform sample are linked by an effective macroscopic modulus  $C^*$  that obeys Hooke's law of linear elasticity,

$$C^* = \langle\sigma\rangle\langle\varepsilon\rangle^{-1}$$

where

$$\langle \varepsilon \rangle = \frac{1}{V} \int \varepsilon(\mathbf{r}) \, d\mathbf{r}$$

and

$$\langle \sigma \rangle = \frac{1}{V} \int \sigma(\mathbf{r}) \, d\mathbf{r}$$

and  $V$  is the volume. The stress  $\sigma(\mathbf{r})$  and strain  $\varepsilon(\mathbf{r})$  distribution in a real polycrystal varies discontinuously at the surface of grains. By replacing the real polycrystal with a "statistically uniform" sample we are assuming that  $\sigma(\mathbf{r})$  and strain  $\varepsilon(\mathbf{r})$  are varying slowly and continuously with position ( $\mathbf{r}$ ).

The best known averaging techniques for obtaining estimates of the effective elastic constants are the Voigt and Reuss averages. The Voigt average is found by simply assuming that the strain field is everywhere constant (i.e.  $\varepsilon(\mathbf{r})$  is independent of  $\mathbf{r}$ ). The strain at every position is set equal to the macroscopic strain of the sample.  $C^*$  is then estimated by a volume average of local stiffnesses  $C(\mathbf{g}_i)$  with orientation  $\mathbf{g}_i$ , and volume fraction  $V_i$ ,

$$C^* \approx C^{\text{Voigt}} = \left[ \sum_i V_i C(\mathbf{g}_i) \right]$$

Reuss average is found by assuming that the stress field is everywhere constant. The stress at every position is set equal to the macroscopic stress of the sample.  $C^*$  is then estimated by the volume average of local compliances  $S(\mathbf{g}_i)$ ,

$$C^* \approx C^{\text{Reuss}} = \left[ \sum_i V_i S(\mathbf{g}_i) \right]^{-1}$$

A physical estimate of the moduli should lie between the Voigt and Reuss average bounds as the stress and strain distributions are expected to be somewhere between uniform strain (Voigt bound) and uniform stress (Reuss bound). Hill (1952) observed that arithmetic mean of the Voigt and Reuss bounds, sometimes called the Hill or Voigt-Reuss-Hill (VRH) average, is often close to experimental values. The VRH average has no theoretical justification. In Figure 1 we present the Voigt, Reuss and Hill averages of a number of rock forming minerals for randomly orientated polycrystals as a function of anisotropy for compressional ( $V_p$ ) and shear ( $V_s$ ) wave anisotropy. The anisotropy is defined here as the  $(V_{\max} - V_{\min})/V_{\text{mean}}$ .

With increasing anisotropy the separation between the Voigt and Reuss bounds increases (Figure 1), which is unacceptable for minerals with a considerable degree of anisotropy.

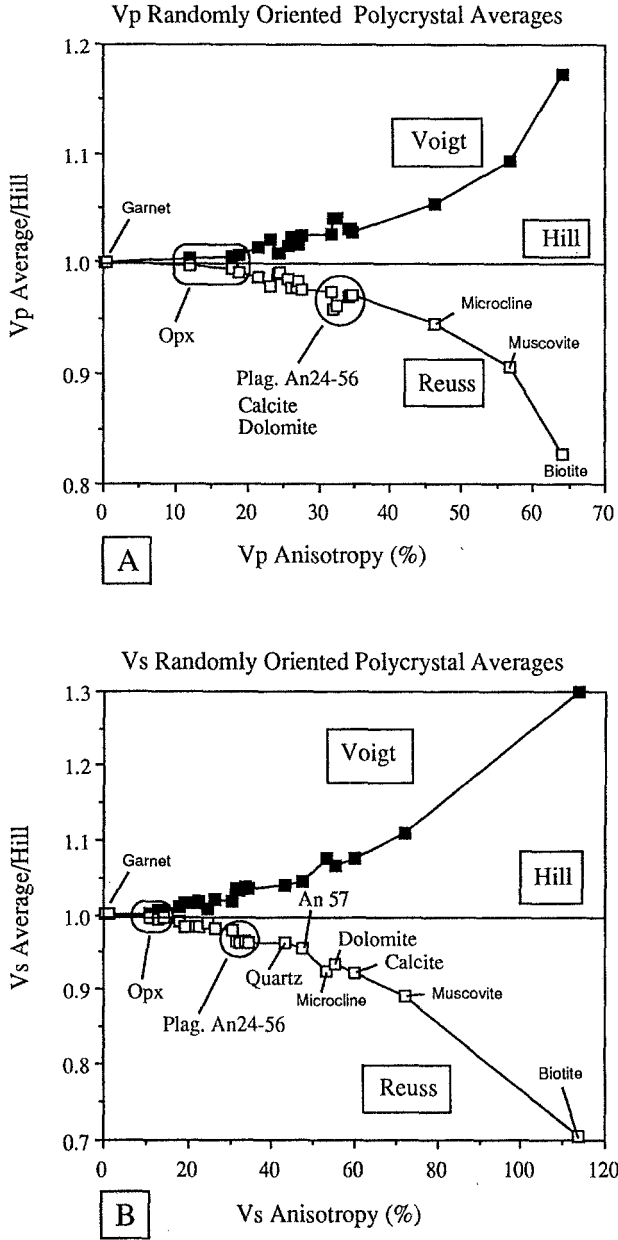


Fig. 1. The Voigt and Reuss averages for 23 different rock forming minerals as a function of anisotropy for  $V_p$  and  $V_s$  seismic velocities.

Four methods have been proposed to account for the non-random distribution of  $C(\mathbf{r})$  (Watt *et al.*, 1976), which we list in order of increasing complexity:

1) First approach uses simple statistical methods based on volume fractions for the calculations of bounds without reference to geometrical details. For polycrystalline samples the most widely used averaging techniques are those originally proposed by Voigt (1928) and Reuss (1929), mentioned above. In Earth sciences the Voigt, Reuss and Hill averages have been widely used for averages of oriented polyphase rocks (e.g. Crosson and Lin, 1971; Baker and Carter, 1972). Although the Voigt and Reuss bounds are often far apart for anisotropic materials, they still provide the limits within which the experimental data must be found (Ono, 1992).

Recently several authors have searched for a geometric mean of oriented polycrystals using the exponent of the average of the natural logarithm of the eigenvalues of the stiffness matrix (Morawiec, 1989; Matthies and Humbert, 1993). Their choice of this averaging procedure was guided by the fact that the ensemble average elastic stiffness  $\langle C \rangle$  should equal the inverse of the ensemble average elastic compliances  $\langle S \rangle^{-1}$ , which is not true, for example, of the Voigt and Reuss estimates. The physical importance of this reciprocal relationship was first suggested by Aleksandrov and Aisenberg (1967) for second order tensors.

A method of determining the geometric mean for arbitrary orientation distributions has been recently developed (Matthies and Humbert, 1993). The method derives from the fact that a stable elastic solid must have an elastic strain energy which is positive, it follows from this that the eigenvalues of the elastic matrix must all be positive. As is well known, the arithmetic mean of a positive scalar  $x$  depending on orientation  $\mathbf{g}$  reads as follows:

$$\bar{x} = \sum_{n=1}^N x(\mathbf{g}_n) f(\mathbf{g}_n) \Delta \mathbf{g}_n \quad \text{with} \quad \sum_{n=1}^N f(\mathbf{g}_n) \Delta \mathbf{g}_n = 1$$

where  $f(\mathbf{g}_n)$  is the ODF (Orientation Distribution Function) and  $\bar{x}$  is the arithmetic mean. The orientation space is discretized into cells of volume  $\Delta \mathbf{g}_n$ . The corresponding geometric mean can be expressed as:

$$\langle x \rangle = \prod_{n=1}^N [x(\mathbf{g}_n)]^{f(\mathbf{g}_n) \Delta \mathbf{g}_n} = \exp(\overline{\text{Ln } x})$$

with

$$\overline{\text{Ln } x} = \sum_{n=1}^N \text{Ln}\{x(\mathbf{g}_n)\} f(\mathbf{g}_n) \Delta \mathbf{g}_n$$

The geometric mean of elastic properties is a generalization of the above relations, which involves the eigenvalues of the matrix representing the elastic tensors. In the present case the elastic tensor is expressed by a  $6 \times 6$  matrix  $C^0$  which links

the symmetric parts of dimension 6 of the stress and strain tensors (the antisymmetric parts of dimension 3 being nil). The components of  $C^0$  are calculated from the conventional elastic constants. For a grain orientation  $\mathbf{g}$  this matrix reads:

$$C^0(\mathbf{g}) = W(\mathbf{g})C^0W(\mathbf{g})^{-1}$$

where  $W(\mathbf{g})$  is an orthogonal matrix. By diagonalizing  $C^0$ , it follows:

$$C^0(\mathbf{g}) = W(\mathbf{g})P^0 \wedge P^{0-1}W(\mathbf{g})^{-1}$$

where  $\wedge$  is a  $6 \times 6$  matrix formed with the eigenvalues of  $C^0$ , which are all positive. Therefore it is possible to introduce the "logarithmic" matrix  $\text{Ln } C^0(\mathbf{g})$  which is equal to:

$$\text{Ln } C^0(\mathbf{g}) = W(\mathbf{g})P^0(\text{Ln } \wedge)P^{0-1}W(\mathbf{g})^{-1} = W(\mathbf{g})(\text{Ln } C^0)W(\mathbf{g})^{-1}$$

where  $\text{Ln } \wedge$  is the  $6 \times 6$  matrix formed with the logarithms of the eigenvalues of  $C^0$ . The components of the corresponding geometric mean of this logarithmic matrix is:

$$[\overline{\text{Ln } C}]_{ij} = \int [W(\mathbf{g})(\text{Ln } C^0)W(\mathbf{g})^{-1}]_j f(\mathbf{g}) d\mathbf{g}$$

This matrix can be diagonalized by the orthogonal matrix  $Q$  and possesses the eigenvalues  $\mu_k$ . Finally the components of the matrix corresponding to the geometric mean can be expressed by:

$$\langle C \rangle_{ij} = \sum_{k=1}^N Q_{ik} \exp(\mu_k) Q_{kj}$$

The geometric mean of the polycrystal elastic constants is given by the

$$C^* \approx C^{\text{Geometric Mean}} = \langle C \rangle_{ij}$$

after conversion of  $\langle C_{ij} \rangle$  back into the conventional form of the elastic constants. Comparison between Voigt, Reuss, Hill and self-consistent estimates show that the geometric mean provides estimates very close to the self-consistent method, but at considerably reduced computational complexity (Matthies and Humbert, 1993). The condition that the macroscopic polycrystal elastic stiffness  $\langle C \rangle$  must equal the inverse of the aggregate elastic compliance  $\langle S \rangle^{-1}$  appears to be a powerful physical constraint on the averaging method.

2) The second set of methods assume a specific geometry. In order to obtain tractable results, particularly in polyphase aggregates of greatly different component moduli, it is necessary to define the specific geometry of the aggregate. Obviously the results of this approach are limited to specific geometries, but

provide solutions for extreme cases (e.g. aggregates containing fluids or voids) which are of great geophysical interest. The most important approach in this area is the “self-consistent” (SC) method (e.g. Hill, 1965). In the SC method the elastic field of each position is approximated to the field of an isolated inclusion in an homogenous matrix. The matrix has the isotropic elastic properties of the polycrystal. The results follow from the solution of a single elliptical inclusion in an infinite matrix with prescribed loads at infinity (Eshelby, 1957). The method notionally takes into account the interactions between inclusions by using the matrix of homogenous properties of the polycrystal.

Various implementations of the SC method have been made for oriented polycrystalline aggregates (e.g. Kröner 1958; Kneer 1965; Gubernatis and Krumhansl 1975). Most practical applications have been based on the scheme proposed by Kneer (1965), for example Morris (1970), Humbert and Diz (1991) and Diz and Humbert (1992). Corrections to this scheme for hexagonal symmetry have been proposed by Gubernatis and Krumhansl (1975) and an alternative method of convergence suggested by Morris (1971). It should be mentioned that the SC scheme gives the exact solution only if the aggregate is perfectly disordered (Ono, 1992), but as there are likely to be correlations between orientations of neighbouring grains, the solution will not be exact for real polycrystals.

3) The third is based on scattering theory, where the elastic modulus is decomposed into a spacial invariant part  $C^0$  and a fluctuating part  $\delta C(\mathbf{r})$ ,

$$C(r) = C^0 + \delta C(\mathbf{r})$$

The solution is found using scattering theory where  $\delta C(\mathbf{r})$  “scatters” the strain field via the “propagator” given by a tensor Green’s function which describes the integral stress and strain fields (e.g. Gubernatis and Krumhansl, 1975; Zeller and Dederichs, 1973).

4) The last method includes a statistical description of the elastic moduli and resulting stress and strain fields. This approach (e.g. Beran, 1971) is the most complete description, but too involved for practical application.

### 3. Special Case of Cracked Polycrystals

Macroscopic elastic properties and seismic velocities have also been calculated for polycrystals with oriented with cracks (e.g. Thill *et al.*, 1969; Anderson *et al.*, 1974; Babuska and Pros, 1984; Crampin, 1987; Sayers, 1988; Sayers and van Munster, 1991; Siegesmund *et al.*, 1991; Siegesmund and Vollbrecht, 1991; Cheng, 1993), using the elastic constants of the cracked aggregate, which are often given in the form

$$C_{ijkl} = C_{ijkl}^0 + C_{ijkl}^1 + C_{ijkl}^2$$

where  $C_{ijkl}^0$  are the moduli of the uncracked material and  $C_{ijkl}^1$  and  $C_{ijkl}^2$  the first order and second order crack induced corrections to the elastic stiffness of

$C_{ijkl}^0$ . For example, Siegesmund *et al.* (1991), used the expressions given by Hudson (1980, 1981) for the first order correction  $C_{ijkl}^1$  in their analysis of a mylonite. The analysis of Hudson requires that  $C_{ijkl}^0$  is isotropic which is not strictly true for the mylonite they studied which had a texture related elastic anisotropy at high pressure. The Hudson analysis may only be strictly applied to low crack densities, where interaction between cracks can be ignored. Ass'ad *et al.* (1992) found that Hudson's method gave good agreement with experiment for crack densities up to 7 percent, but disagrees for higher crack densities. The Hudson method, although only valid to moderate crack densities and parallel cracks, allows some estimate of the effects of dry and fluid filled cracks. A more general method has been formulated by Sayers and Kachanov (1991) which uses a differential scheme that is valid to higher crack densities and can be used for an arbitrary orientation distribution of cracks. These methods assume that the uncracked material is elastically isotropic, where as many measurements show that most rocks have both a crack and texture related elastic anisotropy (see review by Kern, 1990). Schoenberg and Sayers (1993) have recently developed a method which allows the calculation of the effective medium as the sum of the compliance tensor of the unfractured anisotropic background medium and a series of excess compliance tensors. Each excess compliance tensor defines the elastic contribution of a set of parallel fractures, hence multiple fracture sets can be modelled.

#### 4. Practical Aspects of Calculation of Seismic Properties

Orientation of crystals in a polycrystal can be measured by volume true diffraction techniques (e.g. X-ray or neutron diffraction) or individual orientation measurements (e.g. U-stage & Optical microscope, electron channelling or electron backscattered patterns). In a rock with many grains of various orientations, the ensemble can be described by an Orientation Distribution Function (ODF), which is a function  $f(\mathbf{g})$  that quantitatively describes the volume fraction of the sample within an orientation range  $\mathbf{g} \pm \Delta\mathbf{g}$ . The function  $f(\mathbf{g})$  may be developed into a series expansions using generalized spherical harmonics (Bunge, 1982) as

$$f(\mathbf{g}) = \sum_{L=0}^{L_{\max}} \sum_{M=-L}^{+L} \sum_{N=-L}^{+L} C_L^{MN} T_L^{MN}(\mathbf{g})$$

where  $C_L^{MN}$  are the coefficients of the series development of the texture function  $f(\mathbf{g})$ ,  $T_L^{MN}(\mathbf{g})$  are the generalised spherical harmonic functions, and  $L_{\max}$  is the maximum degree used in the expansion.

In the series development method the index  $L$  may be evaluated to infinity. In practice it has to be truncated at  $L_{\max}$  value of  $L$  (see Wagner *et al.*, 1981). Once the  $C_L^{MN}$  coefficients have been calculated they can be used to calculate the pole figures and many other types of representation.



To calculate the seismic properties of a polycrystal, one must evaluate the elastic properties of the aggregate. In the case of an aggregate with a crystallographic fabric, the anisotropy of the elastic properties of the single crystal must be taken into account. For each orientation  $\mathbf{g}$  the single crystal properties have to be rotated into the specimen coordinate frame using the orientation or rotation matrix  $g_{ij}$ ,

$$C_{ijkl}(\mathbf{g}) = g_{ip} \cdot g_{jq} \cdot g_{kr} \cdot g_{lt} C_{pqrt}(\mathbf{g}^0)$$

where  $C_{ijkl}(\mathbf{g})$  is the elastic property in sample coordinates,  $g_{ij} = g(\varphi_1 \phi \varphi_2)$  the measured orientation in sample coordinates and  $C_{pqrt}(\mathbf{g}^0)$  is the elastic property in crystal coordinates.

The elastic properties of the polycrystal may be calculated by integration over all possible orientations of the ODF. Bunge (1985) has shown that integration is given as:

$$\langle C_{ijkl} \rangle^m = \int C_{ijkl}^m(\mathbf{g}) \cdot f(\mathbf{g}) \, dg$$

where  $\langle C_{ijkl} \rangle^m$  is the elastic properties of the aggregate of mineral  $m$  and  $dg = 1/8\pi^2 \sin \phi \, d\varphi_1 \, d\phi \, d\varphi_2$ . Given that we are interested in elasticity, a centrosymmetric fourth order tensor property, only the even part of the texture function  $f(\mathbf{g})$  to  $L_{\max} = 4$  is required (e.g. Humbert and Diz, 1991). Hence the texture information can be determined from relatively few pole figures. The integral  $\int C_{ijkl}^m(\mathbf{g}) \cdot f(\mathbf{g}) \, dg$  can also be solved in several ways. Firstly, it may be obtained directly from the generalized harmonic functions as

$$\langle C_{ijkl} \rangle^m = \sum_{L=0(2)}^4 \sum_{M=-L}^{+L} \sum_{N=-L}^{+L} [1/(2L+1)] C_L^{MN} A_L^{MN*}(ijkl, pqrt) C_{pqrt}(\mathbf{g}^0)$$

where  $A_L^{MN*}(ijkl, pqrt)$  is a library function of rotations for the elastic constants. Note that the single crystal elastic constants are determined in an ortho-normal right-handed reference frame, which for low symmetry crystals is not necessarily the same as the one used to define the Euler angles of the O.D.F., hence an additional rotation may be necessary to bring the elastic reference frame into coincidence with the Euler angle reference frame (see for example Johnston and Wenk, 1986). Secondly the integral may be determined by numerical integration of  $f(\mathbf{g})$  at tabulated values on a grid in Euler space. Thirdly it may be determined by simple summation of individual orientation measurements, viz.

$$\langle C_{ijkl} \rangle^m = \sum C_{ijkl}^m(\mathbf{g}) \cdot v(\mathbf{g})$$

where  $v(\mathbf{g})$  is the volume fraction of the grain in orientation  $\mathbf{g}$ . Finally, there is an interesting method of determining the integral directly from one pole figure in the

case of hexagonal crystal symmetry. In hexagonal crystals the fourth order elastic tensor has axial symmetry about the [0001] axis. Hence to determine the elastic constants for an arbitrary oriented crystal we need only define the orientation of the [0001] (Humbert and Diz, 1991).

Thus instead of  $g(\varphi_1, \phi, \varphi_2)$ , we only need  $g(\varphi_1, \phi, 0)$  or the azimuth ( $\alpha$ ) and inclination ( $\beta$ ) of [0001]. The elastic tensor is therefore given by

$$\langle C_{ijkl} \rangle^m = \frac{1}{2\pi} \int_{\alpha}^{2\pi} \int_{\beta}^{\pi/2} P_{0001}(\alpha, \beta) C_{ijkl}(\alpha, \beta) \sin \beta \, d\alpha \, d\beta$$

where  $P_{0001}(\alpha, \beta)$  is the [0001] pole figure density at azimuth ( $\alpha$ ) and inclination ( $\beta$ ). This result is particularly useful for biotite and muscovite, which are strictly monoclinic, but sufficiently close to hexagonal that their elastic constants have been determined assuming hexagonal crystal symmetry (Alexandrov *et al.*, 1974).

We define the Voigt average of the rock for  $m$  mineral phases as:

$$\langle C_{ijkl} \rangle^{\text{Voigt}} = 1/m \sum \langle C_{ijkl} \rangle^m$$

The final step is the calculation of the three seismic phase velocities by the solution of the Christoffel equation,

$$\text{Det} | \langle C_{ijkl} \rangle^{\text{Voigt}} X_i X_j - \delta_{ik} \rho V^2 = 0$$

where  $X_i X_j$  are the direction cosines of the wave propagation direction,  $\rho$  is the density of the rock,  $\delta_{ik}$  is the Kronecker delta and the three values of  $V$  are the three seismic phase velocities.

To calculate the elastic constants at pressures and temperatures of interest in Earth Sciences the following procedure is used. The single crystal elastic constants are extrapolated to pressure and temperature using the following relationship:

$$C_{ij}(PT) = C_{ij}(P_0 T_0) + (dC_{ij}/dP) \cdot (P - P_0) + (dC_{ij}/dT) \cdot (T - T_0)$$

where  $C_{ij}(PT)$  are the elastic constants at upper mantle pressure  $P$  and temperature  $T$ ,  $C_{ij}(P_0 T_0)$  the elastic constants at reference pressure  $P_0 = 0.1$  MPa and temperature  $T_0 = 25$  °C;  $dC_{ij}/dP$  is the first order pressure derivative and  $dC_{ij}/dT$  is the first order temperature derivative. In using the above relationship, we have assumed a linear variation of  $C_{ij}$  with temperature and pressure. Second order pressure temperature derivatives  $d^2 C_{ij}/dP^2$  and  $d^2 C_{ij}/dT^2$  are only available for a few minerals. The seismic velocities also depend on the density of the minerals at pressure and temperature which can be calculated using:

$$\rho(P,T) = \rho_0 + (\rho_0/K) \cdot (P - P_0) - \alpha \cdot \rho_0 \cdot (T - T_0)$$

where  $\rho(P,T)$  is the density at pressure  $P$  and temperature  $T$ ,  $\rho_0$  is the density at reference pressure  $P_0$  and temperature  $T_0$ ,  $K$  is bulk modulus and  $\alpha$  is the coefficient of thermal expansion, assumed to be isotropic for the present purpose. Ignoring these corrections for density will result in error of the order of 3% at 1 GPa (Watt, 1988).

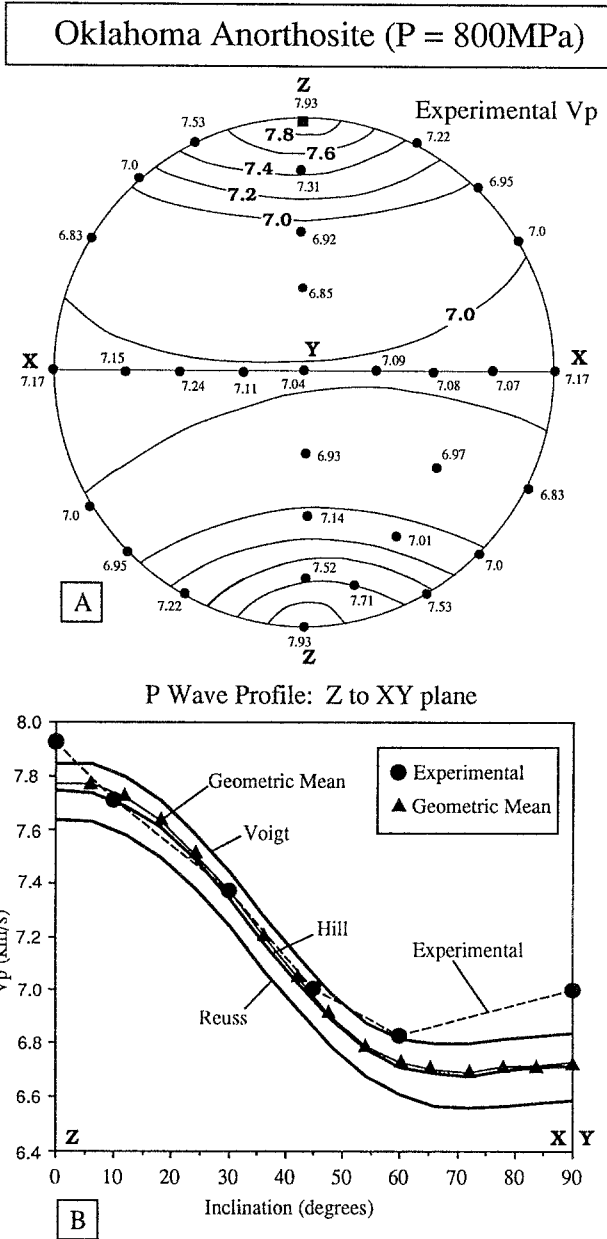


Fig. 2. The seismic properties of anorthosite determined by direct laboratory measurements and calculation using the LPO (after Seront *et al.*, 1993). The laboratory measurements were made at 0.8 GPa and ambient temperature. A) The experimental measurements for  $V_p$  are shown on a stereographic projection with the reference directions X, Y and Z. For  $V_p$  the black dot represents the direction of propagation. B) The comparison between experimental and calculated P wave velocities projected on a plane in zone with the symmetry axis Z. Z is inclination  $0^\circ$  and XY plane is inclination  $90^\circ$ . Calculated values for Voigt, Reuss and Hill show as solid lines. Geometric mean indicated by filled triangles. Experimental data indicated by black dots.

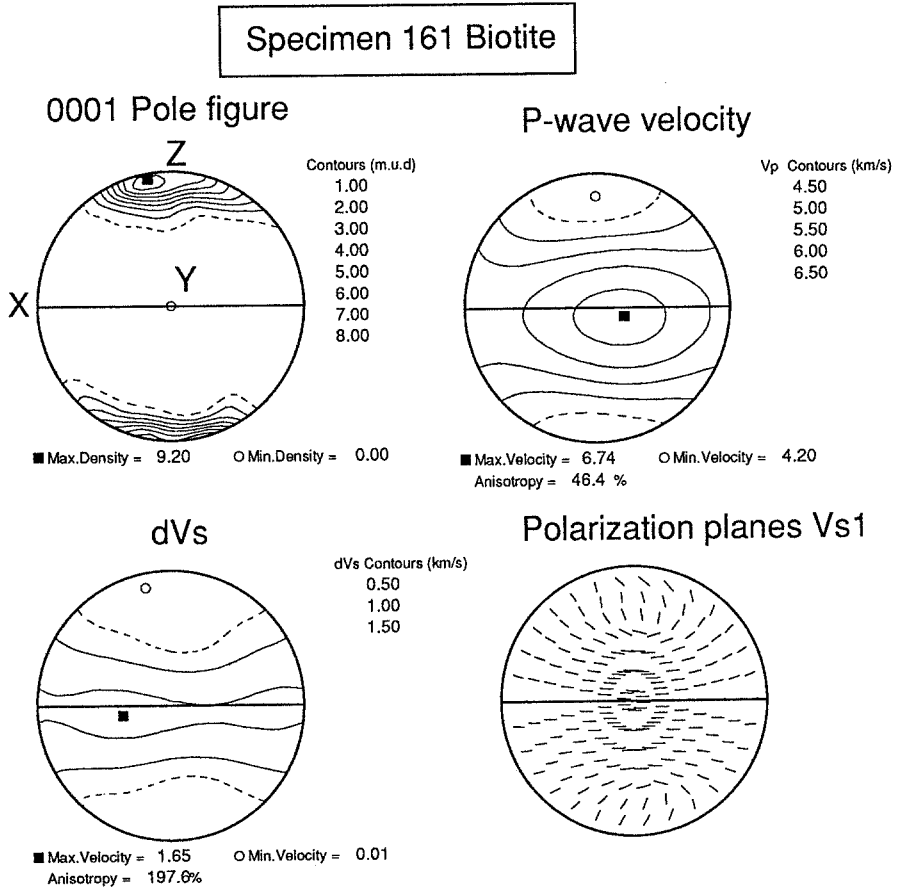


Fig. 3. The (0001) pole figure and seismic properties of specimen 161 composed of biotite. The calculated seismic velocities are for the self-consistent model with spherical grains.

### 5. Application to the Calculation of Seismic Properties to Plagioclase and Muscovite

As our first example we take the work of Seront *et al.* (1993) on polycrystalline plagioclase. They measured the P-wave velocity in 24 directions and the S-wave velocity in 6 directions of an anorthosite sample. The exceptional number of experimental measurements provided a unique test for the Voigt, Reuss, Hill and geometric mean values calculated from the LPO as determined by optical microscopy and assuming isotropy of grain shapes and uniform grain size. The results, in Figure 2, show that P-wave velocities have an axial symmetry about the specimen Z direction, and can be conveniently summarised in an XY profile. The XY profile of P-wave velocities shows that the laboratory measurements agree well with the Hill average and the geometric mean near the Z direction, but diverge in the XY plane. Seront *et al.* (1993) suggested that the poor correlation

in the  $XY$  plane was due to two factors. Firstly, the quality of the single crystal constants measured at room pressure was probably influenced by cleavage cracks inherent in plagioclase. Secondly, the strong grain shape, directly related to the crystallography of the grains may have influenced the experimental results.

As can be seen from Figure 1, micas, represented by muscovite and biotite are among the most anisotropic minerals. They are also very common in the Earth's continental crust and almost always have strong LPOs (e.g. O'Brien *et al.*, 1987). Aggregates containing significant volume fractions of mica have been argued to be the cause of seismic anisotropy in the crust (e.g. Christensen and Szymanski, 1988; Brocher and Christensen, 1990; Kern and Wenk, 1990; Barruol and Mainprice, 1993; Burlini and Fountain, 1993).

We have taken (0001) pole figure data for biotite measured in sample 161 by optical microscopy (kindly provided by G. Barruol) and calculated the seismic properties by several different methods. The (0001) pole figure is shown in Figure 3, the LPO is axial about  $Z$  which is extremely common for micas. The calculated P-wave, shear wave splitting ( $dV_s$ , the difference in velocity of the two polarized S-waves) and orientation of polarization planes of the faster S-wave ( $V_{s1}$ ) for the self-consistent model assuming spherical grains is shown in Figure 3. As the properties are axial we will illustrate them with profile between the  $Z$  specimen direction (inclination  $0^\circ$ ) and the  $Y$  specimen direction (inclination  $90^\circ$ ) in Figures 4 and 5. We have calculated the usual Voigt, Reuss and Hill averages. In addition the geometric mean (Matthies and Humbert, 1993), a self-consistent model (see Diz and Humbert, 1992 for details of the procedure) for spherical grains (axial ratio  $a:b:c = 1:1:1$ ) and oblate grains (axial ratio  $a:b:c = 100:100:1$ ) and a mean velocity model with the same grain shapes have been calculated. The mean velocity model has previously been applied to randomly oriented olivine aggregates by Birch (1972). In this model we have calculated the average velocity as

$$\bar{V} = \frac{\text{total path length}}{\text{total travel time}} = \frac{\sum d_i}{\sum t_i}$$

where  $d_i$  is path length in grain ( $i$ ) for a given crystal shape (e.g. ellipsoid) and  $t_i$  is the travel time in that crystal direction determined from the Christoffel equation. It is assumed that the crystal shape is correlated with the crystal orientation. For mica we have assumed that either the  $c(0001)$  axis is short and  $b$  and  $c$  axes are long (axial ratio  $a:b:c = 100:100:1$ ) or the grains are spherical (axial ratio  $a:b:c = 1:1:1$ ). The results show that, for  $V_p$ , the mean velocity model is close to the Voigt, and the S.C. model for spherical grains and the geometric mean are close to the Hill. For  $V_{s1}$ , the velocity model is close to the Voigt, and the S.C. model for spherical grains and geometric mean are again close to the Hill. For  $V_{s2}$  the velocity model is close to Reuss at small inclinations and close to the Hill at high inclinations, the S.C. model for spherical grains and geometric mean are again close to the Hill. For  $dV_s$  the velocity model is well above all the other

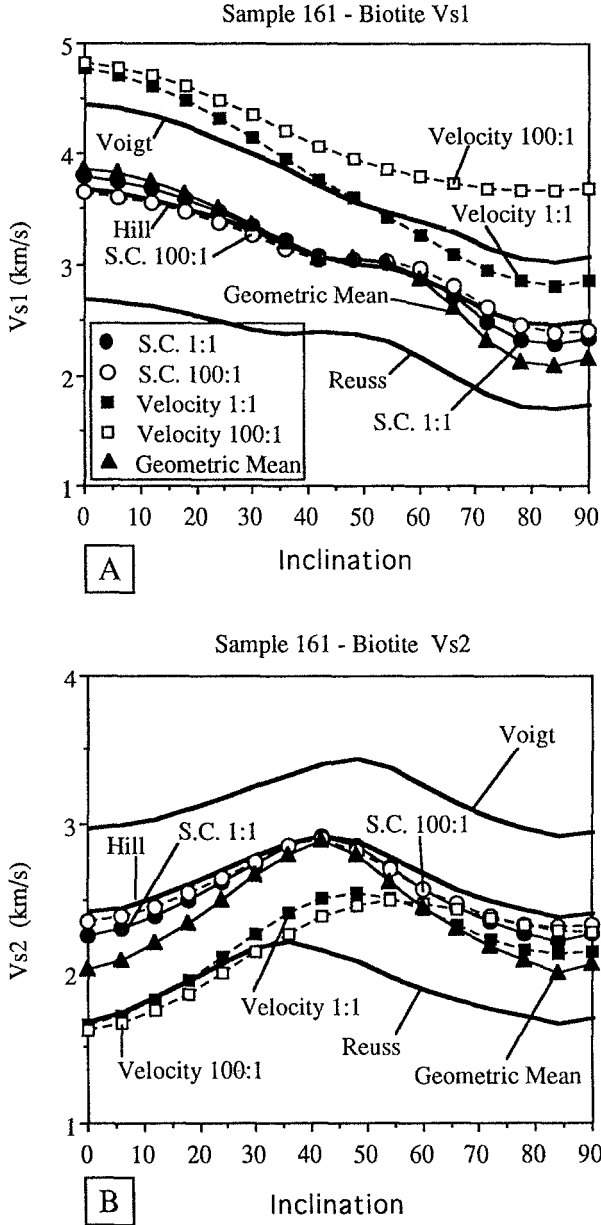


Fig. 4. Profiles from the Z sample direction ( $0^\circ$  inclination) to the XY plane ( $90^\circ$  inclination, see Figure 3) for  $V_p$  and  $dV_s$  for the Voigt, Reuss, Hill, self-consistent (S.C.), geometrical mean and velocity mean models. The S.C. and velocity mean models are shown for spherical ( $a/c = 1:1$ ) and oblate ( $a/c = b/c = 100:1$ ) grain shapes. A) P wave velocity ( $V_p$ ) in km/s; B) Difference in velocity of the two polarized S waves ( $dV_s$ ) in km/s.

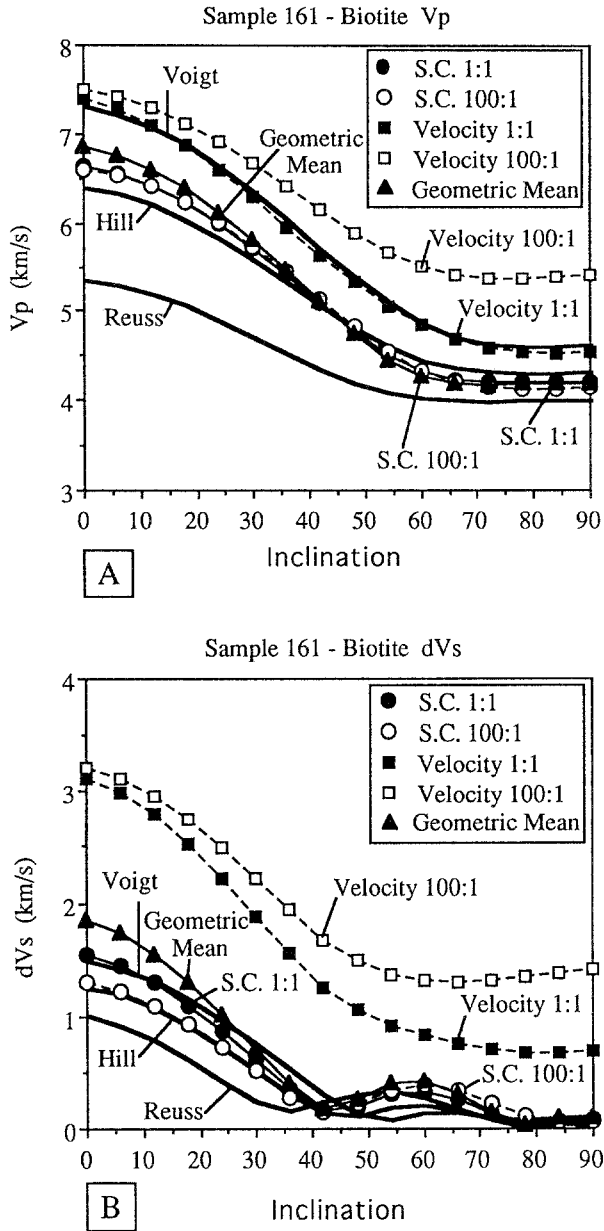


Fig. 5. Profiles from the Z sample direction ( $0^\circ$  inclination) to the Y sample direction (see Figure 3) for  $V_{s_1}$  the fast polarized S-wave and  $V_{s_2}$  the slow polarized S-wave, for the Voigt, Reuss, Hill, self-consistent (S.C.), geometrical mean and mean velocity models. The S.C. and mean velocity models are shown for spherical ( $a/c = 1:1$ ) and oblate ( $a/c = b/c = 100:1$ ) grain shapes. A) Fastest S wave ( $V_{s_1}$ ) in km/s; B) Slowest S wave ( $V_{s_2}$ ) in km/s.

estimates, and the S.C. model for spherical grains and the geometric mean are again close to the Hill. The S.C. model does not show much grain shape effect, whereas the velocity model shows a significant reduction in anisotropy (i.e. the difference between  $0^\circ$  inclination and  $90^\circ$ ). The geometric mean gives virtually identical results to the S.C. model for spherical grains. Given the success of the S.C. model in predicting properties we must conclude that the geometric mean is the best estimate of the seismic properties of the simple averaging methods. The Hill average is also close to the S.C. and geometric mean values, hence it remains a good estimate of seismic velocities, even if it is only a phenomenological result. The effect of grain shape deserves further consideration, for strong textures (e.g. biotite) the grain shape effect appears to be of secondary importance. As pointed out by Birch (1972), the mean velocity model is a "short-wave" approximation, where individual grains are taken into account. In this sense, the fact that the conversion of seismic waves at grain boundaries (e.g. P to S) is ignored means the model must be false. Further, given our initial goal of characterizing a macroscopic sample, this method is microscopic and hence not valid for a macroscopic analysis.

## 6. Conclusions

With increasing elastic anisotropy the classical aggregate averages of Voigt and Ruess are increasingly separated. Comparisons between simple averaging methods (Voigt, Ruess, Hill and geometric mean) and more elaborate self-consistent methods for strongly anisotropic biotite aggregates show that the geometric mean and the Hill average give similar results to the self-consistent methods. The self-consistent method is used to explore the effect of grain shape on seismic velocities of a macroscopic polycrystalline specimen of biotite. The grain shape is shown to have a minor effect for the biotite specimen with a strong lattice preferred orientation. In contrast, the microscopic mean velocity model (Birch, 1972) for the same biotite specimen show important effects for different grain shapes, as might be intuitively expected. The  $V_p$  seismic anisotropy is reduced by the presence of a strong grain shape anisotropy. The mean velocity model is microscopic, seismic wave travel times being evaluated at the grain scale, which is inappropriate for the calculation of macroscopic (specimen scale) properties.

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