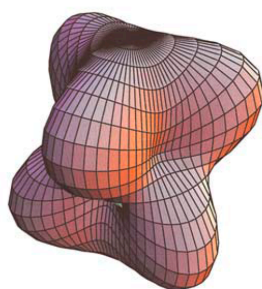


Estimation of anisotropic physical properties of aggregates with preferred crystal orientation with applications to seismic anisotropy

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PART II : Estimation of anisotropic polycrystalline physical properties

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The calculation of the physical properties from microstructural information (crystal orientation, volume fraction, grain shape etc.) is important for mantle rocks because it gives insight into the role of microstructure in determining the bulk properties. A calculation can be made for the in-situ state at high temperature and pressure of the mantle for samples where the microstructure has been changed by subsequent chemical alteration (e.g. the transformation olivine to serpentine) or mechanically induced changes (e.g. fractures created by decompression). The in-situ mantle temperatures and pressures can be simulated using the appropriate single crystal derivatives (see below). Additional features not necessarily preserved in the recovered microstructure, such as the presence of fluids (e.g. magma) can be modeled (e.g. Blackman and Kendall, 1997; Mainprice 1997; Williams and Garnero, 1996). Finally, the effect of phase change on the physical properties can also be modeled using these methods (e.g. Mainprice et al., 1990). Modeling is essential for anisotropic properties as experimental measurements in many directions necessary to fully characterize anisotropy is not currently feasible for the majority of the temperature and pressure conditions found in the Earth's mantle.

In following, we will only discuss the elastic properties needed for seismic velocities, but the methods apply to all tensorial properties where the bulk property is governed by the volume fraction of the constituent minerals. Many properties of geophysical interest are of this type, for example thermal conductivity, thermal expansion, elasticity and seismic velocities. However these methods do not apply to properties determined by the connectivity of a phase, such as the electrical conductivity of rocks with conductive films on the grain boundaries (e.g. carbon). We will assume 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. The local stress and strain fields at every point \mathbf{r} in a linear elastic polycrystal which are completely determined by Hooke's law as follows

$$\sigma_{ij}(\mathbf{r}) = C_{ijkl}(\mathbf{r}) \epsilon_{kl}(\mathbf{r}) \quad (1)$$

where $\sigma_{ij}(\mathbf{r})$ is the stress tensor, $C_{ijkl}(\mathbf{r})$ is the elastic stiffness tensor and $\epsilon_{kl}(\mathbf{r})$ the strain tensor at point \mathbf{r} . The evaluation of the effective constants of a polycrystal would be the summation of all components as a function of position, if we know the spatial functions of stress and strain. The average stress $\langle \sigma \rangle$ and strain $\langle \epsilon \rangle$ of a statistically uniform sample are linked by an effective macroscopic modulus C^* that obeys Hooke's law of linear elasticity,

$$C^* = \langle \sigma \rangle \langle \epsilon \rangle^{-1} \quad (2)$$

where

$$\langle \epsilon \rangle = \frac{1}{V} \int \epsilon(r) . dr$$

and

$$\langle \sigma \rangle = \frac{1}{V} \int \sigma(r) . dr$$

and V is the volume, the notation $\langle \cdot \rangle$ denotes an ensemble average. The stress $\sigma(\mathbf{r})$ and strain $\epsilon(\mathbf{r})$ 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 $\epsilon(\mathbf{r})$ are varying slowly and continuously with position \mathbf{r} .

A number of methods are available for determining the effective macroscopic modulus. We will briefly present these methods which try to take into account an increasing amount of microstructural information, which of course results in increasing theoretical complexity, but yields estimates which are closer to experimental values. The methods can be classified by using the concept of the order of the statistical probability functions used to quantitatively describe the microstructure (Kröner, 1978). A zero order bound is given when one has no statistical information on the microstructure of the polycrystal and for example we do not know the orientation of the component crystals, in this case we have to use the single crystal properties. The maximum and minimum of the single crystal property are the zero order bounds. The simplest and best known averaging techniques for obtaining estimates of the effective elastic constants of polycrystals are the Voigt (1928) and Reuss (1929) averages. These averages only use the volume fraction of each phase, the orientation and the elastic constants of the single crystals or grains. In terms of statistical probability functions, these are first order bounds as only the first order correlation function is used, which is the volume fraction. Note no information on the shape or position of neighboring grains is used. The Voigt average is found by simply assuming that the strain field is everywhere constant (i.e. $\epsilon(\mathbf{r})$ 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 ,

$$C \approx C^{voigt} = \left[\sum_i V_i . C(\mathbf{g}_i) \right] \quad (3)$$

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^* or S^* is then estimated by the volume average of local compliances $S(\mathbf{g}_i)$,

$$C^* \approx C^{Reuss} = \left[\sum_i V_i . S(\mathbf{g}_i) \right]^{-1} \quad (4)$$

$$S^* \approx S^{Reuss} = \left[\sum_i V_i . S(\mathbf{g}_i) \right] \quad (5)$$

$$C^{Voigt} \neq C^{Reuss} \text{ and } C^{Voigt} \neq [S^{Reuss}]^{-1} \quad (6)$$

These two estimates are not equal for anisotropic solids with the Voigt being an upper bound and the Reuss a lower bound. 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 Fig. 7a,b we present the Voigt, Reuss and Hill averages of a number of mantle minerals from Table 1 for randomly orientated polycrystals as a function of anisotropy for compressional (V_p) and shear (V_s) wave anisotropy. 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). Although the Voigt and Reuss bounds are often far apart for anisotropic materials, they still provide the limits within which the experimental data should be found.

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. A method of determining the geometric mean for arbitrary orientation distributions has been 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. 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 $\langle S \rangle^{-1}$ would appear to be a powerful physical constraint on the averaging method (Matthies and Humbert, 1993). However, the arithmetic (Hill) and geometric means are very similar (Mainprice and Humbert, 1994), which tends to suggest that they are just mean estimates with no additional physical significance.

The second set of methods use additional information on the microstructure to take into account the mechanical interaction between the elastic elements of the microstructure. Mechanical interaction will be very important for rocks containing components of very different elastic moduli, such as solids, liquids, gases and voids. The most important approach in this area is the 'self-consistent' (SC) method (e.g. Hill, 1965). The SC method was introduced for materials with a high concentration of inclusions where the interaction between inclusions is significant. In the SC method, an initial estimate of the anisotropic homogeneous background medium of the polycrystal is calculated using the traditional volume averaging method (e.g. Voigt). All the elastic elements (e.g. grains, voids etc.) are inserted into the background medium using Eshelby's (1957) solution for a single ellipsoidal inclusion in an infinite matrix. The elastic moduli of the ensemble, inclusion and background medium are used as the 'new' background medium for the next inclusion. The procedure is repeated for all inclusions and repeated in an iterative manner for the polycrystal until a convergent solution is found. The interaction is notionally taken into account by the evolution of the background medium which contains information about the inclusions, albeit in an homogenous form. As the inclusion can have an ellipsoidal shape, an additional microstructural parameter is taken into account by this type of model.

Several people (e.g. Bruner, 1976; Henyey and Pomphrey, 1982) have remarked that the SC progressively overestimates the interaction with increasing concentration. They proposed an alternative differential effective medium (DEM) method in which the inclusion concentration is increased in small steps with a re-evaluation of the elastic constants of the aggregate at each increment. This scheme allows the potential energy of the medium to vary slowly with inclusion concentration (Bruner, 1976). Since the addition of inclusions to the background material is made in very small increments, one can consider the concentration step to be very dilute with respect to the current effective medium. It follows that the effective interaction between inclusions can be considered negligible and we can use the inclusion theory of Eshelby (1957) to take into account the interaction. In contrast, the SC uses Eshelby's theory plus an iterative evaluation of the background medium to take into account the interaction. Recently Mainprice (1997) has compared the results of SC and DEM for anisotropic oceanic crustal and mantle rocks containing melt inclusions and found the results to be very similar for melt fractions of less than 30%. At higher melt fractions the SC exhibits a threshold value around 60% melt, whereas the DEM varies smoothly up a 100% melt. The presence of a threshold in the SC calculations is due to the specific way that the interaction is taken into account. The estimates of both methods are likely to give relatively poor results at high fractions of a phase with strong elastic contrast with the other constituents as other phenomena, such as mechanical localization related to the percolation threshold, are likely to occur.

The third set of methods uses higher order statistical correlation functions to take into account the first or higher order neighbor relations of the various microstructural elements. The factors that need to be statistically described are the elastic constants (determined by composition), orientation and relative position of an element. If the element is considered to be small relative to grain size, then grain shape and the heterogeneity can be accounted for the relative position correlation function. Nearest neighbors can be

taken into account using 2-point correlation function, which is also called an auto-correlation function by some authors. If we use the "statistically uniform" sample introduced above, we are effectively assuming that all the correlation functions used to describe the microstructure up to order infinity are statistically isotropic, this is clearly a very strong assumption. In the special case where all the correlation functions up to order infinity are defined, Kröner (1977, 1978) has shown that the upper and lower bounds converge for the self-consistent method so that $C^{SC} = (S^{SC})^{-1}$. The statistical continuum approach (e.g. Beran, 1968) is the most complete description and has been extensively used for model calculations (e.g. Beran et al., 1996; Mason and Adams, 1999). Until recently it has been considered too complicated for practical application. With the advent of automated determination of crystal orientation and positional mapping using electron back-scattered diffraction (E.B.S.D.) in the scanning electron microscope (Adams et al., 1993), digital microstructural maps are now available for the determination of statistical correlation functions. This approach provides the best possible estimate of the elastic properties but at the expense of considerably increased computational complexity.

The fact that there is a wide separation in the Voigt and Reuss bounds for anisotropic materials is caused by the fact that the microstructure is not fully described by such methods. However, despite the fact that these methods do not take into account such basic information as the position or the shape of the grains, several studies have shown that the Voigt or the Hill average are within 5 to 10% of experimental values for low porosity rocks free of fluids. For example, Barruol and Kern (1996) showed for several anisotropic lower crust and upper mantle rocks from the Ivrea zone in Italy that the Voigt average is within 5% of the experimentally measured velocity.

THE CALCULATION OF ANISOTROPIC SEISMIC PROPERTIES

Orientation of crystals in a polycrystal can be measured by volume diffraction techniques (e.g. X-ray or neutron diffraction) or individual orientation measurements (e.g. U-stage & Optical microscope, electron channeling or EBSD). An orientation, often given the letter \mathbf{g} , of a grain or crystal in sample co-ordinates can be described by the rotation matrix between crystal and sample co-ordinates. In practice it is convenient to describe the rotation by a triplet of Euler angles, for example $\mathbf{g} = (\phi_1 \phi \phi_2)$ used by Bunge (1982). One should be aware there are many different definitions of Euler angles that are used in the physical sciences, here we will use the definition given by Bunge (1982). The orientation distribution function (O.D.F.) $f(\mathbf{g})$ is defined as the volume fraction of orientations with an orientation in the interval between \mathbf{g} and $\mathbf{g}+d\mathbf{g}$ in a space containing all possible orientations given by

$$\Delta V/V = \int f(\mathbf{g}) d\mathbf{g} \quad (7)$$

where $\Delta V/V$ is the volume fraction of crystals with orientation \mathbf{g} , $f(\mathbf{g})$ is the texture function and $d\mathbf{g} = 1/8\pi^2 \sin\phi d\phi_1 d\phi d\phi_2$ is the volume of the region of integration in orientation space.

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 co-ordinate frame using the orientation or rotation matrix g_{ij} ,

$$C_{ijkl}(\mathbf{g}) = g_{ip} g_{jq} g_{kr} g_{lt} C_{pqrt}(\mathbf{g}^0) \quad (8)$$

where $C_{ijkl}(\mathbf{g})$ is the elastic property in sample co-ordinates, $g_{ij} = g(\phi_1 \phi \phi_2)$ the measured orientation in sample co-ordinates and $C_{pqrt}(\mathbf{g}^0)$ is the elastic property in crystal co-ordinates.

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:

$$\langle C_{ijkl} \rangle^m = \int C_{ijkl}^m(\mathbf{g}) f(\mathbf{g}) d\mathbf{g} \quad (9)$$

where $\langle C_{ijkl} \rangle^m$ is the elastic properties of the aggregate of mineral m . Alternatively it may be determined by simple summation of individual orientation measurements,

$$\langle C_{ijkl} \rangle^m = \sum C_{ijkl}^m(\mathbf{g}) \cdot v(\mathbf{g}) \quad (10)$$

where $v(\mathbf{g})$ is the volume fraction of the grain in orientation \mathbf{g} . For example, the Voigt average of the rock for m mineral phases of volume fraction $v(m)$ is given as

$$\langle C_{ijkl} \rangle^{\text{Voigt}} = \sum v(m) \langle C_{ijkl} \rangle^m \quad (11)$$

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

$$|\langle C_{ijkl} \rangle^{\text{Voigt}} n_j n_l - \rho V^2 \delta_{ik}| = 0 \quad (12)$$

where n is the plane wave propagation direction, ρ is the density of the rock, δ_{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 Earth's mantle the single crystal elastic constants are extrapolated to pressure and temperature using the following relationship:

$$C_{ij}(PT) = C_{ij}(P_0 T_0) + (dC_{ij}/dP) \cdot (P - P_0) + 1/2 (d^2 C_{ij}/dP^2) \cdot (P - P_0)^2 + (dC_{ij}/dT) \cdot (T - T_0) \quad (13)$$

where $C_{ij}(PT)$ are the elastic constants at Earth's 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. The second order pressure derivatives $d^2 C_{ij}/dP^2$ are available for an increasing number of mantle minerals (e.g. olivine, orthopyroxene, garnet, MgO) and first order temperature derivatives seem to adequately describe the temperature dependence of most minerals. Note however when phase transitions occur, the specific changes in elastic constants at pressures near the phase transition will have to be taken into account, for example the SiO₂ polymorphs. The seismic velocities also depend on the density of the minerals at pressure and temperature which can be calculated using an appropriate equation of state (Knittle, 1995). The Murnaghan equation of state derived from finite strain is sufficiently accurate at moderate compression (Knittle, 1995) of the upper mantle and leads to the following expression for density as a function of pressure,

$$\rho(P) = \rho_0 (1 + (K'/K) \cdot (P - P_0))^{1/K'} \quad (14)$$

where K is bulk modulus, $K' = dK/dP$ the pressure derivative of K , ρ_0 is the density at reference pressure P_0 and temperature T_0 . For temperature the density varies as

$$\rho(T) = \rho_0 [1 - \int \alpha_v(T) dT] \approx \rho_0 [1 - \alpha_{av} (T - T_0)] \quad (15)$$

where $\alpha_v(T) = 1/V(\partial V/\partial T)$ is the volume thermal expansion coefficient as a function of temperature and α_{av} is an average value of thermal expansion which is constant over the temperature range (Fei, 1995). According to Watt (1988) an error of less 0.4% on the P and S velocity results from using α_{av} to 1100K for MgO. For temperatures and pressures of the mantle, the density is described for this paper by,

$$\rho(P, T) = \rho_0 \{ (1 + (K'/K) \cdot (P - P_0))^{1/K'} [1 - \alpha_{av} (T - T_0)] \} \quad (16)$$

Attenuation

From a mechanical point of view the seismic attenuation can be modeled by a visco-elastic material with a complex elastic rigidity tensor (C_c) with real (C_{re}) and imaginary (C_{im}) components,

$$C_c = \sigma \varepsilon^{-1} = C_{re} + i C_{im} = \square C \square \exp(i \Phi)$$

where \square modulus of C_c , $i = \sqrt{-1}$, Φ is the phase difference between stress (σ) and strain (ϵ). The quality factor Q is given by

$$Q^{-1} = C_{im} / C_{re} = \tan \Phi$$

The complex elastic rigidity tensor or Q^{-1} can be modelled if one makes some assumptions about the mechanical behaviour for the material. All seismic observations and experimental data on upper mantle rocks show that Q^{-1} is a weak function of frequency (f) (see review by Karato and Spetzler, 1990) with $Q^{-1} = f^{-\alpha}$ where $\alpha=0.1$ to 0.3 . Such a frequency dependence could be modelled for example by either a Maxwell body or a standard linear solid of Zener (1948). Experimental data where the sub-solidus to hyper-solidus temperature range has been explored (e.g. Kampmann and Berckhemer, 1985) show no dramatic change in attenuation with the onset of melting, presumably due to the operation of a solid state mechanism of attenuation. In previous studies of attenuation the standard linear solid has been used either with a single relaxation time (e.g. Mavko 1979; Schmeling, 1985) for melts or a multiple relaxation time for solid state mechanisms (e.g. Anderson and Given, 1982). At present there is no high temperature experimental data for melt containing rocks which have the Debye attenuation peak characteristic of a standard linear solid. In fluid saturated sandstones a Debye attenuation peak is observed at 2000 Hz, whereas in vacuum dried samples no frequency dependence of Q is observed (e.g. Jones, 1986). These results indicate that attenuation mechanism is associated with the interaction of the pore fluids with the solid rock, rather than absorption within the rock frame or liquid. Here I will assume that the medium is a linear viscoelastic body which has the mechanical behaviour of the standard linear solid with a single relaxation time and the energy loss mechanism is melt squirt (e.g. Schmeling, 1985), in doing so I will ignore any solid state mechanisms. Using these two assumptions one can define a low frequency modulus M_l and a high frequency modulus M_h which corresponds in this case to the two pore fluid regimes defined above. For the standard linear solid the maximum amplitude of the Debye peak is given by

$$Q_{\max}^{-1} = \frac{M_h - M_l}{2\sqrt{M_h \cdot M_l}}$$

The elastic moduli (M) associated with the compressional and shear waves in a given propagation direction (x) were calculated from the phase velocities by

$$M(x) = \rho V(x)^2$$

where ρ is the density, $V(x)$ is the compressional or shear wave velocity. The three seismic phase velocities (V_p, V_{s1} and V_{s2} , where $V_{s1} > V_{s2}$) for an elastically anisotropic homogeneous medium are given by the solution of the Christoffel equation

$$\text{Det} \square C_{ijkl} x_i x_j - \delta_{ik} \rho V(x)^2 \square = 0$$

where $x_i x_j$ are the direction cosines of the wave propagation direction, δ_{ik} is the Kronecker delta, C_{ijkl} is the volume averaged elastic constants of the aggregate derived for the effective medium and $V(x)$ is one of the three phase velocities.

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