A continuum theory for lattice preferred orientation

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SUMMARY
A 2-D model for the development of lattice preferred orientation (LPO) in aggregates of crystals (such as high $T/T_m$ olivine) which deform with a single dominant slip system is presented. In two dimensions, an arbitrary LPO can be described by an orientation distribution function (ODF) $g(\phi, t)$, such that $g(\phi, t)\,d\phi$ represents the fraction of crystals for which the orientation of the slip plane lies between $\phi$ and $\phi + d\phi$ at time $t$. A differential equation which describes the evolution of the ODF during an arbitrary deformation history is described. This evolution is controlled by the vorticity number $\lambda(t) = \Omega/\dot{\varepsilon}$ of the deformation, where $2\Omega(t)$ is the vorticity and $\dot{\varepsilon}(t)$ is the strain rate. For $\lambda = 0$ (uniaxial compression or pure shear), the ODF of an initially isotropic aggregate consists of two growing peaks oriented symmetrically about the extensional axis. For $|\lambda| = 1$ (simple shear), the ODF consists of two unequal peaks which migrate relative to the extensional axis, and which eventually merge into a single peak centred on the shear plane orientation. If $|\lambda|$ exceeds a critical value $\sim 1.15$, the ODF periodically returns to its initial isotropic state. The theory gives an excellent fit to data from olivine aggregates deformed in uniaxial compression, and an acceptable fit to data from ice aggregates deformed in simple shear.

Key words: crystalline plasticity, lattice preferred orientation, slip systems

1 INTRODUCTION

When a polycrystalline material such as a rock is deformed, the crystallographic axes of the constituent crystals generally take on a non-random or 'preferred' orientation. The observation and interpretation of lattice preferred orientation (LPO) has important applications in several areas of the earth sciences. In structural geology, for example, LPO is often used to interpret the deformation history of rocks exposed at the surface (e.g. Hobbs 1985). Observations of LPO in ophiolites have been used to infer the pattern of flow beneath ocean ridges (e.g. Nicolas & Violette 1982). Observations of LPO by seismic methods may provide new constraints on the pattern of mantle circulation (Nataf, Nakanishi & Anderson 1984, 1986; Tanimoto & Anderson 1984).

One of the principal mechanisms for the formation of LPO is the mechanism of 'intracrystalline slip' first identified by Taylor (1938). Most common minerals deform by slip on a limited number of planes which have a fixed orientation relative to the crystallographic axes. On the scale of the whole crystal, such a deformation has the form of a continuous simple shear. Now, simple shear is a deformation which has a rotational component: the material rotates relative to the slip plane, and hence relative to the crystal axes. This rotation is equivalent to an opposite rotation of the crystal axes relative to the material. The mechanism of crystallographic rotation by intracrystalline slip is the foundation of the so-called Taylor–Bishop–Hill (TBH) model (Taylor 1938; Bishop & Hill 1951), which has been widely applied to the interpretation of LPO in deformed metals (e.g. Mecking 1985) and rocks such as quartzites (e.g. Lister, Paterson & Hobbs 1978) and carbonates (e.g. Wenk 1985). The TBH model is only applicable, however, if the material has a sufficient number of independent slip systems to accommodate an arbitrary imposed deformation by slip alone. This criterion, due originally to Von Mises (1928), is satisfied for most metals, and for such minerals as quartz and calcite. On the other hand, it is not satisfied for minerals such as olivine, which deforms with a single dominant slip system. The TBH theory can therefore not be used to understand the development of LPO in the upper mantle, where olivine is the most abundant mineral phase.

A model for the formation of LPO in aggregates of crystals with a single dominant slip system has been proposed by Etchecopar (1977) and Etchecopar & Vasseur (1987). In the simplest version of this model (Etchecopar 1977), a specified deformation is applied to a 2-D aggregate of crystals containing only a single slip plane. Because the Von Mises criterion is not satisfied, the aggregate cannot accommodate the imposed deformation by slip alone, and voids and overlaps develop between neighbouring crystals. Etchecopar's model consists of a numerical algorithm which minimizes this misfit between neighbouring grains.

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Unlike the TBH model, Etchecopar's (1977) model is directly applicable to olivine, and gives a good fit to ODFs measured in dunites deformed by uniaxial compression (see Section 4). Nevertheless, Etchecopar's model has serious limitations which motivate the present work. Firstly, the model is difficult to apply in practice, and requires a fairly involved computer simulation even for simple uniform deformations. Secondly, it is a discrete model which can only be applied to aggregates comprising a relatively small number of grains (of order 100). The ODFs predicted by the model thus contain a substantial amount of noise, which tends to become amplified with time. Consequently, it is difficult to apply the model to situations (such as mantle convection) in which material elements experience complex time-dependent deformation histories. For this purpose, a continuum theory for LPO is required, in the form of a partial differential equation which describes the evolution of LPO during an arbitrary deformation history. The aim of this paper is to present such a theory.

2 THE THEORY

In two dimensions, the orientation relative to external axes of a crystal with one slip plane can be described by a single angle \( \phi \), in the range \(-\pi/2 < \phi < \pi/2\). In this paper, \( \phi \) is defined as the angle between the slip plane and a fixed horizontal axis, with \( \phi \) increasing in the counter-clockwise direction. The LPO of an aggregate of such crystals can be described by an orientation distribution function (ODF) \( g(\phi, t) \), such that \( g(\phi, t) \, d\phi \) represents the (area or volume) fraction of crystals having orientations between \( \phi \) and \( \phi + d\phi \) at time \( t \). This ODF satisfies a simple differential equation which can be derived as follows. When a polycrystalline aggregate is deformed, each crystal within it rotates at some rate \( \dot{\phi} \). Let us assume that, for a given imposed deformation, \( \dot{\phi} \) depends only on the crystal's orientation \( \phi \), and not on the orientations of neighbouring crystals (the same assumption, by the way, is implicit in the TBH theory). Now consider an orientation interval \((\phi, \phi + d\phi)\). The rate of change of the volume fraction of crystals with orientations in this interval is

\[
\frac{\partial}{\partial t} [g(\phi, t) \, d\phi].
\]  

(1)

The net flux of crystal volume fraction into this interval is

\[
\dot{\phi}(\phi) g(\phi, t) - \dot{\phi}(\phi + d\phi) g(\phi + d\phi, t).
\]  

(2)

By equating (1) and (2) and taking the limit \( d\phi \to 0 \), we obtain

\[
\frac{\partial g}{\partial t} + \frac{\partial}{\partial \phi} (\phi g) = 0.
\]  

(3)

Equation (3) is the fundamental equation describing the evolution of LPO, but it is useful only if the function \( \phi \) is specified. The quantity \( \dot{\phi} \) clearly must depend on the nature of the deformation experienced by the aggregate. Now in two dimensions, an arbitrary deformation may be completely described by three quantities: the vorticity \( 2\Omega \), the strain rate \( \dot{\varepsilon} \), and the orientation \( \phi_i \) of the axis of maximum instantaneous extension. The meaning of these quantities is shown in Fig. 1 for two common types of uniform deformation, pure shear and simple shear. For a more detailed discussion, the reader is referred to Lister & Williams (1983).

The dependence of \( \dot{\phi} \) upon \( \Omega, \dot{\varepsilon} \) and \( \phi_i \) may be determined by simple arguments. First, if there is no strain (\( \dot{\varepsilon} = 0 \)), each crystal must rotate with the imposed angular velocity \( \Omega \). Second, if there is no externally imposed rotation (\( \Omega = 0 \)), the rate of crystallographic rotation must be proportional to the strain rate \( \dot{\varepsilon} \). This is so because crystallographic rotation occurs by simple shear on a slip plane, and the rotation associated with such a shear is equal to the strain rate (Fig. 1). Finally, the orientation \( \phi_i \) of the extensional axis has no effect on the rotation rate, and may be regarded simply as a reference direction. The rotation rate \( \dot{\phi} \) must therefore have the form

\[
\dot{\phi} = \Omega + \epsilon f(\phi - \phi_i),
\]  

where \( f \) is an arbitrary function. The reader who wishes to see a more rigorous derivation of the same result may consult Appendix A, in which an exact expression of the form (4) is obtained for an idealized model crystal with two independent slip planes.

Our problem has now been reduced to that of specifying the function \( f(\phi - \phi_i) \). Like the ODF \( g(\phi, t) \), \( f \) must be periodic with period \( \pi \). Moreover, the ODF of an olivine
aggregate deformed in pure shear ($\Omega = 0$) is observed to be symmetric about the extensional axis (Etchecopar 1977); that is, $g$ is an even function of $\phi - \phi_i$. Inspection of (3) with $\Omega = 0$ then shows that $f$ must be an odd function of $\phi - \phi_i$. Accordingly, $f$ can be expressed as a Fourier series of the form

$$f = \sum_{n=1}^{-\infty} c_n \sin 2n(\phi - \phi_i),$$

(5)

where $c_n$ are undetermined coefficients which may be freely chosen to match experimental data. A good fit to the available data (Section 4) can be achieved by retaining only the first two terms in (5). In the solutions discussed below, the form used is

$$f = -\sin 2(\phi - \phi_i) + c \sin 4(\phi - \phi_i),$$

(6)

where $c = c_2 = 0.32$.

The expression (6) has a simple physical meaning, which can be understood by recalling Etchecopar's (1977) model for LPO. In this model, the imposed deformation is first divided into a series of small increments. For each increment, the simulation comprises two steps. In the first step, one determines for each crystal the amount of slip and rotation required so that the final shape of the crystal best matches its 'ideal' shape, i.e. the shape it would have if it could deform as a pure continuum. In the second step, additional amounts of slip and rotation are applied iteratively to each crystal so as to minimize the remaining misfit between neighbouring grains. These two steps are effected by minimizing a quadratic sum (Appendix B, equation B1) which is proportional to the square of the differential strain (i.e. the strain relative to the ideal shape) in a crystal. Because elastic energy is proportional to the square of the strain, Etchecopar's minimization criterion can be regarded as a minimum-energy principle.

Although Etchecopar (1977) applied the two steps of this algorithm numerically, an exact analytical expression can be derived for the amounts (or rates) of slip and rotation required so that the final shape of the crystal best matches its ideal shape. The equation for the characteristics is

$$d\theta/d\tau = \lambda + f(\theta),$$

(9)

subject to the initial condition $\theta(0) = \theta_0$. Physically, a characteristic is simply the orientation $\theta$ as a function of time $\tau$ of a crystal with initial orientation $\theta_0$. The solution for the ODF along a characteristic is

$$g(\theta, \tau) = g(\theta_0, 0) \frac{\lambda + f(\theta_0)}{\lambda + f(\theta_n)},$$

(10)

where $g(\theta_0, 0)$ is the initial value of the ODF at $\tau = 0$.

The characteristic equation (9) can be integrated analytically, but the result is too complicated to be useful. It is thus more efficient to obtain solutions numerically. Consider a set of $N$ characteristics $n = 1, \ldots, N$, and let $t_n(m = 0, \ldots, M)$ be the values of the time at which the solution is desired, with $t_0 = 0$. Let $\theta_{nm}$ and $g_{nm}$ be the values of $\theta$ and $g$, respectively, at time $t_n$ along characteristic $n$. To obtain solutions, one first defines a set of $N$ points $\theta_{n0}$ (which need not be equally spaced) in the interval $(-\pi/2, \pi/2)$. Next, the initial ODF $g_{n0}$ is specified at these points. The characteristic equation (9) is then solved for each $n$, subject to the initial condition $\theta(0) = \theta_{n0}$, using a high-order numerical method such as the Runge–Kutta algorithm. This yields the set of numbers $\theta_{nm}$. Finally, the solution is determined from (10), in the form

$$g_{nm} = g_{n0} \frac{\lambda + f(\theta_{n0})}{\lambda + f(\theta_{nm})}.$$  

(11)

Let us now examine the solutions obtained by the methods just described. The most interesting case is that of an initially isotropic (random) orientation distribution, for which $g(\theta_0, 0) = \pi^{-1}$. Consider first the case of pure shear deformation, for which the vorticity number $\lambda = 0$. The evolution of the ODF for this case is shown in Fig. 2. The initial isotropic distribution is shown by the dashed line. The ODF consists of two growing peaks which are orientated symmetrically about the extensional axis, and which slowly migrate towards this axis with time. Because the evolution equation (3) conserves the total crystal volume fraction, the area under each of the curves in Fig. 2 is unity. For $\tau \to \infty$, the two peaks merge into a single, infinitely narrow peak centered on the extensional axis.

The solution of the ODF in simple shear ($|\lambda| = 1$) is shown in Fig. 3. The profiles shown correspond to sinistral shear with $\lambda = 1$; the corresponding profiles for dextral shear ($\lambda = -1$) are obtained by simply reflecting the profiles shown across the extensional axis $\phi = \phi_i = 0$. In sinistral shear, the shear plane orientation is $\phi_i = 45^\circ$. For small values of the dimensionless time $\tau = \varepsilon \tau$, the ODF is identical to that for pure shear, with two peaks oriented
symmetrically about the extensional axis. As time increases, however, these peaks migrate in the direction of the imposed vorticity (i.e. counter-clockwise), and the 'downstream' peak grows at the expense of the 'upstream' one. This stage of the evolution is represented by the curve for $t = 0.5$. As the time increases further, the upstream peak overtakes the downstream peak ($t = 1.0$) and merges with it ($t = 1.5$), yielding a single peak close to the shear plane direction $\phi - \phi_0 = 45^\circ$. For $t \to \infty$, the ODF becomes an infinitely narrow peak which coincides with the shear plane direction.

Figure 3. Same as Fig. 2, but for an aggregate deformed in sinistral simple shear ($\lambda = 1$).

Figure 4. Same as Fig. 2, but for a deformation with vorticity number $\lambda = 2$.

Figure 4 shows the evolution of the ODF for $\lambda = 2$. This value of $\lambda$ corresponds to a deformation whose intrinsic rotation is twice that associated with simple shear. The ODF no longer evolves monotonically, but instead returns periodically to its initial isotropic state. The maximum concentration of the ODF occurs at approximately $t = 1.2$. At $t = 1.8$, the ODF has nearly returned to its initial value (dashed line).

In the solutions obtained above, the initial evolution of the ODF (i.e. two symmetrical peaks) is independent of the vorticity number $\lambda$. The long-term evolution, by contrast, is strongly dependent on $\lambda$. To better understand these two features of the solutions, it is helpful to examine the basic equations more closely. Consider first the initial evolution of the ODF. By evaluating equations (3) and (4) at $t = 0$ with $g = n^{-1}$, we obtain

$$\dot{\phi} \mid _{\phi = 0} = - \left( \frac{\dot{\epsilon}}{\pi} \right) df.$$

Equation (12) shows that the initial growth rate of the ODF is independent of the vorticity $2\Omega$ (and hence of $\lambda$). Physically, this means that a deforming aggregate does not 'know' whether it is rotating or not until some finite time has elapsed. Furthermore, (12) shows that the maximum growth rate of the ODF occurs where the derivative of $f$ is a minimum. For a function $f$ of the form (6), the initial orientations of maximum growth are

$$\phi_{max} = \phi_0 \pm \frac{1}{2} \cos^{-1}\left( \frac{1}{8c} \right).$$

For $c = 0.32$, the two peaks are initially located $33.5^\circ$ to either side of the extensional axis.

To understand how the long-term evolution of the ODF depends on $\lambda$, it is helpful to examine a phase--plane plot of the crystallographic rotation rate $\dot{\phi}$ as a function of $\phi - \phi_0$. The function $\phi$ defined by equations (4) and (6) is shown in Fig. 5 for the values of $\lambda$ used in Figs 2–4. The arrows on
local sense of crystallographic rotation. Stationary points where from equations (4) and (6) with \( c = 0.32 \). Thin vertical arrows indicate the initial orientations of the peaks of the ODF for an initially isotropic aggregate. For several values of the vorticity number \( \lambda \). Curves are calculated from equations (4) and (6) with \( \phi = 0 \) are indicated by solid circles (stable) and open circles (unstable). Thin vertical arrows indicate the initial orientations of the peaks of the ODF for an initially isotropic aggregate.

![Figure 5. Crystallographic rotation rate \( \dot{\phi} \) as a function of \( \phi - \phi_i \) for several values of the vorticity number \( \lambda \). Curves are calculated from equations (4) and (6) with \( c = 0.32 \). Heavy arrows show the local sense of crystallographic rotation. Stationary points where \( \phi = 0 \) are indicated by solid circles (stable) and open circles (unstable). Thin vertical arrows indicate the initial orientations of the peaks of the ODF for an initially isotropic aggregate.](image)

The basic assumption of this approach is that one need not understand the microscopic physics in order to describe the macroscopic behaviour of the system. Accordingly, the microscopic physics appears only in the form of material properties or constants (such as viscosity or elastic modulus) which must be determined by experiment. In the present theory, this role is played by the constant \( c \) (equation 6). As will be shown below, a wide range of experimental data can be fitted by an appropriate choice of this single constant, viz. \( c = 0.32 \). This is a strong indication that the basic assumptions of the theory are correct.

The solutions discussed in the previous section can be compared with measured ODFs for materials which deform by single slip. Because slip plane orientations can vary in three dimensions however, it is necessary to project these orientations onto a reference plane in order to compare them with the 2-D theory presented here. Etchecopar (1977) gives such projected ODFs for olivine, which are derived from the experimental data of Nicolas, Boudier & Boullier (1973) on synthetic dunites deformed in uniaxial compression. Figure 6 compares these projected ODFs (shown as histograms) with the ODFs predicted by the theory (smooth curves). The angle \( \phi \) in this figure represents the projected orientation of the 4, or seismically fast, axis of olivine. Plots are shown for three values of the dimensionless time \( \epsilon_t = 0.29, 0.36 \) and 0.87, which correspond respectively to shortening of 25, 30 and 58 per cent. The fit of the theoretical ODFs \( g(\phi) \) to the histograms \( h(\phi) \) can be measured by a parameter \( \chi \) defined as

\[
\chi = 1 - \frac{1}{2} \int_{-\pi}^{\pi} |g - h| d\phi.
\]

The parameter \( \chi \) ranges from zero when the observed and theoretical curves have no overlap to unity when they coincide exactly. Figure 6 shows that the theory gives an excellent fit to the data, with \( \chi \) values ranging from 0.81 to 0.93. The relatively less good fit for \( \epsilon_t = 0.29 \) appears to be due to the large amount of noise in the data.

It would clearly be desirable to compare the theory with observations from olivine aggregates deformed in simple shear, but such experiments are not yet available. On the other hand, many experiments have been done on deformation of ice aggregates in torsion, which is locally equivalent to simple shear (for references see Burg, Wilson & Mitchell (1986)). Because ice deforms on a single dominant slip plane (the basal plane), it is a useful analogue material for olivine (there are, however, important differences between the two materials; see below). Figure 7 compares projected ODFs for ice aggregates deformed in torsion from Bouchez & Duval (1982) with ODFs predicted by the theory. The fit to the data is less good than in Fig. 6, with \( \chi \) values ranging from 0.58 to 0.76. However, the theory does a reasonably good job of predicting the locations of the peaks of the ODF and the rate at which they migrate with increasing deformation.

The theory can also be compared with ODFs measured in
natural shear zones in glacial ice. Figure 8 compares the theoretical ODFs with projected ODFs given by Bouchez & Duval (1982), based on the data of Hudleston (1977). The fit of the theory to the data is similar to that shown in Fig. 7, with $\chi$ values ranging from 0.64 to 0.77. Again, the theory gives good predictions of the locations of the peaks of the ODF.

Finally, Table 1 compares the fit to the data of the continuum theory with that of Etchecopar's (1977) model. Column 1 shows the measured value of $\dot{\epsilon}$, and column 2 shows the values of $\dot{\epsilon}$ for which Etchecopar (1977) presented results. Although the two values are not always identical, they are close enough to make a meaningful comparison possible. Columns 3 and 4 show the values of $\chi$ for the continuum theory and for Etchecopar's model, respectively. For some values of $\dot{\epsilon}$, Etchecopar (1977) presented two different histograms, depending on the degree of crystal fracturing allowed in the model; the one which provides the better fit to the data is used here. For olivine, Etchecopar's model gives a slightly better fit to the data for $\dot{\epsilon} = 0.29$ and 0.36, but the continuum theory is substantially better for $\dot{\epsilon} = 0.87$. For ice, however, the continuum theory fits the data better than Etchecopar's model for all values of $\dot{\epsilon}$.

Whichever model is used, it is clear from Table 1 that the fit to the data is worse for ice than for olivine. A likely reason for this discrepancy is that the theory does not account for recrystallization, which occurs extensively in deforming ice aggregates. The effect of such recrystallization is to consume grains that are unfavourably oriented for slip (A. Nicolas, J.-L. Bouchez, personal communication). Another possible reason for the discrepancy is that there are two independent slip directions in the basal plane of ice (from which any other direction can be formed by linear combination), but only one dominant slip direction in the (010) plane of olivine. The effects of recrystallization and the additional slip direction are in the same sense: they will cause the ODF to evolve more rapidly for ice than for olivine. This is consistent with the results of Figs 7 and 8, which show that the ODF for ice evolves more rapidly than the theory predicts.

Finally, two important extensions of the theory presented here should be pointed out. The most obvious limitation of this theory is that it is 2-D, whereas all real crystals are 3-D. However, the continuum formulation of this paper can be easily generalized to 3-D by introducing new independent variables (such as the Euler angles) to describe crystal orientation. The generalized evolution equation will still be hyperbolic, and the same numerical methods can therefore be used to obtain solutions. Another desirable extension of the theory is to take into account the effects of
recrystallization, which may be an important factor in the evolution of LPO in the mantle (Karato 1987). In the continuum framework proposed here, recrystallization may be regarded as the replacement of material having one crystallographic orientation by material with a different orientation. This process can be described mathematically by adding an inhomogeneous or 'source' term to the right side of (3) to represent the rate at which material with a given orientation is being produced or destroyed by recrystallization. This extension of the theory, as well as the generalization to 3D, will be the subject of future work.

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REFERENCES


Table 1. Comparison of continuum theory and model of Etchecopar (1977).

<table>
<thead>
<tr>
<th>$\phi$ (Measured value)</th>
<th>$\dot{\varepsilon}$ (Etchecopar's model)</th>
<th>$\chi$ (Continuum theory)</th>
<th>$\chi$ (Etchecopar's model)</th>
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<td>0.29</td>
<td>0.81</td>
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<tr>
<td>0.36</td>
<td>0.39</td>
<td>0.89</td>
<td>0.91</td>
</tr>
<tr>
<td>0.87</td>
<td>0.76</td>
<td>0.93</td>
<td>0.86</td>
</tr>
<tr>
<td>Ice deformed in torsion (experimental)</td>
<td>0.30</td>
<td>0.36</td>
<td>0.74</td>
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<tr>
<td>0.48</td>
<td>0.50</td>
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<tr>
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<td>1.00</td>
<td>0.58</td>
<td>0.48</td>
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<tr>
<td>Ice deformed in simple shear (natural)</td>
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<td>1.35</td>
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Figure 8. Comparison of predicted ODFs for $\lambda = 1$ (smooth curves) with measured ODFs from a natural shear zone in glacial ice (histograms). Histogram in part (a) is an average of histograms III and IV from Fig. 7 of Bouchez & Duval (1982); histogram in part (b) is a similar average of histograms V and X; histogram in part (c) is identical to histogram IX. (a) $\dot{\varepsilon} = 0.47$, $\chi = 0.77$. (b) $\dot{\varepsilon} = 0.70$, $\chi = 0.64$. (c) $\dot{\varepsilon} = 1.35$, $\chi = 0.68$. 

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APPENDIX A: \( \phi \) FOR A CRYSTAL WITH TWO SLIP PLANES

An exact expression for the crystallographic rotation rate \( \phi \) can be derived for a crystal which has two independent slip systems. Let \((x_1, x_2)\) be fixed external Cartesian axes, \((\tilde{x}_1, \tilde{x}_2)\) be internal crystallographic axes, \(\phi\) be the angle between the \(\tilde{x}_1\) axis (=slip plane 1) and the \(x_1\) axis, and \(\beta\) be the (acute) angle between the two slip planes (Fig. 9). Because an arbitrary plane strain has two independent components, it can be resolved into two simple shears whose shear planes coincide with the slip planes. Denote the shear rates on the two slip planes by \(2\dot{\epsilon}_1\) and \(2\dot{\epsilon}_2\). The total strain rate is simply the sum of these two shears, and is described by a strain rate tensor whose components relative to the fixed external axes are

\[
\begin{pmatrix}
-\dot{\epsilon}_1 \sin 2\beta - \dot{\epsilon}_2 \sin 2(\phi + \beta) \\
\dot{\epsilon}_1 \cos 2\beta + \dot{\epsilon}_2 \cos 2(\phi + \beta) \\
\dot{\epsilon}_1 \cos 2\phi + \dot{\epsilon}_2 \sin 2(\phi + \beta) \\
\end{pmatrix}
\]

(A1)

This strain rate tensor must match that of the imposed deformation (assumed incompressible), viz.

\[
\begin{pmatrix}
\dot{\epsilon}_{11} & \dot{\epsilon}_{12} \\
\dot{\epsilon}_{12} & -\dot{\epsilon}_{11} \\
\end{pmatrix}
\]

(A2)

By equating the components of (A1) and (A2), we obtain

\[
\dot{\epsilon}_1 = \frac{\dot{\epsilon}_{11} \cos 2(\phi + \beta) + \dot{\epsilon}_{12} \sin 2(\phi + \beta)}{\sin 2\beta},
\]

(A3a)

\[
\dot{\epsilon}_2 = \frac{\dot{\epsilon}_{11} \cos 2\phi + \dot{\epsilon}_{12} \sin 2\phi}{\sin 2\beta}.
\]

(A3b)

Note that (A3) becomes infinite when \(\beta = 0\) or \(\pi/2\). This is because simple shears on parallel (\(\beta = 0\)) or perpendicular (\(\beta = \pi/2\)) slip planes are not independent, i.e. they give the same contribution to the rate of strain tensor. Such slip planes are therefore unable to accommodate an arbitrary imposed deformation. To determine the crystallographic rotation rate \(\phi\), we write

\[
\Omega^\phi = \Omega^mc - \Omega^me,
\]

(A4)

where \(\Omega^\phi\), \(\Omega^me\) and \(\Omega^mc\) are, respectively, the rotation rates of the crystal axes relative to the external axes, the material relative to the external axes, and the material relative to the crystal axes. (A4) is simply a transitive law for rotation which states that the rotation rate of \(A\) (the crystallographic axes) relative to \(C\) (the external axes) is the sum of the rotations of \(A\) relative to \(B\) (the material) and \(B\) relative to \(C\). The quantity \(\Omega^\phi\) is equal to \(\phi\) by definition, and \(\Omega^me\) is equal to the intrinsic rotation \(\Omega\) of the imposed deformation. The quantity \(\Omega^mc\) is equal to the sum of the rotation rates associated with the two simple shears, or \(-2(\dot{\epsilon}_1 + \dot{\epsilon}_2)\). Thus (A4) can be rewritten as

\[
\dot{\phi} = \Omega + \dot{\epsilon}_1 + \dot{\epsilon}_2.
\]

(A5)

Substitution of (A3) into (A5) gives

\[
\dot{\phi} = \Omega + \dot{\epsilon}_{12} \cos (2\phi + \beta) - \dot{\epsilon}_{11} \sin (2\phi + \beta) \frac{\cos \beta}{\sin 2\beta}.
\]

(A6)

An alternative form of (A6) is obtained by writing

\[
\dot{\epsilon}_{11} = \dot{\epsilon} \cos 2\phi,
\]

(A7a)

\[
\dot{\epsilon}_{12} = \dot{\epsilon} \sin 2\phi,
\]

(A7b)

where \(\dot{\epsilon}\) is the imposed strain rate and \(\phi\) is the orientation of the axis of maximum (instantaneous) extension. Substitution of (A7) into (A6) yields

\[
\dot{\phi} = \Omega - \dot{\epsilon} \frac{\sin (2\phi - 2\phi_i + \beta)}{\cos \beta},
\]

(A8)

which has the same form as (4).
**APPENDIX B: \( \phi \) FOR THE MODEL OF ETCHECOPAR (1977)**

Consider a 2-D crystal whose initial shape is that of an arbitrary \( N \)-sided polygon. Let \( \zeta_i^{(n)} \) be the \( i \)th coordinate (\( i = 1, 2 \)) of the \( n \)th vertex of this polygon, and let the orientation of the slip plane be \( \phi \). Let \( x_i^{(n)} \) be the vertex coordinates of the 'ideal' polygon produced by the imposed deformation. Finally, let \( r_i^{(n)} \) be the vertex coordinates of the polygon produced by a combination of single slip with a shear rate \( 2\dot{\varepsilon}_s \) and rotation with angular velocity \( \phi \) (translation can be ignored with no loss of generality). Our goal is to determine the values of \( \dot{\varepsilon}_s \) and \( \phi \) such that the polygons defined by the coordinates \( x_i^{(n)} \) and \( r_i^{(n)} \) match one another as closely as possible. Accordingly, we seek to minimize the quadratic sum (Etchecopar & Vasseur 1987)

\[
Q = \sum_{n=1}^{N} \sum_{i=1}^{2} [x_i^{(n)} - r_i^{(n)}]^2. \tag{B1}
\]

To derive expressions for \( x_i^{(n)} \) and \( r_i^{(n)} \), consider an infinitesimal deformation increment of duration \( \delta t \). To the first order in \( \delta t \),

\[ x_i^{(n)} = \zeta_i^{(n)} + D_{ij} \zeta_j^{(n)} \delta t, \tag{B2} \]

where \( D_{ij} \) is the velocity gradient tensor of the imposed deformation:

\[
D_{ij} = \begin{pmatrix} \dot{\varepsilon}_s \cos 2\phi_i & \dot{\varepsilon}_s \sin 2\phi_i - \Omega \\ \dot{\varepsilon}_s \sin 2\phi_i + \Omega & -\dot{\varepsilon}_s \cos 2\phi_i \end{pmatrix}. \tag{B3}
\]

In (B2), summation is implied over the repeated subscript \( j \).

Similarly,

\[ r_i^{(n)} = \zeta_i^{(n)} + d_{ij} \zeta_j^{(n)} \delta t, \tag{B4} \]

where \( d_{ij} \) is the velocity gradient tensor for a combination of single slip and rotation:

\[
d_{ij} = \begin{pmatrix} \mp \dot{\varepsilon}_s \sin 2\phi & \pm \dot{\varepsilon}_s (\cos 2\phi - 1) - \dot{\phi} \\ \pm \dot{\varepsilon}_s (\cos 2\phi + 1) + \dot{\phi} & \mp \dot{\varepsilon}_s \sin 2\phi \end{pmatrix}. \tag{B5}
\]

In (B5), the upper sign corresponds to dextral shear (clockwise vorticity) on the slip plane, and the lower sign to sinistral shear. Substitution of (B2)–(B5) into (B1) yields, to within a multiplicative constant,

\[
Q = \sum_{n=1}^{N} \left( (A \zeta_1^{(n)} + (B + C) \zeta_2^{(n)})^2 + [(B - C) \zeta_2^{(n)} - A \zeta_1^{(n)}]^2 \right), \tag{B6}
\]

where

\[
A = \dot{\varepsilon}_s \cos 2\phi_i \pm \dot{\varepsilon}_s \sin 2\phi
\]

\[
B = \dot{\varepsilon}_s \sin 2\phi_i \pm \dot{\varepsilon}_s \cos 2\phi
\]

\[
C = -\Omega \pm \dot{\varepsilon}_s \cos 2\phi_i
\]

To minimize \( Q \), we require

\[
\frac{dQ}{d\dot{\varepsilon}_s} = \frac{dQ}{d\phi} = 0. \tag{B10}
\]

Substitution of (B6)–(B9) into (B10) yields two linear equations which can be solved for \( \dot{\varepsilon}_s \) and \( \phi \). If the initial shape of the crystal is a regular polygon, \( \dot{\varepsilon}_s \) and \( \phi \) are independent of \( \zeta_i^{(n)} \), and are given by

\[
\dot{\varepsilon}_s = \mp \dot{\varepsilon}_s \sin 2(\phi - \phi_i), \tag{B11}
\]

\[
\phi = \Omega \mp \dot{\varepsilon}_s \sin 2(\phi - \phi_i). \tag{B12}
\]

Equations (B11) and (B12) give the rates of single slip and rotation which are produced by an arbitrary imposed deformation defined by the quantities \( \Omega \), \( \dot{\varepsilon}_s \) and \( \phi \). Because the coordinates \( \zeta_i^{(n)} \) do not appear in (B11) or (B12), these expressions are valid for a crystal of any shape whatsoever. Note that (B12) is identical to (A8) in the limit \( \beta = 0 \), which corresponds to a single slip plane.