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Lattice rotation in polycrystalline aggregates and single crystals with one slip system: a numerical and experimental approach

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Abstract—In this study, lattice rotations in polycrystals and single crystals with one slip system have been analysed for pure shear and simple shear by re-visiting previously published data and by conducting new numerical models that are compared with results from experiments on polycrystalline ice. The numerical models are based on the finite-difference method and on the assumption that dislocation glide on one slip system is the dominant crystalline deformation mechanism and is controlled by the critical resolved shear stress law. Such a deformation scheme corresponds to the operation of glide on (0001) in polycrystalline ice used in the physical deformation experiments. The results show that lattice rotation is primarily controlled by the bulk deformation kinematics in both the polycrystalline aggregates and the single crystals. In the single crystals the lattice rotation is entirely consistent with the vorticity of the bulk deformation kinematics, whereas in the polycrystalline aggregates extensive grain interactions significantly modify the local lattice rotations and may even lead to the lattice planes of individual grains rotating in an opposite sense to that of the bulk deformation. These results can reasonably explain the development of crystallographic preferred orientations widely reported in the literature. © 1997 Elsevier Science Ltd

INTRODUCTION

Polycrystalline materials can accommodate large amounts of intragranular plastic deformation and in so doing develop crystallographic preferred orientations. In simple shear, *c*-axis preferred orientations in materials containing one dominant slip system (e.g. quartz and ice) generally exhibit two girdles or maxima slightly asymmetrical with respect to the bulk finite shortening axis, with one being normal to the shear plane (e.g. Bouchez and Pecher, 1976; Lister and Hobbs, 1980; Bouchez and Duval, 1982; Burg *et al.*, 1986; Etchecopar and Vasseur, 1987; Jessell, 1988; Zhang *et al.*, 1994), or one single girdle or maximum normal to the shear plane (e.g. Brunel, 1980; Bouchez and Duval, 1982; Law, 1987; Law *et al.*, 1990). A fabric transition from the bimodal pattern to the single maximum pattern can take place at large shear strains (Bouchez and Duval, 1982; Jessell, 1988). In pure shear, the *c*-axis preferred orientations are usually a small circle or two maxima about the shortening axis (Etchecopar, 1977; Lister and Hobbs, 1980; Wilson, 1982; Zhang *et al.*, 1994).

The development of crystallographic preferred orientations is considered to be the result of lattice rotation that is controlled by both the imposed bulk deformation kinematics and the local grain interaction. The temporal changes of lattice re-orientation behaviour as a function of instantaneous lattice orientation during a progressive deformation history also adds to the complexity of the rotation processes. To understand the mechanisms behind the evolution of various lattice preferred orientation patterns, a detailed analysis of lattice rotation in polycrystalline materials is necessary. Lister (1982) analysed the vorticity related to lattice re-orientation for a number of plastic deformation cases in crystals with several sets of slip systems. The Taylor–Bishop–Hill model (Taylor, 1938; Bishop and Hill, 1951) is based on free lattice spinning of the crystals in a homogeneously deforming polycrystal causing the rotation of individual crystals axes with respect to a reference frame. This is considered to be the result of three rotation components: (1) the bulk stretching axes with respect to the frame; (2) the local stretching axes within individual grains with respect to the bulk stretching axes; and (3) the crystal axes with respect to the local stretching axes. This model can account for the common crystallographic fabric patterns observed in natural materials.

Another important study of lattice rotation is Etchecopar's geometrical model (Etchecopar, 1977), that explicitly describes the lattice rotation of polycrystals with one slip system under simple shear. The results show that all the slip planes rotate towards the shear plane in a way consistent with the rotation sense generated by the simple shearing, except for those oriented in a 30° domain with respect to one end of the shear plane (Fig. 1a). In this orientation domain, the slip planes rotate towards the shear plane but in a direction contrary to the bulk rotation sense of the simple shearing. This observation

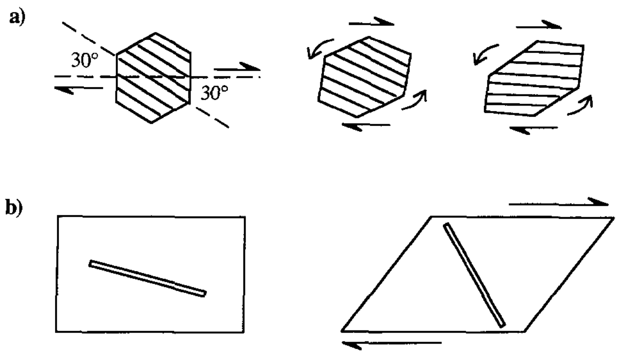

Fig. 1. (a) Slip-plane rotation predicted by Etchecopar (1977) for slip planes with initial orientations at 30° to the simple-shear plane. (b) Rotation of rigid objects of the same orientation in a soft matrix (after Ildefonse and Mancktelow, 1993; Lamb, 1994).

has also been reported in some other studies of fabric development (e.g. Nicolas and Poirier, 1976; Burg *et al.*, 1986). However, it has long been known that in simple shear, material lines rotate following the vorticity of the bulk shearing. Studies on the behaviour of rigid objects in a soft matrix (e.g. Ildefonse and Mancktelow, 1993; Lamb, 1994) also show that the rotation is entirely consistent with the rotation kinematics of simple shearing, even for those initially oriented in the domain mentioned above (Fig. 1b).

These observations suggest that some lattice planes in polycrystalline aggregates, unlike material lines or rigid objects, may rotate in a direction contrary to the imposed vorticity of the bulk deformation in simple shear (Fig. 1a). The mechanism responsible for this rotation behaviour is not clear, and requires further investigation. Moreover, lattice rotation in a single crystal, that will help our understanding of lattice rotation in polycrystals, has not been previously investigated through an experimental approach or mechanical modelling. In this paper we aim to examine lattice rotations that accompany plastic deformation using both numerical and experimental methods. One-slip-system computer models are constructed for both the polycrystal and single crystal situations under pure shear and simple shear, respectively. The numerical results will then be compared with the basal-plane rotation observed in experimentally deformed polycrystalline ice, and finally related to the development of crystallographic preferred orientations.

NUMERICAL RESULTS

Model basis

The two-dimensional one-slip-system numerical models employed here have been constructed using the explicit finite-difference computer code FLAC (Fast Lagrangian Analysis of Continua) of Itasca Consulting Group (Cundall and Board, 1988). The model simulates a crystalline grain as an elastic–perfectly-plastic polygon (matrix) containing an infinite number of parallel slip planes (one slip system) and being approximated by a finite-difference mesh. The simulation of a polycrystalline aggregate can be achieved by considering a collection of polygonal grains, each possessing different initial slip-plane orientations. The theoretical background of the model has been described in Zhang *et al.* (1993, 1994), and the application of the method to modelling of strain and microstructural development in polycrystalline ice (Wilson and Zhang, 1994) has produced results consistent with experimental observation.

The model allows inhomogeneous deformation within individual grains while still maintaining strain compatibility and dynamic stress equilibrium. The polycrystalline deformation can be accommodated by slip on a single-slip system, which conforms to the critical resolved shear stress law (Schmid, 1928), and by elastic–plastic deformation in the matrix which is controlled by a non-associated flow law (Vermeer and de Borst, 1984; Ord, 1991). Slip on the slip planes commences when the resolved shear stress is equal to the critical resolved shear stress (τ_c). Similarly, the matrix deformation switches from elastic to plastic when the maximum shear stress reaches the yielding limit (σ_o). Because τ_c and σ_o are entirely determined by slip-plane cohesion (C_s) and matrix cohesion (C_m), respectively, after zero friction angles are chosen for both the matrix and slip planes, setting $C_m \gg C_s$ leads to $\sigma_o \gg \tau_c$. By so doing, slip on slip planes is made much easier than the matrix deformation in the model so that it accommodates the major part of the imposed bulk deformation.

Material properties defining the crystalline material with a single-slip system must be assigned to the mesh adopted. These include density, elastic moduli, cohesion and friction angle for both the slip planes and matrix material, and slip-plane orientations. The parameters adopted in this study are identical to those used in Zhang *et al.* (1994, table 1), which ensure the domination of the deformation mechanism described above. Numerical bulk deformations for simple shear and pure shear are simulated by specifying appropriate boundary conditions for the mesh and assigning constant displacement rates to the boundaries. Total bulk strain is achieved through a series of bulk strain increments. The accompanying slip-plane rotation is described with the co-ordinate system defining slip-plane orientation illustrated in Fig. 2, and in this way the evolution of slip-plane orientation can be traced throughout the whole deformation history.

Lattice rotation in polycrystalline aggregates

Zhang *et al.* (1994) described a group of numerical polycrystal models, and focused on strain distribution, microstructure and crystallographic preferred orientation development for a number of deformation histories. Here we re-analyse the results of two of their models, for simple shear and pure shear, respectively (see Zhang *et al.*, 1994, figs 2 & 5c & d), concentrating on the features of

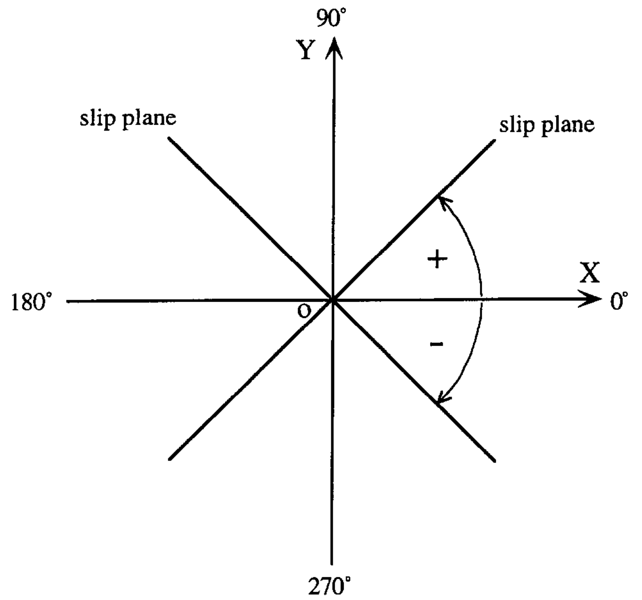

Fig. 2. The definition of slip-plane orientation with respect to X–Y co-ordinates. Orientation angles are positive if measured counter-clockwise from the X axis, but negative if measured clockwise. A negative orientation angle is used when slip-plane rotation cannot be expressed by continuous positive angles, such as a rotation from 30° to 0° to −30°. This orientation and the X–Y reference frame is adopted in the other figures of this paper.

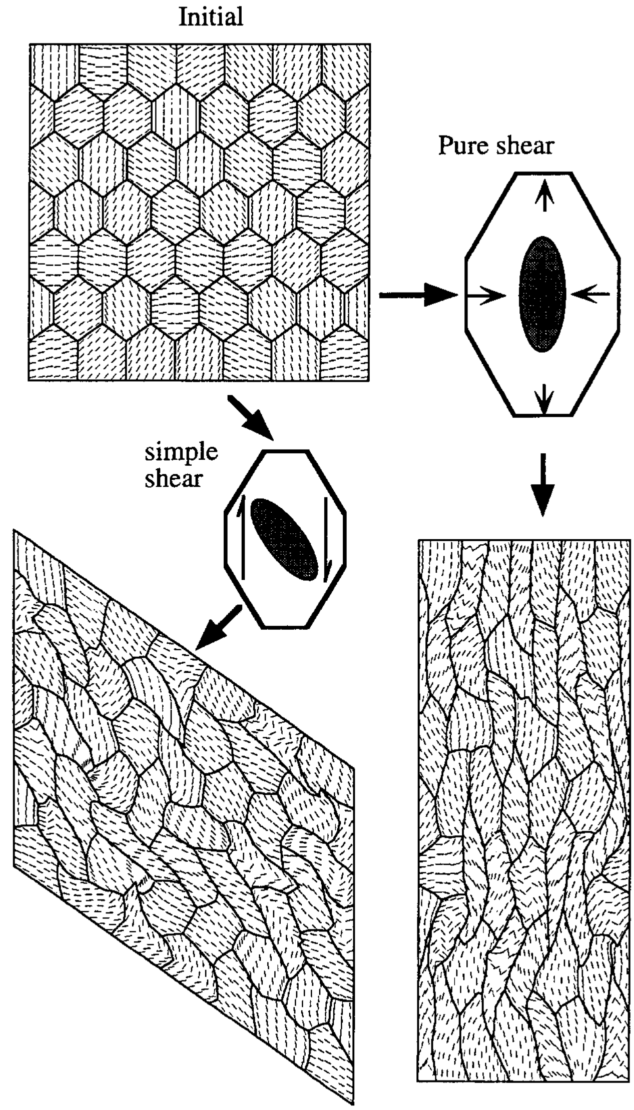

Fig. 3. Schematic presentation of slip-plane traces before and after deformation (simple shear and pure shear) for polycrystalline deformation models (see Zhang *et al.*, 1994 for the details of the model).

progressive lattice (slip-plane) rotation. Figure 3 shows the spatial distribution of slip-plane traces in the simulated polycrystalline aggregate before and after deformation. Polycrystalline deformation, including intragranular strains and inter-grain rotation, has clearly caused significant slip-plane misorientation. The trajectories of progressive slip-plane rotation for a number of uniformly distributed locations in the aggregate are given in Fig. 4.

Pure shearing history. For the pure shearing history (Fig. 4a), slip planes generally rotate towards the bulk extension (elongation) direction. However, the rotation can be clockwise or counter-clockwise, depending on the initial orientation of slip planes with respect to the bulk extension axis. During the rotation process there is a change in the rotation rate for slip planes with higher angles (> 45°) to the bulk extension axis. Most of these slip planes rotate at a larger rate until they reach an orientation of about 25–30° from the bulk extension axis where their rotation rate diminishes. In fact, many slip planes seem to become stabilized at this orientation without showing much further rotation toward the bulk extension axis. The preferred orientations of slip-plane normals resultant from this kind of slip-plane rotation are two maxima slightly asymmetrical with respect to the bulk finite shortening axis (Zhang *et al.*, 1994, fig. 7c).

The principal features of the lattice rotations during pure shear are in agreement with the predictions of theories of plasticity (e.g. Mase, 1970; Nicolas and Poirier, 1976). However, for two special cases of initial orientations, the rotation differs from that anticipated.

(1) Grains with slip planes approximately parallel to the bulk shortening direction (the 0° and 180° orientations in Fig. 2) do not deform such that the slip planes maintain their starting orientations, but rather the slip planes undergo large clockwise or counter-clockwise rotation towards the bulk extension direction (Figs 3 & 4a). This behaviour seems to be related to the initiation of kinking instabilities along the loaded slip planes due to grain interaction from neighbouring grains in a deforming polycrystal (Nicolas and Poirier, 1976). These slip planes are in highly unstable orientations once the instabilities are initiated. Rapid amplification of the instabilities will then lead to kinking of the slip planes within the grains, as widely observed in deformed polycrystals with one dominant slip system such as ice (Wilson *et al.*, 1986). Therefore, the clockwise and counter-clockwise rotation of these slip planes is

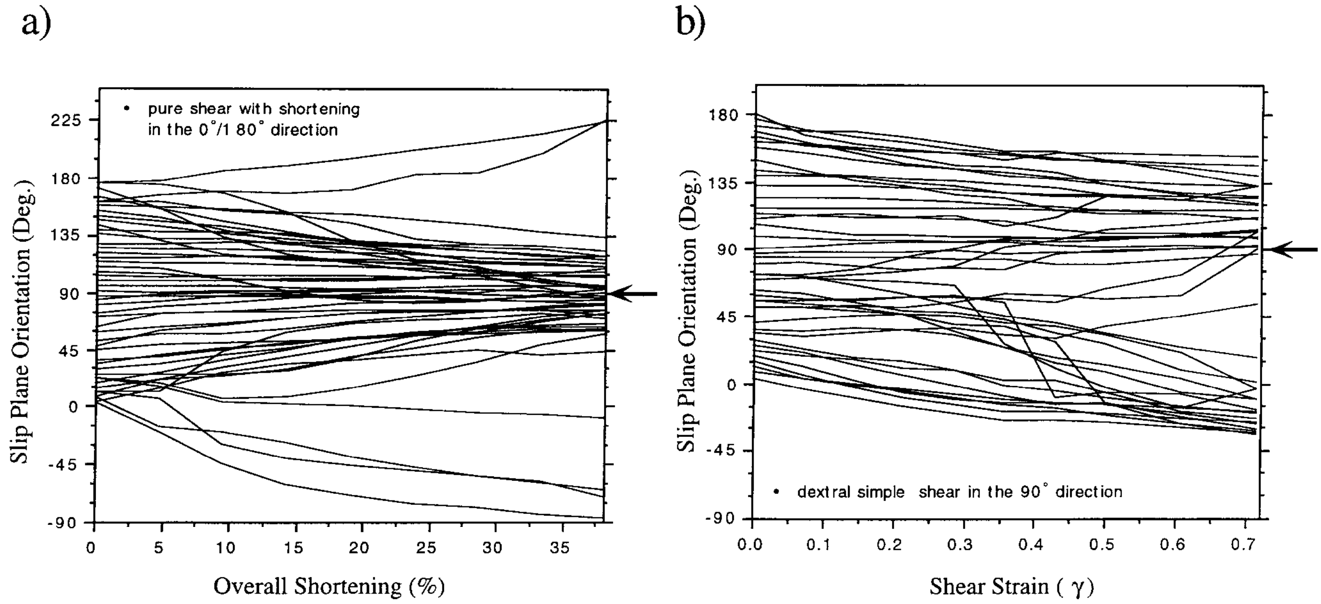

Fig. 4. The re-orientation trajectories of slip planes. These show slip-plane orientation changes with the increase of bulk strain for two numerical models of polycrystalline deformation (see Fig. 3). (a) Pure shearing; the arrow indicates the bulk extension direction. (b) Simple shearing; the arrow gives the shear-plane orientation.

inevitable. This is consistent with the observation that such grains do not behave as 'hard' grains although they have small initial resolved shear stresses on slip planes (Zhang *et al.*, 1994).

(2) Slip planes that are approximately parallel to the bulk extension axis (the 90° orientation in Fig. 2) still undergo a small rotation away from the bulk extension axis (Figs 3 & 4a). This is anomalous because the resolved shear stresses and rotation tensors along the slip planes are close to zero and the slip planes are initially in the most stable position. Such anomalous slip-plane rotation may also be attributed to neighbour grain interactions which can cause small rigid grain rotations or small deviations of the local deformation field from the imposed bulk deformation framework. The behaviour described above can also be observed for the slip planes initially oriented at a small angle (about 30°) to the bulk extension axis (Fig. 4a). Owing to a similar mechanism, these slip planes can rotate past the bulk extension axis or reverse rotation direction when they reach or are close to the bulk extension direction.

Simple shearing history. During the simple shearing history (Fig. 4b), slip planes rotate either towards or away from the shear plane (the 90° orientation), depending on the initial slip-plane orientations. The slip planes can be divided into three major groups according to their dominant rotation behaviour (Fig. 5a).

(1) Slip planes initially oriented in the range of about

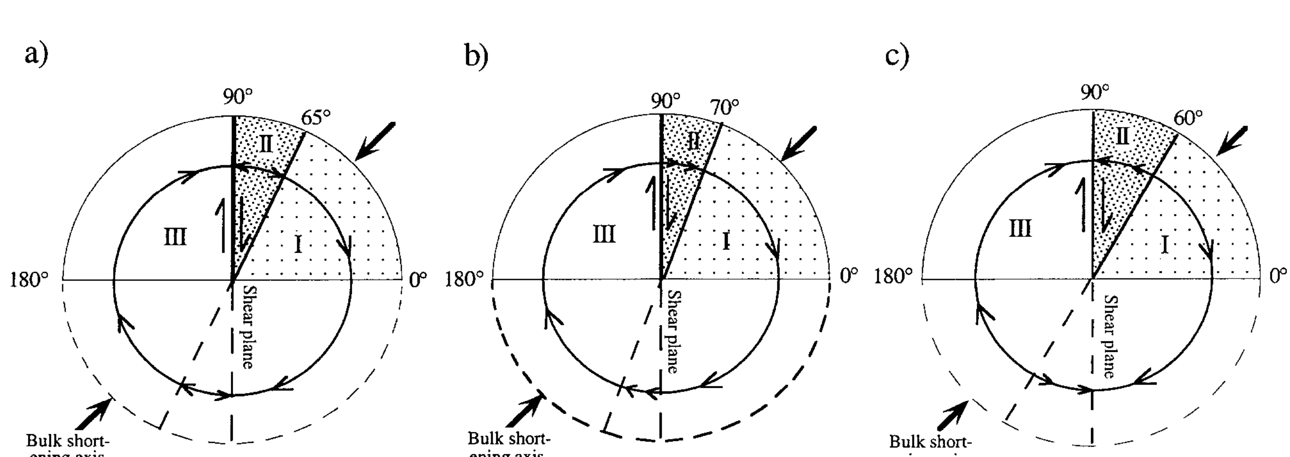

Fig. 5. Classification of slip planes according to their initial orientation and rotation behaviour for the simple-shearing history. I, II and II denote three orientation segments with different rotation features (see text for further description); arrows indicate the rotation directions of slip planes in the segment, and 90° is the shear plane direction. (a) The polycrystal model. (b) The single crystal model. (c) The results of the Etchecopar (1977) model.

0–65° (segment I in Fig. 5) generally rotate clockwise away from the shear plane, but rotate towards the shear plane once they pass the normal to the shear plane. This rotation direction is consistent with the imposed vorticity of the dextral shearing. However, for slip planes initially oriented at a small angle to the bulk shortening axis (the 45° orientation, Fig. 4b), the rotation in the opposite sense can also be observed. This rotation phenomenon is the result of kinking of the slip planes which occurred due to shortening sub-parallel to the slip planes.

(2) Slip planes with the initial orientations of about 65–90° (segment II in Fig. 5) can rotate both counter-clockwise towards the shear plane, in a direction contrary to the vorticity of the shearing, or clockwise away from the shear plane, in a direction consistent with the vorticity of the shearing. The latter differs from the results of the Etchecopar (1977) model for slip planes with such orientations, where it was found that the slip planes of this orientation only rotated towards the shear plane. The reasons for the variations in rotation behaviour reported here will be discussed further below.

(3) Slip planes initially oriented in the range of 90–180° (segment II in Fig. 5) generally rotate clockwise towards the shear plane, in a direction consistent with the rotation kinematics of the dextral shearing.

The shear-plane orientation represents the rotationally stable position for slip planes in simple shear. If the shear strain is sufficiently large, the final orientation of the slip planes is parallel to the bulk shear plane irrespective of the directions in which they rotate. Crystallographic preferred orientation analyses (Zhang *et al.*, 1994, fig. 7d) show that the corresponding slip-plane normal preferred orientations for $\gamma = 0.72$ are two maxima, one normal to the shear plane and the other slightly asymmetrical to the first with respect to the finite bulk shortening axis.

Lattice rotation in single crystals

Numerical experiments for single crystal deformation have been performed which cover a continuous range of initial slip-plane orientations. The constitutive theory and material parameters for these experiments are the same as those for the polycrystalline models. However, a square mesh of 36 elements, all with an identical initial slip-system orientation, is adopted here to simulate a single grain. The boundaries of the grain are constrained, using velocity boundary conditions, so that the grain deforms progressively. The bulk finite deformations achieved in these models are 50% shortening for pure shear and $\gamma = 2.0$ for simple shear. The slip-plane rotation results are summarized (Figs 6 & 7) and discussed below.

Pure shearing history. The trajectories of the slip-plane rotations are entirely towards the bulk extension direction (Fig. 6b), and exhibit an overall simple and regular pattern without the complexities of the polycrystalline model (Fig. 4a). Three different rotation patterns are observed.

(1) For slip planes initially oriented in the range of 20–90° and 90–160° (two 70° segments symmetrical about the bulk extension axis), the rotation curves are approximately straight lines, i.e. the rotation rates are nearly constant.

(2) For slip planes with initial orientations in the range of 0–20° and 160–180° (two 20° segments from the bulk shortening axis), the rotations show a two-stage pattern. The slip planes initially rotate at a small and approximately constant rate, until about 20% bulk shortening, and then the rotations accelerate at larger strains.

(3) Slip planes initially parallel to the bulk shortening axis (the 0° and 180° orientations) or the bulk extension axis (the 90° orientation) remain unrotated throughout the whole deformation history (Fig. 6). This is in clear contrast to the polycrystalline case where the slip planes still rotate. In this case the slip planes fully behave as passive material lines in the deforming grain as they have zero resolved shear stress and do not activate at all throughout the deformation history. The imposed bulk deformation on the grain is actually accommodated by the matrix deformation which, in effect, would be equivalent to the involvement of another deformation mechanism such as diffusion.

Simple shearing history. The slip-plane rotation in the single crystal models (Figs 5b & 7) also display a simple pattern; that is, entirely clockwise rotation towards the bulk shear plane, consistent with the imposed dextral shearing kinematics. In contrast to the polycrystalline models (see Fig. 5a), there is no counter-clockwise rotation. The slip planes in the single crystal models can also be classified into three groups according to their rotation behaviour (see Fig. 5b).

(1) For the slip planes initially oriented in the range of about 0–70° (segment I), the rotation is away from one direction but towards the other direction of the shear plane (the 270° direction).

(2) The slip planes with the initial orientations of about 70–90° (segment II) also rotate away from the shear plane but the amount of rotation is small. The slip-plane orientations remain close to the shear-plane direction even after a bulk shear strain of $\gamma = 2.0$. The slip planes initially parallel to the shear plane (the 90° orientation) remain unrotated.

(3) The slip planes of the third group are initially oriented in the range of 90–180° (segment III). These slip planes rotate towards the shear plane. The larger the initial angle between the slip plane and the shear direction, the larger is the component of rotation.

The major difference between the results of the polycrystal model and the single crystal model lies in the rotation behaviour of the slip planes in segment II. In the

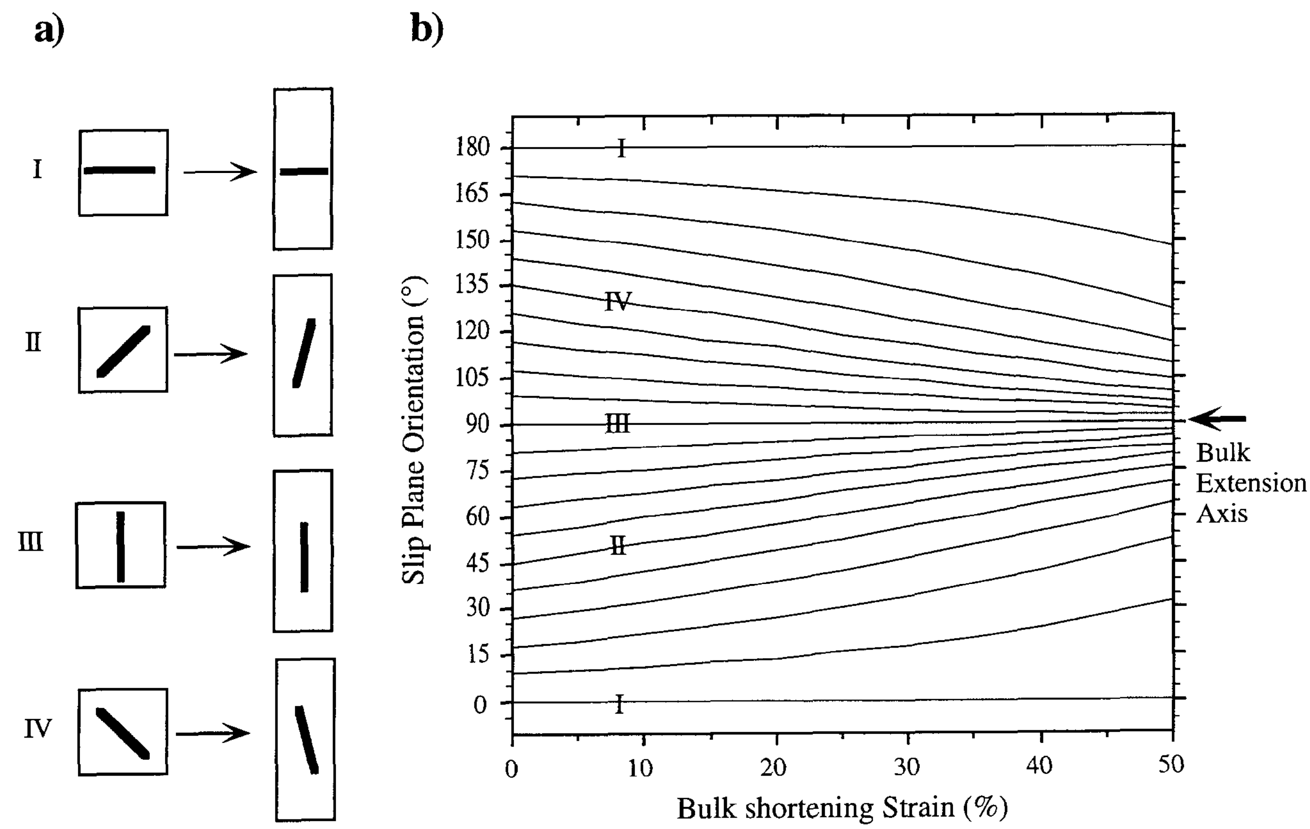

Fig. 6. Slip-plane rotation in single crystals in a pure shear regime. (a) Sketch of the experiments (left column, starting crystals; right column, deformed crystals; thick lines represent slip planes). (b) Re-orientation trajectories.

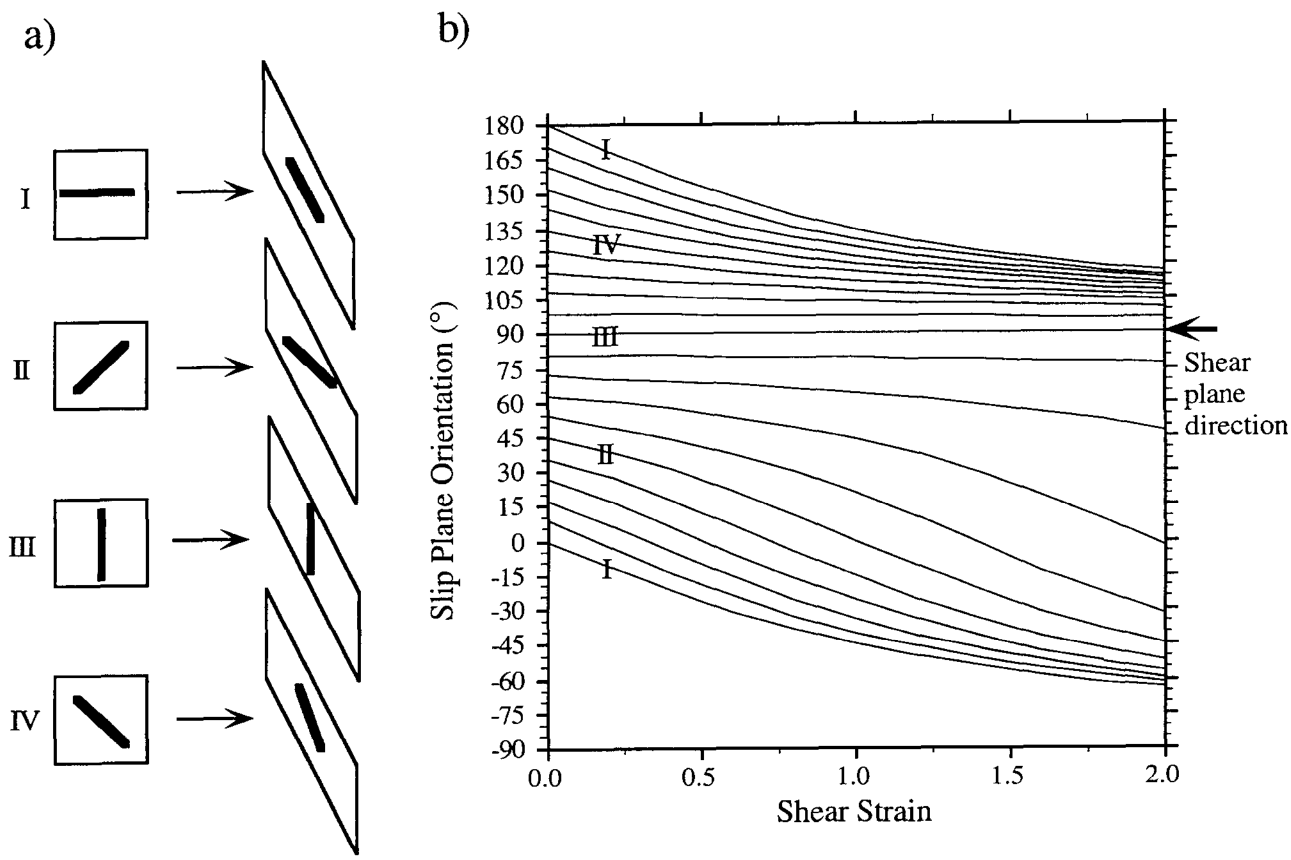

Fig. 7. Slip-plane rotation in single crystals in a simple shear regime. (a) Sketch of the experiments (left column, starting crystals; right column, deformed crystals; thick lines represent slip planes). (b) Re-orientation trajectories.

polycrystal case (Figs 4b & 5a), the slip planes can rotate both towards and away from the shear plane, contrasting with the one-way rotation revealed for the single crystal model.

The slip planes initially parallel to the bulk instantaneous shortening and extension axes (the 45° and 135° directions) behave as passive material lines only in the initial stages when they have zero or small resolved shear stresses and therefore do not activate. The bulk deformation imposed on the grain in the single crystal case must be accommodated by matrix deformation. However, once the slip planes become rotated, and the resolved shear stresses increase to a sufficient level, the slip planes will activate to accommodate bulk deformation.

EXPERIMENTAL DEFORMATION OF POLYCRYSTALLINE ICE

Experimental techniques

Polycrystalline ice has been used as an analogue for deformed quartz-rich rocks to investigate the relationship between crystallographic preferred orientation and microstructural development (Wilson, 1984; Burg *et al.*, 1986; Wilson *et al.*, 1986). The most commonly reported glide system in ice is (0001) with a variety of slip directions (Kamb, 1961). The only dislocations ever observed to participate in plastic deformation have the Burger's vector lying in this plane (Shearwood and Whitworth, 1993). Therefore, there exists an important similarity between ice crystals and the one-slip-system polycrystalline models presented in this study.

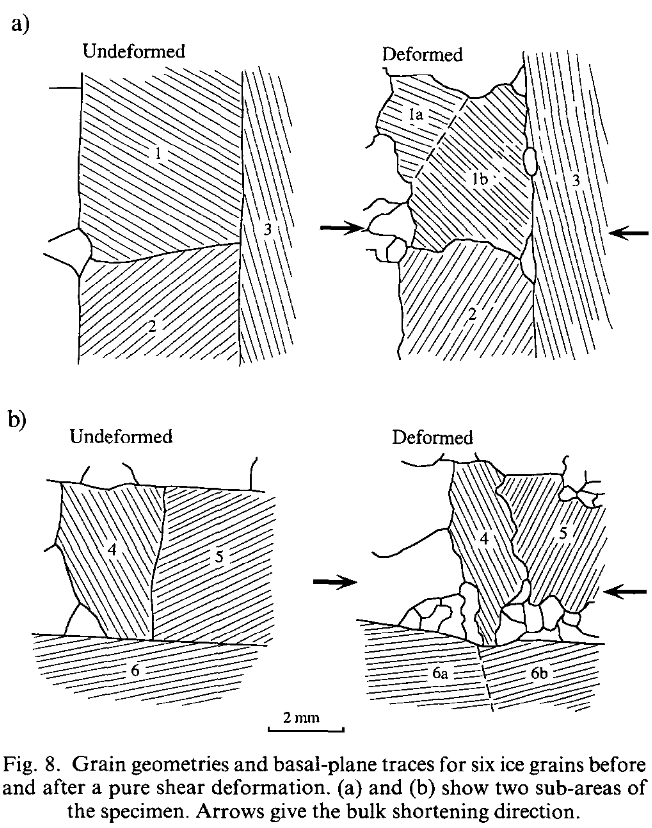

Fig. 8. Grain geometries and basal-plane traces for six ice grains before and after a pure shear deformation. (a) and (b) show two sub-areas of the specimen. Arrows give the bulk shortening direction.

The detailed description of the techniques and the experimental conditions have been given in Wilson (1984) and Wilson *et al.* (1986) for pure shearing, and in Burg *et al.* (1986) for simple shearing. The techniques adopted in these studies involve three major steps. First, a rectangular section of polycrystalline ice about 25×35 mm and 0.7 mm thick is prepared from a refrozen block of sized ice particles and distilled water. The resultant sample consists of approximately equant polygonal grains where the *c*-axis and hence (0001) basal-plane orientations were measured using a universal stage. Second, the ice sample is confined between two fixed glass plates that are part of the deformation apparatus. Finally, the deformation of the sample is carried out on the apparatus under an optical microscope at temperatures below -1°C with the plane-strain conditions ensured. The microstructural development of ice grains in selected areas is recorded on 16 mm and 35 mm video film.

Below we describe the orientation changes of (0001) in ice grains with the basal plane lying perpendicular to the plane of observation in a pure shear and a simple shear experiment, respectively, and compare with the results of the numerical models. It needs to be mentioned that the bulk strains at which basal-plane rotation in ice is described are small; recrystallization in ice becomes severe at higher strain. This somewhat limits the prediction of lattice rotation reported here. For this reason the choice of examples was dictated by areas in the sample that contained grains of the appropriate initial orientation and to areas where the early stages of the deformation did not involve excessive grain-boundary migration.

Experimental observations

Pure shearing history. Figure 8 shows the initial and deformed grain shapes and the orientation change of basal-plane traces for six ice grains, in two sub-areas of the specimen. A prominent feature of the deformed ice polycrystal is that grain shapes have been significantly modified mainly by rotation recrystallization and/or grain-boundary migration. Grain-boundary migration is the dominant recrystallization process occurring along existing grain boundaries or on sub-grain boundaries produced by localized lattice rotation.

Intragranular deformation clearly caused the rotation of basal-plane traces in all grains towards the extension axis of the bulk deformation field, if kinking is not involved. Examples are grains 2–5 (Fig. 8a & b). The basal planes of these grains were initially oriented at 40°, -75°, -62° and 26°, respectively, to the bulk shortening axis, but by ~ 16% bulk shortening these were rotated to the orientations of 60°, -78° to -80°, -65° and 63° to the bulk shortening axis, respectively. The direction of basal-plane rotation for these grains is in qualitative agreement with the results of numerical modelling of the rotations observed in both polycrystals and single crystals.

Where the deformation of an ice grain is accommodated by processes other than basal slip and grain-boundary migration, then the basal planes may rotate by kinking. This can be illustrated by the lattice rotation features of grains 1 (Fig. 8a) and 6 (Fig. 8b) which have the initial basal-plane orientations of $-31°$ and $11°$ to the bulk shortening axis, respectively. The lattice rotation is bi-directional with the basal planes rotated towards the bulk extension axis only in part of the kinked grains (grains 1b and 6b, where the final basal-plane orientations are $-45°$ and $15°$ to the shortening axis). In the other part of the kinked grains (grains 1a and 6a), basal planes rotated in an opposite sense, towards the bulk shortening axis. The final basal-plane orientations for grains 1a and 6a are $-23°$ and $7°$ to the shortening axis. These lattice rotation behaviours are comparable to those observed in the numerical polycrystal model as the result of kinking, due to either grain interaction or special initial slip orientations.

Simple shearing history. The orientation changes of basal-plane traces in seven ice grains in a simple shear experiment are illustrated in Fig. 9. Grains 1, 4 and 7 have initial basal-plane orientations corresponding to the those outlined in group III of Fig. 5(a). After a bulk shear strain of 0.23, the basal planes in grains 1 and 7 rotated towards the shearing plane; the rotation angle is 9° and 3°, respectively. However, the rotation behaviour of grain 4 seems to be influenced by neighbouring grain interaction, that is, the effect of indentation from grains 5 and 6. As such, the major orientation of its basal planes did not change, while the basal planes in a small area near its upper-left boundary showed a slight rotation away from the shearing plane direction. These observations are consistent with the results derived from the present polycrystalline numerical models for grains with this kind of initial lattice orientation distribution, particularly with regard to the significance of grain interactions.

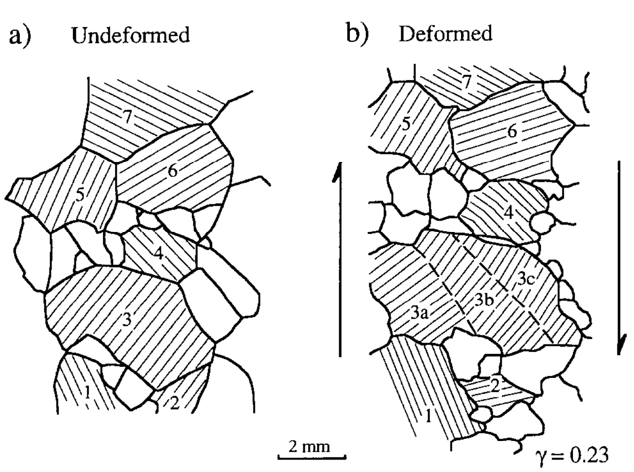

Fig. 9. Grain geometries and basal-plane traces in seven ice grains for the simple shearing ice deformation experiment. (a) Undeformed and (b) deformed.

Grains 2, 3 and 6 (Fig. 9a) represent a group of ice grains with initial basal-plane orientations situated in group I of Fig. 5(a). The rotation observed for grains 2 and 6 and part of grain 3 (i.e. 3a) is clockwise, in a direction consistent with the vorticity of the shearing. This is again consistent with the features revealed by the polycrystalline model. Two sub-areas of grain 3 (i.e. 3b and 3c) exhibit rotation opposite to that for this group of grains. This is due to kinking and can be compared to the rotation behaviour of the kinked grains in the numerical models (see Fig. 3).

Grain 5 is the only ice grain that has an initial basal-plane orientation in group II of Fig. 5(a). During deformation (Fig. 9b) the basal plane did not rotate towards the shear plane as suggested by some previous studies (Nicolas and Poirier, 1976; Etchecopar, 1977; Burg *et al.*, 1986), but rather rotated 8° away from the shear plane in a direction consistent with the rotation vorticity of the shearing. This supports the suggestion of the present numerical models that lattice rotation in these orientations (group II, Fig. 5a) does not have to be towards the shear plane, in a sense contrary to the vorticity of the shearing.

DISCUSSION

Under the same external deformation frame, the lattice rotations in polycrystals and single crystals are not identical. The main differences lie in the rotation behaviour of the slip planes initially oriented in particular orientations. These are slip planes initially parallel and normal to the bulk shortening axis in the case of pure shear, and slip planes initially oriented at about 20–25° to the shear plane (i.e. segment II in Fig. 5a & b) in simple shear.

A fundamental difference between a deforming polycrystalline grain aggregate and a single crystal is that the former involves strong grain interactions while the latter does not (Zhang *et al.*, 1994). This produces lattice rotation differences that may be attributed to the following polycrystalline deformation behaviours.

(1) Grain interaction can initiate kinking instabilities which are geometrically expressed as small lattice rotation, along the slip planes initially parallel to the shortening axis in pure shear. These instabilities facilitate kinking and buckling. As such, the slip planes with this orientation undergo significant clockwise or counter-clockwise rotation in the polycrystalline case. In the single crystal case, however, the slip planes remain unrotated at this initial unstable orientation due to lack of grain interaction, as well as the associated instabilities to break initial perfect balance.

(2) Grain interaction plus kinematic enhancement produce a deviation of the local shortening and extension axes from the bulk shortening and extension axes (see Zhang *et al.*, 1994, fig. 12). As a result, the slip planes with an initial orientation parallel to the bulk extension axis of pure shear will not be exactly parallel to the local extension axis and therefore do not lie in the local rotationally stable position within the polycrystalline aggregate. These slip planes can still experience a small amount of rotation towards their local rotationally stable orientation. This is in contrast to the single crystal situation where the slip planes at this orientation do not rotate at all.

(3) Grain interactions represent a kind of mutual deformation influence among different grains in a polycrystal. Grains with different lattice orientations have different deformabilities, each tending to deform independent of others. However, the condition of strain compatibility requires that their boundaries remain in contact after deformation. This means that the deformation of the boundary areas among neighbouring grains could be a compromise, different from the deformation of their respective grain interiors. Correspondingly, lattice rotation in the boundary areas could change irregularly, reflecting the changes of local deformation features. This probably explains why lattice rotation in polycrystals, combining the effect of local anomalous behaviour, is more complex than in single crystals: in particular, why the rotation of the slip planes oriented in segment II of a simple shearing framework (Fig. 5a) can be both clockwise and counter-clockwise, while the single crystal models (Fig. 5b) suggest that all of the rotation caused by the dextral simple shearing is clockwise.

Another important difference between the polycrystalline model and single crystal model is that the former allows inhomogenous deformation and the latter does not. In polycrystals, a 'hard' grain (with lattice orientations unfavourable for slip) may only undergo small internal deformation plus some rigid rotation, while the bulk deformation is dominantly accommodated by other 'soft' grains. In contrast, a 'hard' grain in the single crystal model must still deform to accommodate the bulk strain. The slip planes in this case rotate as passive material lines, entirely controlled by deformation in the matrix.

Slip-plane rotation associated with single-slip systems in simple shear has been discussed by Etchecopar (1977), and a similar pattern has been described by others (e.g. Nicolas and Poirier, 1976; Burg *et al.*, 1986). The differences between Etchecopar's results (Fig. 5c) and the current models (Fig. 5a & b) mainly occur in segment II. Etchecopar (1977) demonstrated that slip planes oriented in the equivalent of segment II can only rotate counter-clockwise towards the shear plane, in a sense contrary to the rotation vorticity of the dextral simple shear, and to the rotation behaviour reported for material lines and rigid objects in a soft matrix (e.g. Ildefonse and Mancktelow, 1993; Lamb, 1994). The slip planes in other orientations rotate clockwise. We believe that the slip-plane rotation results of the present polycrystalline model more reasonably reflect the true situation. That is, these slip planes dominantly rotate in a way consistent with the vorticity of the shearing, but grain interactions among neighbouring grains could produce contrary rotation.

The pattern of crystallographic preferred orientation can be better understood by taking the progressive nature of lattice rotation into consideration. In simple shear (Figs 4b & 5a), the slip planes initially oriented in segment III (90–180°) and some slip planes in segment II (about 65–90°) rotate progressively towards the shear plane. This re-orientation process results in a re-alignment of slip planes parallel to the shear plane and is therefore responsible for the formation of one of the two *c*-axis girdles or maxima, normal to the shear plane, as widely reported in previous studies of fabric development (e.g. Bouchez and Pecher, 1976; Brunel, 1980; Lister and Hobbs, 1980; Bouchez and Duval, 1982; Etchecopar and Vasseur, 1987; Law, 1987, 1990; Jessell, 1988; Law *et al.*, 1990; Zhang *et al.*, 1994). This girdle or maximum will maintain its orientation throughout the deformation history as slip planes parallel to the shear plane are situated in a rotationally stable position and generally do not rotate away from it.

The other girdle or maximum reported by previous workers for simple shear is slightly asymmetrical to the first with respect to the bulk finite shortening axis. This girdle/maximum appears to be caused by the rotation of slip planes in segments I and II (Figs 4b & 5a). However, such a widely observed asymmetrical fabric pattern may only be the result of progressive lattice rotation at a particular level of shear strain. As shear strain increases, the continued rotation of the slip planes could lead to the migration of this second girdle or maxima toward the girdle/maxima normal to the shear plane. Eventually, this girdle or maximum should disappear at sufficiently high shear strain, and a single girdle/maximum normal to the shear plane would prevail. This interpretation is consistent with the fabrics reported in single-slip-dominant polycrystalline grain aggregates at high shear strains (e.g. Hudleston, 1980; Bouchez and Duval, 1982; Jessell, 1988).

In pure shear, the rotation behaviour of the slip planes that are approximately parallel to the bulk extension axis has important implications for the formation of the corresponding fabrics. The slip planes with these initial orientations still rotate sideways due to grain interactions and the deviation of the local extension axis from the bulk extension axis. As a result, the crystallographic preferred orientations of *c*-axes or slip-plane normals widely reported in the literature are maxima or small circles surrounding the shortening axis (e.g. Nicolas *et al.*, 1973; Lister and Hobbs, 1980; Wilson, 1982; Wenk and Christie, 1991; Zhang *et al.*, 1994), rather than a single maximum parallel to the shortening axis. Another reason for the development of such fabrics in single-slip polycrystals could be due to slip-plane 'lock-up' during rotation, a situation where the resolved shear stress becomes smaller than the critical resolved shear stress and the deformation of the grain stops. Therefore, the slip planes can never reach the extension axis and the 'lock-up' orientation controls the lattice preferred orientation. However, this possibility only applies to constant stress boundary conditions, as in the models of van der Veen and Whillans (1994). There will be no slip-plane 'lock-up' in the cases where finite displacements or finite-strain increments control the deformation, such as in the current model, although further slip-plane rotation or polycrystalline deformation may involve an increase of internal stresses.

CONCLUSIONS

Lattice rotation is primarily controlled by the bulk deformation field both in polycrystals and in a single crystal. For a particular deformation history, the overall directions of lattice rotation in polycrystals and a single crystal are similar, but there do exist differences in the detailed features of lattice rotation trajectories. In polycrystalline aggregates, grain interactions can significantly modify lattice rotation, with the result that the patterns of slip-plane rotation are much more complex than in single crystals. Indeed the slip planes in some grains may rotate in a direction contrary to the vorticity of the bulk deformation kinematics. This is why the slip planes oriented in a domain of about 25° to the shear plane (Fig. 5a, segment II) can rotate both towards and away from the shear plane in simple shear, and why the slip planes with initial orientations parallel to the bulk extension and shortening axes can still rotate in pure shear. In contrast, lattice rotation in the numerically simulated single crystals is entirely consistent with the rotation vorticity of the bulk deformation.

The lattice re-orientation features described here explain the patterns of crystallographic preferred orientations widely reported in the literature; that is, bimodal fabrics for simple shear and perfect–imperfect maxima for pure shear. These are particularly important when intracrystalline lattice rotation processes are considered in aggregates dominated by a one slip system.

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