Pergamon

Journal of Structural Geology, Vol. 16, No. 9, pp. 1315 to 1325, 1994

0191-8141/94 $07.00+0.00

0191-8141(93) E00019-H

The effect of grain-boundary sliding on fabric development in polycrystalline aggregates

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(*Received* 15 *February* 1993; *accepted in revised form* 12 *November* 1993)

Abstract—The influence of grain-boundary sliding on fabric development in polycrystalline aggregates has been numerically modelled using the finite difference computer code FLAC. In the model we allow the co-operation of intragranular slip and grain-boundary sliding, and consider situations involving different proportional combinations of the two mechanisms. The results show that the amount of grain-boundary sliding incorporated in polycrystalline deformation relative to intragranular slip strongly influences fabric development. When the amount is small, grain-boundary sliding significantly reduces grain interaction but still ensures the dominance of intragranular deformation. Correspondingly, crystallographic preferred orientations associated with well-evolved microstructures, are even better developed in comparison with those obtained without grain-boundary sliding. When the amount of grain-boundary sliding is increased, however, polycrystalline fabric development is effectively weakened. In the extreme situation where grain-boundary sliding dominates, a total absence of crystallographic preferred orientation and microstructures results. The introduction of grain-boundary sliding weakens the dependence of intragranular deformation upon the lattice orientation of grains. With the increase of grain-boundary sliding, intragranular strains become smaller and more homogeneous. The distribution of strain is dominantly determined by the distribution of grain-boundary sliding.

INTRODUCTION

GRAIN-BOUNDARY sliding (GBS) is one of the most important strain accommodation mechanisms operating in deforming polycrystalline aggregates, particularly at high temperatures and low strain rates (Langdon & Vastava 1982, Ranalli 1987). Results of metallurgical studies (e.g. Ashby & Verrall 1973, Shariat *et al.* 1982, Langdon & Vastava 1982, Tvergaard 1988) even show that GBS alone can accommodate a major part of the deformation in metals. However, the influence of GBS on fabric development in polycrystals has been very unclear, except that it is generally assumed that GBS causes the weakening or absence of crystallographic preferred orientation (e.g. Law 1990). Also, very little is known about the true nature of GBS in minerals and rocks. A great number of the previous theoretical studies of fabric development have been based on the plastic deformation scheme involving intragranular slip alone (e.g. Etchecopar 1977, Lister *et al.* 1978, Harren & Asaro 1989, Tharp 1989, Wenk *et al.* 1989, Zhang *et al.* 1994) or with recrystallization (e.g. Jessell 1988a,b, Jessell & Lister 1990). The results of these models may lose predicative ability in deformational environments involving GBS.

In this paper, therefore, we aim to explore the role of GBS in polycrystalline fabric development, using the finite difference computer code FLAC (Cundall & Board 1988, Board 1989, Itasca Consulting Group 1991). Three different deformation-mechanism combinations will be examined here, varying from a small amount of GBS incorporated with intragranular slip to the dominance of GBS. The results will be compared with those achieved in a previous model not involving GBS (Zhang *et al.* 1994).

MODEL OUTLINE

FLAC provides an algorithm for frictional and cohesive interfaces to exist between two or more portions of continuum grids (Board 1989, Itasca Consulting Group 1991). These interfaces can be used to simulate the effects of joints, faults and other geological discontinuities, upon which sliding and separation are allowed. We use the FLAC interface logic to model grain boundaries. Therefore, the theoretical basis of the current

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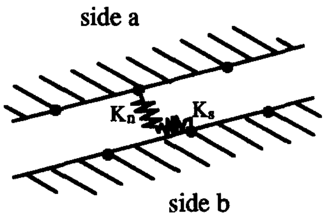

Fig. 1. Sketch of a grain boundary which is simulated as an interface connected by shear stiffness (K_s) and normal stiffness (K_n).

model is essentially an advancement of that described in Zhang *et al.* (1993, 1994) from a GBS-free case to the incorporation of GBS. More specifically, a polycrystalline domain is simulated here as a collection of grains with one slip system, separated by grain boundaries which are allowed to slide; the operation of slip planes is still assumed to follow the critical resolved shear stress law (Zhang *et al.* 1993, 1994).

Each grain boundary in the model is approximated as a series of normal springs and shear springs between two opposing planes which initially contact each other (Fig. 1), and is defined through the specification of grid nodes which may interact (see Board 1989 and Itasca Consulting Group 1991 for a detailed description). This contact logic in FLAC for each side of a grain boundary (interface) is similar to that employed in the distinct method. The material properties needed for a grain boundary are normal stiffness (K_n), shear stiffness (K_s), cohesion (C_i), tensile strength (T) and friction angle (ϕ_i); ϕ_i has been taken to be zero to achieve the best sliding effect. The normal and shear stiffnesses determine the normal and shear displacements of the opposing planes, respectively, and therefore control the normal force (F_n) and shear force (F_s) in the normal and tangential directions on the boundaries. Sliding along a grain boundary is assessed according to the following criterion:

$$|F_s| \geq F_{s\,max} = C_i L + F_n \tan \phi_i$$
$$= C_i L \qquad (\text{for } \phi_i = 0),$$

where $F_{s\,max}$ is the maximum shear force allowed on grain boundaries and L is the effective contact length of a grain boundary. If the above criterion is satisfied (i.e. $|F_s| \geq F_{s\,max}$), grain-boundary sliding then occurs and F_s is set equal to $F_{s\,max}$. Under this formulation, using smaller values of shear stiffness and grain boundary cohesion will make GBS easier, and the adoption of larger normal stiffness can prevent the overlap of grain boundaries. The tensile strength is also checked for each step of the calculation for grain boundaries. If the normal force (F_n) is tensile and exceeds the strength, separation occurs. This causes the formation of vacancies.

Because of the nature of GBS, the swapping of grain neighbours could occur during deformation. Therefore, the boundaries of grains which have a potential to come into contact must be specified as interacting grain boundaries, although they initially may not be in contact. By doing this it can be ensured that a pair of grains will start to interact when they come into contact. Otherwise they will not recognize each other and overlaps then take place.

In the current model, intragranular slip and GBS are two competing deformation mechanisms. They both can possibly become the dominant mechanism in a deforming polycrystal, depending on the material properties and boundary conditions adopted in the simulations. Different deformation-mechanism combinations can be simulated by using different model specifications. It should be pointed out that, as in the previous model of Zhang *et al.* (1994), a small amount of elastic deformation of the matrix material which is assumed to exist between slip planes is also involved here.

All the numerical experiments to be described in the following sections started from the polycrystalline specimen illustrated in Fig. 2. It must be mentioned that this starting configuration, including mesh details and slip-plane initialization, is identical to that used in Zhang *et al.* (1994). We chose this design simply for the convenience of comparing the results between the models with and without GBS. Furthermore, the previous designation of grain (i,j) is also used here, identifying the grain at grain row i and column j in the specimen (see Fig. 2b). The indices i and j are counted from the bottom-left corner.

THE MODEL INVOLVING A SMALL AMOUNT OF GBS

The material properties used in the present model (Table 1) are identical to those adopted in Zhang *et al.* (1994) except that the parameters for grain boundaries are added. In order to avoid grain-boundary overlaps and to make sliding possible, a much larger normal stiffness (1.5×10^{12} GPa m^{-1}) than shear stiffness (2.2×10^6 GPa m^{-1}) is used here. Grain-boundary cohesion

Table 1. Material properties

Density	2647 kg m^{-3}	(Clark 1966)
Shear modulus	4.23×10^{10} Pa	(Clark 1966)
Bulk modulus	4.64×10^{10} Pa	(Clark 1966)
Matrix cohesion	2×10^{10} Pa	
Slip-plane cohesion	2×10^5 Pa	
Matrix and slip-plane frictions	0°	
Normal stiffness (K_n)	1.5×10^{12} GPa m^{-1}	
Shear stiffness (K_s)	2.2×10^6 GPa m^{-1}	
Grain-boundary cohesion	2×10^5 Pa	
Boundary tension strength	4×10^5 Pa	
Grain boundary friction	0°	

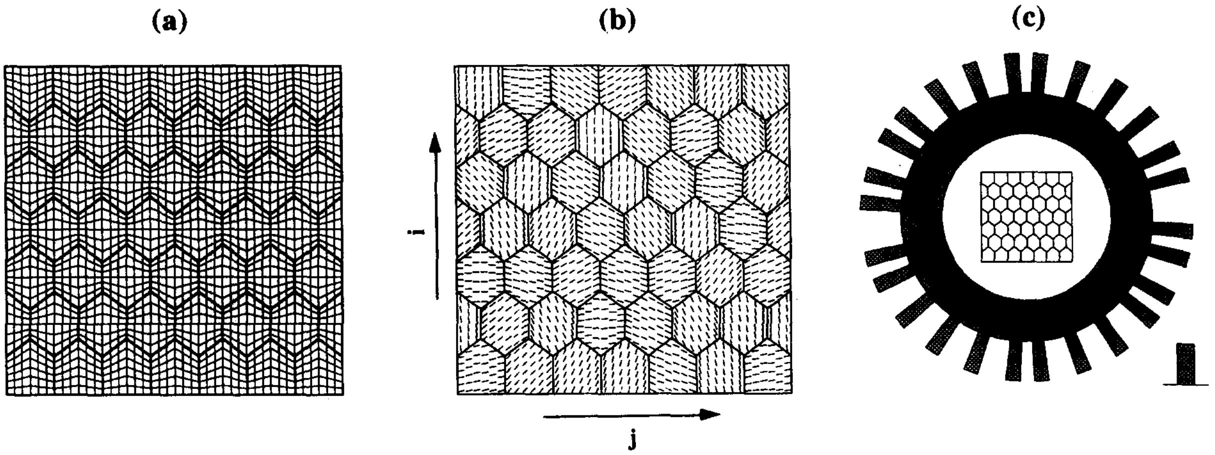

Fig. 2. Specification of the numerical polycrystalline specimen. (a) The finite difference mesh. (b) Initial slip-plane traces in the specimen; arrows indicate the sequences of increasing grain row numbers (*i*) and column numbers (*j*). (c) The initial orientation distribution of slip-plane normals with respect to the specimen orientation.

and friction are chosen as 2×10^5 Pa and 0°, respectively, equal to slip-plane cohesion (critical resolved shear stress) and friction, respectively. This specification theoretically allows both GBS and intragranular slip to occur with equal ease; however, as will be revealed later by the results, the amount of GBS in this situation is small. A tensile strength of 4×10^5 Pa is also adopted for grain boundaries.

Three deformation histories, axial shortening, pure shearing and simple shearing, are simulated here. The resulting preferred orientations of slip-plane normals are presented in Fig. 3 (left column). We can see that, in comparison with the results of Zhang *et al.* (1994) (Fig. 3, right column), the patterns of preferred orientations are relatively strengthened. For axial shortening and pure shearing, the two-maxima pattern of preferred orientations are more strongly developed symmetrically about the overall shortening axis; the average strengths of the two maxima are 7.23 and 9.82%, respectively, compared to 6.8 and 8.0% for the model without GBS. Besides, the included angles between the two maxima are generally larger than those for the corresponding GBS-free model. For simple shearing, the two-maxima configuration is also more marked, with one maximum normal to the shearing plane and the other symmetrical to the first about the maximum finite shortening direction.

The distributions of strain ellipse axes are shown in Figs. 4(a),(b) & (c). It is noted that the polycrystalline aggregates simulated here have experienced significant intragranular deformation which is accommodated by intragranular slip. The grains with an initial equiaxed geometry have been mostly deformed into non-equiaxed shapes. The distribution of deformation is clearly inhomogeneous. However, intragranular strain inhomogeneity is much less severe than in the previous model with GBS (see fig. 10 in Zhang *et al.* 1994). This is because grain boundaries are no longer fully adhesive and some sliding between neighbouring grains is possible. The GBS reduces neighbouring grain interaction and helps to solve the compatibility problems. As a result, the variation of strain near grain boundaries and intragranular strain inhomogeneity are reduced. The distribution of inter-grain inhomogeneous strains is dominantly related to the starting lattice orientation. The grains showing high strain are mostly those with deformation-favourable lattice orientations (see Zhang *et al.* 1994), similar to the situation in the GBS-free models. However, this inter-grain strain inhomogeneity is somewhat affected by GBS. In the areas of the specimens with larger GBS (e.g. the areas near the free boundaries of the specimen in the axial shortening case), grains overall show smaller strains.

Intragranular microstructures (Figs. 4d, e & f) are also well developed here, including subgrains, kink–subgrain structures (see Zhang *et al.* 1994), undulatory lattice orientations and flattened grains. These are generally similar to those developed in the model without GBS (Zhang *et al.* 1994). However, one difference is that those subgrains and local shear zones that are developed in the model without GBS and are closely related to grain interactions have been almost eliminated by the introduction of GBS. Some examples are grains (2,2) and (6,6) in the axial shortening and pure shearing cases and grains (3,6) and (4,6) in the simple shearing case (see Figs. 4d, e & f, with reference to Fig. 2b); these grains do not show the formation of subgrains (intra-grain lattice misorientation) whereas their counterparts in the previous model developed clear subgrains (Zhang *et al.* 1994, fig. 5).

It is evident from Fig. 4 that GBS has occurred extensively in the deformed polycrystalline specimens, but the amount of GBS is generally small. It is characterized by the small local shifting of neighbouring grains along boundaries and does not create any large grain migration. Even after a large bulk deformation, each of the grains remains in contact with the same neighbours it started out with. This further indicates that GBS in the model described here only accommodates a small amount of the bulk deformation. The other competing strain-accommodation mechanism, intragranular slip, still dominates, as shown by the development of large

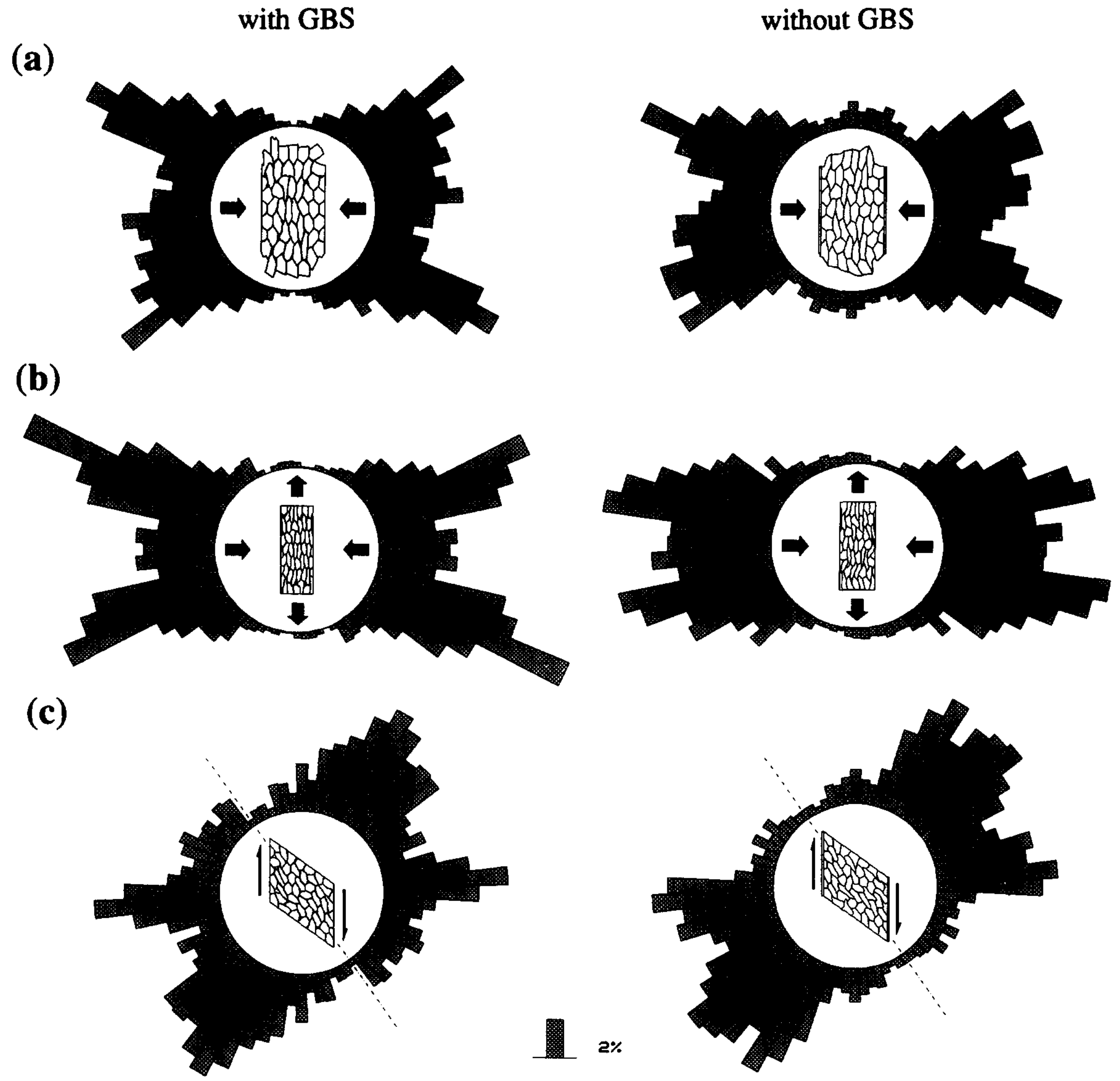

Fig. 3. Final orientation distribution of slip-plane normals with respect to the orientation of the deformed specimens: (a) 29% bulk axial shortening; (b) pure shearing, 38% bulk shortening; (c) simple shearing, $\gamma = 0.72$. Left: the model with GBS; right: the model without GBS (after Zhang *et al.* 1994).

intragranular deformation. There are three possible reasons for the limited contribution of GBS, which theoretically should operate with the same ease as intragranular slip according to the model specifications. (1) The geometrical alignment of grains with respect to the bulk shortening direction is not favourable for boundary sliding in axial shortening and pure shearing histories (see Fig. 5a). When grains try to slide along their boundaries, they block each other, and severe compression arises across the boundaries normal to the bulk shortening direction. Switching the bulk shortening axis is shown to facilitate GBS (Fig. 5b, and see below). (2) The deformation boundary conditions do not allow a large amount of GBS to occur in specimens consisting of closely packed hexagonal equiaxed grains, without the involvement of other process such as intragranular deformation or diffusion, particularly in the case of simple shearing. (3) If grain boundaries are treated as extra slip planes, volumetrically they are quite insignificant.

An accompanying consequence of GBS is the formation of vacancies between neighbouring grains in deforming polycrystalline specimens (Fig. 4). The most favourable locations for vacancy formation seem to be original grain triple junctions where tensile stress can be easily caused by GBS. The overall volume of vacancies generally increases with increasing bulk deformation, and also more vacancies form near the free boundaries or extension boundaries of specimens (according to the bulk deformation frame). The persistent formation of vacancies has been shown to be possible in real materials (Ree 1988). However, in rock involving active fluids and transportation of matter, the situation should be quite different. Any nucleated vacancies could be soon filled with material transferred by the fluids.

THE MODEL WITH ENHANCED GBS

It has been indicated that the mutual blocking effect of grains in the models just described, caused by the combination of grain-boundary alignment and the bulk deformation frame, is one factor leading to limited GBS. To

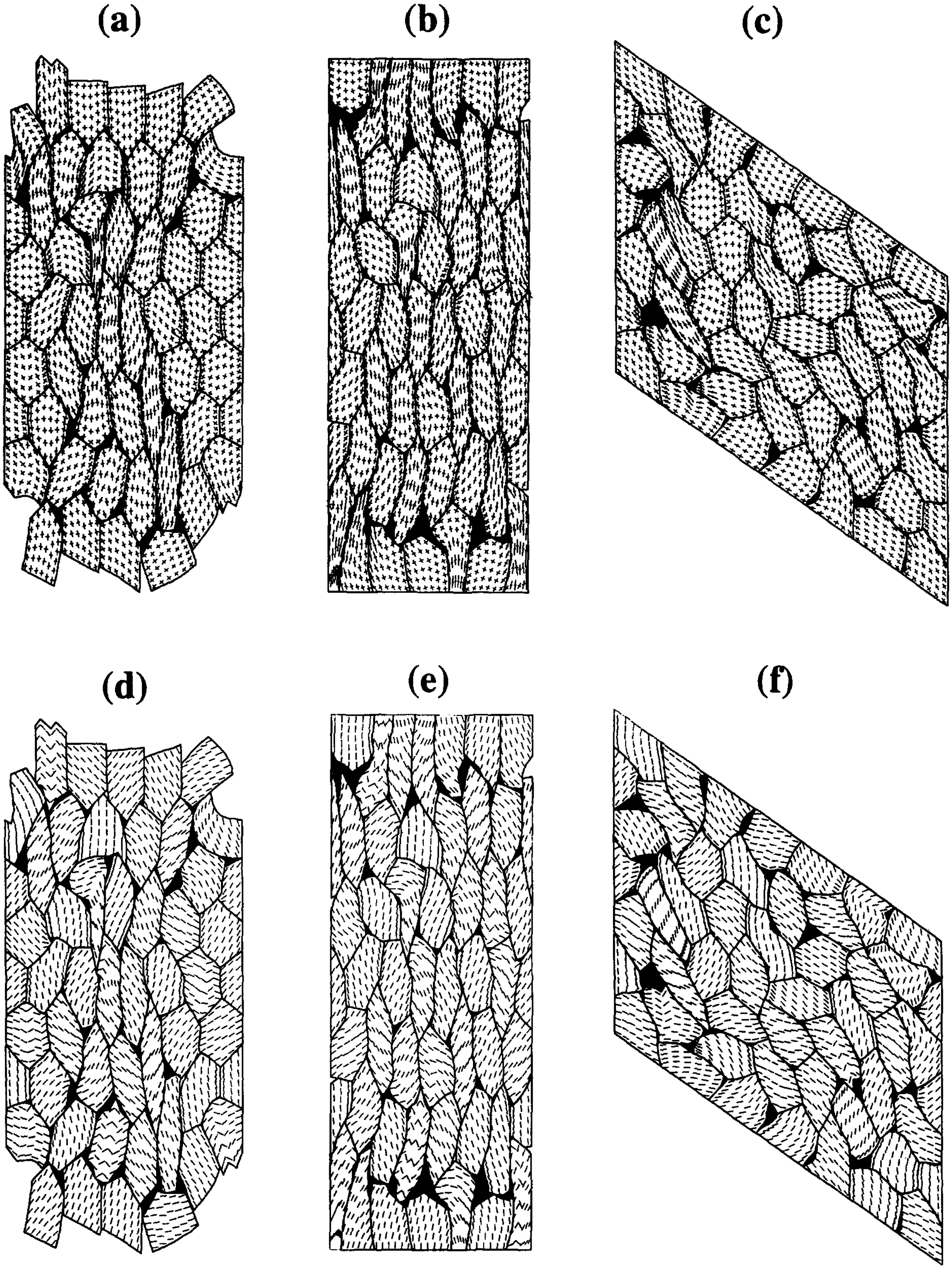

Fig. 4. Strain ellipse axis distribution (a, b & c) and final slip-plane trace distribution (d, e & f) in deformed specimens for the model involving a small amount of GBS. Left: axial shortening; middle: pure shearing; right: simple shearing (see Fig. 3 for corresponding bulk strains).

lessen this effect and enhance GBS, we have repeated the simulation of axial shortening and pure shearing with the same specimen (Fig. 2) and material properties (Table 1) but with the bulk shortening axes switched (Fig. 5).

After the same bulk finite strains, the results show that GBS has been intensified both in the axial shortening and pure shearing deformation histories (Fig. 6). GBS is no longer limited to creating only small local shiftings of neighbouring grains; its operation now results in large

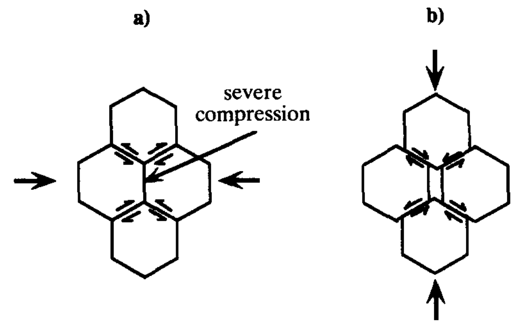

Fig. 5. The patterns of grain-boundary sliding for two situations involving different bulk shortening directions. (a) The horizontal bulk shortening axis: harder GBS. (b) The vertical bulk shortening axis: easier GBS.

grain migrations in the deformed specimens. Some grains eventually switch neighbours. For example, grains D1 and D3 are not initially neighbours of grains B1 and B3, respectively (Fig. 6a). But these two pairs of grains have become neighbours by the end of the deformation (Figs. 6b & c). GBS has caused the migration of these grains past a number of intermediate grains (grains C1, C2, C3 and C4). The formation of inter-grain vacancies is also intensified as a result of enhanced GBS, demonstrated by a visible increase of vacancy volume (compare Fig. 7a with Figs. 4a & b). The favoured locations for vacancy formation are again grain triple junctions, and also grain boundaries making low angles to the bulk shortening axis.

Corresponding to the increase of GBS, the intragranular strains (Fig. 7a), although still significant, are generally smaller than those for the models with a small amount of GBS (see Figs. 4a & b). More grains show small deformation and weak flattening, including even some grains with deformation-favourable slip-plane orientations. Higher strains mostly occur in grains where GBS is relatively weak and also where slip-plane orientation is relatively favoured over intragranular slip, while small strain is the general feature of grains involving larger GBS and vacancy formation. Strains are still characterized by being inhomogeneous. Within single grains, however, they tend to be more uniform in magnitude. Therefore, as GBS is enhanced, the partitioning of bulk deformation between intragranular slip and GBS changes, and the role of intragranular slip is considerably weakened.

The fabric also varies with the strengthening of GBS. Microstructures such as kink–subgrain structures, as revealed by final slip-plane traces (Fig. 7b), are more poorly developed than in the limited-GBS model (see Figs. 4d & e). The formation of undulatory lattice orientations seems to be more favoured. These features are particularly evident in those grains which experienced large GBS. Lattice preferred orientations (Fig. 7c) are also much less well developed than in the limited-GBS model (Fig. 3, left column) and the non-GBS model (Fig. 3, right column). The distributions of slip-plane normals only exhibit two quite obscure maxima roughly symmetrical about the bulk shortening axis, especially in the axial shortening case. From the results described here, we can conclude that intensified GBS weakens fabric development in polycrystalline aggregates.

SIMULATION OF DOMINANT GBS

The dominance of GBS as a strain-accommodation mechanism requires that GBS operates much more easily than intragranular deformation. We have simulated this situation by changing some material properties so as to achieve an easier sliding along grain boundaries and a high rigidity for the intragranular material. More specifically, easy GBS is guaranteed by using smaller shear stiffness and grain-boundary cohesion (6.6×10^3 GPa m^{-1} and 2×10^2 Pa, respectively), and on the other hand, larger shear modulus (4.23×10^{11} Pa), bulk modulus (4.64×10^{11} Pa), and matrix material and slip-plane cohesions (both 4×10^{11} Pa) ensure that intragranular deformation is very difficult. The simulation is only performed for the pure shearing history.

The results show that the predominance of GBS was indeed achieved in this case (Fig. 8a, and also Fig. 6a). Significant GBS has led to the extensive rigid migration

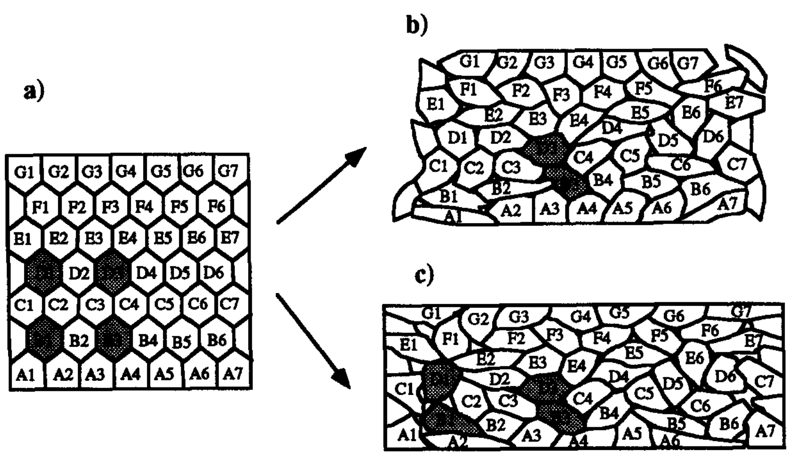

Fig. 6. Variation in position of labelled grains for the model with enhanced GBS. (a) Starting positions; (b) & (c) end positions for axial shortening (29% bulk shortening) and pure shearing (39% bulk shortening), respectively.

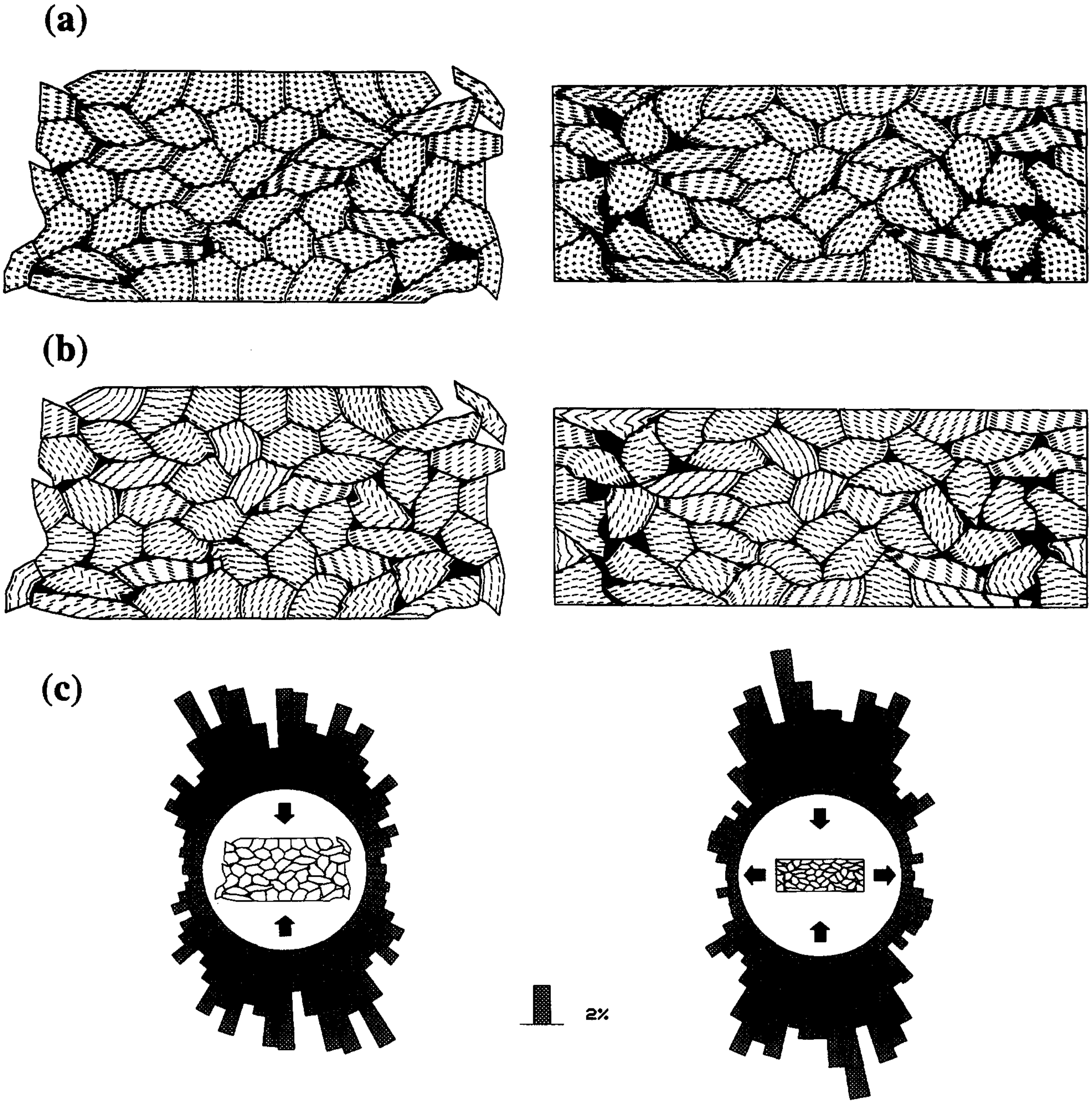

Fig. 7. (a) Strain ellipse axes, (b) final slip-plane traces and (c) the final orientation distributions of slip-plane normals for the model with enhanced GBS. Left, axial shortening; right, pure shearing; (see Fig. 6 for corresponding bulk strains).

of grains and vacancy formation in the specimen subjected to a 36% bulk shortening, particularly in the areas near the borders of the specimen. The whole specimen seems to have behaved like a group of loaded but undeformable grains, with each sliding toward any possible locations according to the local grain configuration and the bulk deformation condition. Some grains (such as grains A2, C2, D2 and F2 in Fig. 8a) have migrated a considerable distance to become adjacent to totally new neighbouring grains. This phenomenon could be compared with that of steel balls in a box under loading.

The deformation configuration (Fig. 8b) generated from a dominant GBS is clearly different to those obtained previously (cf. Figs. 4b and 7b). The imposed bulk deformation is accommodated almost entirely by GBS. All the grains remain roughly in their original equiaxed shapes and exhibit very small, nearly homogeneous intragranular strains. The distribution of this small intragranular deformation is totally independent of the initial lattice orientation of the grains, but is somewhat dependent upon the distribution of GBS. Slightly higher strains occur in those grains subjected to small GBS (e.g. grains in the central area of the specimen, Fig. 8a). Relatively higher strains are also observed in the grains near the extension boundaries of the specimen. This is purely because of the constraint of the boundary there, which does not allow large boundary sliding.

Fabrics developed with dominant GBS are also obviously different from those achieved in the previous simulations. Final slip-plane traces (Fig. 8c) display very simple intragranular microstructures. Subgrains and

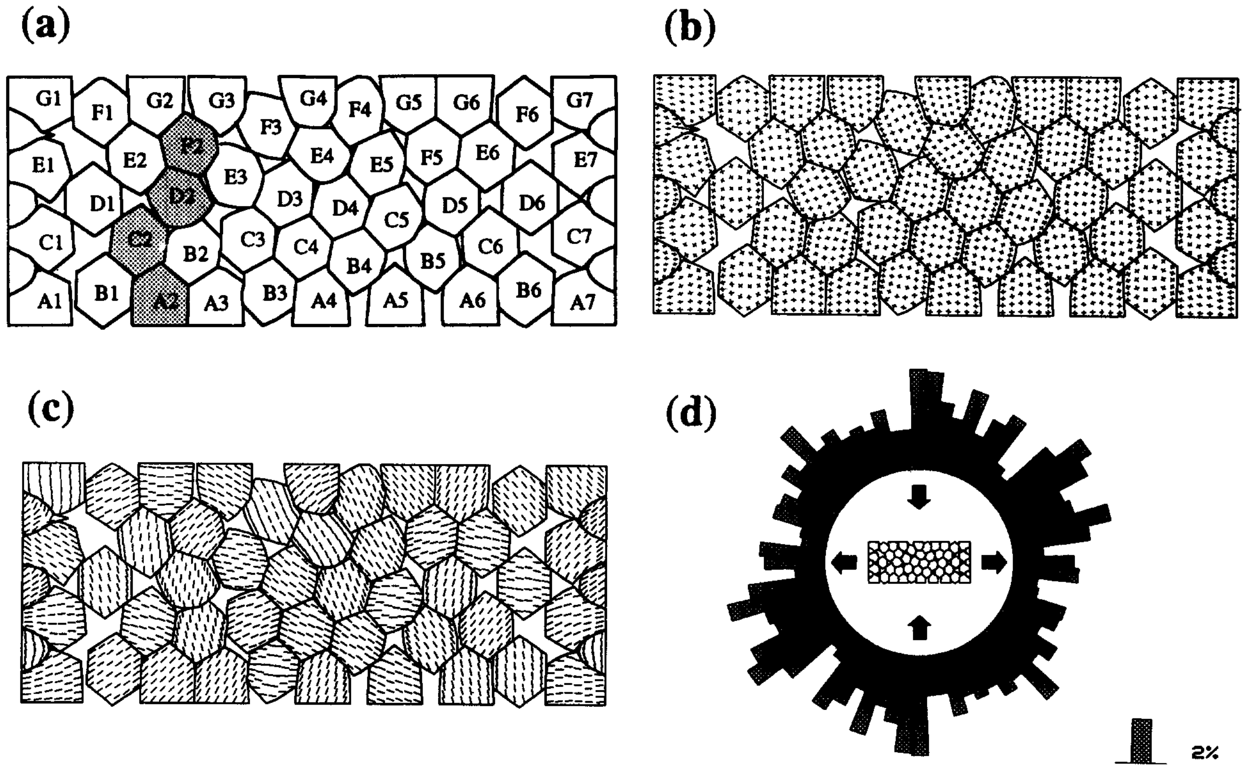

Fig. 8. The results of a model with dominant GBS (pure shearing, 36% bulk shortening). (a) grain positions; (b) strain ellipse axes; (c) slip-plane traces; and (d) the orientation distribution of slip-plane normals.

kink–subgrain structures, which are generally well developed in the previous simulations are totally absent here. Corresponding to the lack of microstructural patterns, the final orientation distribution of slip plane normals (Fig. 8d) also does not show any preferred orientations. A number of small peaks may be recognizable, but they are situated over the whole range of orientations. This basically uniform pattern contrasts sharply with the strong crystallographic preferred orientation development in the situation where minor GBS operates (see Fig. 3).

DISCUSSION

By introducing different amounts of GBS into the deformation of polycrystalline aggregates, this study has produced a varying sequence of crystallographic fabric patterns. The development of microstructures and lattice preferred orientations weakens with the strengthening of GBS, and is totally absent where GBS dominates. This is certainly consistent with the general assumption about the role of GBS made by structural geologists (e.g. Boullier & Gueguen 1975, Etheridge & Vernon 1981, Wenk 1985, Law 1990). However, what is unexpected is that stronger crystallographic preferred orientations are developed in the model involving a small amount of GBS than in the model without any GBS. We believe that this outcome is very important because it reveals the other aspect of GBS's influence on rock fabric development.

To understand why a small amount of GBS facilitates the development of crystallographic preferred orientation, we need to examine the process of GBS as well as its effects on intragranular deformation. As stated previously, GBS in the limited-GBS model only causes small local shiftings between neighbouring grains (Fig. 4), and does not give rise to large grain migration. In terms of deformation partitioning, this GBS is only capable of taking up a very small part of the imposed bulk deformation, and the major part is still accommodated by intragranular slip. Correspondingly, intragranular deformation, which is critical to lattice preferred orientation development, is still very strong in most grains. This is obviously similar to the model with no GBS involvement. However, an important change created by the introduction of a small amount of GBS is that grain interaction is significantly reduced because of the possibility of small adjustments between neighbouring grains. Strain compatibility is no longer such a severe problem between neighbouring grains, and each grain can deform relatively independently of neighbouring grains according to its own lattice orientation. If we imagine the extreme, GBS would seem to be nonexistent but every grain would deform separately from the others through intragranular slip. As such, both the intragranular deformation of single grains and the fabric of the whole specimen in this reduced grain interaction case should be better developed than in the non-GBS model (Zhang *et al.* 1994), in which grain interaction is always strong and some form of strain compatibility between neighbouring grains must always be obtained.

GBS plays a different role in the situation involving significant GBS (Fig. 7) or dominant GBS (Fig. 8).

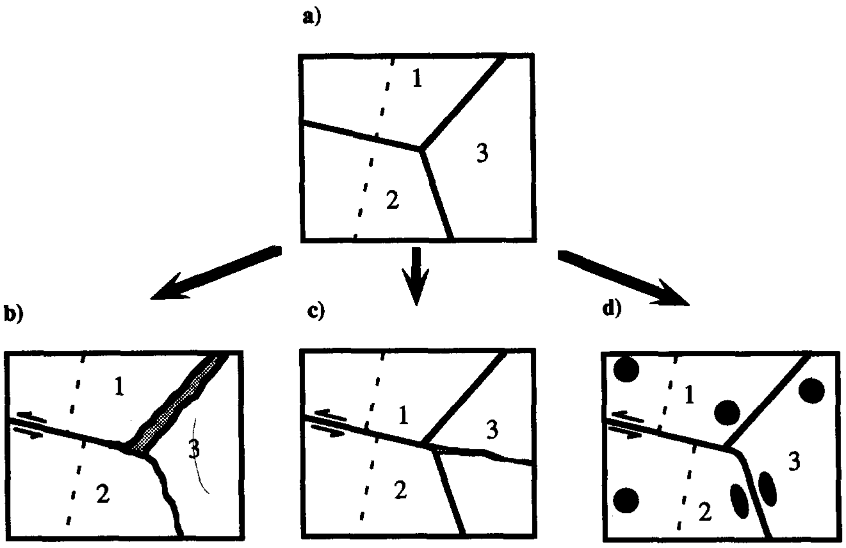

Fig. 9. Examples of the mechanisms which facilitate grain-boundary sliding. (a) Starting pattern; (b) diffusional flow; (c) micro-fracturing; and (d) intragranular plastic deformation.

Certainly, GBS still reduces grain interactions, but it also accommodates a significant or major part of the bulk deformation so that the intragranular deformation is small. As a result, fabric development must be poor.

The current model suggests that intragranular deformation (slip) prevails over GBS when both have similar operating thresholds and when there are no material transfer or brittle processes involved. Unlike diffusion-accommodated GBS, which is generally associated with superplastic flow in metals (e.g. Gifkins 1976, Langdon & Vastava 1982, Shariat *et al.* 1982), the GBS simulated here is characterized by fully mechanic offsets along grain boundaries. This type of GBS is not a self-sufficient mechanism to create large macroscopic strains. In the process of CBS, grains will tend to shift with respect to each other and vacancies must be continually formed. This is hardly possible in a tightly confined mosaic package of hexagonal equiaxed grains with an exclusive operation of GBS, since there is no space to accommodate the formation of vacancies and there are no other mechanisms to remove the mutual blockings of neighbouring grains. Significant intragranular deformation therefore must be involved for the full accommodation of the imposed bulk strain.

It might be argued that the relationship between GBS and intragranular deformation, suggested by this model, is a specific feature of the two-dimensionality of the model. The involvement of a third dimension will add one extra degree of freedom for the accommodation of strain and GBS. This could mean that GBS will become easier than in the two-dimensional case. However, the dominance of GBS over intragranular deformation seems to be still unlikely for a densely-packed three-dimensional polycrystal if the active deformation mechanisms only include GBS and dislocation glide. Ree (1994) has analysed GBS in experimentally deformed octachloropropane samples. His results show that the strain accommodated by GBS is generally small compared to intragranular strain. This is consistent with the prediction of the current model.

The dominance of GBS is successfully simulated in an extreme model (see Fig. 8). However, we must point out that this scheme of achieving large GBS through increasing grain rigidity is very unlikely for geological materials owing to the involvement of unrealistic material properties in the model. For the dominant involvement of GBS in realistic materials, there must be extra mechanisms to accommodate GBS. The simultaneous or alternative co-operation of a few deformation mechanisms is often possible in the case of real deformation. For example, at least three deformation mechanisms (intragranular slip, mechanical GBS and brittle fracturing) can be recognized in experimentally deformed ZnS (see TEM micrographs in Davidson 1989). Diffusional mass transfer has also been proved to be an efficient GBS accommodation mechanism (e.g. Shariat *et al.* 1982, Ree 1994). The activity of GBS could then be greatly intensified and become significant through the help of these co-existent mechanisms. This is because the mutual blocking of neighbouring grains during GBS can always be easily overcome by other mechanisms such as diffusional flow or local melting (Fig. 9b), micro-fracturing (Fig. 9c) (also see Langdon & Vastava 1982) and intragranular plastic deformation (Fig. 9d), so that GBS can proceed mechanically and geometrically. With respect to the development of crystallographic preferred orientations, processes like diffusional flow, local melting and micro-fracturing may not make much contribution. Intragranular plastic deformation, which is the case in the current models, does however greatly facilitate fabric development while accommodating GBS.

It has been shown that inter-grain vacancies form as a result of GBS. This is in agreement with the experimental observations by Ree (1988, 1994). However, we need to mention that the formation of vacancies in the pure shearing and simple shearing deformations actually involves a slight decrease in the areas of single grains. The boundary conditions of both deformations require the maintenance of area of the specimen throughout deformation, while the formation of vacancies requires an increase of area. This means that either a decrease in the areas of single grains or grain overlaps must occur. Because the current model does not allow grain overlap, a forced decrease of grain area is numerically incorporated, particularly in the central part of the specimen, which is most distant from the extension-dominated borders. Mechanically, this area decrease is achieved by elastic volume contraction allowed by the currently-adopted Poisson's ratio of 0.14. This phenomenon may be viewed as coinciding with the effect of deformation in the third dimension, which could be one of the reasons for the grain size decrease in deformed real materials (Ree 1994).

The effect of grain boundaries or the influence of grain mesh size should be minimal in the model presented here. This is probably justified for three main reasons. First, the results of the previous GBS-free model (Zhang *et al.* 1994) indicate that the effect of grain mesh size is small and does not result in a change of fabric pattern. Second, grain interactions at their boundaries is weaker in the present GBS model than in the model without GBS because of the easier achievement of strain compatibility. This means a reduced strain variation near grain boundaries, and hence a reduced grain boundary effect. Third, the deformation feature of grain boundaries is essentially determined by the bulk deformation frame. It has been shown that grain boundaries become dominantly oriented parallel to the bulk extension (elongation) direction (Zhang *et al.* 1994). A grain boundary will be subjected to compression–sliding if normal to or at a high angle to the bulk shortening axis, but subjected to extension–sliding if parallel to or at a low angle to the shortening axis. The normal and shear stress components on grain boundaries which control the above situations are also dependent upon the local stress tensors, which dominantly reflect the bulk deformation frame. This suggests that if there is a boundary effect, it should be consistent with the main stream of the polycrystalline deformation under the specified bulk deformation condition.

CONCLUSIONS

(1) The amount of GBS involved in polycrystalline deformation influences fabric development in polycrystalline aggregates. When only a small amount of GBS is involved, the preferred orientations of slip-plane normals are even better developed than in the situation without any GBS, showing stronger two-maxima patterns. Intragranular microstructures are also well developed.

(2) This enhanced fabric development is thought to result when the introduction of a small amount of GBS largely decreases grain interaction but does not accommodate much of the imposed bulk strain. The intragranular deformation of grains is still dominant and is relatively independent of strain in neighbouring grains.

(3) Enhancing GBS weakens fabric development. In the extreme, the dominance of GBS results in the absence of preferred orientations and intragranular microstructures. Intragranular deformation is very limited.

(4) The introduction of GBS weakens the dependence of intragranular deformation upon the lattice orientation of grains. With the increase of GBS, intragranular strains become smaller and more homogeneous. The distribution of strain is dominantly determined by the distribution of GBS. Grains involving larger GBS show smaller strains.

Acknowledgements—Peter Hudleston and two anonymous reviewers are thanked for their critical and constructive comments on the initial version of the manuscript. A. Ord, C. J. L. Wilson and W. D. Means are also thanked for their important help in the various stages of the work.

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