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Microstructural shear criteria associated with grain-boundary sliding during ductile deformation

M. R. DRURY

Instituut voor Aardwetenschappen, Rijksuniversiteit Utrecht, Budapestlaan 4, 3584 CD Utrecht, The Netherlands

and

F. J. HUMPHREYS

Department of Metallurgy and Material Science, Imperial College, London SW7 2BP, U.K.

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Abstract—Experimental studies on rock analogues are described which establish that certain microstructures (diamond grain structures, tabular grain structures and asymmetric grain-boundary bulges) can be used to determine (i) if deformation was coaxial or non-coaxial and (ii) the sense of shear in zones of non-coaxial deformation. Mechanisms for the development of the structures are described which involve the linked operation of grain-boundary sliding and migration.

INTRODUCTION

CRITERIA for distinguishing coaxial from non-coaxial deformational histories and the sense of shear in zones of non-coaxial strain are of current interest to geologists (White *et al.* 1980, Simpson & Schmid 1983, Lister & Snoke 1984).

In this contribution we describe results from experimental studies on deformation of some rock analogues, and consider the development of some types of microstructure that can be used as shear criteria in mylonites and other tectonites. These microstructures are defined by preferred grain-boundary orientations and particular grain shapes. They include diamond grain structures, tabular grain structures and particular types of grain-boundary bulges.

The materials used in this study were a solid solution alloy of the f.c.c. metal aluminium containing 5% magnesium and sodium nitrate ($NaNO_3$) which is isostructural with calcite (Tungatt & Humphreys 1981a, 1984). The experiments were run at temperatures of $T = 0.6$–$0.9\ T_m$ (where T_m is the absolute melting temperature) and $\dot{\varepsilon} = 10^{-2}$–$10^{-6}\ s^{-1}$. More detailed descriptions of the conditions are given elsewhere (Tungatt & Humphreys 1981a, 1984, Drury & Humphreys 1986). Under these conditions the rock analogues deformed predominantly by dislocation-creep mechanisms (Poirier 1985) with the occurrence of subsidiary grain-boundary sliding. In Al5%Mg the grain-boundary sliding accounted for 10–15% of the imposed deformation (Drury & Humphreys 1986).

The methods used to calculate the amount of strain accommodated by sliding are described elsewhere (Drury & Humphreys 1986). It should be noted that these methods do not take account of any stretch of the grain boundary, such a stretch will alter the magnitude of the displacement of a marker line across the boundary. For the equiaxed polygonal microstructures described here, this effect is likely to be small for a low-strain deformation.

The microstructural shear criteria described here are potentially useful in rocks that have deformed by the same mechanisms, for example quartz, olivine and calcite mylonites and other tectonites.

It is important to establish from experimental studies, first, the reliability of a particular microstructural shear criterion and second, the stability of the microstructure with respect to resetting by small strains at the end of the deformational history.

GEOMETRY OF GRAIN-BOUNDARY BULGES AS SHEAR CRITERIA

Microstructures

Irregular grain boundaries are commonly developed during high-temperature ductile deformation due to the occurrence of non-uniform grain-boundary migration.

In aluminium alloys containing 2–5% Mg in solid solution, the geometry of the bulges depends upon the orientation of the grain boundary with respect to the stress axis (Fig. 1a). In uniaxial compression tests bulges along boundaries subparallel or subperpendicular to the stress axis have a symmetrical 'zig-zag' geometry. Bulges along inclined boundaries are asymmetric with the sense of asymmetry the same as the local sense of sliding along the grain boundary. The shear sense along boundaries can be determined in this material from displacements of stringers of second-phase particles across the boundaries.

This structure develops after strains of $\varepsilon = 0.05$–0.1.

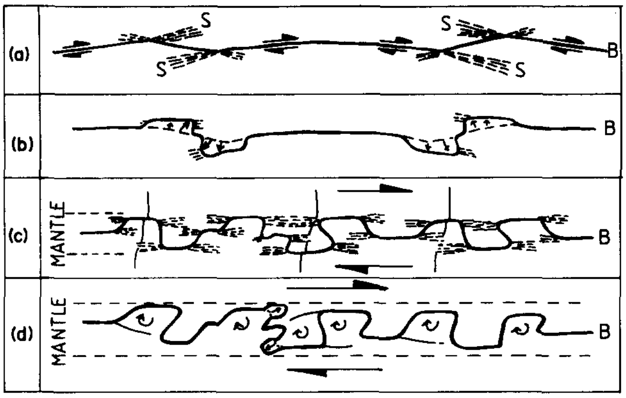


Fig. 2. Mechanism of formation of asymmetric bulges. (a) Deformation at the grain boundary B is accommodated by sliding and by non-uniform intragranular strain S adjacent to irregularities. (b) Local grain-boundary migration consumes zones of high defect density S, producing asymmetric bulges. The initial asymmetry depends upon the prior geometry of the irregularity. (c) Further deformation along the irregular boundary is accommodated by sliding along short segments and shear in the grain mantle. (d) Shear in the mantle modifies the shape of the bulges, amplifying the asymmetry of bulges with the same sense of shear as the sliding. Bulges with the opposite sense of asymmetry will be sheared to a more symmetrical geometry.

At high strains ($\varepsilon > 1.0$) the grains are highly flattened and most grain boundaries are subperpendicular to the stress axis. The grain-boundary bulges at this stage are then predominantly of the 'zig-zag' type.

Mechanisms

A model for the development of the grain-boundary bulges is shown in Fig. 2. In Al5%Mg, grain-boundary sliding accommodates 10–15% of the imposed deformation (Drury & Humphreys 1986). At low strains sliding is easy along most sections of the grain boundary. Adjacent to irregularities and at triple points some non-uniform intragranular deformation must occur to accommodate the sliding displacements. This non-uniform strain will provide the driving force for local grain-boundary migration. The geometry of the local migration will reflect the geometry of the intragranular strain which depends upon the geometry of the initial irregularity and the sense of shear across the boundary (Fig. 2a & b). Once grain-boundary bulges are developed they will become asymmetric as they are sheared in the mantle adjacent to the grain boundary (Fig. 2c & d).

This model accounts for the relationship between bulge geometry and sense of sliding along boundaries and is consistent with the small strains required to develop the structure.

So far tests have only been conducted in uniaxial compression. Grain-boundary bulge geometries are predicted for simple shear in Fig. 3. Examples of symmetrical and asymmetrical bulge geometries in some ribbon-quartz mylonites are shown in Fig. 1(b) & (c). These indicate late coaxial deformation in a quartzite from the Cap de Creus shear zones (Garcia Celma 1982) (which is also suggested by the development of two sets of shear bands), and sinistral shear in a quartzite from the Darling fault zone (Bretan 1985) (which is also suggested by the asymmetry of quartz fabrics).

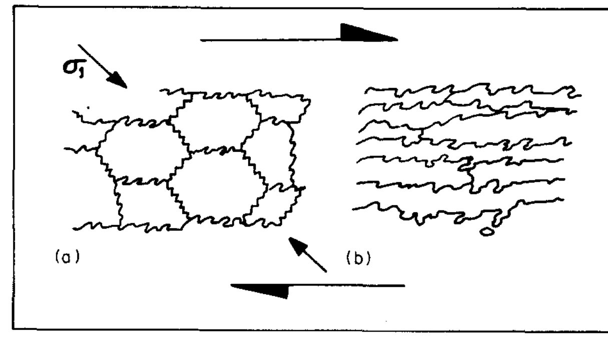


Fig. 3. Predicted geometry of grain-boundary bulges (developed by the mechanism shown in Fig. 2) for simple shear. (a) Low strain and (b) high strain.

DIAMOND AND TABULAR GRAIN STRUCTURES AS SHEAR CRITERIA

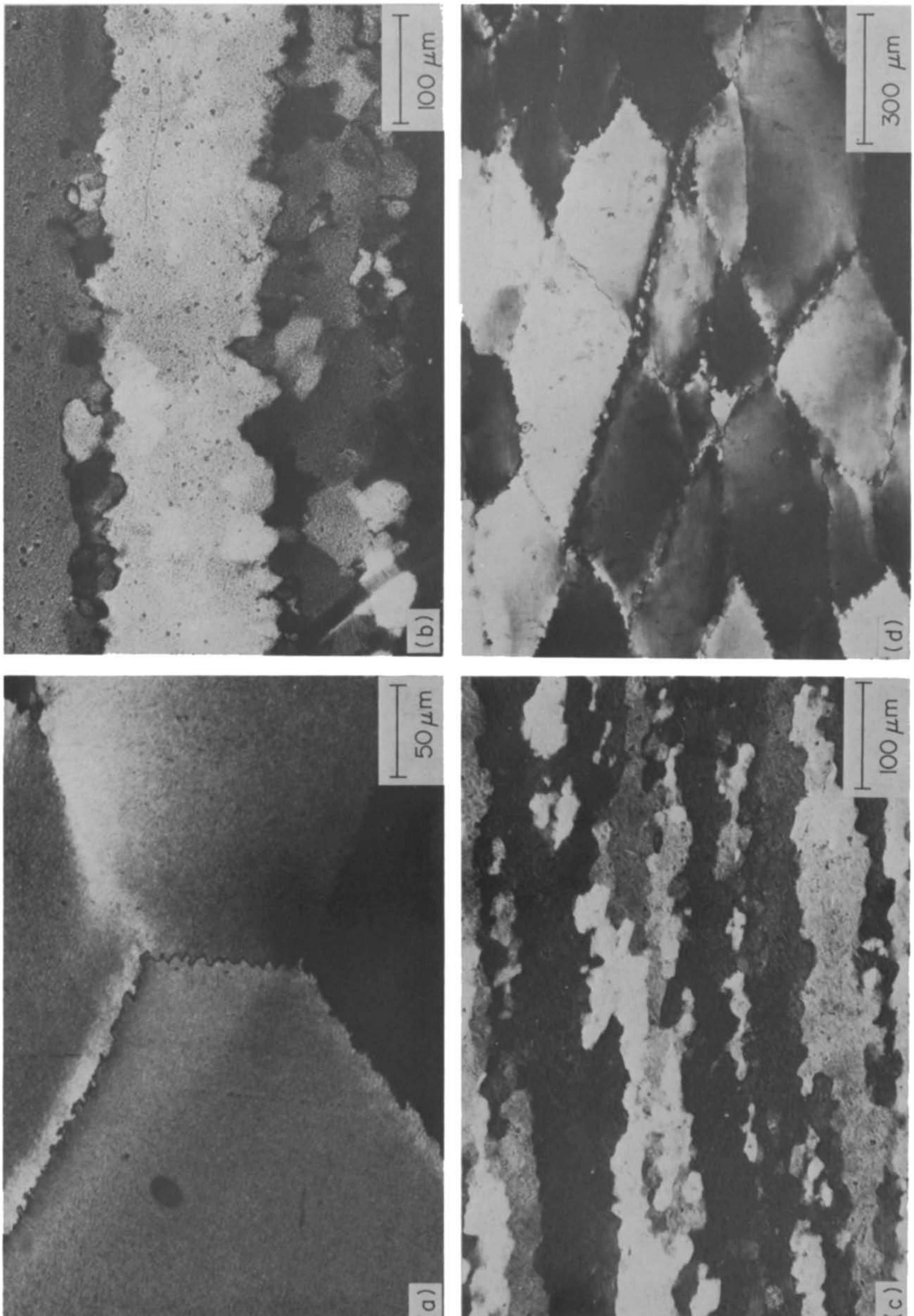
Microstructures

These structures are defined by preferred orientations of grain boundaries or grain-boundary envelopes. Diamond grain structures are developed during coaxial deformation and can be divided into two types. Type M has preferred alignments at ±45° to the compressive stress axis (Singh *et al.* 1977, Tungatt & Humphreys 1981a) (Fig. 4a). Most of the boundaries have this preferred orientation, which develops after small strains of $\varepsilon = 0.01$–0.2. The structure remains stable to high strains.

Type M diamond grain structures are commonly developed during cyclic deformation of metals and also have been reported during single-phase experimental deformation of Zn,Cu (Singh *et al.* 1977), sodium nitrate, camphor (Tungatt & Humphreys 1981a, 1984), calcite (Schmid *et al.* 1980), bischofite (Urai in press) and clinopyroxene (Boland & Tullis 1986) and in naturally deformed quartz (Lister & Dornsiepen 1981, Lister & Snoke 1984, Van den Eeckhout 1986).

A related structure to a type M diamond grain structure but with different alignment of grain boundaries has been described in simple shear tests on calcite (Fig. 4b)

Fig. 1. (a) Reflected light micrograph of specimen of Al5%Mg deformed to $\varepsilon = 0.16$ at $T = 400°C$, $\dot{\varepsilon} = 2 \times 10^{-3}\ s^{-1}$. Symmetrical zig-zag bulges develop on boundaries perpendicular and parallel to the compression axis, and asymmetrical bulges on inclined boundaries. (b) Grain-boundary bulges in quartz-ribbon mylonites from a dextral shear zone (Cap de Creus, NE Spain, Garcia Celma 1982), suggesting a late component of coaxial deformation across the zone. (c) Grain-boundary bulges in quartz-ribbon mylonites from a sinistral shear zone (near the Darling fault zone, Western Australia) suggesting no kinematic changes during the late stages of ductile deformation in the zone. (d) Type N diamond grain structure in Al5%Mg deformed to $\varepsilon = 0.5$ at 400°C, $\dot{\varepsilon} = 2 \times 10^{-3}\ s^{-1}$.


(a)
50 μm
(b)
100 μm
(c)
100 μm
(d)
300 μm

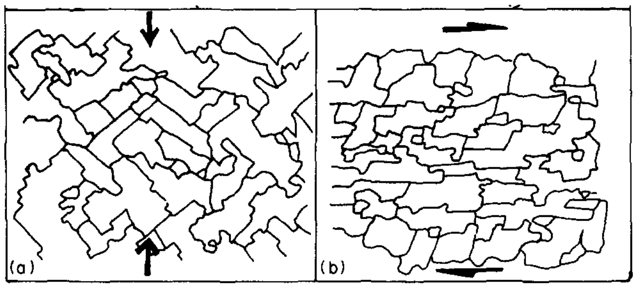


Fig. 4. Type M diamond and tabular grain structures. (a) Coaxial deformation and (b) simple shear deformation.

by Panozzo (1986). It is suggested that this microstructure be termed a type M tabular-grain structure. In this case the boundaries are aligned at 0 and 70° to the shear plane with grains displaying tabular to parallelogram shapes.

The second type of diamond grain structure will be termed type N. It is characterized by preferred orientations of grain-boundary envelopes at 60–70° to the stress axis in uniaxial compression tests (Fig. 1d). This type of structure has only been observed in aluminium–magnesium alloys and sodium nitrate (Drury & Humphreys 1986, Humphreys & Drury 1986). It differs from the type M structure in five respects:

(i) The preferred orientations of grain-boundary envelopes differ.

(ii) There are a lower percentage of boundaries with preferred orientation.

(iii) Moderate strains are required (ε = 0.4–0.5) to develop the structure.

(iv) The structure is not stable at high strains.

(v) Type M structures occur under conditions where extensive grain-boundary migration occurs, while in type N structures old grains are partially preserved.

Mechanisms

The development of diamond and tabular grain structures can be attributed to the interaction between grain-boundary sliding and migration (Walter & Cline 1968, Wigmore & Smith 1971, Nix 1975, Singh *et al.* 1977). The driving force for migration is the reduction of stored energy that is built up as a result of grain-boundary sliding. Three different mechanisms of this type could produce preferred grain-boundary alignments.

(A) Nix (1975) equated the elastic energy of a grain boundary that had undergone sliding to that of a shear crack. He suggested that grain-boundary migration would occur to minimize the stored energy, which for a 'crack' of given length is a minimum at ±45° to the compressive stress axis.

This mechanism can account for type M diamond grain structures that develop very rapidly as soon as stress is applied to the material. Camphor provides an example of this behaviour (Tungatt & Humphreys 1981b).

(B) Walter & Cline (1968) have shown that diamond grain structures can develop when the driving force for migration is provided by non-uniform intragranular

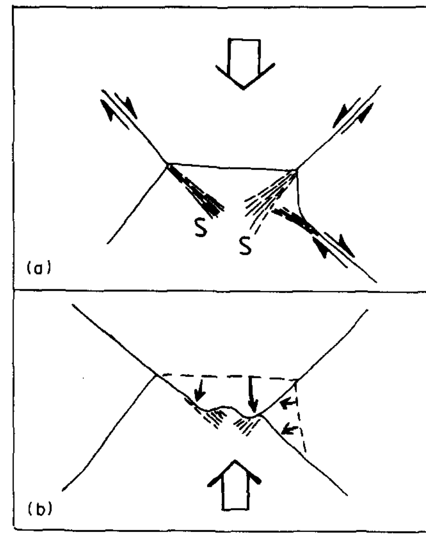


Fig. 5. Development of type M diamond grain structure. (a) Grain-boundary sliding occurs along boundaries subjected to a high shear stress. Zones of accommodation strain S develop at the triple points. (b) Grain-boundary migration consumes the zones of high strain (S), thus aligning the boundaries at ±45° to the compression axis.

strain caused by accommodation of grain-boundary sliding at triple points (Fig. 5). When this mechanism operates strains of ε = 0.1–0.2 are required for the structure to develop.

(C) Humphreys & Drury (1986) have shown that new high-angle boundaries can develop in zones of sliding accommodation-strain at triple points (Fig. 6). If these new boundaries link across old grains diamond shaped grains will form (in uniaxial compression).

Type M diamond grain structures are formed by mechanism (A) or mechanism (B). In Al5%Mg, where type N structures occur, there is microstructural evidence for the occurrence of mechanisms (B) and (C). It should be noted that if the development of new grain

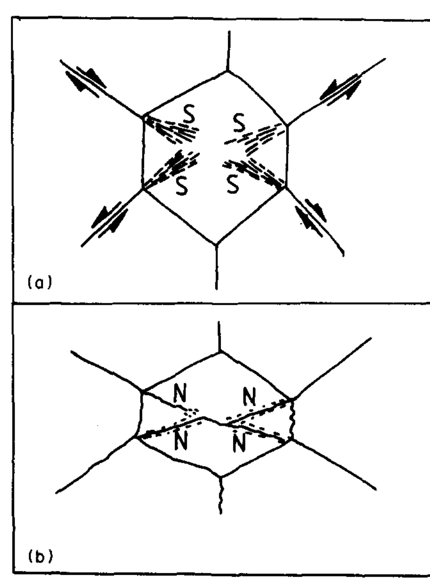


Fig. 6. Development of type N diamond grain structure. (a) Zones of accommodation strain S develop at triple points ahead of sliding boundaries with high shear stress. (b) With increasing strain new high-angle boundaries N form in the deformation zones, thus dividing the grain into flattened diamond shapes.

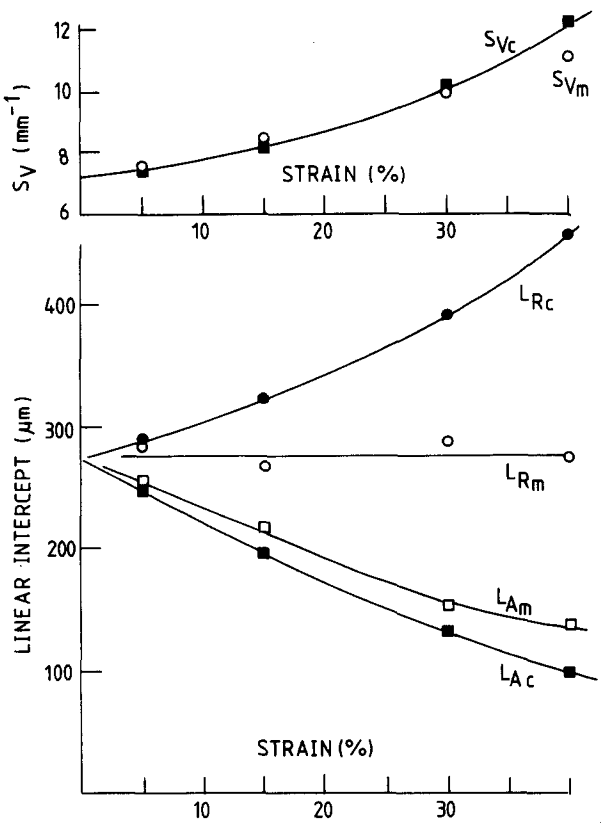


Fig. 7. Measurements of grain-boundary area per unit volume, S_V, as a function of increasing strain in Al5%Mg, for T = 400°C, $\dot{\varepsilon} = 2 \times 10^{-3}$ s^{-1}. S_{Vc}—theoretical increase of S_V with passive strain of a grain-boundary network. S_{Vm}—measured value of $S_V = (1/L_A + 1/L_R)$ (Underwood 1969). L_{Am}—mean linear intercept of grain size parallel to compression axis. L_{Rm}—mean linear intercept of grain size perpendicular to the compression axis. L_{Ac}—theoretical value of axial linear intercept for a passively strained boundary network. L_{Rc}—theoretical value of radial linear intercept for a passively strained boundary network.

boundaries in triple point deformation zones was the dominant mechanism then there should be a significant increase in the grain-boundary envelope area per unit volume (S_V), with increasing strain.

Measurements of S_V with increasing strain show an increase (Fig. 7), but this is not significantly greater than that expected due to the distortion of the passive grain-boundary network (Hartley & Unal 1983). This suggests that the grain-boundary migration mechanism (B) is as important as the new grain-boundary formation mechanism (C).

SUMMARY AND CONCLUSIONS

Studies on some rock analogues have provided experimental evidence for the validity of certain shear criteria associated with preferred grain-boundary alignments and grain-boundary bulge geometry.

Diamond grain structures are indicative of coaxial deformation, while tabular grain structures indicate non-coaxial deformation and the sense of shear (see Panozzo 1986). Type M structures develop at low strains ($\varepsilon \cong$ 0.1–0.2), are stable to high strains and provide information on the last ($\varepsilon \cong 0.2$) strain increment, while type N structures require larger strains ($\varepsilon \cong 0.5$) to develop, and are not preserved at high strains ($\varepsilon > 0.8$). They are thus only useful as shear criteria at low to moderate strains.

If consistent sets of asymmetric or symmetric grain-boundary bulges are developed, then these provide information on the shear regime during the last ε = 0.05–0.01. These structures can be readily reset during later deformation. This type of shear criterion should be used with caution because there are other mechanisms for the development of grain-boundary bulges (Bailey & Hirsch 1962), although these should not produce any particular asymmetry along a boundary.

It is emphasized that all of the structures described develop when deformation is accommodated predominantly by intragranular dislocation creep. Grain-boundary sliding only accounts for 10–20% of the imposed deformation, but has a significant effect on microstructural development.

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