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The dislocation structures responsible for the optical effects in some naturally-deformed quartzes

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The optical features in naturally deformed quartzites, namely undulatory extinction, deformation bands, deformation lamellae and sub-grains, can be related to dislocation structures in the quartz grains. Dislocation walls forming mosaics of sub-grains are the principal cause of all the optical features. The irrational deformation lamellae common in metamorphic quartzes are sub-grain walls; only those which lie on slip planes are slip lines and these are normally emprinted (superimposed) on sub-grain structures. The dislocation structures are indicative of recovery and thus optical features cannot be used as stress or strain gauges.

1. Introduction

Natural polycrystalline quartz often exhibits deformation features when viewed under crossed polarizers or in phase contrast conditions in the petrological microscope. Sander [1] in an early review of this subject recognized three distinct features which he termed "deformation lamellae", "undulatory extinction" and "ruptured quartz". There have been many subsequent studies of this subject and it is often difficult to correlate these because of the inconsistent use of nomenclature, much of which is caused by the failure of some authors to include photomicrographs of the features they described.

The term "undulatory extinction" for slight gradational variations in the extinction position in a grain as if the lattice was bent, remains in use. Basically the same can be said of "deformation lamellae" which are closely-spaced planar features. Some lamellae in natural tectonites are brown and these have been referred to as "Boehm lamellae" which Spry [2] regarded as a separate type of lamellae, although no such distinction is to be found in most recent works [3, 4]. Spry [2] also classified healed fractures as lamellae but Carter and Friedman [5] have listed the diagnostic differences between fractures and lamellae, so these two features need not be confused.

The term "ruptured quartz" is no longer used. Sander [1] described such quartz as consisting of discrete fragments with a slight misorientation relative to one another. He noted that while some fragments had an equant shape, most were needle-like and parallel to the undulatory extinction. The former have a counterpart in deformed metals and are now referred to by their metallurgical name, "sub-grains" [6] and this term has been used consistently in the literature. The same cannot be said of the "needle-like fragments". Riley [7] noted that they were similar in appearance to deformation bands in metals and so used this term (i.e. "deformation band"). However, he did not include a photomicrograph of them, but did refer to their similarity to structures recorded by Adams [8] in hydrothermal vein quartz. These were growth features (fibres) and not formed by a deformation.

The deformation bands described by Riley [7] have also been referred to as "extinction bands" [9, 10], "kink bands" [11] and "deformation lamellae" [12]. These terms, however, have been used in other senses, "kink band" and "deformation band" for the commonly observed misorientation between adjacent deformation lamellae [13, 14] and "extinction band" and

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"deformation band" for any banded feature including undulatory extinction [2, 5]. Christie *et al* [11] differentiated between banded features in naturally and experimentally deformed quartz, the former were referred to as "deformation bands" and the latter as "kink bands" because they could be directly related to slip processes. This differentiation is no longer adhered to and in a recent review Carter [3] described all banded features in quartz as "extinction bands", but similar features in olivine as "kink bands".

When describing the optical features present in the quartzes used in this work, the terms "undulatory extinction", "deformation lamellae", "sub-grain" and "banded extinction feature" will be used. The last encompasses any banded optical feature and it is hoped to determine which of these features are long sub-grains, deformation bands or kink bands by electron microscopy.

The above optical features have long been associated with deformation and so one finds that deformation lamellae and bands are now classified as textural features due to slip [2]. However, the processes by which these features form within the quartz lattice are not clearly understood. Bailey *et al* [15] proposed that undulatory extinction resulted from bend gliding. Although they observed also that "submicroscopic" sub-grains were very common in naturally deformed quartzes which exhibited undulatory extinction, they concluded that the sub-grains represented areas of polygonization within the bent lattice and did not relate the undulatory extinction to the sub-grains. Their envisaged polygonization process was essentially similar to that proposed by Cahn [16] for the annealing of metals. Carter *et al* [17] and Christie *et al* [11], as a result of experimental deformation studies, extended the concept of Bailey *et al* [15] and stressed a direct relationship between the optical deformation features and dislocations. Thus they interpreted deformation lamellae as arrays of edge dislocations formed by slip, undulatory extinction as the result of bend gliding due to parallel edge dislocations of the same sign on basal slip planes, and the deformation and kink bands as the result of the polygonization of these edge dislocations. Furthermore, they emphasized that the optical features in naturally deformed quartz would result from similar dislocation arrangements. However, subsequent electron microscopic studies [18-20] have demonstrated that the lattice defects responsible for optical lamellae in laboratory deformed quartz depend upon the deformation process. If the quartz was deformed rapidly, as in many of the experiments by Carter *et al* [17], the lamellae resulted from twinning, whereas if the deformation was at slower rates, and especially if the sample was stress-annealed after deformation, the lamellae formed from the walls of tangled dislocations which divided the lattice into sub-grains [21]. Neither of these views concurred exactly with the observations of White *et al* [22] who noticed an absence of twinning and the presence of walls of individual dislocations forming sub-grains in the natural quartz.

It appears from the literature that there is a relationship between undulatory extinction, banded optical features and polygonization. The author felt that a detailed electron microscopy study of quartzes in natural tectonites might not only indicate what lattice defect structures are responsible for these optical effects, but also clarify the nomenclature difficulties related to this subject. The results of this study are reported in the following sections.

2. Experimental procedures

Petrological thin sections were prepared from several regionally metamorphosed quartzites and veins. All the thin sections were examined under crossed polarizers and areas showing a specific optical characteristic were marked and prepared for electron microscopy by ion-bombardment as described by Champness and Lorimer [23]. Wherever possible, areas with a large single grain greater than 1 mm in diameter were chosen, as this is the internal diameter of the copper electron microscope grid to which the specimen is attached. All of the thinned samples were examined in a conventional 100 kV EM6G electron microscope and foils selected from these were subsequently viewed in a 1000 kV EM7 microscope. The latter instrument has three important advantages over the former: firstly, a specimen thickness of several microns is transparent to the electron beam; secondly, the rate of beam damage in the quartz is greatly reduced; thirdly, there is a continuous range of magnifications from 64 to 1.6×10^6 times available. Thus extensive areas can be examined at magnifications similar to those obtained in the petrological microscope, thereby permitting direct comparisons to be made between optical and electron micrographs. Moreover, composite micrographs showing in detail the defects over several hundred square microns can be constructed.

TABLE I Quartzes selected

Sample	Optical feature	Locality
A1	An annealed texture without evidence of any deformation.	A quartz vein in high grade gneisses (amphibolite facies). Olary, South Australia.
A2	Simple undulatory extinction.	Mylonite. Assynt, Scotland.
A3	Segmented undulatory extinction	Sheared quartz vein in slates. Ballarat, Victoria. Sample collected away from the shear.
A4	Banded extinction features.	Dalradian schists. Scotland.
A5	Deformation lamellae.	Moine schists. Scotland.
A6	Sub-grains.	Granulite, Scourie, Scotland.
A7	Undulatory extinction and deformation lamellae.	Same vein as A3, but collected from position adjacent to the shear.

3. Quartzes selected

The quartzes used in this study are listed in Table I and micrographs of the optical features

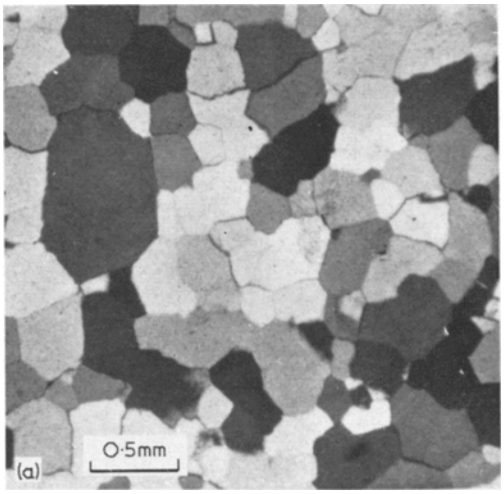


Figure 1a

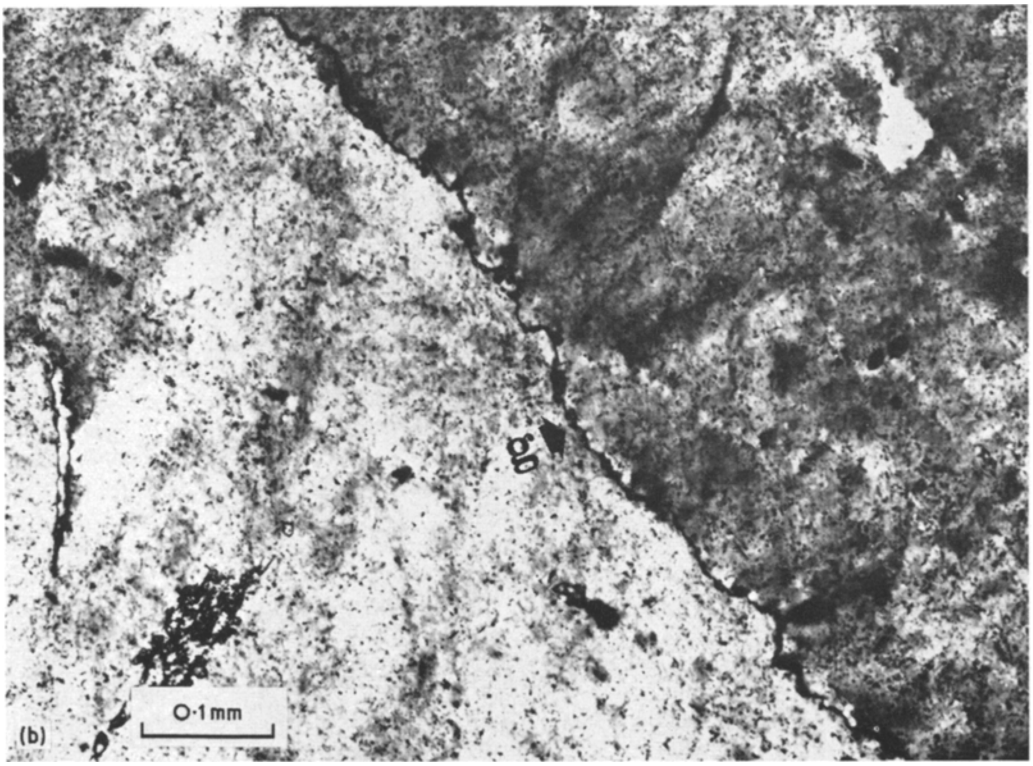
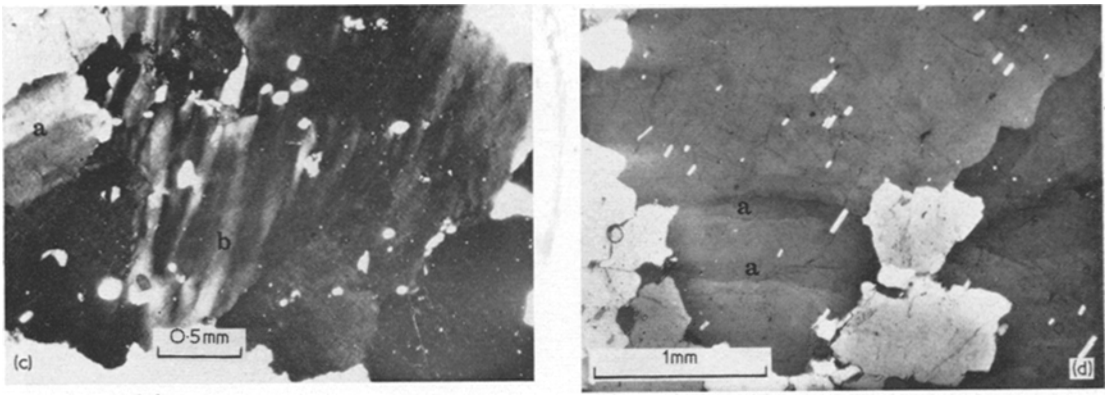
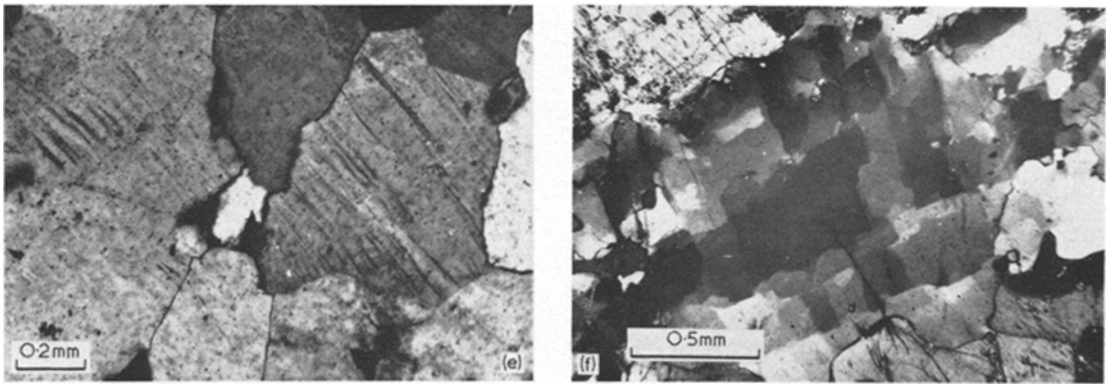


Figure 1b



Figures 1c and d



Figures 1e and f

Figure 1 Optical micrographs of some of the quartzes. (a) Specimen A1 with an annealed texture. (b) Specimen A3 showing segmented undulatory extinction. g is a serrated grain boundary. (c) Specimen A4 exhibits banded extinction features, a is an area of undulatory extinction and b are deformation bands. (d) Specimen A4. The banded extinction features marked a, are long prismatic sub-grains. (e) Specimen A5. Deformation lamellae. (f) Specimen A6. Sub-grains.

are shown in Fig. 1. At least two, and as many as six foils, were prepared from each sample.

Continuous undulatory extinction was rare in quartzites with a grain size of at least 1 mm; in most of these grains the undulatory extinction was banded or segmented. The former effect was more common in fine-grained quartzites and was present in all grains in sample A6. Banded extinction features were prevalent in most coarser grained quartzites and these ranged, even in a single specimen, from simple banding of the undulatory extinction to well developed narrow sub-grains, elongated parallel to the *c*-axis of the host grain (Figs. 1c and d).

4. Dislocation structures

All of the quartzes contained dislocations, even specimen A1. No twinning was observed in any of the foils viewed. Dislocations were present throughout the whole of each grain in specimen A1, with only the occasional wall of dislocations (Figs. 2a and b). The misorientation across these walls could not be detected in selected area diffraction patterns. However, the maximum misorientation (ϕ) can be calculated from the spacing (h) between the adjacent constituent dislocations by assuming that the dislocations are pure edge and that the Burgers vector of a unit dislocation in quartz will be approximately 5 Å [24] by applying the equation

$$\frac{b}{h} = 2\sin\left(\frac{\phi}{2}\right) = \phi \text{ (for small angles)} .$$

Thus the misorientation across the low angle

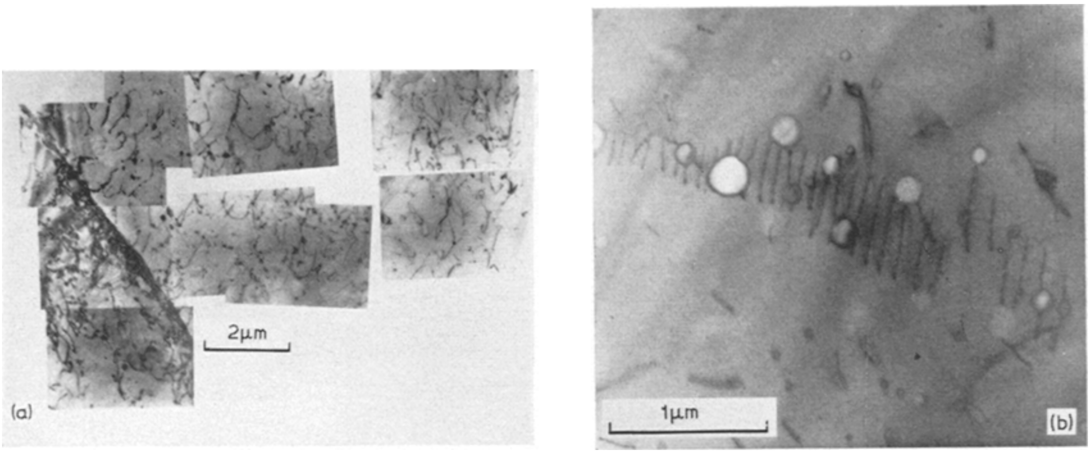


Figure 2 Dislocation structures in quartz without any optical evidence of deformation. (a) A typical dislocation structure; 1000 kV. (b) Dislocations in a low-angle boundary; 100 kV.

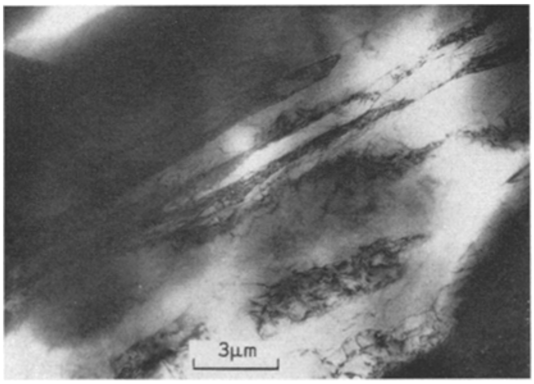


Figure 3 The narrow prismatic sub-grains in quartz with undulatory extinction; 1000 kV.

boundary in Fig. 2b, where *h* is approximately 1200 Å, is 0.3° and would not be detected in an optical microscope.

The most prominent sub-structure in other samples (Figs. 3 to 8) was the development of bowed and stepped dislocation walls which, although along irrational lattice planes, approximated to the prism, rhomb and base (in order of descending frequency). They divided the grains into sub-grains of differing sizes and shapes which varied not only in a given rock, but also within a single grain (Fig. 6a). The misorientation between adjacent sub-grains could be detected in selected area diffraction patterns as thickened or split Kikuchi lines and normally ranged from 1 to 5°. Individual bowed and tangled dislocations and dislocation loops were present in the interiors of all sub-grains in all specimens. Differences in the dislocation structures that could be attributed to a given metamorphic environment were observed and will be the subject of a future publication.

The quartz with simple undulatory extinction contained long, narrow prismatic sub-grains of the type shown in Fig. 3. The walls were not always as closely spaced as this and could be up to several microns apart (see Fig. 8). The narrow sub-grains were often banded together with adjacent bands separated by a region of coarser sub-grains, as in Fig. 3. The quartz with banded extinction features also contained similar narrow sub-grains but differed in that these were enclosed by larger and more misorientated prismatic sub-grains (Fig. 4a). The bands which optically exhibited a sharp contact were simply long thin sub-grains (Fig. 4b). Not all of the specimens had prismatic sub-grains. Specimen A3 contained small equant sub-grains (Fig. 5) and specimen A6 (Figs. 6a and b) also showed these, but they were enclosed by larger approximately equant sub-grains which had a greater misorientation across their boundaries and which corresponded in size to the optical sub-grains in that specimen.

The deformation lamellae in specimen A5 corresponded to long, almost parallel walls of dislocations which formed long basal sub-grains with slight, but detectable, relative misorientations (Figs. 7a, b and c). The occasional prismatic wall of dislocations was also present and was cut

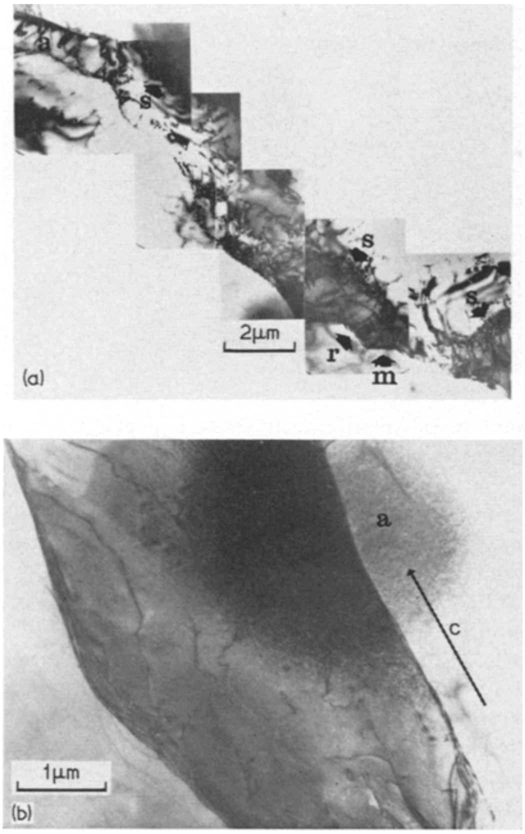


Figure 4 Electron micrograph from quartz with banded extinction features (area b, Fig. 1c). (a) Narrow prismatic sub-grains, s, enclosed by larger prismatic sub-grains. The walls of the large sub-grains approximate to prism (m) and rhomb (r) planes. The sub-grain tapers at a, and this effect can be seen optically (Fig. 1c); 800 kV. (b) A large prismatic sub-grain which is seen as such optically (e.g. Fig. 1d). Area a is beam damage resulting from bringing the beam to a point focus on that area. The trace of the *c*-direction is marked. The foil is approximately parallel to a $\{11\bar{2}0\}$ section; 800 kV.

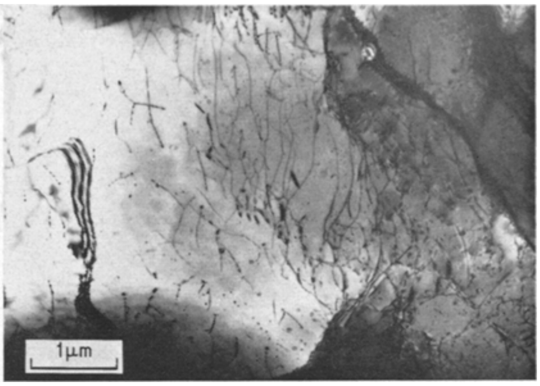


Figure 5 Dislocation structures in quartz with segmented undulatory extinction; 100 kV.

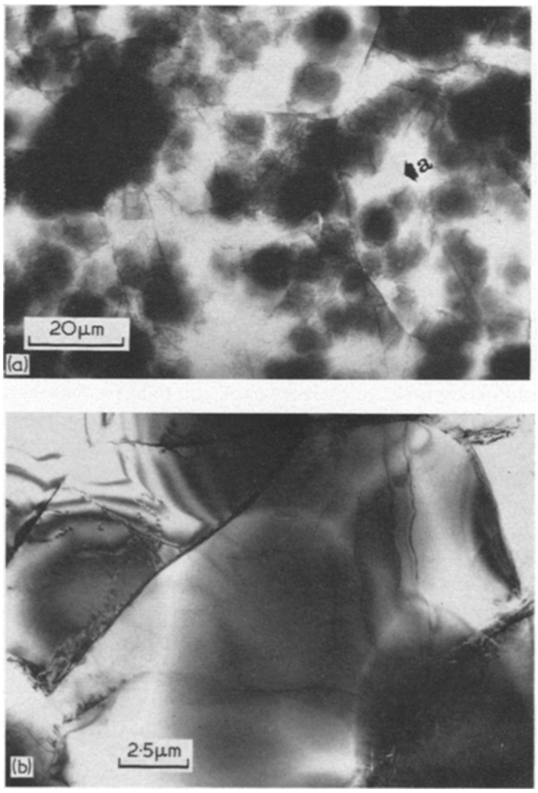
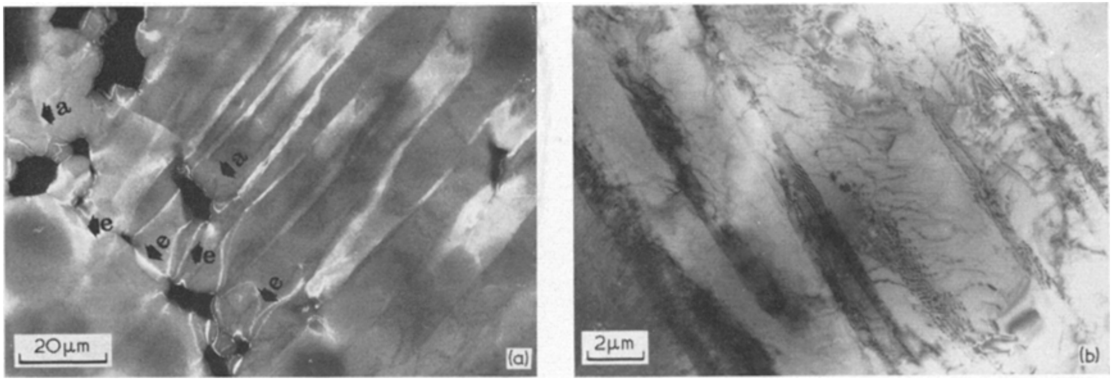


Figure 6 Electron micrographs of quartz with sub-grains. (a) The boundaries of the large sub-grains which exhibit a large size range are clearly visible. A rutile needle, a, cuts across several sub-grains; 1000 kV. The dark areas are "hillocks" formed during thinning. (b) Smaller sub-grains which occur within the large ones; 1000 kV.

by the basal walls. Inclusions occurred along the basal sub-grain walls. The dislocation walls corresponding to the lamellae in specimen A7 were along a rhomb plane and were straight and parallel. They cut across a well-developed structure of prismatic sub-grains and only terminated within a grain at a bubble (Fig. 8).

5. Discussion

The optical deformation features in quartz can be related to the dislocation sub-structures, in particular to the development of sub-grains. Dislocations are present in the grains of specimen A1 but there are few walls of dislocations and those present have introduced only slight misorientations into the grains. Specimens with



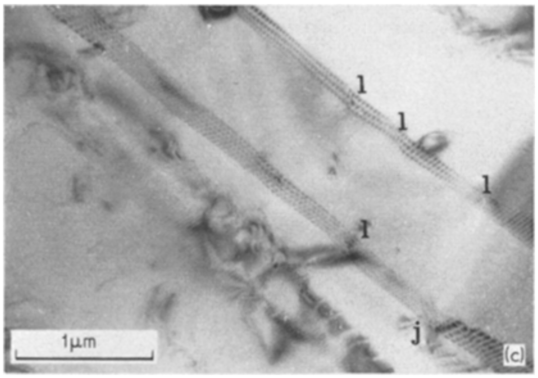


Figure 7 Electron micrographs from quartz with deformation lamellae. (a) Low magnification dark field micrograph showing that the deformation lamellae are narrow basal sub-grains. Adjacent sub-grains are imaged as alternating bright and dark bands and indicate that there is an opposite sense of misorientation across adjacent walls. The sub-grains are inclined at approximately 15° to the (0001) plane and cut across irrational prismatic dislocation walls, a. The bright bands such as those marked e, adjacent to the holes in the foil (black areas) are extinction contours and are diffraction effects; 1000 kV. (b) A bright field micrograph showing the dislocations forming the sub-grain walls; 1000 kV. (c) The walls at a higher magnification. Ledges, l, along the walls and a junction of three walls, j, are marked. The individual dislocations are aligned parallel to a ⟨11$\bar{2}$0⟩ direction; 1000 kV.

optical deformation effects may have similar tangles of dislocations throughout their grains and in other cases may be almost free from them. More noticeably, they have many more walls of dislocations. Thus it is the lattice misorientation across the sub-grain walls and not the development of dislocations throughout a grain that is responsible for the optical effects.

The bending of the lattice to form undulatory extinction in metamorphic quartzes is not accomplished by bend gliding. but by the progressive misorientation introduced by almost parallel walls of dislocations*. The former requires the even distribution of parallel edge dislocations of a similar sign throughout a grain as postulated by Carter *et al* [17] and observed in their laboratory deformed quartzes by McLaren *et al* [20]. Most of the dislocations in the prism walls lie in a ⟨11$\bar{2}$0⟩ or a ⟨11$\bar{2}$3⟩ direction, and if such dislocations have an edge component [20, 24], an effective lattice rotation about an *a*-axis, as recorded by Bailey *et al* [15], is to be expected. A systematic misorientation

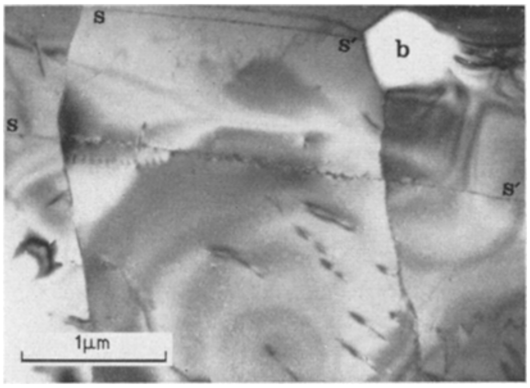


Figure 8 Dislocation structures in quartz which has lamellae developed approximately perpendicular to the undulatory extinction. Dislocations lie along rhomb slip planes, ss′, and cut across prismatic sub-grains . b is a bubble.

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*Note added in proof. Recent observations by the author have shown that undulatory extinction can also form as the result of lattice distortion caused by the strains induced by forests of (0001)⟨11$\bar{2}$0⟩ dislocations in those grains of a quartzite that have undergone little recovery, i.e., deformation in the grains was limited to the initial (primary) stage of creep.

will require the predominance of dislocations of the one sign in all the prismatic walls of a given grain. Quartz during low-grade metamorphic conditions is in the α-phase field and, as α-quartz is piezoelectric, not only will the individual grains be charged during deformation but also the dislocations [25] and so the predominance of dislocations of the one sign is to be expected. Therefore, as a result of such conditions, the lattice is systematically bent at each sub-grain wall. The net result is seen in the optical microscope as undulatory extinction.

The dislocation structures in the quartzes with banded extinction features are basically similar. If the prismatic sub-grains are not equally developed throughout a grain, banded undulatory extinction is formed. Banded extinction features similar to those described by Riley [7] result when larger prismatic sub-grains enclose the smaller sub-grains; however, if the larger ones are free from the smaller, they are seen as long sub-grains. These features can be distinguished from each other optically as *banded undulatory extinction* has diffuse edges, *deformation bands* are more sharply delineated and have undulatory extinction effects within them, and *larger sub-grains* are sharp-edged but without internal undulatory extinction. The dislocation structure of the deformation bands is similar to that of kink bands [26, 27]. However, as pointed out by Christie *et al* [11] they arise from different deformation processes. It will be shown in the proceeding section that the dislocation structures are formed by a recovery rather than a slip process and the bands are therefore "deformation bands". The term "extinction band" should not be used as it is limited to the geological literature, whereas "deformation band" is used throughout the many branches of materials science.

The segmented undulatory extinction results from small equant sub-grains and so there is not the predominance of prismatic walls and hence no systematic bending of the lattice. The optical microscope therefore picks up the net result of a more random lattice misorientation formed by several underlying sub-grains that would occur in a petrological slide which is 30 μm thick.

A comparison of the electron micrographs from specimens A5 and A7 indicates that there are two types of deformation lamellae; those in Fig. 8 are slip planes which appear to be the result of a late high strain-rate period of deformation and have been emprinted on a typical prismatic cellular dislocation structure. It is probable that these slip planes represent a very late movement on the shear adjacent to which quartz A7 was collected. The slip planes are not related to the undulatory extinction which is the optical expression of the prismatic sub-grains.

The second type of deformation lamellae, which are the most common in natural tectonites, are not slip planes but dislocation walls that form narrow basal sub-grains. This explains the lenticular shape, the discontinuous and irrational habit and the visible misorientations between adjacent lamellae which characterize this type of lamellae [2, 13]. In their present form, they are not the products of an echelon slip or rotation by another slip system [11] but of recovery. The lamellae may initially have been basal slip planes formed during a previous episode of rapid deformation and have their present appearance because of later recovery. The manner in which they cut across the prism wall in Fig. 7a supports the possibility of their having been slip planes. The small steps in the basal dislocation walls (Fig. 7c) and the irregular form of the walls certainly indicate the probability that the walls have moved since their formation [28, 29]. In spite of this, they are similar in appearance to the prismatic dislocation walls and may have a similar origin as will be discussed in the following section.

Some of the basal sub-grains are so narrow (Figs. 7a and b) that their constituent walls would be difficult to resolve as individual lamellae in a normal petrological microscope. It is possible that many of the properties attributed to lamellae, such as their having a finite width and a different refractive index and extinction position from those of the host grain [13], are in fact those of a very narrow sub-grain. The lamellae are visible in the optical microscope as phase objects [18]. The brownish colour of some lamellae is consistent with Tyndall scattering of the transmitted light by inclusions (or bubbles) along the dislocation walls [30]. If the prismatic walls of dislocations (Fig. 7a) are sufficiently abundant, undulatory extinction will be formed approximately perpendicular to the lamellae as observed in specimen A7. This effect has been described frequently in the literature and the undulatory extinction in such cases is regarded as being the result of polygonization of the dislocations formed by slip, traces of which remain as lamellae [5]. However, the manner in which the dislocation walls responsible for the lamellae cut across prismatic walls would indicate that, in some quartzes at least, the lamellae and undulatory extinction are the separate products of two distinct types of deformation and are therefore unrelated. It would appear from the preceding observations that the straight lamellae formed along known basal slip planes during experimental deformation [4, 17] or in natural deformations such as in impact areas [31] and by rapid movements along faults, are true slip, or possibly twin [20], features. However the lamellae in most metamorphic quartzes are sub-grain walls.

The sub-grains visible in the optical microscope can be related directly to those which in electron micrographs are bounded by dislocation walls with significant misorientations (much greater than 1°) across them. Smaller sub-grains are formed within the larger by low angle boundaries of 1° or less. These cannot be detected individually in the optical microscope, but their presence may be indicated by the development of segmented undulatory extinction within the large sub-grains.

6. Origin of the dislocation structures

The basic dislocation structures in all naturally deformed quartzes which were studied consisted of dislocation walls forming mosaics of sub-grains. This, together with the irregularity and bowing out of the individual walls, and the abundance of bowed and tangled dislocations and dislocation loops throughout the grains, are all indicative of recovery processes and are consistent with creep [32]. Evidence for a change from a creep process to one with a higher strain-rate could be seen in some samples, however, in such instances, the basic creep structure remained present. The optical deformation features and grain boundary structures in metamorphic quartzes are exactly those that are produced in metals and ceramics by creep [33]. For obvious reasons undulatory extinction is not possible in metals although the requisite sub-grain structures may be formed during creep [28]. These results indicate that creep may be an important process during crustal deformation.

7. Geological implications

From the preceding section it follows that if the dislocation structures in metamorphic quartzes are basically recovered structures, the deformation structures exhibited by such quartzes are recovered (creep) structures and are not the result of slip and polygonization as discussed by Carter *et al* [17] and Christie *et al* [11]. So the effect of recovery processes should be considered when interpreting petrofabric data, especially if it is derived from deformation features in the quartzes. Carter *et al* [17], as a result of experimental deformation studies, proposed a technique whereby the orientations of principal stress axes of a deformation could be determined from the deformation lamellae. The method assumes that deformation lamellae are slip planes and this assumption is not universally true in natural tectonites, as in most cases they are sub-grain walls and their present position and attitude within a quartz grain is due to recovery and not slip.

The optical strain features cannot be used as strain or stress gauges. Undulatory extinction, deformation lamellae and bands and sub-grains in the metamorphic quartzes are formed by essentially similar dislocation structures. Thus, it is not possible to use them as evidence of progressive strain increments or to say that any one of them indicates a particular amount of strain [34]. Even quartzes without any optical evidence of deformation can contain large numbers of dislocations. The coarse sub-grain structure, as in specimen A6, however, is a more recovered structure than the sub-grain structure producing deformation bands or undulatory extinction. Hence, the variation of these features throughout a given specimen or grain for which temperature and pressure conditions were constant during deformation, may correspond to variations in the internal lattice stresses similar to those in crept polycrystalline metals [32].

The presence of sub-grains within sub-grains in many quartzes makes the estimation of former natural stresses from the size of visible sub-grains [35] very difficult. Only the sub-grains with large misorientations are visible in the petrological microscope whereas the techniques of electron microscopy and etching which were used by metallurgists to formulate the relationship between the applied load and the size of the sub-grains [32] revealed all the sub-grains. Therefore, for this method of stress determination to be applicable to natural conditions, even leaving aside the likely complexity of natural creep processes [33], the size of all sub-grains must be taken into account.

8. Conclusions

1. Undulatory extinction in natural quartzes results from the effective bending of the lattice by elongated prismatic sub-grains.
2. Deformation bands are zones of small prismatic sub-grains enclosed by larger prismatic sub-grains. If the former are absent, the large prismatic sub-grains are visible optically as sub-grains free from undulatory extinction and are not deformation bands.
3. Most deformation lamellae in natural quartz tectonites are basal sub-grain walls. Only those that lie along a slip plane are slip lines and indicate a period of high strain-rate deformation. Petrofabric techniques using lamellae should be limited to those lamellae that are slip-planes.
4. Optical deformation features in quartz cannot be used as stress or strain gauges.
5. Electron microscopy can be used to decipher past deformation events in quartz.

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