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INTERACTIONS OF TWIN BOUNDARIES AND DISLOACTIONS IN SOLAR SILICON

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ABSTRACT

Most solar materials grown under the JPL program contain twin boundaries (e.g. EFG and WEB). These twin boundaries interact with dislocations during:
(i) Plastic deformation during cool-down
(ii) Stress relaxation during formation of the diffused junction.
In (i) the twin boundaries restrict the movement of dislocations resulting in higher residual stresses being froozen in into the ribbon In (ii) the twin boundaries act as "concentrators" of dislocations which lead to the formation of sub-boundaries, which. when penetrating a junction. lead to junction defects. For these reasons it is important to understand the mechanism of interaction.
TEM and EBIC were used to study changes in the defect structure which occured when rapidly grown, edge defined film fed growth silicon ribbons were processed at high temperatures. Twin boundaries, which comprise the major structural defects in the ribbons were found to act as strong obstacles to dislocation glide. The impedance of dislocation glide, possible mechanisms for slip transfer across twins, and implications for the mechanical and electrical properties of the silicon ribbons are discussed. A model is developed which explains both twin-induced grain boundary formation during recovery of the microstructure and also the generation of microtwins and second order twin joins by glide-induced twinning processes.

1. INTRODUCTION

A variety of crystal growth techniques have been developed to grow silicon in the form of thin ribbons suitable for low cost solar cells. One of the most advanced ribbon technologies is edge defined film fed growth. EFG (for recent reviews see KALEJS. MACKINTOSH and SUREK 1980. or WALD 1981). Since low production costs can only be achieved by growing large silicon crystal sheets at high speed, the sheets inevitably are cooled very rapidly. (High growth rates require large thermal gradients at the liquid solid interface; establishement of such gradients requies rapid cooling). The result is that high thermal stresses are frozen into the ribbon.

The time for cooldown is very short. much shorter then the duration of the typical heat-treatment required for formation of the p-n junction. This has two important consequences. The first one is that any obstacle which restricts the movement of dislocations during cooldown will lead to a higher residual stress (since climb processes are too slow to be effective). Secondly, when the specimen is reheated during junction formation. the combination of high internal froozen in stresses and elevated temperatures leads to a extensive rearrangement of the defect structure during diffusion ("recovery"). The material properties of EFG ribbons. including their electrical properties, therefore change during processing. (As minority carrier devices, the performance of solar cells is controlled by the minority carrier lifetime which depends both directly (recombination at crystal defects) and indirectly (decoration with impurity atoms) on the defect structure). Other important problems in EFG ribbons resulting from partial recovery during the short time of growth are ribbon buckling, ribbon breakage. and considerable material inhomogeneities (KALEJS et al. 1980).

The defect structure of as-grown EFG ribbons consists predominantly of dislocations and coherent twins, mainly present in the form of microtwins (see e.g. AST, CUNNINGHAM and STRUNK 1982). Most of the twin boundaries are perpendicular to the {110} surfaces and parallel to the <112> growth direction. This defect structure, which invariably develops during growth, has been termed the equilibrium defect structure (WALD 1981). The subject of this work is the recovery of EFG silicon after different annealing treatments.

Two basic reactions of dislocations with twin boundaries (introducing two Shockley partials or a Frank and a Shockley partial) have been found in fcc metals (see e.g. PUMPHREY and BOWKETT 1971, FORWOOD and HUMBLE 1975, or DINGLEY and POND 1979). It will be shown that the same reactions occur in silicon, which has strong directional bonds, and that these reactions are the key to understanding the behaviour and properties of the silicon ribbons. The most comprehensive and systematic investigation of process-induced defects on a similar type of silicon ribbon, by YANG, SCHWUTTKE and CISZEK 1980, was mostly concerned with the classification of these defects with respect to influences on the electrical properties. Consequently, these authors did not present a model accounting for all their observations. We find that twins are strong barriers to the glide of all types of dislocations. In agreement with the observations of HOWELL, NILSSON and DUNLOP 1978 in stainless steel, we observe the development of "near-twin" boundaries. In addition small and large angle grain boundaries were found. The observations led to the formulation of several mechanisms for twin-induced grain boundary formation with the intent to explain the polygonization-like features found in this material. The model can account for the formation of sub-boundaries at the relatively low dislocation densities (10^4 cm^{-2} to 10^8 cm^{-2}) typical for EFG silicon.

2. EXPERIMENTAL

The material investigated was mainly conventional high speed EFG silicon with low oxygen content ($< 10^{16} cm^{-3}$). It has a relatively high average dislocation density ($10^7 cm^{-2}$ to $10^8 cm^{-2}$) and is therefore well suited to the study of dislocation/twin boundary interactions. High residual stresses provide a strong driving force for recovery during heat treatments. The ribbons used for this work experienced different heat treatments: (I) the usual junction diffusion at 950°C for 30 minutes, (II) a ten minutes or one hour anneal at 1200°C prior to diffusion and (III) heat treatments up to 90 minutes at 950°C after the phosphorus diffusion process. The crystal sheets were ground down mechanically to a thickness of 100 um and 3 mm discs were cut out by ultrasonic drilling, selecting the areas of interest optically. The final thinning of TEM samples was done by ion beam milling. Investigations were carried out using a JEOL 200 CX scanning transmission electron microscope operated at an accelerating voltage of 200 kV. To study large scale changes and to compare the electrical properties of defects, the electron beam induced current (EBIC) technique was applied, using the diffused junction for charge collection. The EBIC investigations were carried out on a JEOL 733 scanning electron microscope using a special specimen holder and an additional preamplifier (Keithley 427).

3. RESULTS AND DISCUSSION

The TEM inspection of processed silicon ribbons revealed that twin boundaries and the more frequently occurring microtwins (thin lamellae with twin relation to the matrix) are strong obstacles to dislocation glide (compare YANG et al. 1980). Pile-ups of glide dislocations are formed and an increasing density of dislocations develops in and around the twins. Examples of this are shown in fig. 1. The dislocations are only partly incorporated into the twin boundary. but when this happens the incorporated dislocations usually decompose into partials. Very often the perfect dislocations in the crystal are forced to react with each other to form dense three-dimensional networks adjacent to the twin planes. This may depend on the local stress level or stress distribution and on the relative positions of the microtwins. The retarding force of coherent twin boundaries on gliding dislocations has a strong influence on the recovery processes and therefore has to be taken into account. Considering the fact that the glide planes on both sides of coherent twin boundaries have common lines of intersection, <110>, and that one half of the possible 1/2<110> Burgers vectors (those parallel to the twin plane) are common in both crystals, on first sight the barrier action seems to be unexpected. <u>To understand this problem one has to look in detail at the slip transfer mechanism and to differentiate between the Burgers vectors in the plane of the twin boundary and those inclined at 60° to it</u>. A theoretical consideration of some possible transfer and dislocation reaction mechanisms can be found in the paper of HARTLEY and BLACHON 1978.

3.1. Interaction of dislocations with twin boundaries

It is generally accepted that dislocations in silicon glide in a dissociated state (ALEXANDER 1979). When the leading partial of any dissociated glide dislocation runs into a twin boundary. it cannot pass through on its own, because if it were to glide into the twinned crystal and move along the mirror image of its original glide plane it would produce a high energy stacking fault with a stacking sequence AA. (The twinning operation reverses the allowed <112> shear directions in glide planes inclined to the twin/mirror plane). However. several direct (single dislocation) interaction mechanisms are possible. There are three basic possibilities to be considered:

(I) The leading partial may transform to a Shockley partial glissile in the twin boundary and a stair rod dislocation.

(II) The dislocation may constrict under the applied stress and may then be transferred.

(III) The leading partial may pass through the twin boundary introducing a stair rod dislocation and an extrinsic stacking fault in the twinned crystal, i.e. two Shockley partials coupled together have to be created on adjacent glide planes (see HIRTH and LOTHE 1982). The elastic strain energy of these two dislocations is comparable with the strain energy of a single Shockley partial. However. the core energy contribution to the total energy will be increased.

In all three cases the dislocation has to overcome an energy barrier. which, together with the total energy achieved after the interaction with the twin boundary, determines the probability of the reaction.

The case of dislocations with Burgers vector parallel to the twin plane will be considered first. Such dislocations have to become screw dislocations - if not already in a screw orientation - in order to interact with the twin boundary. Reaction (I), resulting in decomposition in the twin boundary. is the most probable of the three alternatives, since the stair rod dislocation of the type 1/6<110> that is created has a relatively low energy - one third the energy of a Shockley partial. The dislocation reaction proceeds in two steps: the leading partial transforms into a Shockley partial and a stair rod, and the trailing partial then reacts with the stair rod to form another Shockley partial glissile in the twin plane. Since the trailing partial and the Shockley formed by decomposition of the leading partial repel each other. the latter is caused to glide away from the stair rod by the approach of the former and hence the process of decomposition can occur without any constriction. The two product Shockley partials are independent glissile DSC dislocations whose Burgers vectors lie in the twin plane. They introduce steps in the twin plane of opposite sign (see e.g. SCOTT and GOODHEW 1981), but are not connected by a stacking fault. The energy of the perfect dislocation is less in this decomposed state than in the former dissociated state.

The energy barrier for case (II), constriction. is about three times that for reaction (I). After constriction the dislocation may decompose as in (I) or it may be transferred into the twinned crystal with an interchange of the leading and trailing partials. The estimation of the energies involved in case (III) is difficult, since little is known about either the contribution of the core energy in dislocation reactions or the influence of a twin boundary on such reactions (HIRTH and LOTHE 1982). However. it is expected that the core energies are important contributions to the total energy in such a localized configuration. Thus the partly transferred dislocation (comprising three Shockley partials, a 1/18<112> stair rod and an intrinsic and extrinsic stacking fault) might give rise to an energy barrier comparable to that for constriction. This kind of transfer would result in a dissociated screw dislocation with an extrinsic stacking fault which would have a higher energy than the original dislocation. Note that on reaching the next twin plane. the transformation back to an intrinsic stacking fault would be energetically favourable.

As shown in fig. 2 the incorporation of glide dislocations into the twin plane is the more common process (compare e.g. PUMPHREY and BOWKETT 1971. or DINGLEY and POND 1979), although there is evidence for dislocation transfer in silicon (probably during the early stages of processing or during growth.

where the ribbons experience high stresses). The Shockley partials introduced into the twin boundary may glide in the same or opposite directions depending on the resolved shear stress on the twin plane. Examples of glide dislocations at the very moment of decomposition in a twin boundary can be found in fig. 10 (see arrows).

Fig. 2 is a selection of micrographs taken to analyse the structure of "near-twin" boundaries. After the conventional phosphorus diffusion the material was annealed for 30 minutes at 950°C. Since the microtwin under investigation is inclined to the surface of the specimen, the dislocation sets on both sides appear shifted relative to each other. The thickness of the microtwin is about 50 nm. The micrographs have been taken near the $(0\bar{1}1)$, $(1\bar{1}1)$ and $(\bar{1}\bar{1}1)$ poles, the line of intersection of the microtwin with the surface being parallel to [011]. With a few exceptions due to more complex reactions, all the dislocations imaged were clearly identified as Shockley partials. All three 1/6<112> Burgers vector types possible in the $(\bar{1}\bar{1}1)$ twin boundary were found. They are very likely the result of the decomposition of all three possible types of glide dislocations with Burgers vectors in the twin plane. The average separation of the partial dislocations of about 170 nm found in this case is controlled by the number of absorbed dislocations. At each arrow in fig. 2 there are two Shockley partials, separated by only 13 nm. with Burgers vectors of $+1/6[2\bar{1}1]$ and $+1/6[\bar{1}21]$ respectively. The dislocation between these "dipoles", and the ones adjacent have the Burgers vector +1/6[112]. The sign of the Burgers vectors could not be established but the fact that the "dipoles" and the single dislocations are parallel and equidistant suggests that the total Burgers vector of the "dipole" is 1/6[112], corresponding to the positive Burgers vector in each case. This arrangement of partials seems to be the result of dislocation decomposition followed by the absorption of another dislocation (with a different Burgers vector) between the first pair of Shockley partials after they have moved apart. Since Shockley partial dislocations introduce steps in the twin plane. the two dislocations comprising the "dipole" lie on different $(\bar{1}\bar{1}1)$ planes in the twin boundary and therefore cannot combine but appear to be slightly mutually repulsive. It is interesting to note that the line directions of the partial dislocations do not correspond to the intersections of the glide planes with the twin plane. The dislocations discussed are tilted 10° to 15° toward the screw orientation of those Shockley dislocations which have the dominant Burgers vector type 1/6[112].

The microtwin studied was found in the interior of a thin microtwin bundle. Since the vast majority of the dislocations absorbed in this microtwin have Burgers vectors parallel to the twin planes, it is suggested that the <u>microtwins nearer to the edge of the twin bundle act as a "dislocation filter"</u>, holding back dislocations with other Burger vector orientations. In addition. this observation demonstrates the ability of dislocations with Burgers vectors parallel to the twin plane to pass through. probably by an indirect mechanism involving two or more dislocations (see section 3).

We consider now the interaction between a twin boundary and a glide dislocation whose Burgers vector is inclined to the twin plane. If the dislocation passed unchanged into the twinned crystal it would have a Burgers vector of the type $1/6\langle 114\rangle_T$ (where the subscript T (twin) indicates vectors in a coordinate system mirrored at the (111) plane with respect to that of the matrix). Since 1/6<114> is not a translation vector of the lattice, the twin plane is a much higher barrier to dislocation transfer in this case. The dislocation with a 1/6<114> Burgers vector can dissociate into a Frank and a

Shockley partial according to (see e.g. FORWOOD and HUMBLE 1975):

$$1/2[110] \longrightarrow 1/6[\bar{1}\bar{1}\bar{4}]_T \longrightarrow 1/3[\bar{1}\bar{1}\bar{1}]_T + 1/6[11\bar{2}]_T$$

$$1/2[110] \longrightarrow 1/3[111] + 1/6[11\bar{2}] \, . \tag{1}$$

This reaction can be seen as a decomposition into partial dislocations with Burgers vectors parallel (Shockley) and orthogonal (Frank) to the boundary, which are common vectors in both crystals.

The decomposition in eq. (1) will proceed via either a case (I) or case (II) mechanism depending on the angle between the Burgers vector of the leading partial and the twin plane, which can be 28.1° (type A) or 70.5° (type B). The decomposition of type A partials has been treated above. The decomposition of a type B leading partial would create a stair rod of the type 1/3<110>, giving rise to an energy barrier higher than that for constriction. For either type of leading partial, the final result is a sessile Frank and a glissile Shockley partial. Since they exert no force on each other, it depends on the shear stress component on the twin plane whether they will separate or not. The energy of the decomposed dislocation equals that of the constricted dislocation.

The direct transfer (case III) is energetically less favourable than for dislocations with a Burgers vector in the twin plane. The Burgers vectors of the stair rod dislocations introduced by transfer of the leading and trailing partial are 1/18<112> and 1/9<112>. They are parallel and do not cancel, but sum up to a Shockley partial with a Burgers vector in the twin boundary. This partial is attractive to the transferred dissociated dislocation with an extrinsic stacking fault. Even neglecting the core energies of the five Shockley partials involved, the total energy of this transferred dislocation is well above that of a constricted dislocation. Thus for inclined Burgers vectors mechanisms (I) and (II) will be favoured, although none of the reactions is energetically favourable or even neutral, since in each case the final energy level is at least that of a constricted dislocation.

As for dislocations with Burgers vectors lying in the twin plane, <u>the partial dislocations create steps in the twin boundary, but no stacking fault</u>. The important difference in this case is the introduction of a sessile perfect dislocation or a sessile Frank dislocation. The decomposition reaction is shown in fig. 3, in a material with only the short term diffusion treatment. The microtwin investigated has a thickness less than 10 nm and is separated by at least 50 um from the next twin defect. The twin lies on the $(1\bar{1}\bar{1})$ plane. Dislocations of two slip systems on either side of the microtwin are piled up due to the formation of sessile Frank dislocations. The Frank dislocations in front of the pile-ups (arrows) are nearly extinguished using the (220) reflection (g b x l = 0).

YANG et al. 1980 observed similar pile-ups and interpreted them as the reaction of a perfect 60° dislocation with a Shockley partial in the twin to form a Frank partial. This Frank partial was assumed to dissociate into a sessile Shockley partial and a stair rod dislocation. The latter reaction is unlikely and was not observed. The former reaction is energetically favourable, but its probability is low, since only one of the six Shockley partial Burgers vectors allowed in the twin plane can create the Frank dislocation. Furthermore the complicated stepped structure of the twin plane lowers the probability of this reaction. The analysis (see fig. 3) showed the simple decomposition to be more likely, since the Burgers vectors of the observed pairs of Shockley and Frank partials could be summed to the Burgers vector of the perfect dislocations in the corresponding pile-up.

3.2. Influences on the material properties

All the interaction mechanisms discussed result in a considerable resistance to dislocation motion and recovery of the material. (This resistance may be increased by the presence of other dislocations in the twin boundaries and the complex interactions that result.) The mechanical properties of EFG ribbons are strongly affected by these mechanisms. For instance, impeding of recovery by dislocation glide forces stress relief to occur by another mechanism, deformation twinning. Thus considerable areas of the ribbons are covered by microtwins. frequently arranged in dense twin bundles. Microtwin separations of 0.1 um and less can often be found. However- the barrier action of twins and microtwins has additional effects on the material properties besides the observed high brittleness of EFG silicon at low temperatures (compare section 3.5.). Coherent twin boundaries have been shown to be electrically inactive (YANG et al. 1980. STRUNK, CUNNINGHAM and AST 1981). However. once the twins collect dislocations they can influence the efficiency of solar cells. In such cases, with high dislocation densities in the twin boundaries (see e.g. in fig. 1), very strong recombination activity is expected. Defects of this type are imaged in fig. 4 by the EBIC technique in the scanning electron microscope (see e.g. LEAMY 1982). In this imaging mode, electron/hole pairs are injected by the scanned high energy electron beam (in this case 30 keV) and are separated at the diffused p-n junction of the solar cells. They give rise to a current in the external circuit of the detection system modulating the intensity of the synchronously scanned cathode ray tube. Minority carriers recombining at an electrically active defect result in a local reduction of this current and cause the visible dark contrast.

Fig. 4 is an EBIC micrograph of a piece of solar cell. Since it is known that dislocation-free coherent twin boundaries have negligible EBIC contrasts (see e.g. STRUNK et al. 1981), only the twin boundaries with collected dislocations appear as straight dark lines. The spotted background is caused by the dispersed dislocations. Within dense twin bands the crystal is shielded against the penetration of glide dislocations. Thus areas with significantly higher local collection efficiencies are produced. Two such dense twin bands (bright contrast), which were optically observed to contain many microtwins. can be seen in fig.4. This influence of twin bands may be further demonstrated by the TEM micrograph in fig. 5. taken at the very edge of a dense twin bundle. The material was untreated except for the standard diffusion procedure. Within the limitations of a TEM inspection, the dense twin band did not contain any dislocations. As discussed later such "border twins" may have an important function. The effect of dislocation-free areas is, however. limited by the relatively high density of dislocation sources in the material. most of which appear to reside at the surfaces. Twin spacings of a few microns seem to be sufficiently large to permit dislocations to enter. This conclusion may be drawn from the observation of dislocations with Burgers vectors out of the twin planes in between microtwins of twin bundles. The only other explanation for their presence could be the indirect transfer of such dislocations. This dislocation transfer is possible by the interaction of a Frank partial with either of the two Shockley partials that will produce a dislocation glissile in the $\{111\}_T$ glide plane containing the Frank partial. For example:

$$1/3[\bar{1}\bar{1}\bar{1}]_T + 1/6[\bar{1}\bar{1}2]_T \longrightarrow 1/2[\bar{1}\bar{1}0]_T . \qquad (2)$$

Such reactions, especially repeated reactions, have a relatively low probability. The necessary Burgers vectors, with "negative sign", can be introduced by dislocations with a Burgers vector in the twin plane. The complicated stepped structure of the twin boundary and the possibility of annihilation of Shockley partials reduces the likelihood of this reaction (equation (2)) but it has a considerably higher probability in single twin planes. where the dislocations can be introduced from both sides.

3.3. Twin-induced formation of grain boundaries

In this section further consequences of the interaction between dislocations and twin boundaries are discussed. Models and suggestions are presented to explain our own observations and also those published in earlier papers. The accumulation of dislocations at twin boundaries has an important consequence: each dislocation collected results in a small misorientation of both crystal parts out of the perfect twin relation. Hence, twin boundaries such as those shown in fig. 1, are in fact small angle grain boundaries superimposed on the twin boundaries, which are usually referred to as "near-twin" boundaries (compare e.g. HOWELL et al. 1978). Measurements of Kikuchi line shifts at such planar defects showed a rotation out of the perfect twin relationship of typically a few tenths of a degree. (The values fluctuate. since the ribbons are very inhomogeneous.) The orientation relationships observed range from pure tilt through various combinations to nearly pure twist. The "boundary" in fig. 2 for instance appears mainly to be a twist boundary. The residual stress level after growth. and as a consequence the number of dislocations incorporated during recovery, depend on the growth conditions and seem to increase with the growth speed.

Evidence exists that the mechanisms described above also operate during growth of the ribbons. As mentioned before. the majority of twins in the material are parallel to the <112> growth direction. once steady state conditions are reached (for more details see e.g. WALD 1981). Occasionally it is observed that twin bands, such as those shown in the optical micrograph of fig. 6, are slightly inclined, or tilted, with respect to each other. Such tilts can simply be understood by the collection of dislocations in the twin planes as discussed above. However, careful measurements of the tilt angles reveal a continuous increase of the tilt angle along the growth direction. This indicates that there may be a cumulative effect during the ribbon growth. A perfect growth twin may collect dislocations close to the solid/liquid interface, forcing the crystal to grow a "near-twin" boundary. As growth proceeds, this boundary may collect more dislocations, increasing the tilt angle and so forth. If the misorientation becomes too large, the "near-twin" boundary may dissociate into a perfect twin boundary and a grain boundary.

Recent investigations (YANG et al. 1980. AST et al. 1982. GLEICHMANN, CUNNINGHAM and AST 1984) have shown that the main change in EFG ribbons during processing is the generation of low angle grain boundaries. The boundaries investigated in these papers have been mainly of the tilt type. The measured tilt angles have ranged up to about 5^o. Since grain boundary formation was reported even in materials having only an average dislocation density of 10^4 cm^{-2}, the local concentration of dislocations via twin boundary-dislocation interactions is an essential step to initiate polygonization. Whether the pile-up arrangement shown in fig. 1b is an initial stage in this process is not yet clear.

The process-induced grain boundaries (discussed in the previous paragraph) may also be introduced by releasing superimposed boundaries from their twin boundary matrix. It is likely that the net Burgers vector of the dislocations introduced into a twin boundary will be inclined to the (111) boundary plane. This creates a shear stress on the boundary plane. The superimposed low angle grain boundaries are forced to develop in the (111) twin plane where they are asymmetric and with increasing dislocation density the energy of the grain boundaries starts to play an important role. Thus a driving force exists to move the superimposed boundary out of the twin plane towards a symmetric orientation with a lower grain boundary energy. This driving force could be strong enough to initiate a process of boundary emission at sufficient high temperatures (compare also AST, CUNNINGHAM and GLEICHMANN 1984). At the border of the twin band in the lower section of fig. 6, some small angle grain boundaries appear to break away from the twin planes (arrows). The emission of a grain boundary may be demonstrated in the optical micrograph of fig. 7.

There is a fourth mechanism for creating grain boundaries, via "dissolution" of microtwins by the absorption of suitable dislocations. The mechanism is a possible explanation for the formation of subsurface grain structures as described by RAO. CRETELLA, WALD and RAVI 1980 or KALEJS 1983. Such structures develop in thicker ribbons, probably due to the higher temperature difference between the surface and the ribbon volume causing higher thermal stresses. Support for this mechanism is provided by the observation that the formation of the subsurface grain structure is accompanied by the dissolution of twin bands which previously ran from surface to surface. This may be ascribed to decomposing glide dislocations introducing steps in the twin boundaries. In the case of dislocations with Burgers vectors in the twin plane. two glissile Shockley partials are created. By moving these partials apart the thickness of the microtwin can be reduced by one layer. Repeated absorption of such glide dislocations removes successively more of the defect, and may remove it completely. Under realistic conditions, however. complex dislocation interactions will impede the twin destruction. Examples for such complicated interactions can be found in figs. 1 and 2.

Dislocations with Burgers vectors parallel to the twin plane are more easily transferred, and this allows one possible twin dissolution mechanism to occur. The interaction energy of partial dislocations introduced between two barriers (e.g. sessile dislocations) increases with their number. After a certain density of partials has developed between the barriers, the energy of constriction becomes less than that of introducing two more partials into the twin boundary. and therefore subsequent incoming dislocations will be transferred. Once they reach the "empty" back surface of the microtwin they can remove the microtwin layer by layer. All the dislocations with other types of Burgers vectors left behind at the front surface of the microtwin form a grain boundary. Microtwins with shielded back surfaces, such as the border twins of dense twin bundles, are more likely to be converted into grain boundaries in this way. Since many microtwins are only a few atomic layers thick, an appreciable fraction of twins may be removed by this mechanism.

Further investigations are needed to show which of the suggested mechanisms for releasing or generating grain boundaries are more likely. For all the grain boundary formation mechanisms discussed above, twin boundaries are essential and each mechanism can be described as twin-induced.

3.4. Interactions between grain boundaries

The inspection of ribbons with ten minute or one hour anneal at 1200°C prior to diffusion indicates that the formation of small angle grain boundaries still does not represent a final configuration of the defect structure. Following such a pre-anneal at 1200°C the material contains several complicated large angle grain boundaries (GLEICHMANN et al. 1984). The results up to now suggest that these large angle boundaries are not formed by the continued accumulation of glide dislocations. Instead, several individual low angle boundaries may react with each other and form more complex boundaries. The orientation relationship across such boundaries appears to be more or less accidental and cannot be described by a low index rotation axis. The EBIC micrograph of a ten minute pre-annealed solar cell is given in fig. 8. It may demonstrate the interaction of small angle grain boundaries with each other.

In some cases it was observed that the boundary plane of a large angle grain boundary is the {111} plane of one of the crystals. This points to an important influence of twins on the movement of grain boundaries and may also explain the very complex orientation relationships between the grains often found. Fig. 9 is an example of the reaction of a large angle grain boundary with twins. The plane of the figure on the side of the microtwins is near {100} and across the boundary it is about 10° out of a {112} orientation. The boundary reaches the first microtwin and "absorbs" it (mark A). At the second microtwin the boundary tilts into the twin orientation, merges with the thin microtwin and continues as a more complex large angle grain boundary (mark B). Further work has to be done to reveal the details of such boundary reactions.

3.5. Glide-induced twinning

Finally, another dynamic interaction process between dislocations and twin boundaries will be discussed. As reported by STRUNK, CUNNINGHAM and AST 1981, the electrical activity at twin boundaries is strongly enhanced at intersections between twins of different orientation (second order twin joins). An example of such a second order twin join is given in fig. 10. The origin of the Shockley partial dislocations in the thin microtwin lamella inclined to all the others may not in each case be due to the direct incorporation of glide dislocations, visible in the very beginning of decomposition (see arrows). Similar electrical behaviour was reported by CUNNINGHAM, STRUNK and AST 1982 at the intersections of stacking faults linking the twin boundaries of microtwins. Both defect types discussed in these papers seem to have the more or less regular arrangement typical of a glide band distribution in a deformed material. Although no special investigations have been done so far a possible model for their formation will be proposed.

It was shown in eq. (1) that a dislocation with a Burgers vector inclined to the twin plane can introduce a sessile Frank dislocation and as a consequence lead to a dislocation pile-up (see fig. 3). Since the effective stress on the leading (perfect) dislocation in the pile-up is the applied stress multiplied by the number of dislocations in the pile-up, very high stresses may be produced during cooling of the ribbons. Under these high stresses the leading dislocation in the pile-up may react with the Frank dislocation according to:

$$1/3[111] + 1/2[110] \longrightarrow 1/6[552] . \qquad (3)$$

The Burgers vector of the reaction product transferred to the twinned lattice is $1/2[\bar{1}\bar{1}\bar{2}]_T$. This type of dislocation has often been described in the literature on small angle grain boundaries in silicon and germanium (see e.g. BOURRETT and DESSEAUX 1979, CUNNINGHAM and AST 1983). In addition CUNNINGHAM and AST 1983 observed the generation of microtwins at dislocations of this type. The dislocation is unstable and dissociates into three partial dislocations according to:

$$1/2[\bar{1}\bar{1}\bar{2}]_T \longrightarrow 1/6[\bar{1}\bar{1}\bar{2}]_T + 1/3[00\bar{1}]_T + 1/3[\bar{1}\bar{1}\bar{1}]_T . \qquad (4)$$

One important feature of this dissociation is that the initiating Frank dislocation is recreated and can again react with the next glide dislocation in the pile-up. The Shockley partial created is glissile on a glide plane inclined to the twin and if the stress level is high enough, it can move away to release the stress concentration. As discussed above, such a partial dislocation is likely to be stopped at the next twin plane on its glide path. Otherwise, the stacking fault length depends on the stress distribution. The energy necessary to generate subsequent layers of the developing microtwin by glide of Shockley partials is much less than the energy required to form the initial stacking fault. The Shockley partials increase the thickness of the microtwin by another layer by moving a step across. The continued operation of this mechanism requires dislocation climb and hence elevated temperatures. The brittleness of the material at lower temperatures in combination with the observation of crack formation at twin bands seems to support this explanation.

Fig. 11 shows the rarely observed example of the termination of a thin microtwin lamella within the crystal. Though no completely decisive analysis of the closely spaced dislocations at the very end could be achieved, their contrast behaviour is consistent with that of Shockley partials. The Shockley dislocations which are still bowed out on their way to the end have been clearly identified to be of the same type as expected from the straight dislocations at the tip.

SUMMARY

During growth and subsequent heat treatments of EFG silicon ribbons, the grown-in defect structure recovers by the plastic deformation; this recovery process is impeded by the presence of grown-in twins. The main mechanism considered is the interaction of glide dislocations with coherent twins and microtwins. The twin boundaries are barriers to dislocation motion and usually force the dislocations to decompose into partial dislocations lying in the twin plane. In the case of Burgers vectors parallel to the twin plane. decomposition produces two glissile Shockley partials, otherwise a sessile Frank and a Shockley dislocation are introduced. In the latter case the main consequence is a dislocation pile-up giving rise to low temperature brittleness with crack formation at the twin plane. A mechanism is proposed which can lower the stress concentration at a pile-up via glide-induced twinning at high temperatures.

With respect to electrical properties, two effects are considered: (I) the change in character of the twins from a neutral to a recombination-active state due to the collection of dislocations, (II) the shielding of large crystal areas from the injection of recombination-active dislocations. The collection of dislocations at twins can cause the formation of grain boundaries and several possible mechanisms for releasing or generating these boundaries are discussed.

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FIGURE CAPTIONS

Fig. 1: TEM micrograph showing the accumulation and incorporation of glide dislocations at microtwins.

Fig. 2: TEM analysis of a "near-twin" boundary resulting from the decomposition of glide dislocations into two Shockley partials in the twin plane (Burgers vectors parallel to the plane). The arrows indicate closely spaced (13 nm) Shockley partials (see text).

Fig. 3: TEM micrograph of the pile-up formation due to decomposition of glide dislocations with Burgers vectors inclined to the twin plane.

Fig. 4: EBIC micrograph taken from a solar cell containing recombination active twins (decorated with dislocations) and dense twin bands with high local collection efficiency.

Fig. 5: TEM micrograph of the edge of a dense microtwin bundle. Note the absence of dislocations inside the band.

Fig. 6: Optical micrograph of twin bands slightly tilted with respect to each other. The arrows indicate small angle grain boundaries developing at the lower band edge.

Fig. 7: Optical micrograph showing the emission of a small angle grain boundary from the edge of a twin band.

Fig. 8: EBIC micrograph of the interaction of grain boundaries in a solar

cell which was ten minutes pre-annealed at 1200°C prior to diffusion.

Fig. 9: TEM micrograph showing the interaction of a large angle grain boundary with microtwins (arrows see text).

Fig. 10: TEM micrograph of a second order twin join formed by microtwins with different orientations. The arrows mark regions of decomposing glide dislocations with Burgers vectors parallel to the twin.

Fig. 11: TEM micrograph showing a very thin developing microtwin ending within the crystal.

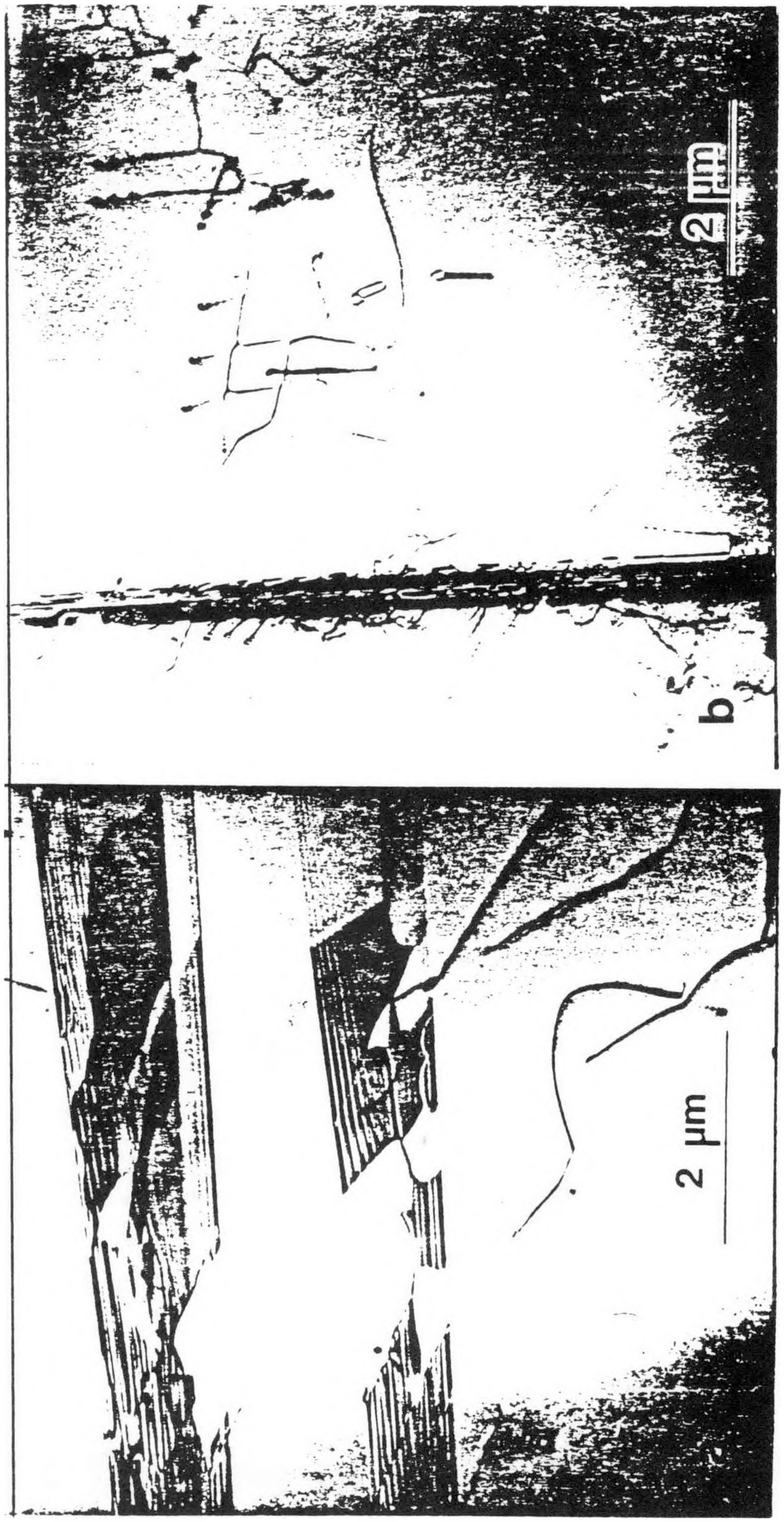
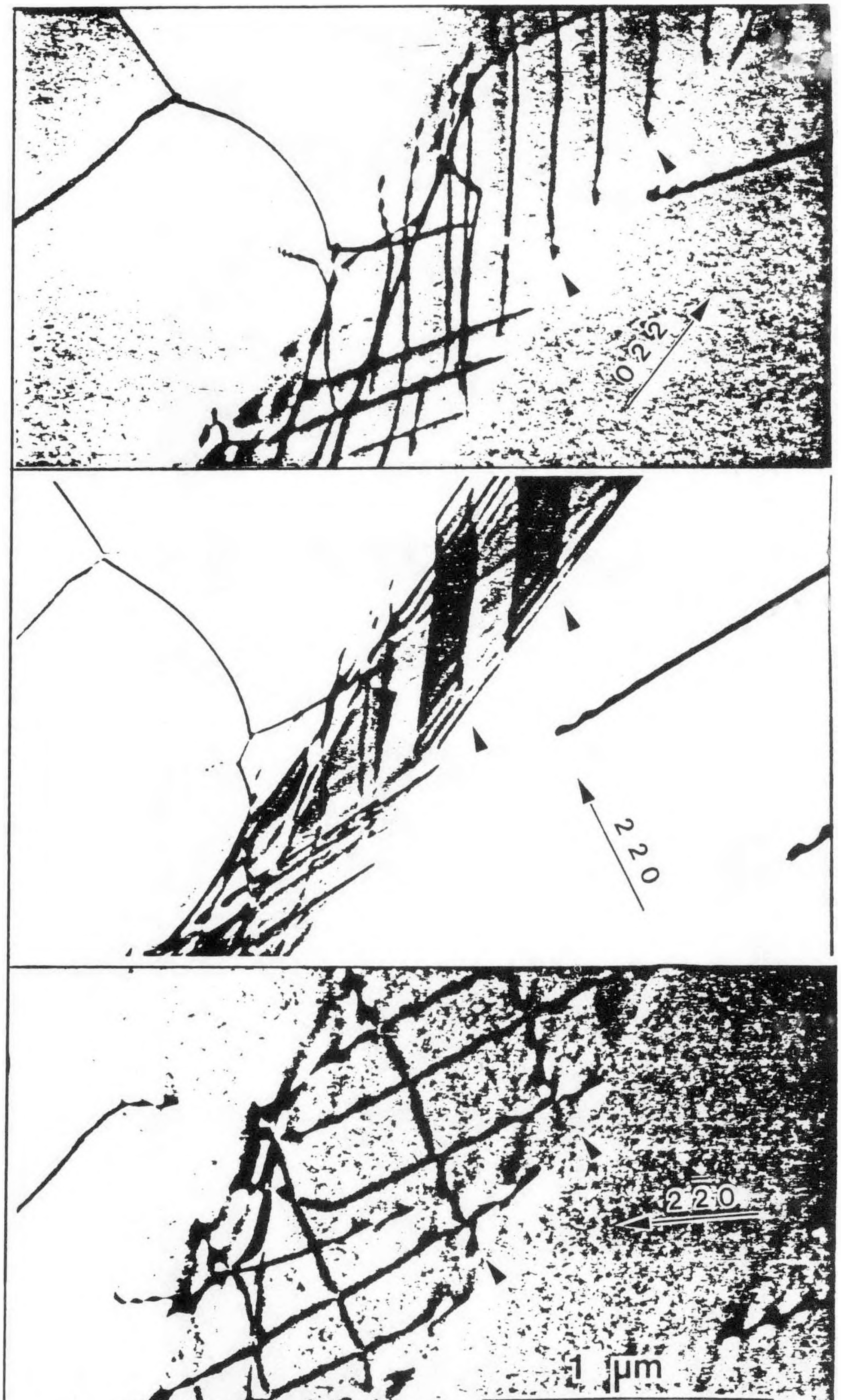


Figure 1



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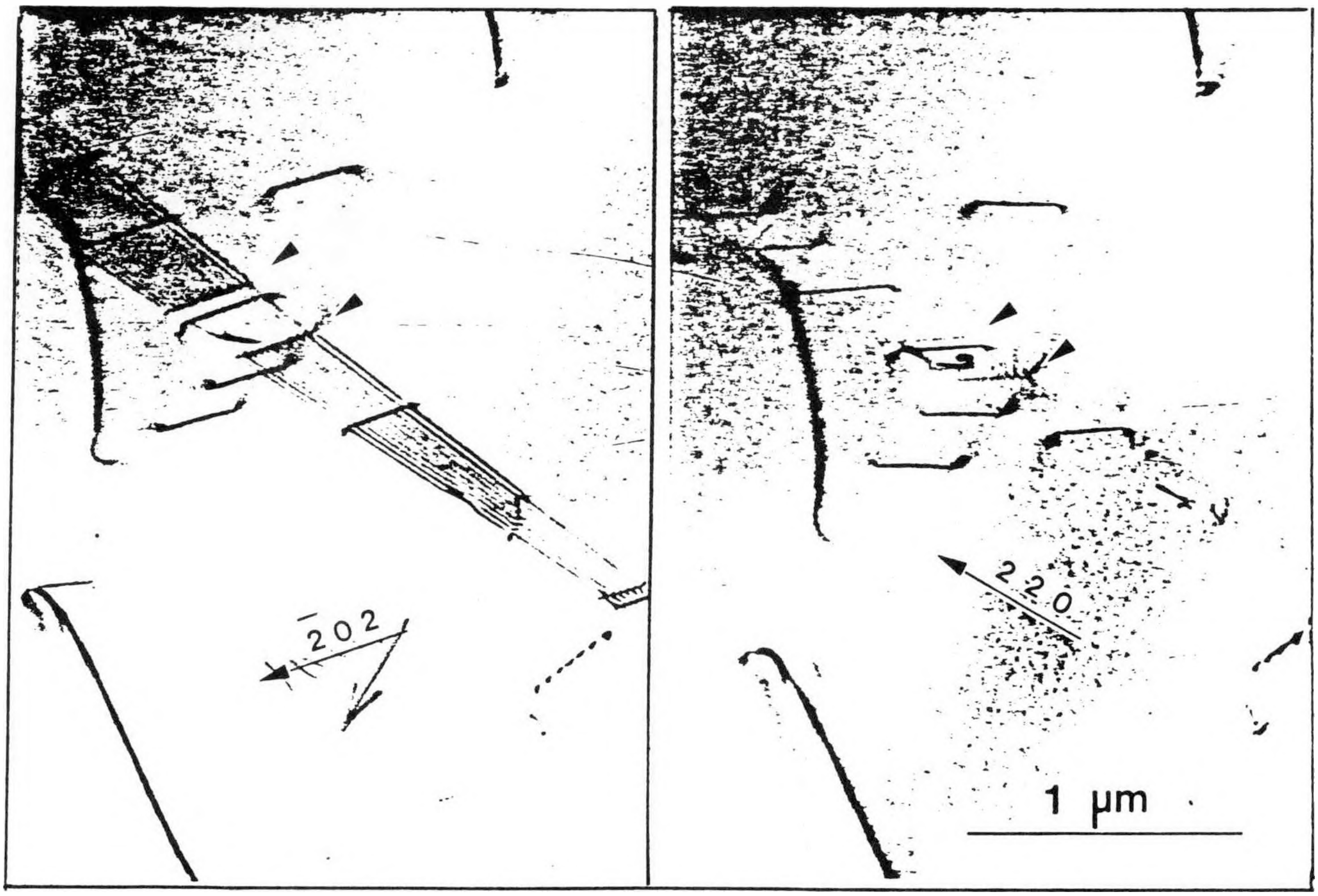
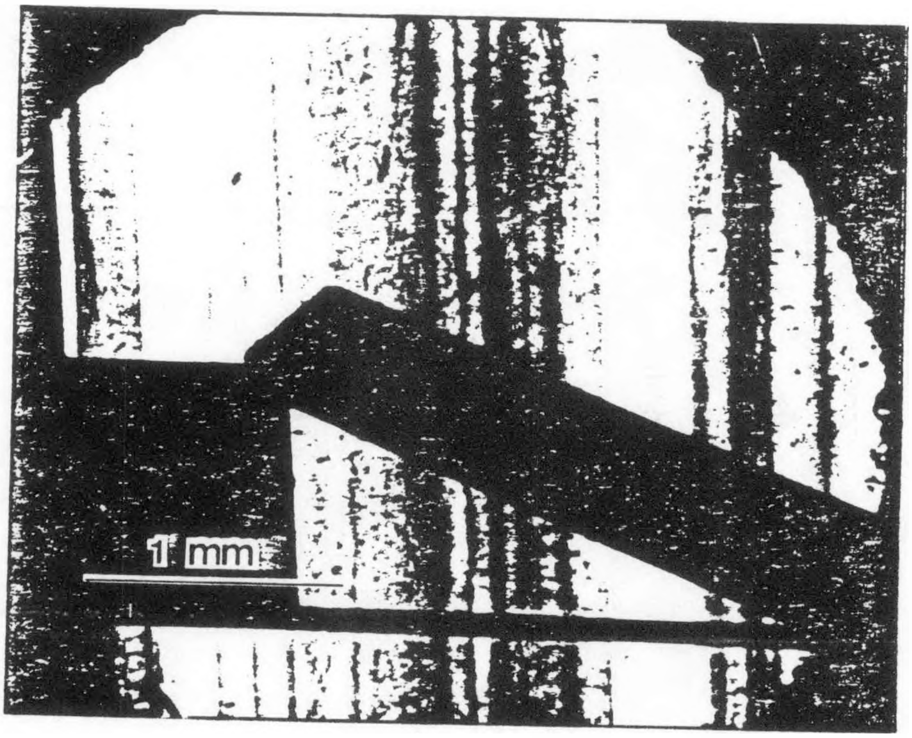


Figure 3

Figure 4



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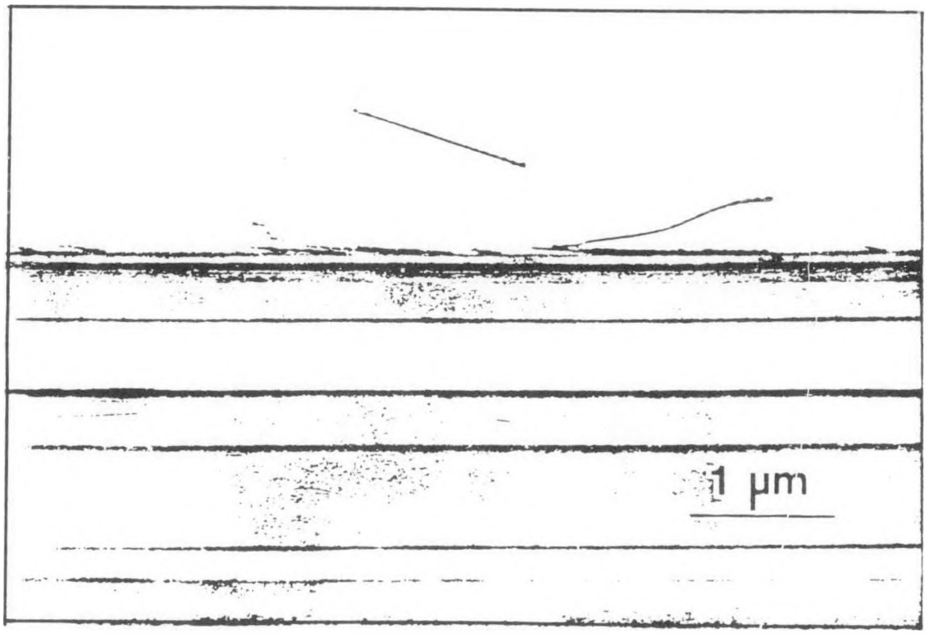

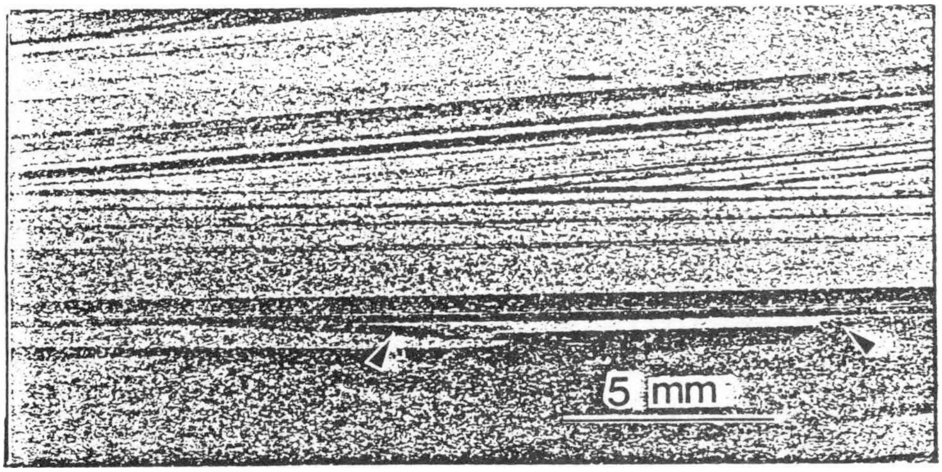

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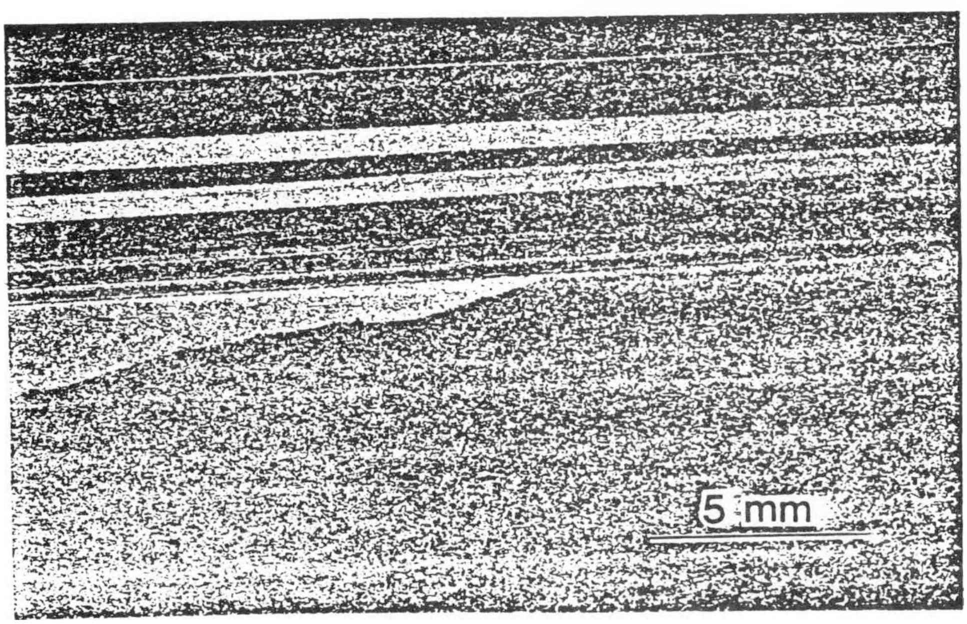

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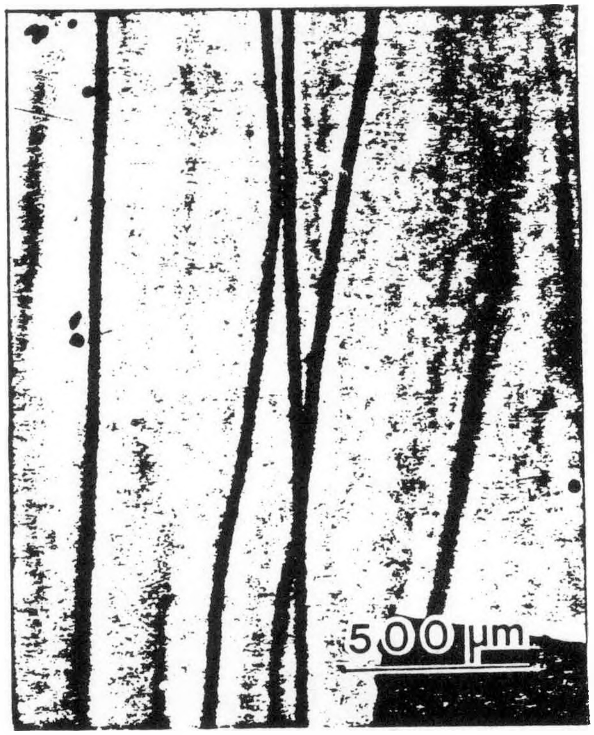

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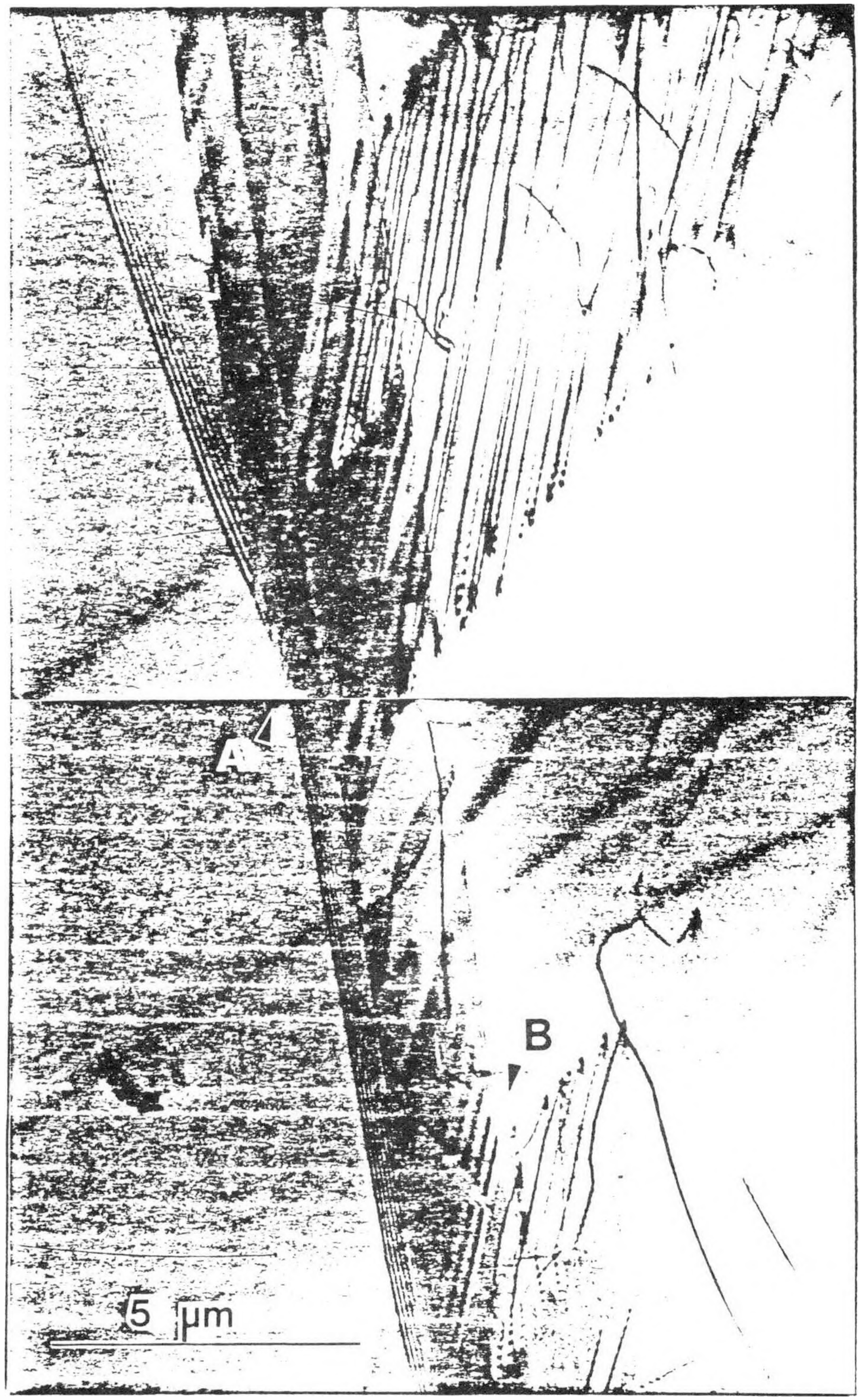

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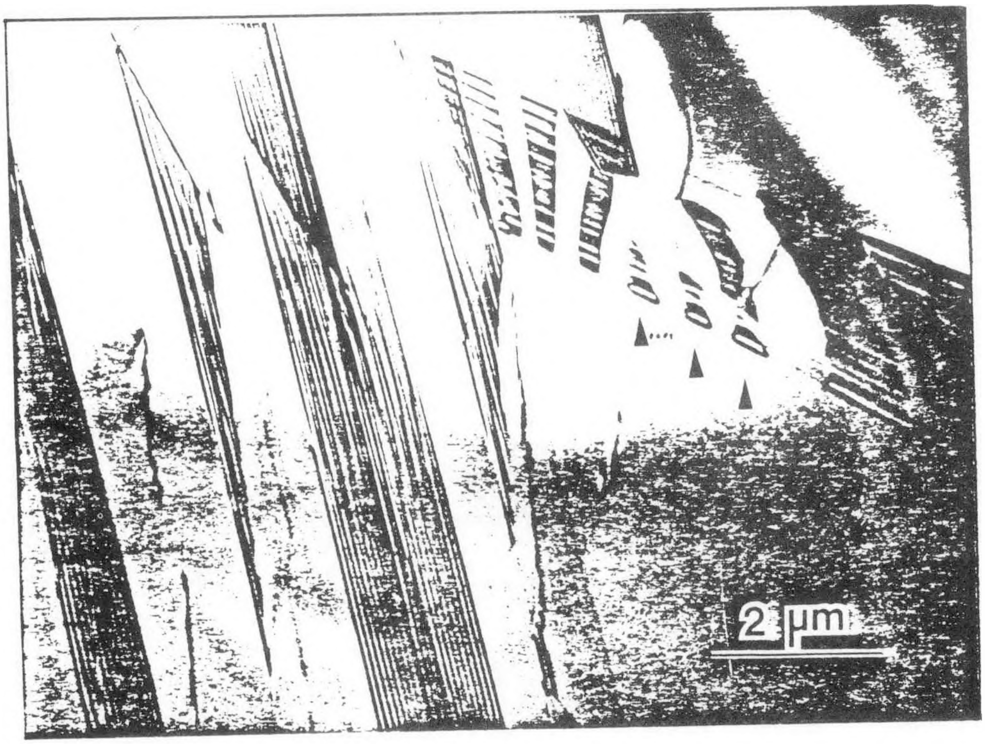

Figure 10

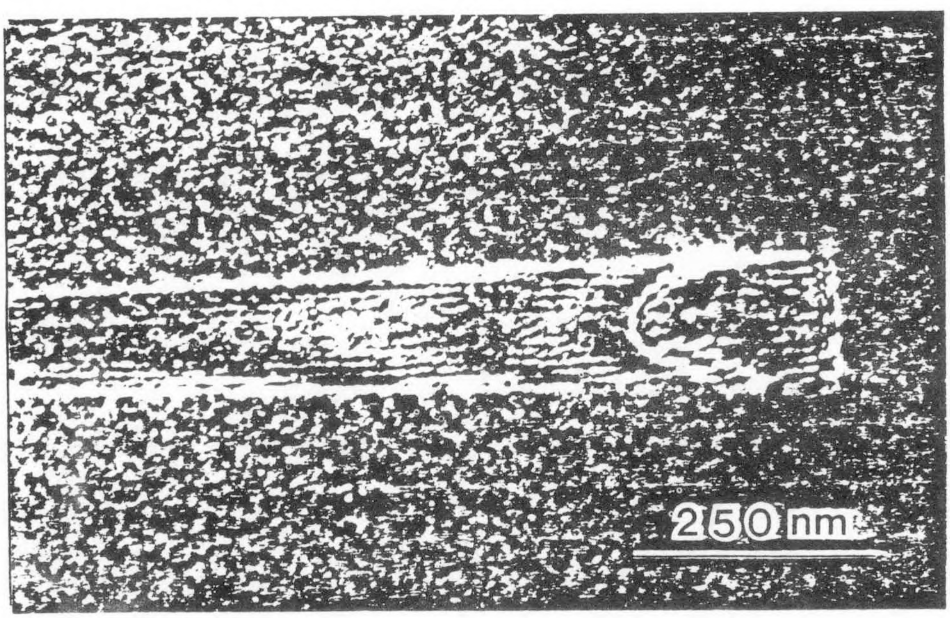

Figure 11

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