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ORIGIN AND MULTIPLICATION OF DISLOCATIONS

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ORIGIN AND MULTIPLICATION OF DISLOCATIONS

A Review Presented at the
AIME Western Metals Congress,
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1. INTRODUCTION

Although the concept of the dislocation was introduced in 1934 by Taylor(1) Orowan(2) and Polanyi,(3) it was not until the early part of the 1950's that more detailed considerations of the theory were well developed.(4-6) At this time the experimentalists were still far behind the theoreticians but over the past ten years the gap between theory and experiment has been almost completely reduced, mainly as a result of careful etch pit studies (e.g., see references 7- 10) and direct observations of dislocations by electron and x-ray metallography.(9, 11, 12) Whilst it is now well known that dislocations really exist in crystals, there is still considerable debate as to how they came to be present in the first place. The debate centers around whether dislocations are nucleated homogeneously or heterogeneously.

From elasticity theory, the self energy of a dislocation line is ~ 5 eV per interatomic distance, i.e., about five times larger than the formation energy of a row of vacancies. This means that dislocations are not created easily in a perfect lattice. For example, a stress $\approx G/30$ would be required to nucleate a dislocation homogeneously (G is the shear modulus). Consequently, heterogeneous nucleation is the most likely process

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for formation of dislocations. A number of possibilities have been suggested, viz., (i) dislocation loops formed from condensation of vacancies during crystal growth (ii) dislocation nucleation and multiplication from impurities, grain boundaries surfaces, and multiplication of dislocations already present by thermal and mechanical stresses, and (iii) dislocations produced as a result of impurity segregation during solidification.

Since the density of dislocations is observed to increase by several orders of magnitude during deformation, it became clear that multiplication must occur continuously as slip proceeds. With the introduction of the concept of the Frank-Read source in 1950 it was thought that the problem of multiplication was solved. However, although Dash(7) observed classical Frank-Read sources sometimes in silicon, little or no evidence for their importance has been obtained from experiments on ionic and metallic crystals. Recent work using the electron microscope has demonstrated the importance of impurities and grain boundaries as sources and in this paper qualitative considerations are given to the various possible mechanisms which may account for the origin and multiplication of dislocations. Examples illustrating the various possibilities have been obtained by transmission electron microscopy.

2. DISLOCATION SOURCES

2.1 Dislocations Formed from Vacancy Aggregates

The equilibrium concentration, c, of vacancies in a crystal increases with temperature as $c = A \exp(-E_f/kT)$, where A is an entropy factor (1-10 for metals) E_f the formation energy of a vacancy (e.g., for Al, $E_f = 0.76$ eV), k is Boltzmann's constant and T the absolute temperature. At the melting point c is ~ 10^{-4} for FCC metals. If cooling from the melting point occurs fast enough to retain all these vacancies in the crystal so that they do not escape to sinks (surfaces, boundaries, dislocations) supersaturations of the order of 10^9 are possible. Typical quenching speeds to achieve this supersaturation are 10^4-10^6°C/min., which is considerably faster than the cooling rates occurring during normal solidification. However, the local concentration at the solid-liquid interface is such that there will always be an excess of vacancies behind this interface. If there are enough vacancies present, they will tend to cluster together and precipitate, forming dislocation loops when the temperature has fallen such that the local supersaturation is high enough for a critical number of vacancies to nucleate a loop (e.g., see reference 13). The critical temperature corresponding to this condition is quite low(15) (~ 150°C for Al, 380°C for Cu). Elbaum(14) and Jackson(15) have shown conclusively that, except for very small crystals, there is insufficient supersaturation of vacancies during crystal growth to nucleate dislocation loops. These supersaturations are only attained by special quenching experiments or by irradiation of materials by α-particles, neutrons, or electrons. Figure 1 is an example of dislocation loops formed in a quenched Al alloy. Furthermore, in the presence of impurities nucleation of loops is more difficult because impurities trap vacancies, thereby effectively reducing the supersaturation.(13)

Chalmers(16) suggested that vacancies would be trapped at the solid-liquid interface. As the interface advances during freezing, more vacancies will be trapped until eventually they collapse to form a dislocation half loop with the ends of the part-dislocation loop terminating at the interface. As the interface advances, the dislocations increase in length. If the local stresses are high enough, multiplication may occur. Jackson(15) pointed out that such dislocation loops could only be formed if the growth rate is faster than a few mm/sec, which is again larger than the freezing rates attained in practice.

It now seems to be generally agreed that formation of dislocations from collapsed vacancy aggregates does not occur during solidification, so that dislocations must be nucleated by other mechanisms. However, if dislocations already exist in the crystal, the total length of dislocation line can be increased by climb or glide during cooling. For example, as a result of climb, edges become jogged and screws transform into helices.(13)

2.2 Dislocation Networks Formed During Solidification

There are three main kinds of substructure (which can be observed with the light microscope) formed in crystals grown from the melt, viz., dendritic, cellular and lineage structures.(14, 17, 18) Since a nucleus of solid is formed homogeneously only when the liquid is supercooled sufficiently, a nucleus once formed is surrounded by supercooled liquid and will grow dendritically provided a reverse temperature gradient or supercooling persists. The tip of the dendrite may be bent by mechanical disturbances, gas evolution, convection currents, or as a result of strains due to segregation of solute atoms to the liquid which solidifies last. Consequently, this dendrite can acquire slight misorientations with respect to its neighbors.

These misorientations can be matched when the dendrites meet each other by the formation of edge dislocation tilt boundaries, screw dislocation twist boundaries, or subboundaries containing mixed dislocations. Such networks give rise to the so-called lineage or mosaic structure in solidified crystals. Examples of mixed and twist boundaries are shown in Figs. 2 and 3.

It appears that dislocations can thus be formed as soon as the first solid is nucleated and a perfect crystal results only if these can be eliminated and the formation of subsequent dislocations prevented.

If segregation of impurities occurs, the last traces of liquid to solidify will have a different composition from the initially solidified dendrite. This usually means that the lattice parameters of both will also be different. As a result of the gradual change in lattice parameter across the freezing solid, a system of edge dislocations may be set up as sketched in Fig. 4. Similar substructures can be formed around particles when precipitation occurs in the solid state. However, experimentally there is not a significant change in dislocation density between crystals grown with and without the cellular impurity substructure and a large difference in density would be expected if this were an important mechanism.(14, 15)

In any case of a solid growing on a solid already containing dislocations, then at the growing face dislocations existing in the substrate may propagate into the new crystal since a dislocation must terminate at a free surface or in other dislocations of different directions (at nodes). In principle, it is possible to grow dislocation-free crystals if the formation of new dislocations during and after growth is prevented. So far, only the covalent crystals Si and Ge(20) have been grown perfectly and no success has yet been reported for metallic and ionic crystals.

If the surface of a seed crystal or substrate is stepped, the discontinuity may be accommodated upon subsequent growth by the generation of dislocations or stacking faults. This is particularly true if impurity atoms are adsorbed on the surface. Recent experiments on vapor deposition of silicon(22) have shown that oxygen is mainly responsible for the growth faults commonly observed in epitaxial deposits. Figure 5a shows an example of these faults and Fig. 5b the suggested effect of oxygen as nucleation sites for the nucleation of the faults.

If two widely misoriented dendrites meet, a large angle grain boundary will be formed. Such a boundary can contain a large number of dislocations, particularly at steps in the boundary.(19) Figure 6a is an example of such a stepped boundary. If the local stress is high enough, these dislocations can be emitted from the boundary, thereby, eliminating the step. Figure 6b is an example of a boundary source that has emitted five dislocations.

The stresses necessary for nucleation and multiplication during cooling probably originate from: (1) Local stresses due to dislocation arrays already formed in the solid; these stresses are probably the main cause for propagation of a small angle boundary into newly solidified layers(21) (2) Stresses due to segregation and atomic misfit, e.g., by differential thermal contraction (3) Thermal stresses due to nonlinear temperature gradients -- particularly if cooling is done rapidly. These stresses are likely to cause multiplication of the existing dislocations. For example, if the thermal stress at the interface is deliberately increased, an increase in dislocation density is observed.(20)

It seems that stress is often the most important cause of dislocations formed during growth from the melt and so the critical stress to move a dislocation must be an important factor. This is borne out by the fact that crystals of silicon and germanium can be produced free of dislocations.(20) Bonding in these crystals is covalent and very strong so that the Peierls stress is very high and dislocations in the diamond lattice are thus relatively immobile.

2.3 Heterogeneous Nucleation of Dislocations from Impurities

Gilman(23) subjected LiF crystals to short stress pulses (1-10 μ sec long) and found that the following heterogeneities lead to dislocation nucleation: (a) cleavage steps (b) dislocation loops (c) glide bands (d) inclusions (e) as-grown, and induced precipitates. Here, we shall consider nucleation at inclusions and precipitates.

A precipitate may act as a small punch inside the crystal in two ways: (1) by differential thermal contraction as the solid cools (2) as a result of "chemical stresses" arising from a localized excess (or depletion) of point defects associated with the removal of solute atoms from the matrix around the particle. The classical example of punching was provided by the experiments of Jones and Mitchell,(24) where prismatic dislocation loops and helicoidal dislocations were shown to emanate from glass spheres purposely introduced into AgCl crystals. Since this work, many examples of heterogeneous nucleation of dislocations from impurities have been observed.

In a metal containing precipitates or inclusions the coefficients of thermal contraction of inclusions are usually less than those of metals, so that the dislocation loops resulting from punching should be of the interstitial prismatic kind. Figure 7 shows an example of these loops observed in a Cu-Ag alloy quenched from 1065°C. They diminish in size with distance from the source so that they must be interstitial loops since the interstitials are gradually eliminated by combination with the vacancies retained in the alloy by quenching. If the loops were of the vacancy kind, they would expand by climb (due to the addition of vacancies) with increasing distance from the source. Figure 8 shows a similar example of dislocations punched out from grain boundary precipitates on both sides of the boundary.

The shapes of prismatic loops formed by a punching mechanism depends upon the shape of the particle from which the loops are nucleated.(23) Spheres or platelets can evolve circular loops, whereas, rods can make circular or elongated loops.

Consider now the case of partially coherent precipitates, i.e., precipitates whose interface with the matrix consists of a grid of dislocations(25) (as in Fig. 4). If the local stress is high enough, some of these interfacial dislocations may be emitted from the particle. Since the stress required to make a dislocation glide is inversely proportional to its free length, large precipitates are the most efficient nucleation sites. An example of a large precipitate which has nucleated many dislocations is shown in Fig. 9. A particle containing 1000 atoms in diameter would produce heterogeneous nucleation at a stress of $\sim G/100$, where G is the shear modulus. If all the dislocations are formed from particles, there must be $\sim 10^6$-10^8 particles/cm^3 in order to account for the observed dislocation densities. It is possible that in metals these particles are refractory oxides which are formed during melting prior to solidification. However, such particles are not usually observed in pure crystals.

Bardeen and Herring(26) proposed that an edge dislocation could give rise to dislocation loops by climb, as shown in Fig. 10a. If there is an excess (or depletion) of vacancies in the region around AB, the line AB moves down and out to form a loop which represents a plane of missing atoms. It should be noted that the climb source shown occurs by expansion of the dislocation normal to the Burgers vector, unlike the Frank-Read source (Fig. 10b) which operates by expansion of the line into loops by glide parallel to the Burgers vector. The source of the original dislocation in the Bardeen-Herring mechanism can be at a precipitate. Climb sources have recently been observed by a number of workers(27-29) and Figs. 11a, 11b are examples.

A Bardeen-Herring source will operate on a dislocation of length ℓ when(26)

$$\ell n \frac{c}{c_o} > \frac{G\ b^4}{KT\ell}$$

where c/c_o is the vacancy supersaturation. For typical values of G, b for FCC metals and taking $\ell \sim 200$ Å at 200°C, a source operates if the supersaturation is $\sim 10^2$. Such vacancy supersaturations can be attained by moderate cooling speeds during solidification and could also arise locally around the particles simply due to the removal of solute atoms from the matrix surrounding the precipitate.

In conclusion, it appears that impurity particles and grain boundaries are the most probable sites of dislocation nucleation in crystals. The stresses to operate such sources arise both from thermal stresses and localized non-equilibrium vacancy concentrations during cooling. Many researchers have also shown that surface damage caused by handling or by impurities falling onto the surfaces also introduces dislocations into crystals.(30, 31)

3. DISLOCATION MULTIPLICATION

3.1 Introduction

Plastic deformation occurs by the motion of mobile dislocations in a crystal. Not all the pre-existing dislocations are mobile, however, because some may not lie in glide planes and some may be pinned by impurities. If the initial number of mobile dislocations is small, yield points are observed in the stress-strain curves.

The plastic strain rate is usually expressed by

$$\gamma = b\ell v$$

where ℓ is the average length of moving dislocation/cm^3 and v is the average dislocation velocity. Both ℓ and v depend on stress, strain, temperature and impurities. The ratio ℓ/ρ, where ρ is the dislocation density does not remain constant during the deformation. Therefore, dislocation multiplication and nucleation of fresh dislocations must occur as the mobile dislocations pass through the crystal.(32)

One of the first direct experimental investigations of dislocation multiplications was carried out by Wilsdorf(33) on stainless steel specimens which were deformed whilst under observation in the electron microscope. Besides obtaining a rare example of a classical Frank-Read source, Wilsdorf observed dislocations nucleating from grain and twin boundaries, dislocation networks, precipitates, and as a result of dislocation interactions during glide.

3.2 The Frank-Read Mechanism and its Modifications

As was mentioned early, the Frank-Read mechanism as originally conceived in 1950 has not been observed frequently enough to account satisfactorily for the multiplication of dislocations. In the original model a length of dislocation line ℓ pinned at its ends can rotate around the pinning points producing an unlimited number of new dislocation loops (Fig. 10b). The stress required to operate such a source varies inversely as ℓ. For the observed yield stresses of most crystals, ℓ must be $\sim 1\ \mu$. The climb source depicted in Figs. 10a and 11 is analogous to the Frank-Read source, but is likely to operate only under special circumstances as described in section 2.3.

Except for the direct nucleation of dislocation loops, all examples of multiplication are really modifications of the Frank-Read model.

Let us consider any obstacle to the path of a moving dislocation as shown in Fig. 12.(33) Edge dislocations (Fig. 12a) become held up at the obstacle until they start bowing around until an appreciable screw orientation can be attained (at A). The screws then cross-slip to B above the obstacle, eventually leading to the formation of a prismatic loop DE behind the particle. This loop can glide on its prismatic surface. When screws encounter the obstacle (Fig. 12b), cross-slip from A to B may eventually lead to the operation of a Frank-Read source at CC. Typical obstacles which can give rise to multiplication are precipitates, subboundaries, and strongly pinned grown-in dislocations. Figure 13 shows a possible example of multiplication near precipitates since the density of dislocations near the precipitates is much greater than elsewhere.

When the obstacles are not randomly distributed, parts of the dislocation may eventually meet. If both segments are on the same glide plane, they will annihilate since the Burgers vectors are opposite in sense. If the segments are on parallel planes, those in screw orientation will tend to cross-slip together and annihilate. However, if the segments are of edge character, a dipole will be formed (Fig. 14). The dipole is stable when the two glide planes are separated by less than a critical value d_c but if d is $> d_c$, the dislocations can cross over one another (Fig. 14). The critical separation is given by

$$d_c = \frac{Gb}{8\pi(1-\nu)\tau}$$

where τ is the local resolved shear stress, ν is Poisson's ratio, and G, b have their usual meanings. The continuation of cross-over can lead to multiplication.(32) Figure 15 is an example of dislocation dipole formation and cross-over. It is thought that jogs on screw dislocations resulting from intersections or by absorption of point defects are mainly responsible for the cross-over mechanism. The interaction between gliding dislocations, sub-boundaries, or immobile dislocations is another possible origin of cross-over and multiplication.(32) The double cross-slip mechanism is important only if the stacking fault energy of the material is not too low. When the stacking fault energy is low, each dislocation is dissociated into two partials separating a stacking fault. Cross-slip or bowing of a dislocation out of its original plane can only occur if the two partials come together by constriction and this requires more energy the more widely separated are the partials (i.e., the lower the stacking fault energy). Consequently, dislocations in these materials (e.g., copper alloys and some stainless steels) rarely leave their original slip planes (Fig. 16).

In all the pure metals so far examined the stacking fault energies are not low (e.g., Al ~ 200 ergs/cm^2, Ni ~ 80 ergs/cm^2, Au ~ 40 ergs/cm^2) and the dislocation arrangements during deformation are complicated. Tangling and formation of densely populated dislocation cell walls are common features in the deformation of both BCC and FCC crystals (e.g., Figs. 17a, 17b). As the strain increases, the separation between dislocations in the tangles decreases as the dislocation density increases. In favorable situations some segments in the tangle may bow out and be released or may act as a Frank-Read source. Figure 17 shows examples of dislocation sources at cell walls in Nb and Ni. Since the critical stress for this mechanism to operate depends on the lengths of dislocation segments in the tangle, i.e., on the cell size, the flow stress varies inversely with the cell size. Kuhlmann-Wilsdorf(35) has recently discussed these effects in some detail to explain work hardening.

It has already been shown that in polycrystals grain boundaries act as sources of dislocations. It is now felt that the operation of grain boundary sources is one of the most significant factors controlling the effect of grain size upon strength.(19) It is also observed that the dislocation density for the same plastic strain and same grain size is independent of alloy composition and stacking fault energy.(36, 37) Since the double cross-slip mechanism is unlikely to operate in the low stacking fault energy materials, it appears that multiplication by cross-over (which does not necessarily involve cross-slip) is probably an important general multiplication mechanism.(32)

CONCLUSIONS

Dislocations appear to be formed easily in metals even when the most careful preparation techniques are employed. The origin of dislocations appears to be most satisfactorily explained by heterogeneous nucleation and multiplication due to stresses arising during solidification, particularly at grain boundaries and impurities. Multiplication of dislocations during plastic strain readily occurs by a number of processes essentially similar to the Frank-Read mechanism as soon as a dislocation starts to move. In polycrystals, grain boundaries appear to be the most common sources of dislocations. The differences in behavior between metals of different crystal structures, ionic and covalent crystals is not well formulated at the present time. More experimental work on the formation and growth of slip bands, e.g., by correlation of surface slip markings with the direct observations of dislocation arrangements in the bands, is essential before a complete understanding is to be obtained.

Acknowledgments

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Figure Captions

Fig. 1 Dislocation loops formed in Al-5% Mg solid solution after quenching from 550°C.

Fig. 2 A mixed dislocation sub-boundary with a strong tilt component due to a large number of parallel edge dislocations in Al-5% Mg solid solution.

Fig. 3 Twist dislocation sub-boundaries consisting of crossed grids of screw dislocations in Nb. Precipitation has occurred on part of the boundary.

Fig. 4 Schematic illustration showing the formation of edge dislocations at the interface between two crystals of different lattice parameters.

Fig. 5a Growth faults in epitaxially deposited silicon in [111] orientation. (Courtesy J. Appl. Physics)

5b (110) section through a scale model illustrating the effect of oxygen at the substrate surface in causing intrinsic (I) and extrinsic (II) faults in the deposited layer. (Courtesy J. Appl. Physics)

Fig. 6a A stepped high angle boundary in Nb containing many dislocations.

6b Showing the operation of a dislocation source at a high angle grain boundary in Nb.

Fig. 7 Showing prismatic dislocation loops punched from an impurity at A. Notice the loops diminish in size with distance from the source. The loops are thus of the interstitial kind. Cu-$\frac{1}{2}$% Ag quenched from 1065°C.

Fig. 8a,b Showing dislocations punched out on opposite sides of a grain boundary from precipitates (probably Mg_3Al_2) in Al-5% Mg quenched from 550°C. The specimen has been tilted a few degrees from (a) to (b) in order to bring each side of the boundary into contrast.

Fig. 9 A particle in stainless steel operating as a complex Frank-Read source.

Fig. 10a Bardeen-Herring source:(26) Showing the creation of a dislocation ring from an edge dislocation pinned at A, B. The slip plane is normal to the page. There is an extra plane of atoms below AC, B which grows by creating vacancies in neighboring planes by successive steps AC_1B, AC_2B, etc. The loops meet at C_5 and C_6 enabling the line AC_5B to create another ring. (Courtesy J. Wiley and Sons)

10b Frank-Read source. The slip plane is parallel to the page.

Fig. 11a Climb sources in quenched Al-5% Mg alloy. The sources are interfacial dislocations at the particle-matrix interfaces. Successive loops lie on a prismatic surface (they are not coplanar). Parts of the loops intersect the free surfaces at A.

11b Similar to 11a but the source configuration is more complicated due to dislocation interactions.

Fig. 12 Dislocations moving around an obstacle by cross-slip(34) (a) Edges approaching obstacle (b) Screws approaching obstacle. The arrows indicate the direction of the Burgers vector. (Courtesy J. Inst. Metals)

Fig. 13 Creation of loops and dislocation multiplication at precipitates in Nb plastically deformed 1% in tension.

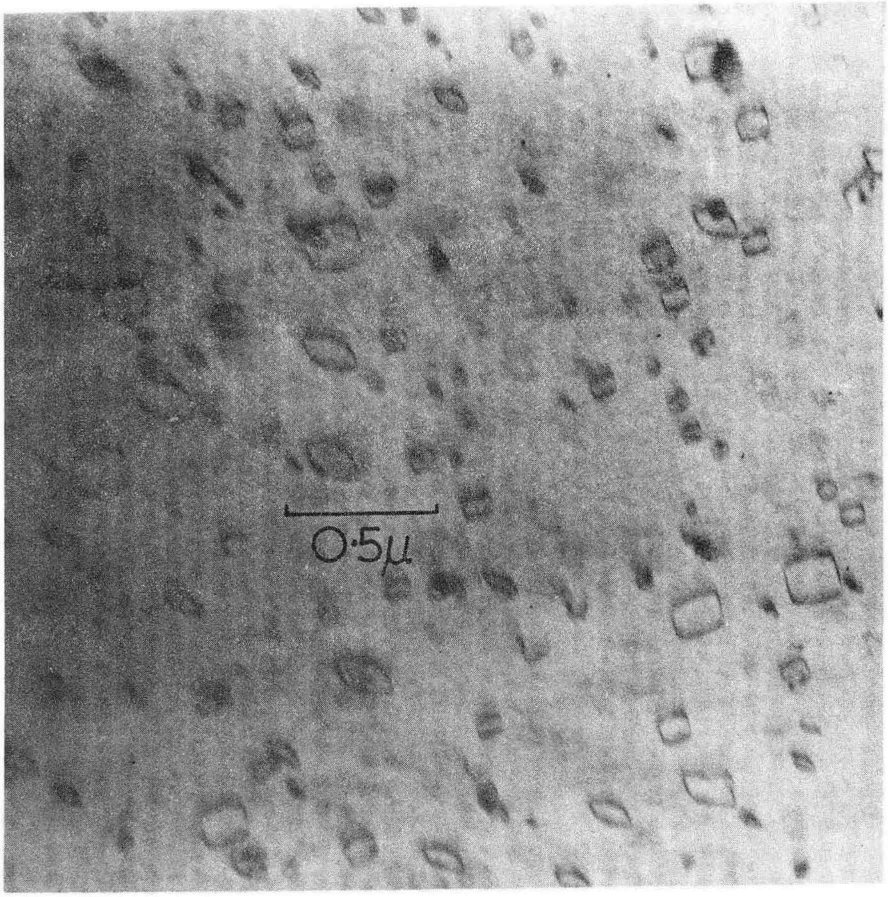
Fig. 14 Showing motion of a dislocation through a crystal containing uniformly dispersed obstacles. (a, b, c) possible successive configurations (d) annihilation (e) pair formation (f) cross-over. (Courtesy of J. Washburn(32))

Fig. 15 Examples of profuse dislocation interactions in Nb after 10% tensile strain. The cross-overs produce local tilts in the crystal leading to changes in contrast. Many of the dislocations are of opposite sign.

Fig. 16 Typical coplanar arrangements of dislocations in materials of low stacking fault energy. Specimen is Cu-33% Zn deformed 5% in tension ($\gamma \simeq 2.5$ ergs/cm^2).

Fig. 17a Cell structure of dislocations in Ni deformed 20% in tension. Notice bowing of loops from cell walls.

17b Similar to 17a but in this case the specimen is Nb.



ZN-3684

Fig. 1.

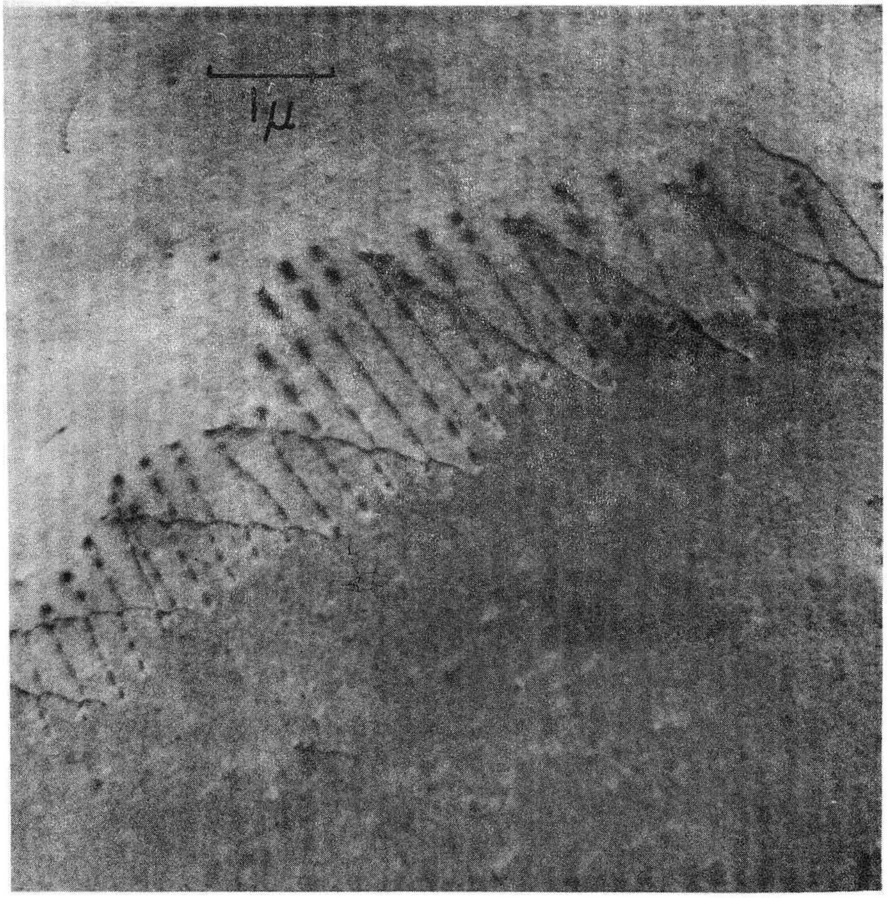


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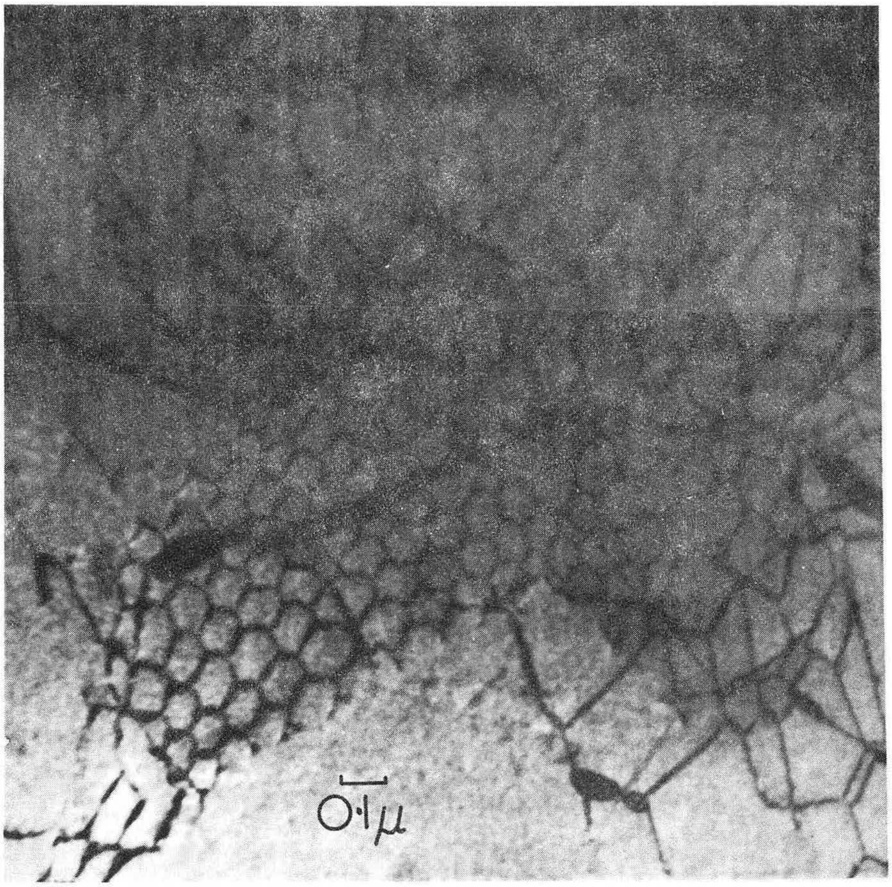
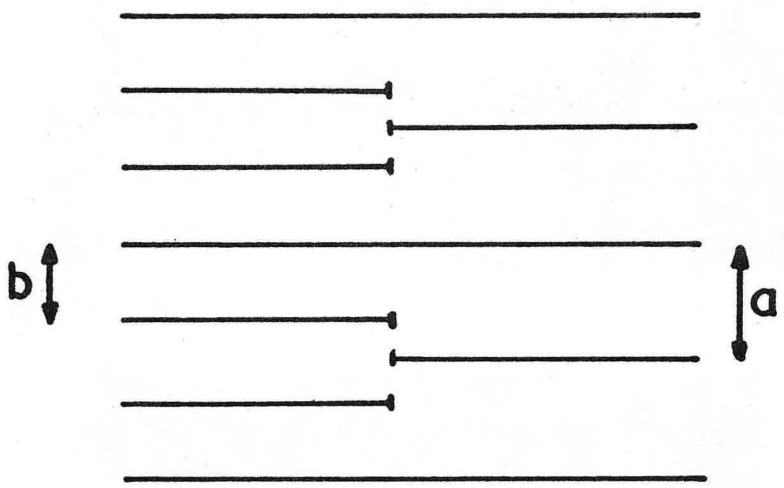
Fig. 2.



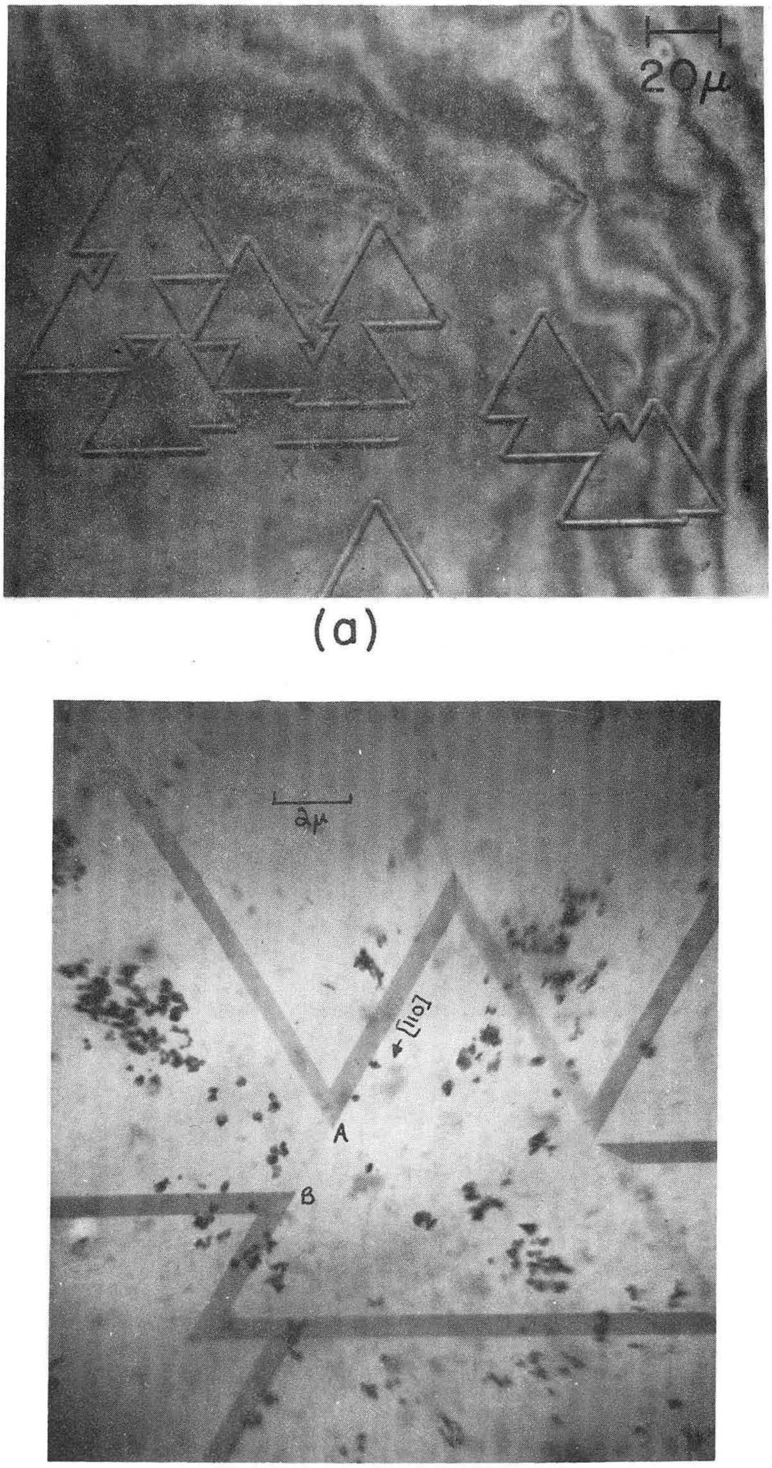
ZN-3691

Fig. 3.



MU-30120

Fig. 4.

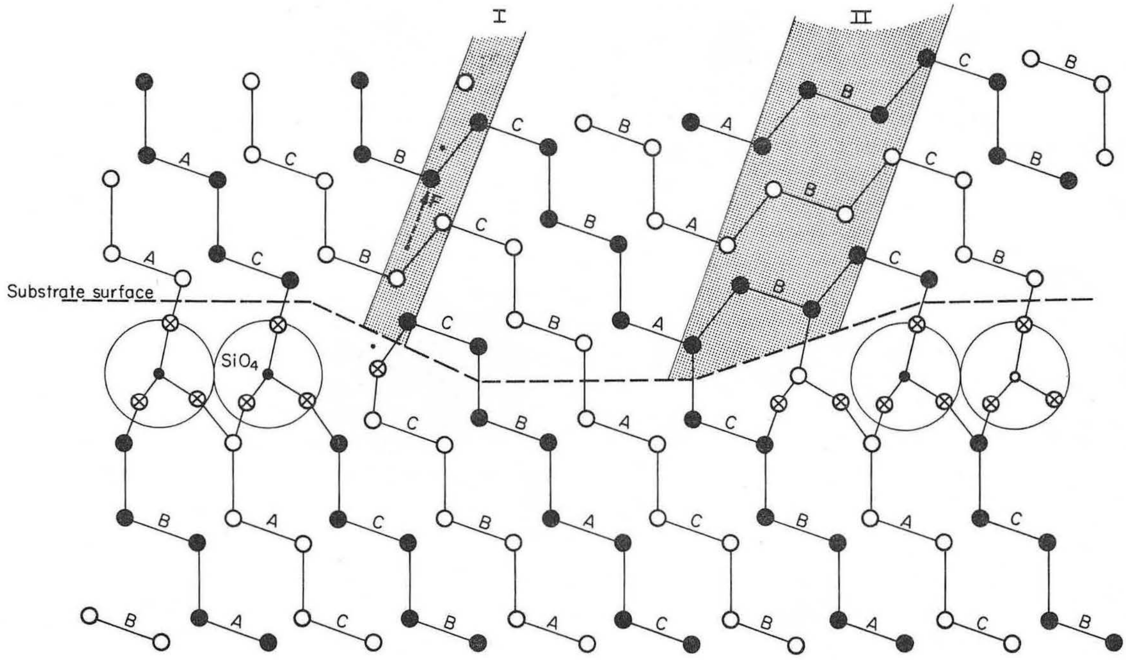


(a)

(b)

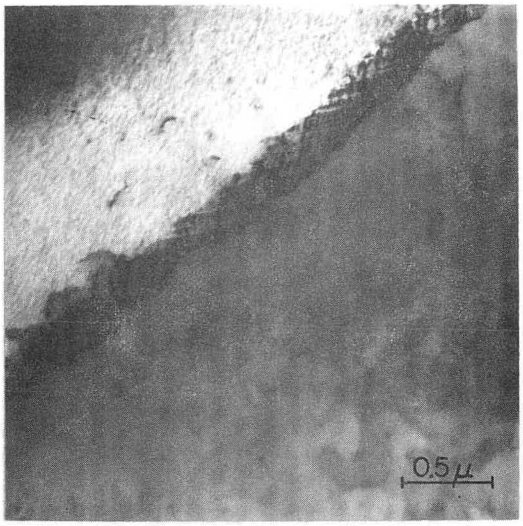
ZN-3237

Fig. 5a

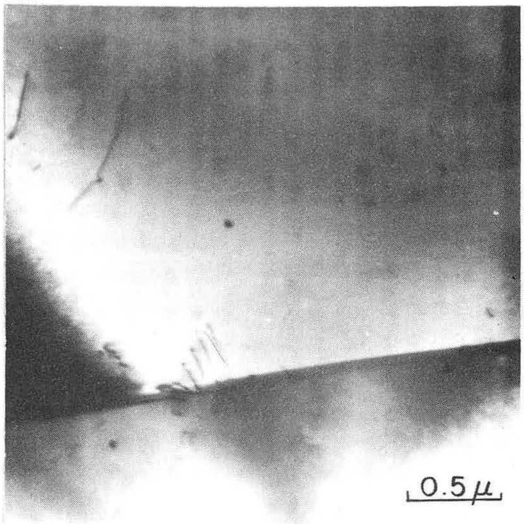


MU-27531

Fig. 5b



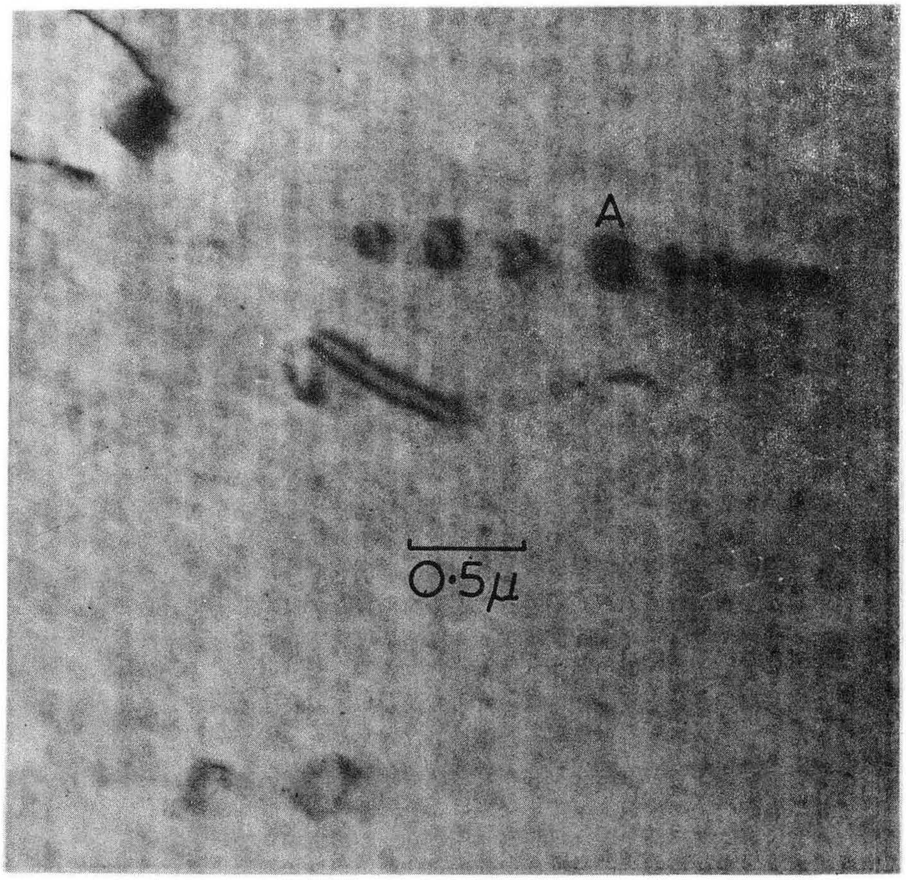
6 (a)



6 (b)

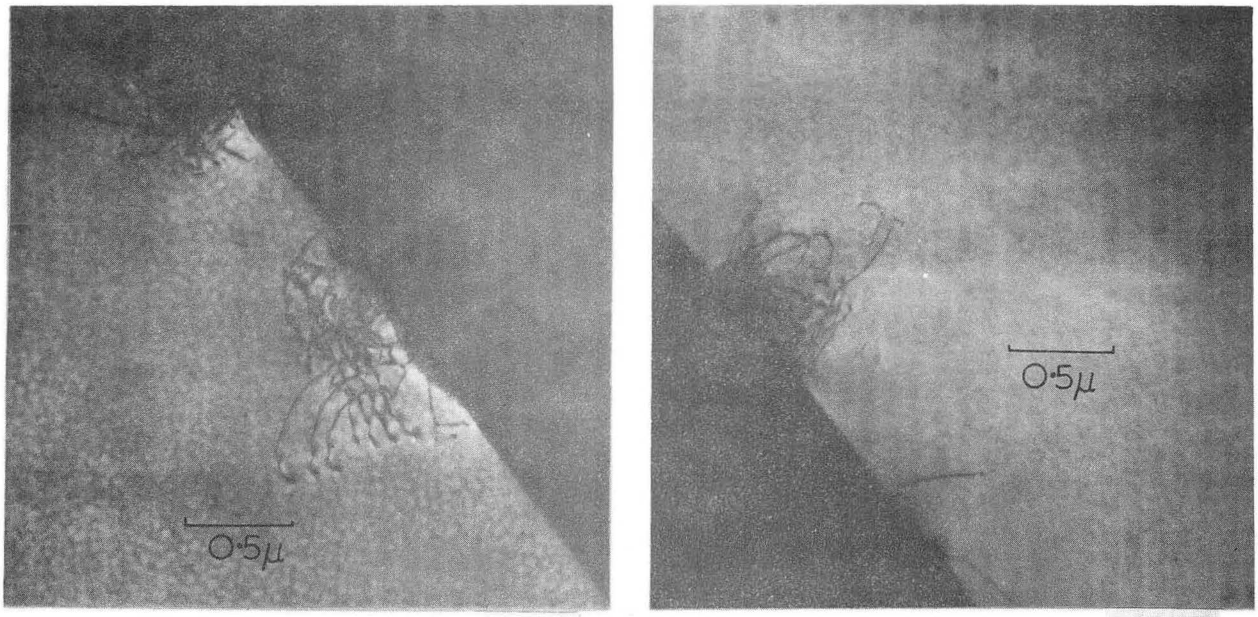
ZN-3683

Fig. 6



ZN-3690

Fig. 7

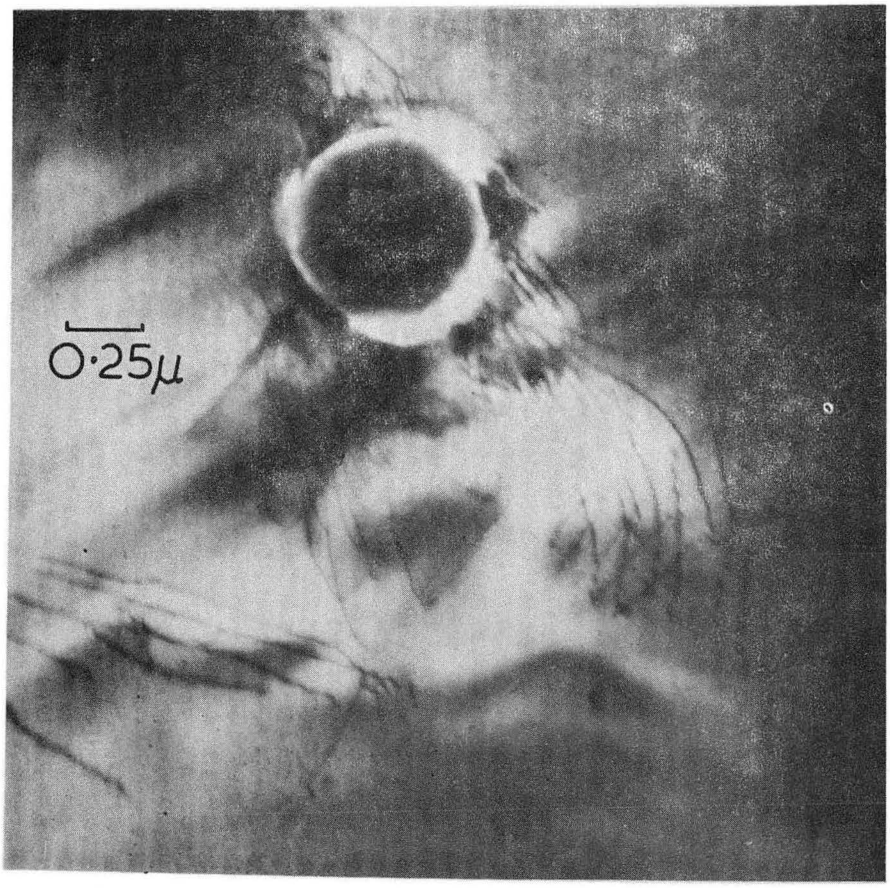


8 (a)

8 (b)

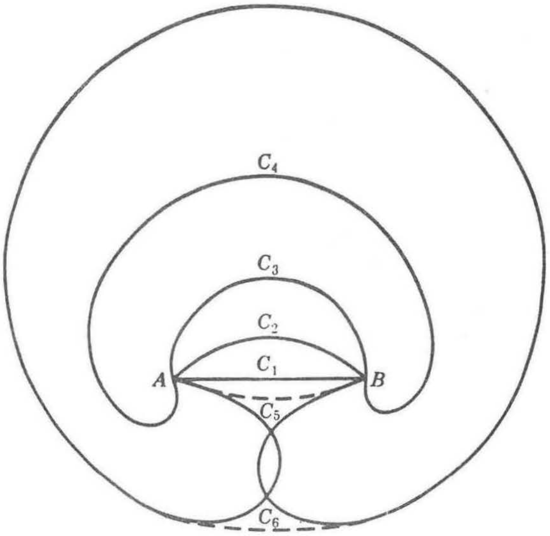
ZN-3681

Fig. 8



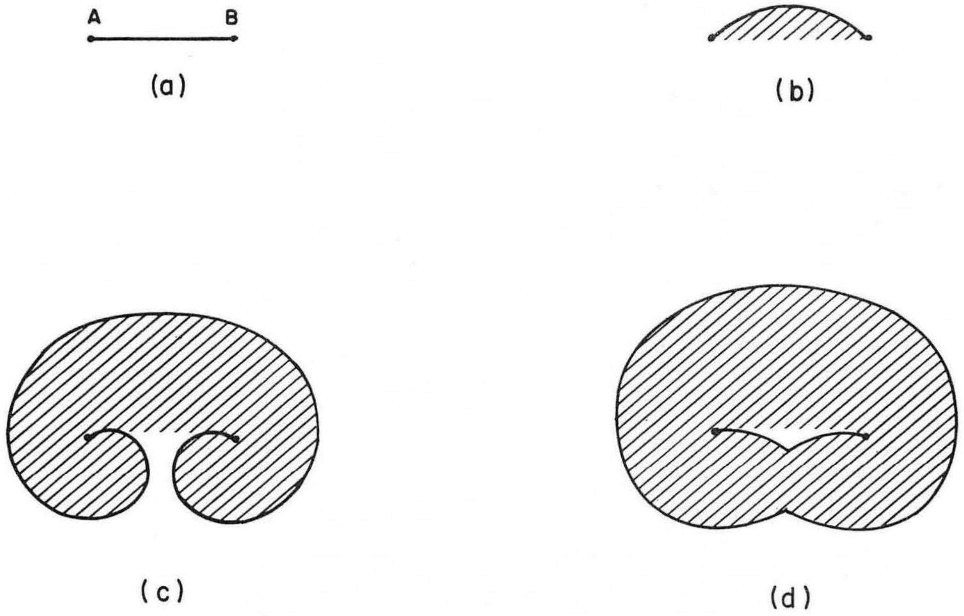
ZN-3689

Fig. 9



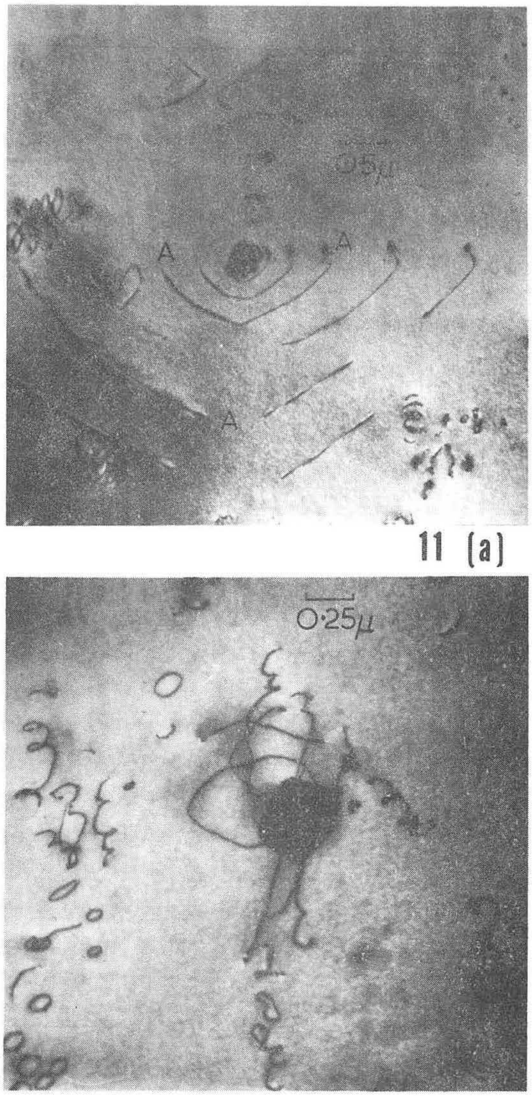
MU-30122

Fig. 10a



MU-27036

Fig. 10b

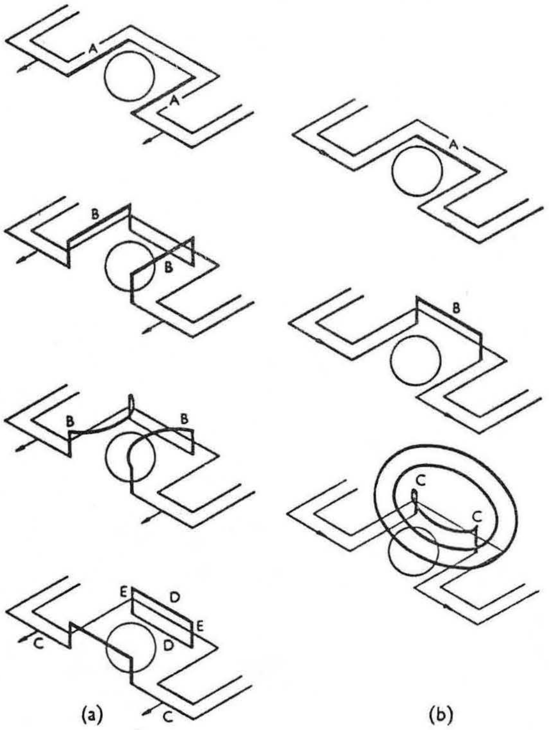


11 (a)

11 (b)

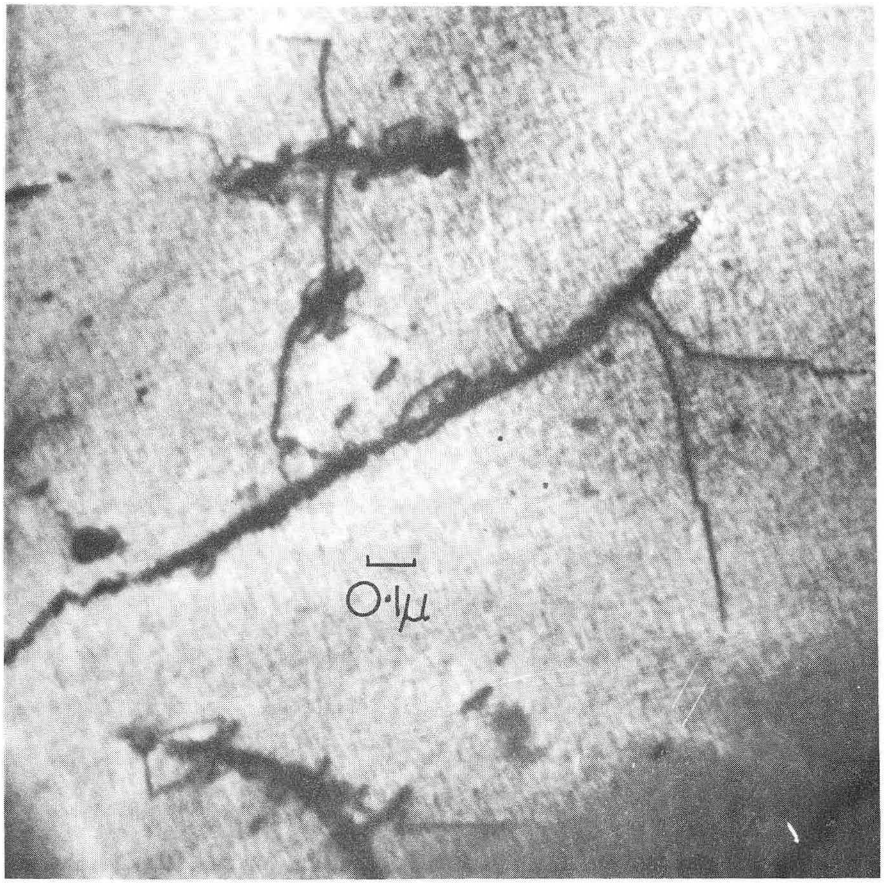
ZN-3680

Fig. 11



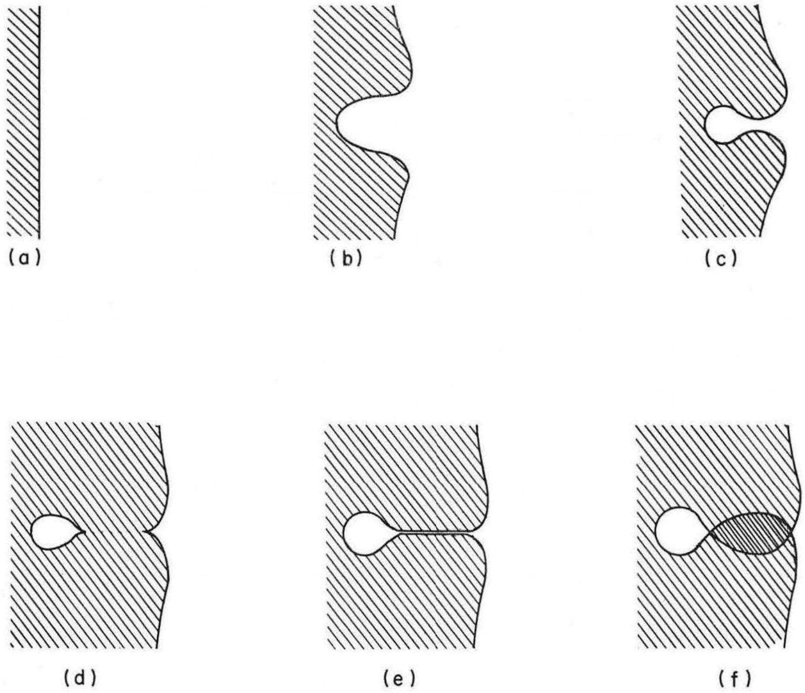
MU-30121

Fig. 12



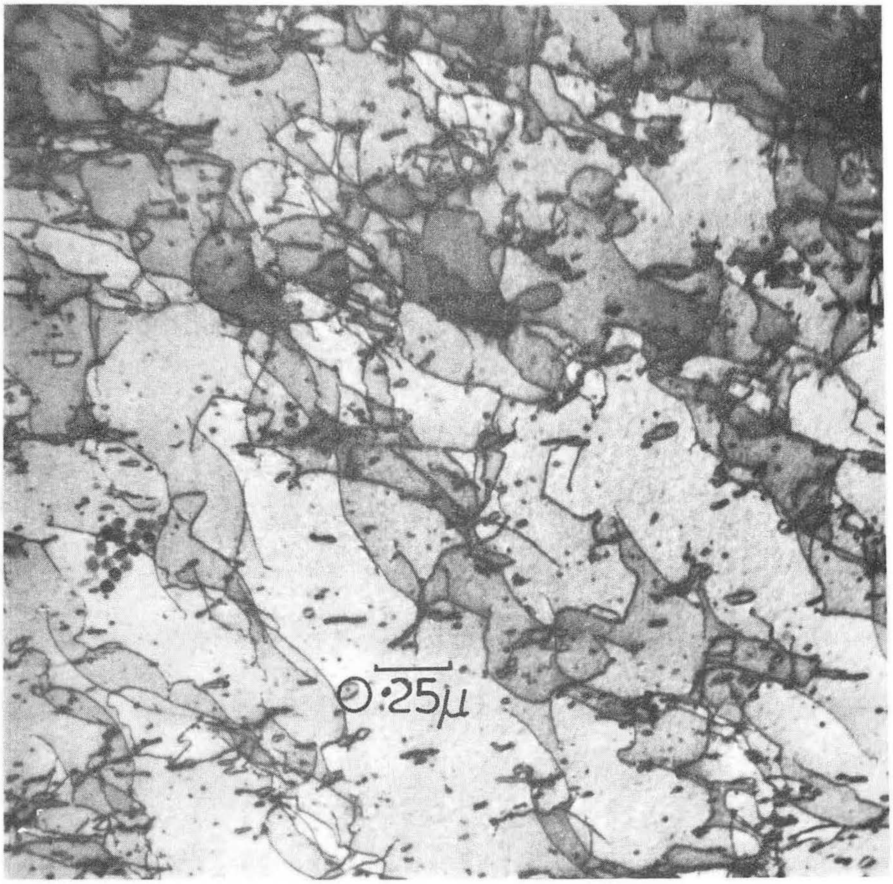
ZN-3688

Fig. 13



MU-27037

Fig. 14

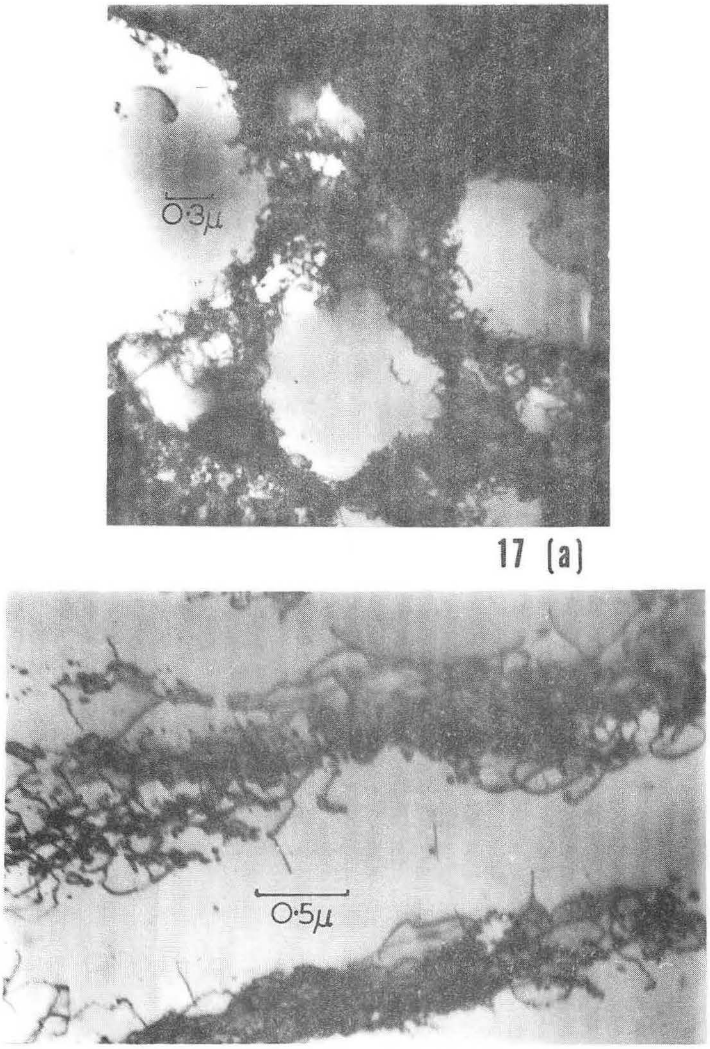


ZN-3686

Fig. 15

ZN-3687

Fig. 16



17 (a)

17 (b)

ZN-3682

Fig. 17