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# DISSOCIATION AND PLASTICITY OF LAYER CRYSTALS

P. DELAVIGNETTE

CEN-SCK, Mol, Belgique

**Résumé.** — Le mécanisme de déformation des cristaux lamellaires idéaux se fait exclusivement par glissement de dislocations sur le plan de base, il n'y a pas d'emmêlement de dislocations conduisant à un écrouissage. Des défauts de structure préexistants comme des boucles de dislocation de Frank ou des dislocations non basales de croissance peuvent conduire à un durcissement. Dans des cristaux lamellaires non idéaux, un système de glissement secondaire peut être activé, ce qui peut donner lieu à un écrouissage.

**Abstract.** — The deformation process in an ideal layer crystal proceeds exclusively by dislocations gliding along the basal plane. No tangling of the dislocations is expected. Structural defects present before deformation are responsible of hardening and work hardening. This is the case for Frank dislocation loops and non-basal grow-in dislocations. In non ideal layer crystals, a secondary glide system may sometimes be operative, giving rise to work hardening.

**1. Introduction.** — A layer crystal consists of layers of atoms whose binding energy within the layers are relatively strong, these layers are generally all similar, while binding energy of atoms between the different layers are relatively weak, therefore essentially of the van der Waals type. These layers may sometimes consist of multilayered blocks of atoms, strongly bound and therefore undeformable.

The plastic deformation of a layer structure will essentially proceed by glide of dislocations along planes parallel to the layers, they are called the basal plane. Their Burgers vectors will be parallel to the basal plane, these are called basal dislocations. This is the exclusive mode of deformation of an ideal layer crystal. The deformation mode of real crystals may vary from this one up till more isotropic modes, where different glide systems may be simultaneously operating. The layer crystals are limited to those for which the predominant mode of plastic deformation is by glide of basal dislocations in the basal plane.

Cleavage and growth properties of layer crystals are easily deduced from these properties. They will often easily cleave on the basal plane. Thin crystal foils are therefore readily prepared for transmission electron microscopy. In many cases also layer crystals grow in thin foils, which can be directly usable in transmission electron microscopy, without any subsequent mechanical or electrochemical treatment.

The dissociation of perfect dislocations into partials is not an essential character of a layer crystal although it is typical. Even in the simplest layer structures, the stacking of each layer or block of layers may generally be accomplished in different approximately equivalent ways, only one of which is the correct stacking. Since

the binding forces between layers are of the weak van der Waals type, the energies associated with the wrong stackings will be small and the dissociation of the dislocations in two or more partials will be a common rule. This is the reason why the most complex dissociations of dislocations have generally been observed in layer crystals.

## 2. Glide of basal dislocations in the basal plane. —

**2.1. — DISSOCIATION OF THE DISLOCATIONS.** — Only few layer crystals show perfect dislocations. It is, for example the case for  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  where the deformation mode is clearly predominantly of the layer type, figure 1, the glide dislocation doesn't show any dissociation [1]. On the contrary, in the majority of the layer crystals, the dissociation occurs in two or more

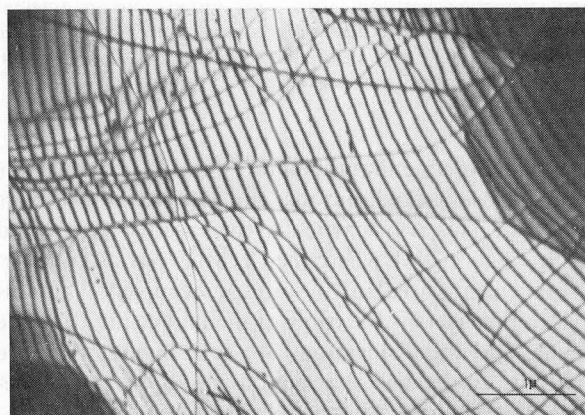


FIG. 1. — A family of basal dislocations in  $\text{Bi}_2\text{Te}_3$  arisen from an invisible source. This family interacts with several isolated dislocations in the same or in neighbouring glide planes.

partials. A detailed account is given in a preceding contribution (Amelinckx). Let us however recall some essential points.

The dissociation of dislocations can be discussed with reference to

*a)* the two-dimensional unit cell of the atomic arrangement in both layers between which glide occurs, we will call it here the unit cell in the glide plane, it allows a determination of the Burgers vectors of the partial dislocations since the hard sphere model is a good basis for describing the glide movements ;

*b)* the two-dimensional unit cell of the structure projected on the basal plane, which may be a multiple of the unit cell in the glide plane, we will call it here the unit cell of the layers, it determines the number of partials necessary to restore the perfect crystal structure.

In structures based on close packed layers, where the two-dimensional unit cell in the basal planes contains only one atom per atomic layer, the dissociation may occur in two partials. This is the case for the structures of the types  $\text{CdI}_2$ ,  $\text{MoS}_2$ ,  $\text{GaS}$ , etc. A similar dissociation occurs in other structures like graphite, figure 2 [2].

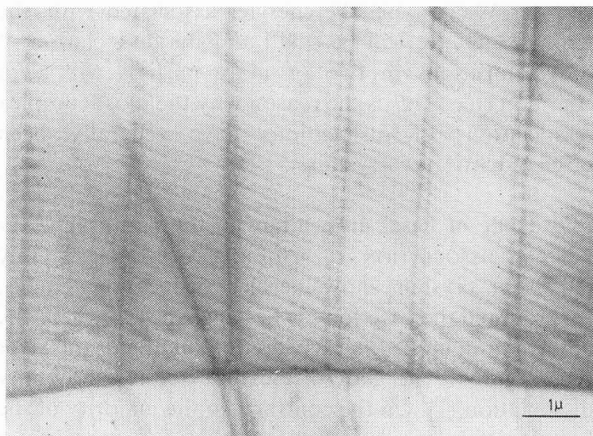


FIG. 2. — Dislocations dissociated in two partials in graphite, and interacting elastically with other dislocations in different basal planes. The dislocations are emitted from the edge of the crystal along a cleavage step. Such sources are often observed in activity in transmission electron microscopy.

It is also possible that the unit cell in the glide plane is simple close packed, but that the unit cell of the layers is larger. This is in particular the case for  $\text{CrCl}_3$  and  $\text{CrBr}_3$ , figure 3 [3], where the Cr layers have a compact arrangement with  $\frac{1}{3}$  of the sites unoccupied. The unit cell of the layers is the triple of the unit cell in the glide plane, and the dislocations are split in four or more partials. A detailed description has been given elsewhere (Amelinckx, this symposium). Finally the dissociation type of talc (its structure can be described by the stacking of multilayered blocks) gives a still more complex example since in that case *a)* both atomic

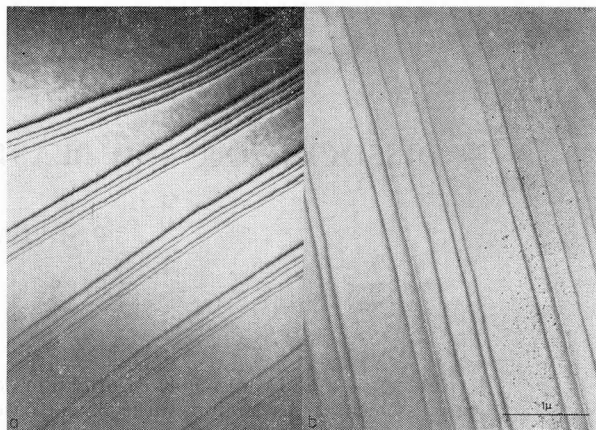


FIG. 3. — Dislocations in (a)  $\text{CrBr}_3$  and in (b)  $\text{CrCl}_3$ . The ribbons are clearly made of six partials, which is the most common dissociation type in these structures, although a dissociation in four partials is also possible.

planes between which glide occurs have a complex structure giving rise to the dissociation of the dislocations in four or more partials, figure 4b) the real situation is still more complex since, while a consideration of each layer separately leads to a hexagonal symmetry, the structure is in fact monoclinic. The dissociation of the dislocations in talc has been observed, but a detailed model has never been given, essentially because part of the stacking fault energies are so small that it has been impossible to distinguish the perfectly stacked regions from the faulted regions.

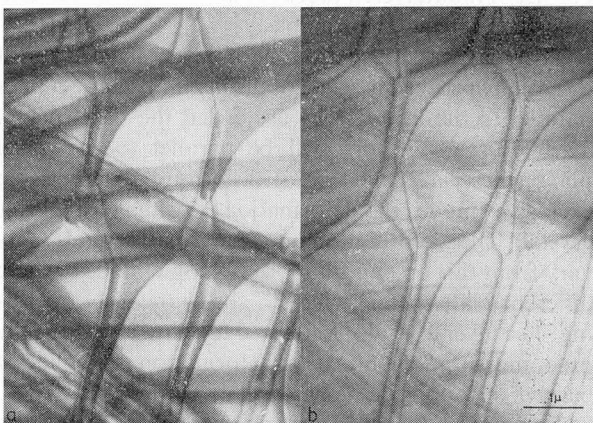


FIG. 4. — Dislocation nodes in talc. The contrast shows clearly here a grouping of the dislocations in four partials, although it has not been possible to give a detailed model of the dissociation.

**2.2 DISLOCATION SOURCES.** — The plastic deformation of ideal layer crystals proceed by glide of basal dislocations in the basal plane. This needs two conditions.

**2.2.1 The displacement of the dislocations.** — The glide of dislocations is generally an easy movement since the binding forces between the layers are weak. If the movement of the dislocations is hindered by any



obstacle, there is hardening of the crystal. If the dislocations in movement during the plastic deformation are hindering each other, there is work hardening. These mechanisms will be studied.

### 2.2.2 A multiplication mechanism for the dislocations.

— The Frank-Read mechanism or any other related mechanism doesn't account for a sufficient multiplication mechanism for the dislocations in layer crystals since non-basal dislocations or other pinning points are generally too rare or absent. Moreover, to our knowledge, there has been no observation of such sources in layer structures by transmission electron microscopy, although the conditions for their observation are ideal since the electron transparent specimens, thin foil shaped, doesn't modify the deformation mechanism of bulk crystals. The deformation proceeds in the foil plane, a complete extension of the dislocation sources would be observed. On the other hand, it has often been observed that dislocations are emitted into the crystal from the boundaries, generally from the non-basal surfaces of the crystals, along the steps. Families

of all parallel dislocations all with the same Burgers vector may be emitted and glide together in the crystal under favourable stress, figure 2. It appears that the emission energy for a dislocation at the crystal surfaces is generally very low in the layer crystals. Such sources are operative in the microscope even under the slightest influence of the electron beam heating or by the stresses introduced in the thin foil by a thinny contamination layer on the crystal surface under the electron beam influence.

2.2.3 *Network formation.* — Dislocations emitted from two independent sources may intersect and form dislocation networks. The intersection and the network formation is generally a factor of work hardening. It will be shown that this is not the case in layer structures.

Two intersecting perfect dislocations situated in the same glide plane in a hexagonal layer crystal will form a pair of nodes, the same as it has been described in F. C. C. metals, for example (the K and P nodes of Frank). If the dislocations are dissociated in two partials, they will form extended and contracted nodes, figure 5. The detailed mechanism of intersection of dislocations has been studied [2] for a large variety of possibilities in graphite. The intersection of the extended dislocations **BA** and **CA** will be given in example, figure 6. At large dis-

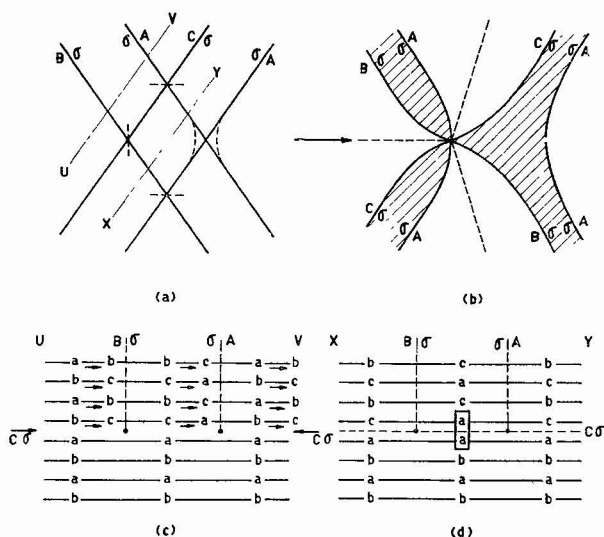


FIG. 5. — Intersection of two dislocations with the formation of one extended and one contracted node (b). The stacking sequences along two lines marked UV (c) and XY (d) is also shown. The region of high stacking fault energy «a over a» shown in (d) must be eliminated, this is done by complete shrinking of this area.

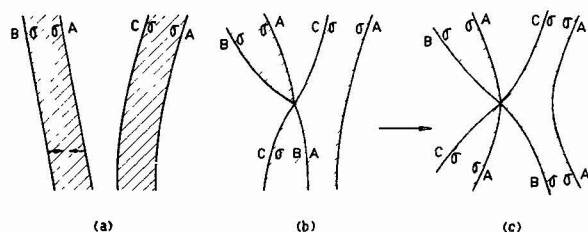


FIG. 6. — Proposed mechanism effectively occurring for the intersection of two extended dislocations **BA** and **CA**. The intersection is only possible after recombination of one of the extended ribbons. Here the recombination of the ribbon **BA** is presented in (b).

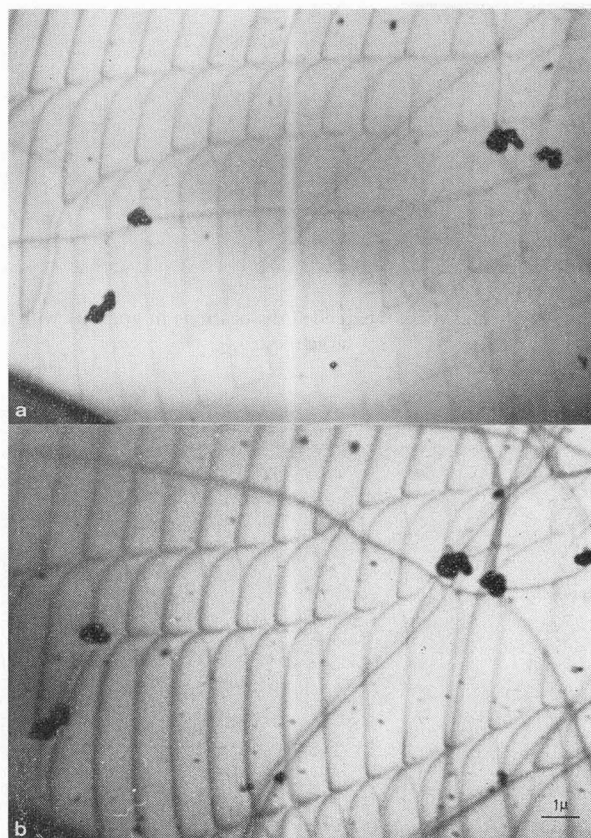


FIG. 7. — Two successive stages in the formation of a network in graphite. The process is repetitive, the network is glissile. The impurities reveal that all the network has moved between both photographs.

tances, the dislocations repel each other, they will intersect only if they are forced to meet under an external stress. At shorter distance, the two internal dislocations  $\sigma A$  and  $C\sigma$  cannot cross each other since otherwise a region of high stacking fault energy (stacking «  $a$  » over «  $a$  ») would be created, which is supposed to be forbidden, figure 6a. One of the extended ribbon is therefore forced to recombine under the stress, say  $B\sigma + \sigma A \rightarrow BA$ . The perfect dislocation  $BA$  will cross without difficulty the partial dislocation  $C\sigma$ , since their Burgers vectors are perpendicular, figure 6b. The dislocation  $BA$  will dissociate again after crossing, according to the new stacking situation :

$BA \rightarrow \sigma A + B\sigma$  giving rise to the final situation figure 6c.

The process of the network formation has been observed in graphite during its formation, figure 7. Successive photographs show that the same process is repeated after each intersection. This process can be explained on the basis of the intersection mechanism presented before. It is repetitive and the glissile dislocations all in the same glide plane create after crossing a glissile dislocation network. An example of dislocation network in graphite is shown in figure 8 for low dislocation densities, for higher dislocation densities it looks like figure 9.

If, on the other hand, the dislocations are perfect like in  $Bi_2Te_3$ , hexagonal networks are formed, figure 10. The network formation mechanism in crystals where the dissociation of the dislocations is more complex will be essentially the same. It is clear that areas for which the stacking fault energies are higher will be narrower, this is observed on the

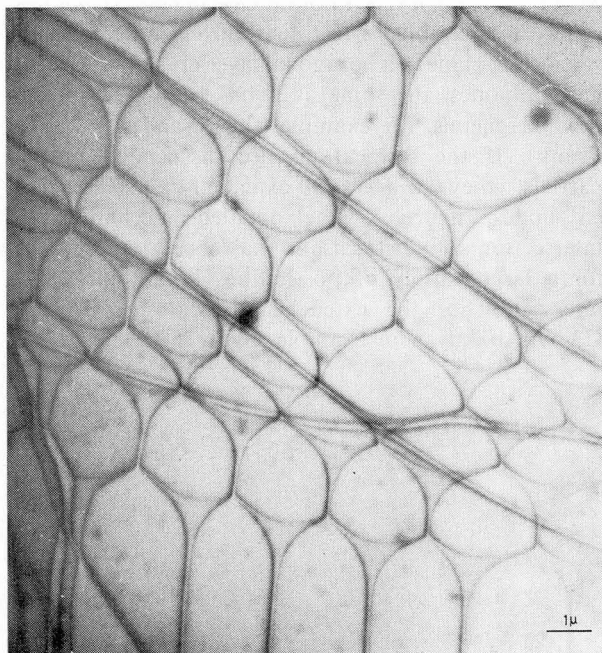


FIG. 8. — Network of extended dislocations in graphite with a large mesh.

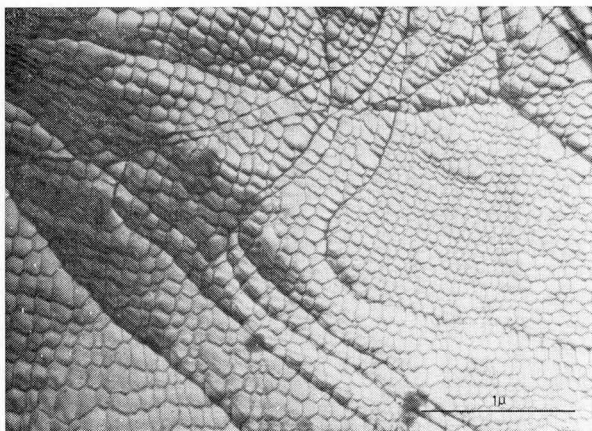


FIG. 10. — Hexagonal network of perfect dislocations in  $Bi_2Te_3$ .

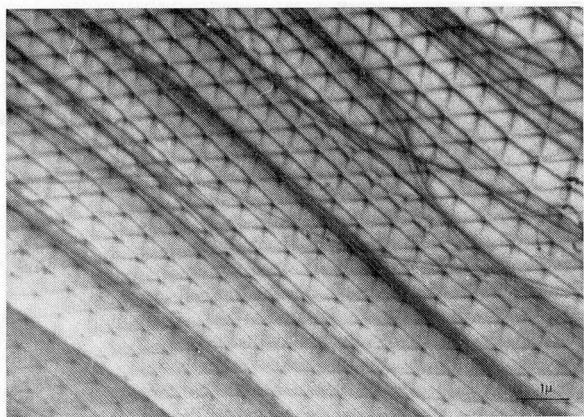


FIG. 9. — Network of extended dislocations in graphite with a small mesh. Perfect and faulted areas are no more distinguishable by their relative surface. It appears as a triangular network.

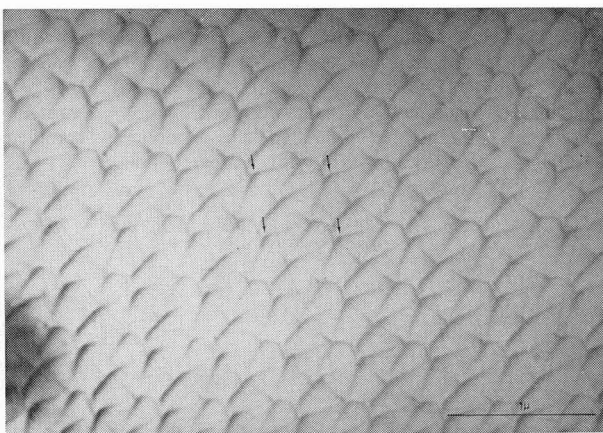


FIG. 11. — Network of partial dislocations in  $CrCl_3$ . The surface of the image is divided by the dislocations in six different kinds of regions, whose areas are varying like the inverse of their stacking fault energies. The largest areas correspond to the perfect stacking.

networks in  $\text{CrCl}_3$ , figure 11, and  $\text{CrBr}_3$ . An example of dislocation nodes in talc is shown on figure 4.

All these networks are glissile and can freely move under stress, as it is often observed. Introduction of other basal dislocations in the two dislocation sources forming the network doesn't modify its glissile character. Network formation is not a factor of work hardening.

**2.2.4 Pseudo-networks.** — The situation is slightly different if two dislocations are crossing in parallel planes. Dislocations or dislocation segments in two neighbouring planes will attract or repel according to their Burgers vectors. Pairs of attractive dislocations will freely glide as an entity if no reaction is possible, they may freely separate again under favourable stress. Triple ribbons in graphite, figure 12, have been explained by this mechanism. It is a quite different model than that of triple ribbons in F. C. C. structures. Other singularities of dislocation networks in graphite have been explained on the same basis, figure 13. If on

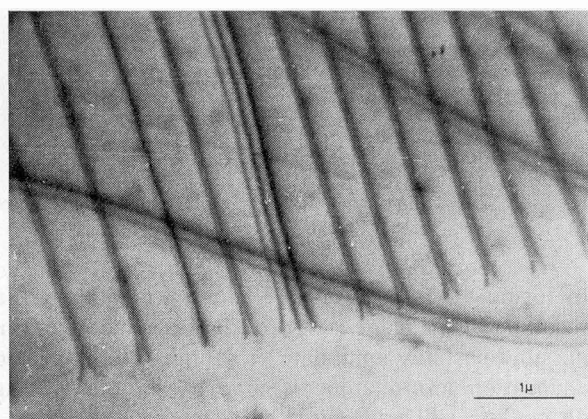


FIG. 12. — A family of extended dislocations in graphite including a triple ribbon, which is formed by the interaction of two extended dislocations in different planes.

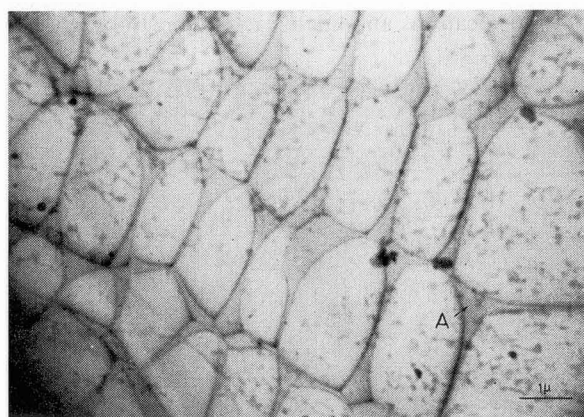


FIG. 13. — Dislocation network in graphite formed by the interaction of dislocations in different glide planes. A dipole is shown in A. It is formed by the strong interaction and the superposition of two opposite partial dislocations in different glide planes. Its contrast is very weak or it is invisible, it is essentially revealed by the marked angle formed by the visible dislocations.

the other hand a reaction is possible between the dislocations in different glide planes, either if a secondary glide plane exists or if the conditions for climb are fulfilled, a jog is then formed, which is responsible of work hardening. This mechanism is studied elsewhere.

**3. Interaction of basal deformation dislocations with non-basal dislocations.** — The plastic behaviour of a layer crystal can be considerably modified by the introduction of non-basal dislocations. We will distinguish two cases: first dislocations with non-basal Burgers vectors, situated in the basal plane, e. g. Frank loops, then dislocations with non-basal Burgers vector, not situated in the basal plane, e. g. grown-in dislocations.

**3.1 FRANK LOOPS.** — Graphite irradiated in a reactor or quenched may show after suitable thermal treatment circular loops situated in the basal plane and exhibiting a stacking fault contrast. They are resulting from the agglomeration of point defects within each basal plane. Their Burgers vector can be described by a two phases process: first an agglomeration of point defects in the basal plane gives rise, after collapse, to a dislocation loop with a Burgers vector of the type  $\frac{1}{2}c$  (half the unit vector along the  $z$  axis), secondly, if a high energy stacking fault is formed, a shear process is eventually needed to restore a stacking fault with a lower energy, the vector of this shear is the same as the Burgers vector of partial dislocations. Similar type of loops have also been described in  $\text{Sb}_2\text{Te}_3$ . Here they are created in order to accommodate deviations of the stoichiometry. Vacancy loops are generated in the Te planes for a composition  $\text{Sb}_2\text{Te}_{3-\epsilon}$ .

Frank loops are sessile in layer structures and they are strongly interacting with glissile basal dislocations through their basal component of the Burgers vector. The loops are therefore responsible of the hardening of the material. A basal dislocation crossing a loop in the same plane or in neighbouring planes will be attracted or repelled, figure 14, but may eventually cross the loop. If the stacking sequence in the loop is modified by the passage of the dislocation, it can be restored by a new shear in the loop. The dislocation after crossing the loop is unchanged. There is therefore no further work hardening.

A Frank loop of purely edge character would have no significant interaction with basal moving dislocations, unless possible modifications of the stacking sequence in the loop region.

**3.2 GROWN-IN DISLOCATIONS.** — It is well-known that natural graphite contains a certain concentration of non-basal dislocations situated in a non-basal orientation. They have been introduced during the growth of the crystal. Although they have never been detected by transmission electron microscopy, their revelation by etch pitting technique makes no doubt [4]. Such dislocations are easily overlooked in electron



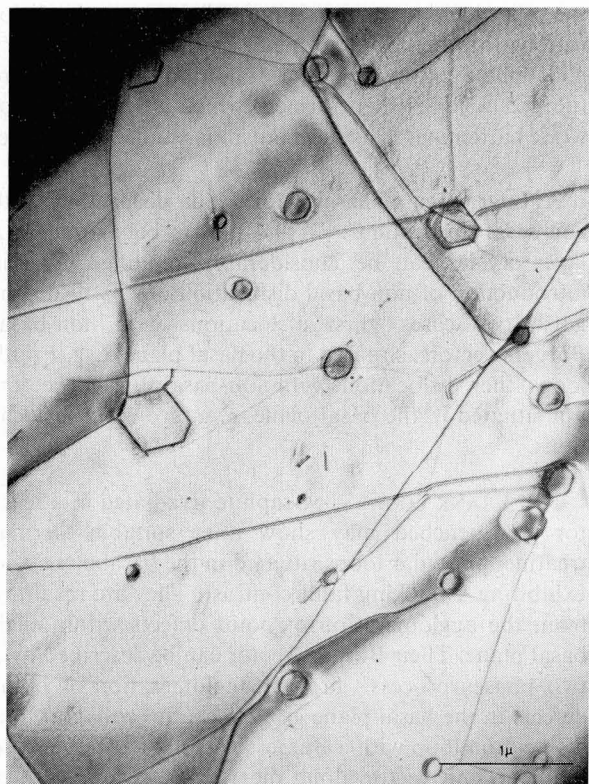


FIG. 14. — Diamond shaped dislocation loops in  $\text{Sb}_2\text{Te}_3$  formed of vacancy loops in the Te layers. The dislocation loops are strongly interacting with the basal dislocations.

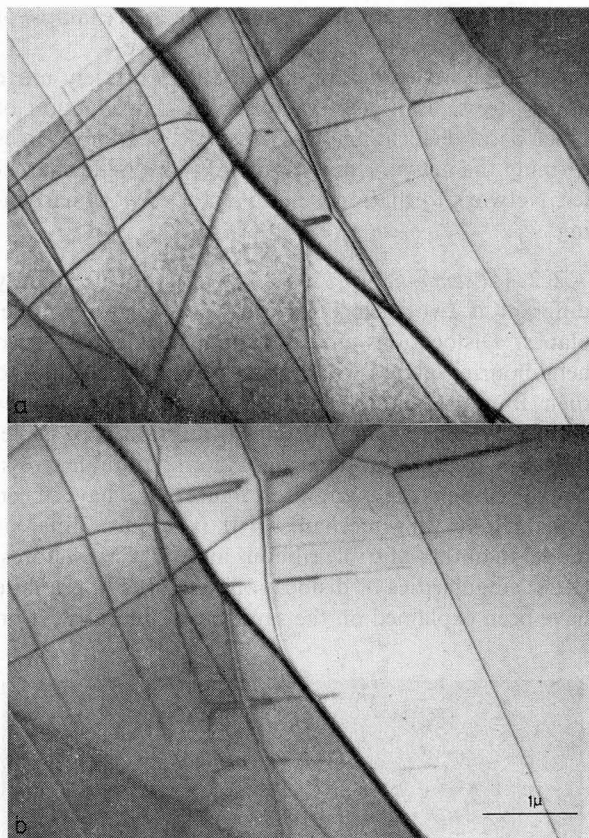


FIG. 15. — Moving dislocations in  $\text{SnS}_2$  leaving trails of dislocation dipoles.

microscopy since they are systematically out of contrast in the most common orientations (horizontal orientation of the foil), only large tilting angles can bring them in contrast.

The intersection of basal dislocations with this type of non-basal dislocations is the first example of a mechanism of work hardening in layer crystals. Jogs are formed in the basal dislocations when they are crossing a forest of non-basal dislocations. This mechanism is well known, let us recall a few of its characteristics. The heights of the jogs are given by the lengths of the non-basal Burgers vectors. In an ideal layer crystal and if the applied stress is high enough, the moving basal dislocation will leave trails of dipoles connecting the jogs in the moving dislocations to the forest of non-basal dislocations, figure 15. Further deformation results in lengthening of these dipoles. They are formed of two basal dislocations of opposite Burgers vectors given by the Burgers vector of the moving dislocation, the separation of the two dislocations of the dipole is equal to the Burgers vectors of the non-basal dislocations.

Strictly speaking, there is no formation of a jog in the basal dislocation and a dipole, but the glide dislocation is trapped at the non-basal dislocation and cannot cross it. Under the stress the movement will proceed anyhow, this is possible only by lengthening of the glide dislocation which adopts its most stable configuration

by forming the long dipoles. If climb is possible or if a secondary glide plane exists, the dislocation dipoles can possibly partially annihilate or change into elongated dislocation loops, a jog is then left in the moving dislocation, still hindering subsequent movement.

Such dipoles have a typically faint and narrow contrast in transmission electron microscopy, since at distances from the dipole larger than the separation distance of both its dislocations, the strain fields of both dislocations annihilate each other. In practice the

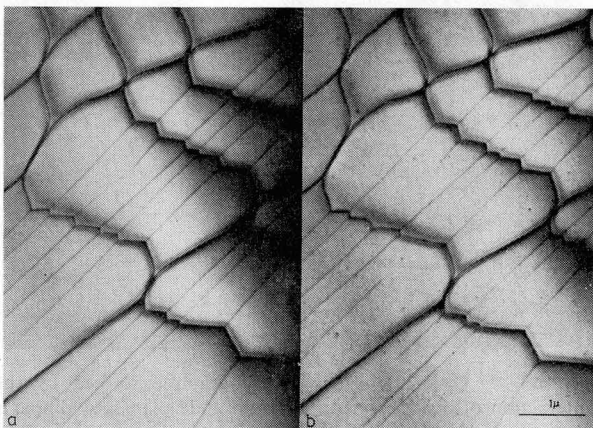


FIG. 16. — Multiple dipoles in  $\text{SnS}_2$  introduced in the crystal by crossing of glide dislocations with a forest of grown-in dislocations.

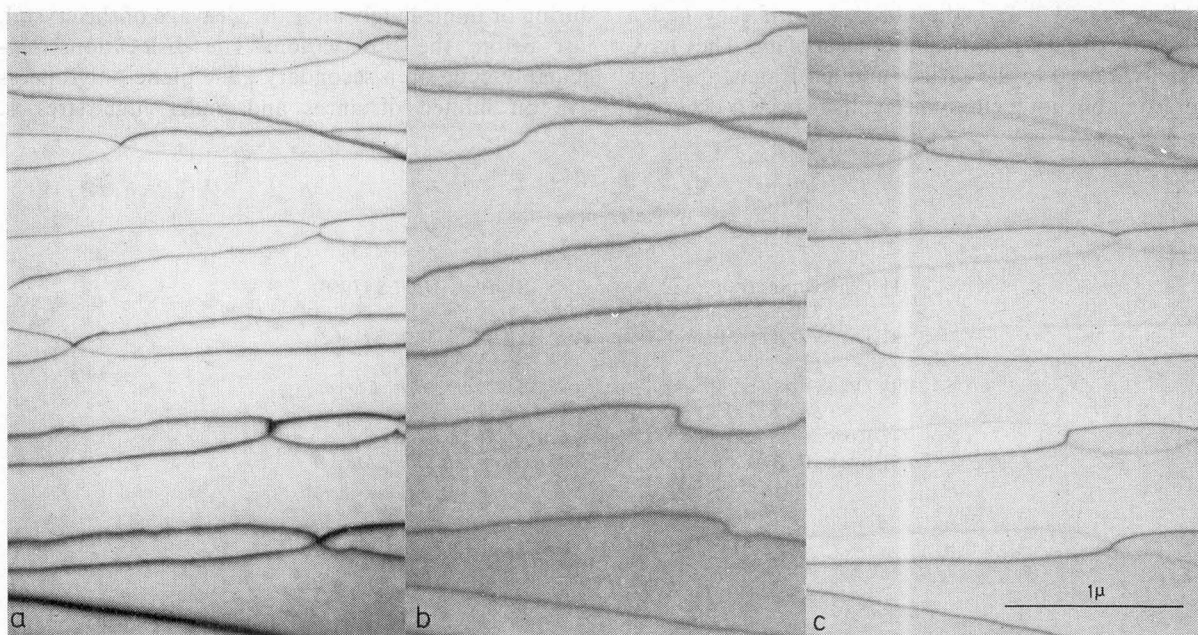


FIG. 17. — Extended and contracted jogs in  $\text{SnS}_2$  taken in different contrast conditions for the determination of Burgers vectors.

contrast will even completely disappear if the two dislocations are in neighbouring planes, the dipole is then revealed only by its strong interaction at its ends, which is a much better marker of its presence than its image. Although these dipoles are made of glissile dislocations, they will generally not glide since they must join the non-basal dislocation to the jog in the basal dislocation, moreover any stress doesn't result in an appreciable force exerted on a dipole. Figure 13 in A shows dipoles in graphite which have been introduced exclusively by basal dislocations interacting in the basal planes. It can be easily disentangled by further separation of the dislocations, since in particular there has been no jog formation. Figure 16, on the other hand, is an example of dipoles introduced by the crossing of basal dislocations with a forest of non-basal dislocations. Such dipoles have not been observed in graphite.

The dipoles are hindering further movements of the dislocations, they form a factor of work hardening in layer crystals.

**4. Movements of basal dislocations on a secondary glide plane.** — If different glide planes are simultaneously operating, cross slipping, jogs formation, locks formation, etc. are possible. These dislocation interactions are no more fundamentally different in the layer crystals than in other crystals. These deformation mechanisms are common to other structures, they have been extensively studied, in particular for F. C. C. metals and alloys of low stacking fault energy. They are more adequately described elsewhere and are directly applicable to non ideal layer structures. Some of these situations have been described for  $\text{SnS}_2$  [5]. Figure 17

shows some extended and contracted jogs in  $\text{SnS}_2$  ribbons, the different contrasts allow a Burgers vector determination. From the limited extension of the faulted regions in the non-basal planes, it is concluded that its stacking fault energy is high. These jogs are responsible of a considerable work hardening of the crystal.

The dislocations in  $\text{Bi}_2\text{Te}_3$  on figure 18 are cut in numerous segments. These dislocations lie essentially in

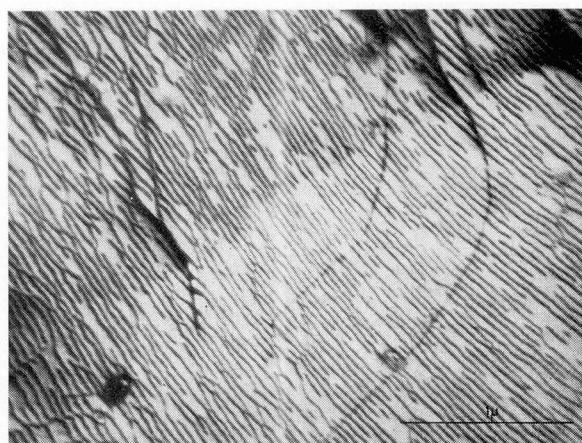


FIG. 18. — Dislocation fragments in  $\text{Bi}_2\text{Te}_3$  in a glide plane lying close to the surface. Parts of the dislocation segments have moved to the surface presumably by glide on a secondary glide plane.

a basal plane situated close to the surface of the foil. Their aspect shows clearly that the dislocations are attracted to the surface of the foil and they would have



all disappeared before the observation if they had a possibility of easy glide in a non-basal plane. They have partially moved to the surface and left fragments. This is presumably not a climb mechanism since it occurred during or immediately after the cleavage of the crystal, just before the observation. The dislocations presumably glide on a secondary glide plane only operative on limited distances and under high stresses.

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