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The Geometry of Lattice Planes. II. Crystallography of Edge Dislocations

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A crystallographic procedure is given for constructing a dislocation of given Burgers vector in any crystal structure. The theory is applied to glissile dislocations in the c.p.h. and diamond structures, and to sessile dislocations in the f.c.c. and b.c.c. lattices.

Introduction

Given that a dislocation has the form of a straight line lying in a particular lattice plane, referred to hereafter as the slip plane, with a prescribed Burgers vector \mathbf{b} , where \mathbf{b} is a lattice vector in this plane, it is well understood that there are two degrees of freedom at our disposal in the construction of the dislocation and three in its crystallographic description. For the direction of the dislocation line may be that of any lattice vector \mathbf{d} in the slip plane, and the dislocation plane* may be any lattice plane (other than the slip plane) containing \mathbf{d} ; if \mathbf{p} is any lattice vector in the dislocation plane (other than \mathbf{d}), a map of the plane \mathbf{p} , \mathbf{b} —referred to hereafter as the elevation plane—provides the most convenient and suggestive picture of the lattice distortion. It is the purpose of the present paper to analyse how the crystallographic construction of the dislocation depends on the choice of the dislocation plane, to show how the description depends on the choice of the elevation plane, and to apply the results to the more general dislocation consisting of a sequence of straight-line segments of differing directions. The analysis is extended to any crystal structure, however complex, and should hence provide the theory of dislocations with a rigorous crystallographic setting which is at present lacking.

Crystallographic construction

According to the preceding considerations, we set up a triplet of vectors \mathbf{b} , \mathbf{d} , \mathbf{p} at any lattice point \circ of

* This may be formally defined as the lattice plane parallel to which half-planes are inserted or removed.

the dislocation line: \mathbf{b} is a given lattice vector in the slip plane; \mathbf{d} lies in the slip plane, but is otherwise arbitrary, and defines the dislocation line through \circ ; \mathbf{p} does not lie in the slip plane, but is otherwise arbitrary, together with \mathbf{d} defining the dislocation plane and together with \mathbf{b} defining the elevation plane. The slip properties of the dislocation depend only on \mathbf{b} . For a given \mathbf{b} , the construction of the dislocation depends on the choice of the dislocation plane. In the simplest possible case, the vectors \mathbf{b} , \mathbf{d} , \mathbf{p} constitute a primitive triplet. This implies that the stacking pattern of the dislocation planes along \mathbf{b} is

... 1 1 1 1 1 ...;

removal or insertion of a half-plane does not alter this stacking at distances far removed from \circ , and hence enables us to construct the dislocation in the usual manner (Cottrell, 1953). The stacking pattern of the elevation planes along \mathbf{d} is

... 1 1 1 1 1 ... ,

so that the map of only one such plane suffices for a complete description of the lattice distortion. Finally, to follow the disturbance along the dislocation line, a map of the slip plane is also necessary.

If \mathbf{b} , \mathbf{d} , \mathbf{p} do not constitute a primitive triplet, e.g. the parallelepiped defined by them contains a lattice point in the interior or on one of the sides, it is convenient to consider three distinct possibilities for the situation of this point:

- (1) It lies in the parallelogram \mathbf{d} , \mathbf{p} , as illustrated in Fig. 1(a). In this case the stacking of the elevation planes along \mathbf{d} is

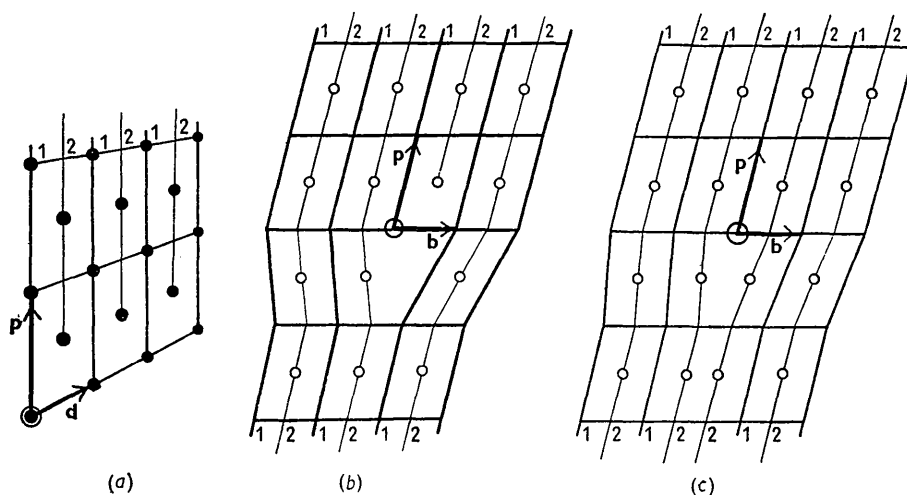


Fig. 1. (a) Dislocation plane showing ... 1 2 1 2 ... stacking of elevation plane traces. (b) Elevation plane showing removal of two half-planes. (c) Stacking 1 2 1 2 2 1 2 produced by removing one half-plane.

... 1 2 1 2 ... ,

so that the maps of two successive such planes are required for a complete description. On the other hand, the stacking of the dislocation planes along **b** is still

... 1 1 1 1 ... ,

so that the usual construction of removing or inserting a half-plane suffices.

(2) It lies within the parallelogram **b**, **p**, as illustrated in Fig. 1(b), in which case the stacking of the dislocation planes along **b** is

... 1 2 1 2 1 2

Removal or insertion of a half-plane alters this stacking to

... 1 2 1 2 2 1 2 1 ... ,

and hence produces a dislocation of Burgers vector **b/2**. The new stacking is energetically unfavourable except in certain special cases, so that the existence of a dislocation of this kind* is most improbable. Removing or inserting two half-planes restores the stacking

... 1 2 1 2 ... ,

as illustrated in Fig. 1(b), and hence produces a dislocation of Burgers vector **b**. As regards the elevation planes, their stacking along **d** is

... 1 1 1 1 ... ,

so that only one map is required.

(3) It lies within the interior of the parallelepiped and not on one of the sides. In this case the stacking of the dislocation planes along **b**, and of the elevation planes along **d**, is

... 1 2 1 2 ... ,

* Such dislocations are referred to as imperfect dislocations since **b/2** is not a lattice vector.

so that a combination is required of the construction (1) and of the description (2).

We now show how to construct a dislocation of Burgers vector **b**, which (Fig. 2) consists of a sequence

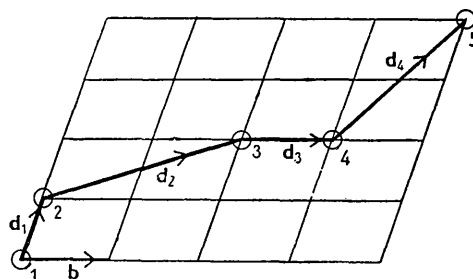


Fig. 2. Dislocation line including pure screw segment O_3O_4 .

of straight-line segments. At the point O_n , initiating the segment O_nO_{n+1} having the direction of the lattice vector \mathbf{d}_n , we examine the parallelepiped defined by \mathbf{b} , \mathbf{d}_n , \mathbf{p} ; if this is primitive, we remove or insert the strip of dislocation plane \mathbf{d}_n , \mathbf{p} standing on O_nO_{n+1} ; if it contains a lattice point L in the interior, we must also remove or insert the parallel strip passing through L . The vectors \mathbf{b} , \mathbf{p} are the same for each initiating point O_n , i.e. the elevation planes are parallel for each segment of the dislocation line, thus enabling us to follow completely the alteration in structure from one segment to the next. An interesting restriction on \mathbf{d}_n is suggested by the analysis, viz. that the number of interior points within the parallelepiped \mathbf{b} , \mathbf{d}_n , \mathbf{p} should be constant for the dislocation line, e.g. if \mathbf{b} , \mathbf{d}_1 , \mathbf{p} is primitive we should expect \mathbf{b} , \mathbf{d}_2 , \mathbf{p} and all succeeding triplets to be primitive. This follows from the consideration that an elaborate physical mechanism would be required for varying the number of parallel strips of dislocation plane to be removed or inserted on

passing from one segment to the next.* The extreme case $\mathbf{d}_n \parallel \mathbf{b}$ is possible, and defines a segment $O_n O_{n+1}$ of pure screw orientation; the extreme case $\mathbf{d}_n \cdot \mathbf{b} = 0$ defines a segment $O_n O_{n+1}$ of pure edge orientation; intermediate cases may be regarded as the superposition of pure screw and pure edge orientations.

Examples of c.p.h. and diamond dislocations

If the structure consists of two interpenetrating lattices, an A -lattice and a B -lattice, we take \mathbf{b} , \mathbf{d} , \mathbf{p} to be lattice vectors of the A -lattice and emanating from an A -point; no matter how \mathbf{b} , \mathbf{d} , \mathbf{p} are chosen, there always exists on B -point within the parallelepiped \mathbf{b} , \mathbf{d} , \mathbf{p} so that, in general, at least two half-planes must be removed to maintain a constant Burgers vector \mathbf{b} along a dislocation line. Sometimes we can arrange for the B -point to fall within the parallelogram \mathbf{d} , \mathbf{p} ; in this case, the stacking of the dislocation planes along \mathbf{b} is

$$\dots 111111\dots,$$

and therefore only one removal or insertion suffices. To determine such planes, referred to hereafter as AB -planes, we make use of the following theorem: if the A -lattice is referred to a primitive unit cell \mathbf{a} , \mathbf{b} , \mathbf{c} which contains a B -point at $x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$, the A -plane (hkl) passes through B -points if $hx + ky + lz$ is an integer (Jaswon & Dove, 1955). Thus the c.p.h. structure may be referred to a primitive hexagonal unit cell, with a B -point at $[\frac{2}{3}, \frac{1}{3}, 0, \frac{1}{2}]$, in which case the AB -planes are $(\bar{1}\bar{2}10)$, as illustrated in Fig. 3(a); these are singly stacked along the direction of the slip vector $\mathbf{b} = [1, 0, 0, 0]$ lying in the basal plane (0001) ,

* Formal geometry alone does not, of course, determine the crystallographic direction of least energy for a given \mathbf{b} , but is an important factor which should be taken into consideration.

as illustrated in Fig. 3(b), and hence qualify as the most likely dislocation planes for this mode of slip. The intersection of $(\bar{1}\bar{2}10)$ with (0001) defines the dislocation direction $\mathbf{d} = [1, 0, \bar{1}, 0]$. As is apparent from Fig. 3(a), the stacking of the dislocation planes along \mathbf{d} is

$$\dots 1212\dots$$

so that maps of two successive such planes are necessary (Fig. 3(c)). Since $(\bar{1}\bar{2}10)$ are the only AB -planes in this structure, any deviation from the direction $[1, 0, \bar{1}, 0]$ implies the removal of at least two parallel strips of dislocation plane corresponding to the new segment, and is hence unlikely, bearing in mind the considerations of the preceding paragraph. If so, the restriction to the straight line $[1, 0, \bar{1}, 0]$ may be removed only by introducing segments of pure screw orientation.*

The diamond structure may be referred to a f.c.c. structure cell, with a B -point at $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$, in which case the AB -planes are $(\bar{1}\bar{1}0)$ (Fig. 4(a)). These are perpendicular to (111) , and singly stacked along the direction of the vector $\mathbf{b} = \frac{1}{2}[1, 0, \bar{1}]$, which qualifies as the most likely slip vector (Fig. 4(b)).

As shown in Fig. 4(a), no less than three successive elevation maps are required for a complete description. An alternative possibility for slip is $\mathbf{b}' = \frac{1}{2}[2, \bar{1}, \bar{1}]$, but this should not be expected to compete with \mathbf{b} for the following reasons: (1) $\mathbf{b}' > \mathbf{b}$, so that the energy associated with \mathbf{b}' exceeds the energy associated with \mathbf{b} . (2) The AB -planes $(\bar{1}\bar{1}0)$, which are the most likely dislocation planes, are triply stacked along \mathbf{b}' but only singly stacked along \mathbf{b} (Fig. 4(b)). (3) Unlike the case with the f.c.c. lattice, the reaction path

* The planes $(11\bar{2}0)$, $(\bar{2}110)$ are crystallographically equivalent to $(\bar{1}\bar{2}10)$; the former intersects the basal plane along $\mathbf{d}' = [1, \bar{1}, 0, 0]$ and is singly stacked along $\mathbf{b} = [1, 0, 0, 0]$. This means that segments of direction \mathbf{d}' are also allowed.

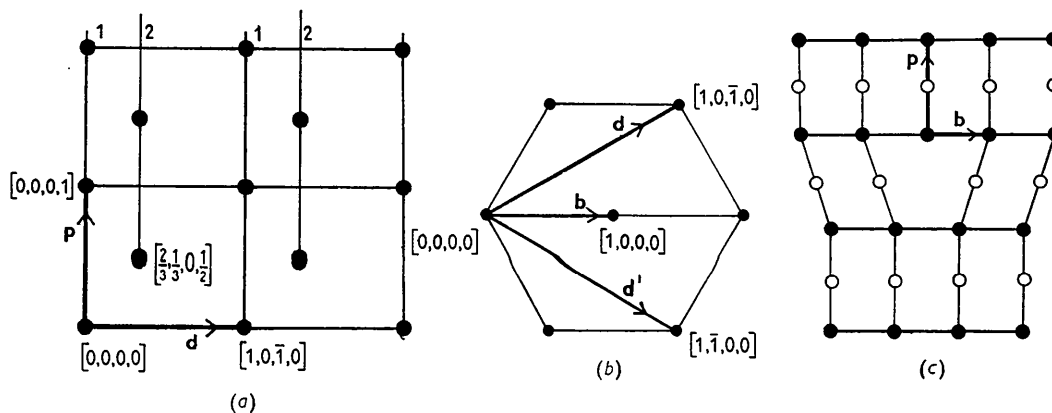


Fig. 3. (a) Map of c.p.h. $(\bar{1}\bar{2}10)$ plane showing arrangement of A - and B -points and consequent $\dots 1212\dots$ stacking of elevation planes.

(b) C.p.h. (0001) plane showing Burgers vector $\mathbf{b} = [1, 0, 0, 0]$ and dislocation line $\mathbf{d} = [1, 0, \bar{1}, 0]$. The direction \mathbf{d}' is crystallographically equivalent to \mathbf{d} , defining the alternative dislocation plane $(11\bar{2}0)$.

(c) Filled circles define map of the first of a pair of c.p.h. elevation planes; open circles are the projection of the second of the pair along the direction \mathbf{d} .

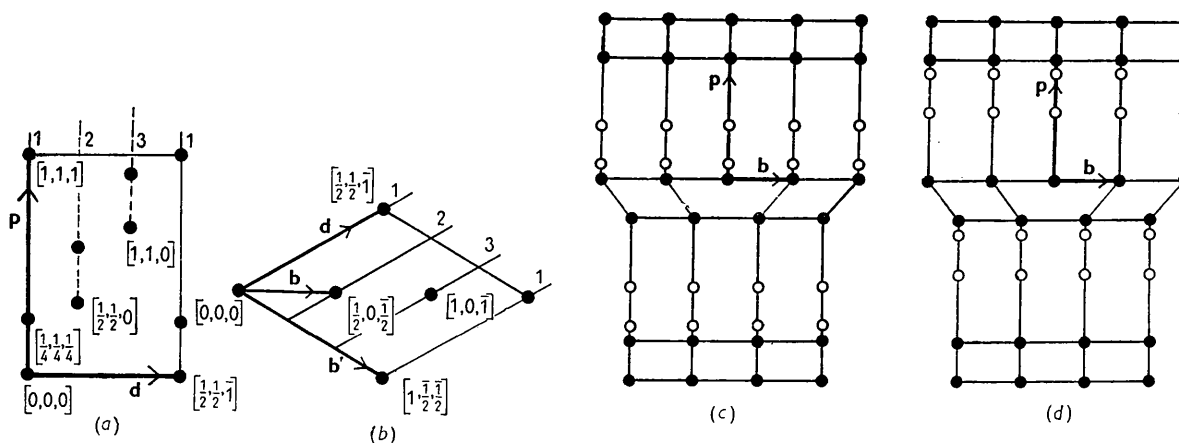


Fig. 4. (a) Diamond ($1\bar{1}0$) dislocation plane showing arrangement of A- and B-points and ... 1 2 3 1 2 3 ... stacking of elevation planes.

(b) Diamond (111) slip plane showing ... 1 2 3 1 2 3 ... stacking of dislocation plane traces along $\mathbf{b}' = \frac{1}{2}[2, \bar{1}, \bar{1}]$, and ... 1 1 1 ... stacking along $\mathbf{b} = \frac{1}{3}[1, 0, \bar{1}]$.

(c) Second plane of the triplet of elevation planes projected (open circles) on to the first (filled circles) along the direction \mathbf{d} .
 (d) Third plane of the triplet projected (open circles) on to the first (filled circles) along \mathbf{d} .

for $[2\bar{1}\bar{1}]$ glide has no advantage compared with $[10\bar{1}]$ glide. It may be remarked, however, that the elements (111) $[21\bar{1}]$ yield the minimum macroscopic shear which could twin the lattice.

No clear-cut evidence has ever been presented for the occurrence of plastic deformation in diamond; at elevated temperatures, slip on $\{111\}$ planes has been reported for germanium and silicon, but the slip direction has not yet been decisively determined (Maddin & Chen, 1954). This suggests that potentially glissile dislocations \mathbf{b} or \mathbf{b}' exist in diamond, but are rendered immobile by various physical factors which are particularly dominant at low temperatures. Discussion of these factors lies outside the scope of the present paper.

Imperfect dislocations

Under certain circumstances we may construct dislocations for which \mathbf{b} is not a lattice vector. These fall into two main classes, sessile dislocations and non-sessile dislocations. Perhaps the best known example of the former class is provided by Frank's dislocation of Burgers vector $\mathbf{b} = \frac{1}{3}[1, 1, 1]$ in the f.c.c. lattice, for which an elevation plane is mapped in Fig. 5. The dislocation planes are (111), of which the stacking pattern along their normal is

$$\dots 1\ 2\ 3\ \dots;$$

removing a half-plane 2 alters this to

$$\dots 1\ 2\ 3\ 1\ 3\ 1\ 2\ 3\ \dots$$

in the lower half-crystal, thereby producing a monolayer twin fault 3 1 3. This dislocation is energetically feasible, but is incapable of movement except, possibly, by the mechanism of vacancy diffusion. Unlike the case with glissiles, the physical properties of a sessile dis-

location—as well as its crystallographic structure—depend very critically on the choice of the dislocation plane. Another example is provided by Cottrell's sessile dislocation $\mathbf{b} = \frac{1}{3}[1, 1, 2]$ in the b.c.c. lattice. Here the dislocation planes are (112), of which the stacking pattern along the normal is

$$\dots 1\ 2\ 3\ 4\ 5\ 6\ \dots;$$

inserting two extra half-planes 12 alters this to

$$\dots 5\ 6\ 1\ 2\ 1\ 2\ 3\ 4\ 5\ 6\ \dots$$

in the upper half-crystal, thereby producing a monolayer twin fault 2 1 2. An alternative, equivalent, procedure, is to remove the four half-planes 3 4 5 6, thereby altering the stacking to

$$\dots 5\ 6\ 1\ 2\ 1\ 2\ 3\ 4\ \dots$$

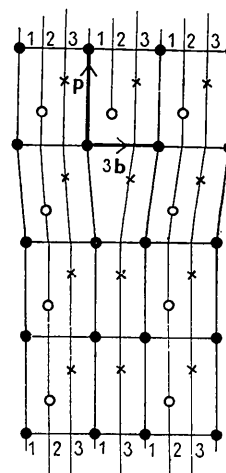


Fig. 5. F.c.c. ($1\bar{1}0$) plane, this being an elevation plane for the sessile dislocation $\mathbf{b} = \frac{1}{3}[1, 1, 1]$, ($\mathbf{p} = \frac{1}{3}[1, 1, 2]$).

in the lower half-crystal and again producing a twin fault. To generalize these results to planes of normal stacking pattern

$$\dots 1\ 2\ 3\ 4 \dots n \dots,$$

we may form a sessile either by inserting two extra half-planes or by removing $n-2$.

A complementary pair of half-dislocations, E and N , separated by a stacking fault of monolayer twin, are illustrated in Fig. 6. The dislocation E is constructed by inserting an extra half-plane and, in the usual way, allowing the atoms on its right-hand side to relax to

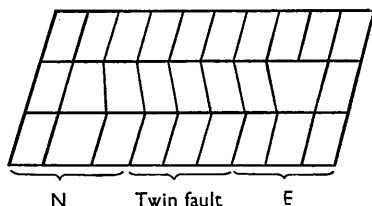


Fig. 6. Extended dislocation consisting of a complementary pair of half-dislocations, E and N , separated by a monolayer twin fault. E contains an extra half-plane, but not N .

the equilibrium configuration characteristic of the perfect crystal; on the left hand side, however, the atoms are allowed to relax only as far as the alternative equilibrium configuration characteristic of the twinned crystal, this being maintained over a certain distance, as shown. The passage of such a dislocation through the crystal leaves in its wake a monolayer twin, which could be formally produced by a homogeneous translation $\lambda\mathbf{b}$ of the upper half-crystal: \mathbf{b} is the unit lattice vector in the twinning direction, and $\lambda/d_{(hkl)}$ the twinning shear. The dislocation N contains no extra half-plane, nor is it deficient in a half-plane, its function being to connect the monolayer twin on its right with the perfect crystal on its left. Its Burgers vector is evidently $(1-\lambda)\mathbf{b}$.

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On the Structure of the Crystal Form C' of n -Hendecanoic Acid

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The crystalline C' -form of n -hendecanoic acid, $C_{10}H_{21}COOH$, is monoclinic with $a = 9.622$, $b = 4.915$, $c = 34.18$ Å and $\beta = 131^\circ 17'$. Space group $C_{2h}^2-P2_1/a$; four molecules in the unit cell. The investigation was carried out at $23^\circ C.$, which is only $5^\circ C.$ below the melting point of the acid. The chains are packed in the common orthorhombic way, but there are large distortions: the chains are probably bent and twisted helically.

Introduction

Normal fatty acids with an odd number of carbon atoms can occur in three polymorphic forms called A' , B' and C' . The crystal structure of the first two have been described by von Sydow (1954*a*, *b*, 1955*b*).

According to Stenhagen & von Sydow (1953) the crystalline C' -form is only stable just below the melting point, and the temperature interval of stability decreases with increasing chain length. Thus a short acid would be more favourable from the X-ray technical point of view, having a relatively wide interval at a more suitable temperature. n -Hendecanoic acid was chosen, the C' -form of which, according to Garner & Randall (1924) and de Boer (1927), exists between the melting point and a temperature between $12.5^\circ C.$ and $17^\circ C.$

Preparation of crystals

The n -hendecanoic acid was obtained from Prof. E. Stenhagen and his collaborators. Its m.p. was $28.0-28.4^\circ C.$

The C' -form is always obtained at temperatures between $17^\circ C.$ and $28^\circ C.$, but the macrocrystalline shape is strongly dependent on the mode of crystallization. Crystallization from the melt always gives conglomerates of crystals which often contain supercooled liquid acid. In order to get crystals suitable for X-ray work, different solvents were tried. Crystallization from carbon tetrachloride solution gave the best crystals, although not very good. They were always twinned, which mostly could be detected in polarized light, and they were often bent owing to their softness near the melting point. Like all the other crystal