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Twinning Properties of Lattice Planes

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A novel crystallographic analysis is undertaken of atomic movements in deformation twinning of metals. Body-centred cubic metals, indium and mercury are treated in detail, and it is established that the operative twinning mode always involves the smallest possible homogeneous shear which could twin the lattice. An analogous criterion is developed for multiple lattices.

Introduction

Twinned crystals are usually analysed in terms of four crystallographic twinning elements K_1, K_2, η_1, η_2, which are well known (Schmid & Boas, 1950; Hall, 1954) and which require little detailed description here. K_1 denotes the composition or twinning plane, and K_2 denotes the second undistorted plane associated with K_1; η_1, η_2 denote directions lying respectively in K_1, K_2 perpendicular to the line of intersection of K_1 and K_2 (Fig. 1). Mechanical twinning is

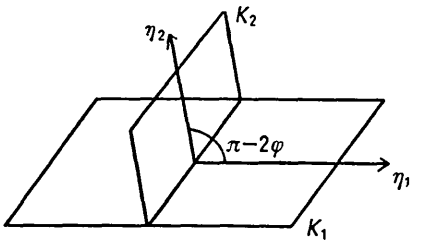

Fig. 1. K_1 denotes the twinning plane, and η_1 the shear direction. K_2 denotes the second undistorted plane.

achieved by a homogeneous macroscopic shear parallel to K_1 along the direction η_1 (referred to hereafter as the shear or twinning direction), the amount of the shear being given by $S = 2\cot 2\varphi$, where 2φ denotes the angle between η_1 and η_2. The plane perpendicular to K_1 passing through η_2 (and hence also through η_1) is termed the plane of shear. In all metals, with the exception of certain twinning modes of α-uranium, an examination of the crystal structure reveals that the plane of shear is a plane of symmetry of the crystal. However, contrary to what is sometimes stated, there is no obvious reason why this should be the case. There are two distinct kinds of twinning, referred to as first and second. In twinning of the first kind, K_1 is rational, and may be regarded as the plane of an imagined mirror which reflects the structure of the twin into that of the matrix. In twinning of the second kind, K_1 is irrational, but η_1 is rational, and may be regarded as the direction of an imagined axis about which a rotation of 180° transforms the structure of the twin into that of the matrix. For any given mode

$$K_1=(hkl),\quad K_2=(h'k'l'),\quad \eta_1=[UVW],\quad \eta_2=[U'V'W'],$$

there exists theoretically a conjugate or reciprocal mode

$$K_1=(h'k'l'),\quad K_2=(hkl),\quad \eta_1=[U'V'W'],\quad \eta_2=[UVW],$$

involving the same macroscopic shear. From the macroscopic point of view, there should be nothing to choose between a mode and its conjugate, but in certain crystal structures only one of the pair is found to be operative. As far as we are aware, no mechanical twinning has ever been substantiated in f.c.c. metals and in diamond. Mechanical twins have been reported in germanium and silicon under special conditions of temperature and loading, but the data are not sufficiently precise to allow a definitive assignment of the twinning elements. Apart from these cases, twinning has been established in all other metals as a possible mode of plastic deformation.

In the present paper, we undertake a new crystallographic treatment of twinning of the first kind by projecting the crystal on to K_1; in effect, we examine the stacking properties of the crystal planes parallel to K_1. This enables a very clear picture to be obtained of the atomic movements required for twinning, and one which is more elegant and powerful than the usual picture obtained by mapping on to the plane of the shear. In spite of its simplicity and relevance, such an approach has never before been systematically pursued. The method is first applied to simple lattices, i.e. those defined by the crystal structures of the b.c.c. metals, indium and mercury, for in these cases mechanical twinning may be achieved by a shear which is homogeneous on the atomic scale. Projecting on K_1 reveals the following property of the operative twinning direction η_1: of all the possible homogeneous shears parallel to K_1 that twin the lattice, the shear along η_1 has the smallest magnitude. This result is not unexpected, but, as far as we are aware, has never been explicitly proved or even stated. The analysis

is then extended to examine the factors which determine the choice of K_1. Given any lattice plane K, projecting on K enables us to deduce the homogeneous twinning shear of smallest magnitude parallel to K, the amount of this hypothetical shear being denoted $\mathscr{S}$. Applying an inequality theorem proved in the text, we arrive at the following significant conclusion: for a given lattice, $\mathscr{S}$ attains a minimum value S on the planes of indices K_1 and K_2. Accordingly, the operative mode in a lattice may be predicted by means of a simple, formal, geometrical requirement, that of minimum homogeneous twinning shear. This result may be readily understood in terms of the theory of dislocations. The mobility of a dislocation depends critically on the ratio of its Burgers vector, **b**, to the interplanar spacing, d, and increases as b/d decreases (Cottrell, 1953). In the present context b/d is to be identified with $\mathscr{S}$, so that the minimum value of the ratio is given by S.

Mechanical twinning in a multiple lattice, e.g. that defined by the c.p.h. crystal structure, cannot be completely homogeneous on the atomic scale, so that an extension of the analysis is required. This is effected by introducing a new notion, that of the semi-homogeneous shear, which may be roughly described as a shear homogeneous on the finest possible scale compatible with producing a twinned configuration; a rigorous definition is given in the text. The magnitude and direction of the semi-homogeneous shear are defined to be those of its homogeneous component, the latter being identified with the macroscopic twinning shear. On this basis a quantitative theory of multiple lattices may be developed. Projecting on K_1 reveals the following property of the operative twinning direction η_1: of all the possible semi-homogeneous shears parallel to K_1 that twin the crystal, the shear along η_1 has the smallest magnitude. As a corollary, given a composition plane, but not the shear direction, theoretical analysis should suffice to determine the latter, and hence also the magnitude of the twinning shear. For instance, a plane $(10\bar{1}1)$, of ill-defined shear direction η_1, has been reported by Schiebold & Siebel (1931) as operative in magnesium. A high shear value, 1·066, has been deduced for this mode on the assumption that η_1 may be identified as the line of intersection of $(10\bar{1}1)$ and of the perpendicular plane of symmetry $(1\bar{2}10)$. The present method, however, indicates a shear of amount 0·353 along the irrational direction '$[\bar{1}2\bar{2}\bar{1}]$'. This latter value seems much more reasonable, and renders the reported occurrence of the mode less remarkable. In the one other case where an application of the method leads to an irrational twinning direction, i.e. '$[3\bar{7}2]$' for the α-uranium (112) mode, this is found to be in complete agreement with the experimental observations of Cahn.

There remains the important problem of discovering the factors which determine the choice of K_1 in a multiple lattice. This problem, and various particular problems of twinning, will be taken up in a later paper.

Body-centred cubic metals, indium and mercury

Twinning in a simple lattice is illustrated schematically in Fig. 2. Using a convenient and obvious notation, successive parallel lattice planes are denoted $\ldots\bar{3}, \bar{2}, \bar{1}, 0, 1, 2, 3, \ldots$. The composition plane K_1 is identified with the plane 0. We now translate plane 1, parallel to K_1, so that it becomes the mirror image of plane $\bar{1}$ with respect to K_1 as mirror plane. The translation vector in question is denoted **T**, and will be referred to as a twinning translation. Such a translation is not unique, for if **L** is any lattice vector parallel to K_1, then **T**+**L** is also a twinning translation. To remove ambiguity, we define **T** to be the smallest possible twinning translation of plane 1, i.e. $T<|\mathbf{T}+\mathbf{L}|$; **T** can be picked out at sight by projecting plane 1 on to plane $\bar{1}$. The vector **T** formally determines a shear $S = T/d$ (d is the interplanar spacing) which always accords, both in magnitude and direction, with the experimentally determined macroscopic shear. As regards the succeeding lattice planes, the most plausible assumption we can make is that each plane moves in essentially the same way, namely by undergoing a translation **T** relative to its predecessor. These movements constitute a homogeneous shear S which twins the lattice, and which may be identified with the macroscopic twinning shear. Bearing in mind the minimum property of **T**, we are led to the conclusion given in the introduction.

As an example of the projection technique, a b.c.c. (112) plane is mapped in Fig. 3. Each symbol ● marks the position of a lattice point in the plane, with co-ordinate parameters as attached. The symbol ○ denotes the projection of a lattice point of the succeeding parallel plane, and may be regarded as obtained by a shift (Jaswon & Dove, 1955) along the

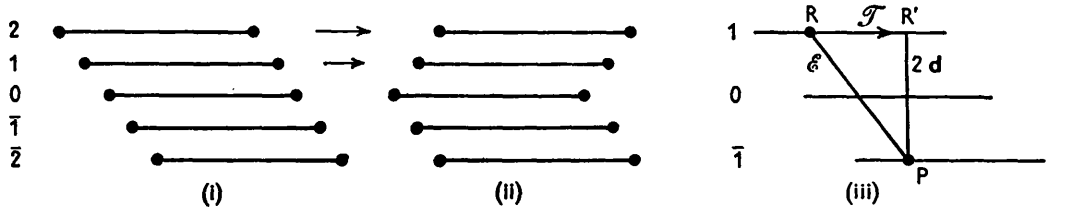

Fig. 2. (i) Original stacking. (ii) Twin configuration. (iii) Twinning translation of plane 1. (Schematic.)

dashed line, as indicated. A shift of double the amount leads to the point marked ①, which denotes the projection of a lattice point of the next succeeding parallel plane. It is convenient to identify these three suc-

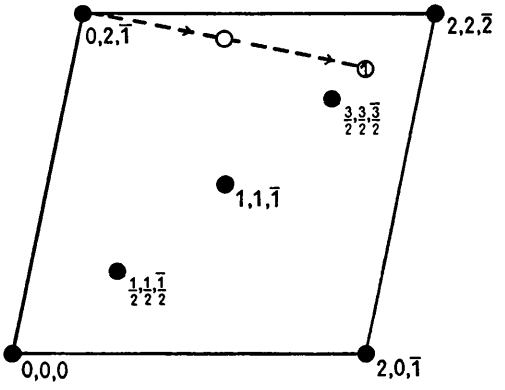

Fig. 3. B.c.c. (112) plane. ① ≡ [⅝, ⅝, 5̄/8].

cessive lattice planes with the planes $\bar{1}$, 0, 1 respectively of Fig. 2. We now seek the minimum translation which carries plane 1 over plane $\bar{1}$, i.e. so that it becomes the mirror image of plane $\bar{1}$, with respect to the mirror plane 0. This implies that the projection ① of a lattice point of plane 1 must be brought into coincidence with the nearest neighbouring lattice point ● of plane $\bar{1}$. Referring to Fig. 3, it will be seen that the translation in question is defined by the movement

$$① \rightarrow [\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{\bar{3}}{2}],$$

whence

$$\mathbf{T} = [\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{\bar{3}}{2}] - [\tfrac{5}{3}, \tfrac{5}{3}, \tfrac{\bar{5}}{3}] = [\tfrac{\bar{1}}{6}, \tfrac{\bar{1}}{6}, \tfrac{1}{6}];$$

accordingly, since

$$d_{(112)} = 1/\sqrt{6},$$

$$T = 1/\sqrt{12},\ S = T/d_{(112)} = 1/\sqrt{2},\ \eta_1 = [\bar{1}\bar{1}1].$$

The conventional deduction of this well known result compares unfavourably with the present deduction in that a knowledge of η_1 is assumed at the outset, i.e. the plane of shear is identified as the plane of symmetry perpendicular to K_1. No justification is given for this identification, which, as already noted, has almost certainly proved misleading when applied to the magnesium $(10\bar{1}1)$ mode. Mapping on to K_1 brings out clearly the essential factor which determines the choice of η_1.

We now compare S with the hypothetical homogeneous twinning shears parallel to other lattice planes. This is most conveniently done indirectly, by making use of the inequality theorem. The theorem may be proved by reference to Fig. 2(iii), in which is illustrated the traces of three successive parallel lattice planes $\bar{1}$, 0, 1, together with a lattice point P in plane $\bar{1}$ and its nearest neighbouring lattice point R in plane 1; the vector PR is referred to as $\boldsymbol{\mathscr{E}}$. Plane 1 may become the image of plane $\bar{1}$, with respect to the mirror plane 0, by undergoing the twinning translation $\mathscr{T} = RR'$, where R' lies directly over P; $\mathscr{T}$ is evidently the smallest possible twinning translation of plane 1. If $\mathscr{S}$ is the hypothetical twinning shear defined by $\mathscr{T}$, we have

$$\mathscr{S}^2 = \mathscr{T}^2/d^2 = (\mathscr{E}^2 - 4d^2)/d^2 = \mathscr{E}^2/d^2 - 4,$$

i.e.

$$1/d^2 = (\mathscr{S}^2+4)/\mathscr{E}^2,$$

where d is the interplanar spacing. Now replacing $\boldsymbol{\mathscr{E}}$ by $\mathbf{E}$, where $\mathbf{E}$ is the smallest possible lattice vector, we obtain the inequality

$$1/d^2 \leq (\mathscr{S}^2+4)/E^2,$$

satisfied by the $\mathscr{S}$, d of any lattice plane (hkl). As a corollary, for any prescribed value of $\mathscr{S}$, e.g. $\mathscr{S} = 1$, the inequality places a restriction on $1/d^2$, and hence on the planes (hkl) satisfying the inequality.

In the b.c.c. lattice,

$$\mathbf{E} = [\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}],\ E^2 = \tfrac{3}{4}a^2;$$

also

(i) $a^2/d^2 = 4(h^2+k^2+l^2)$ if $h+k+l$ is odd,

(ii) $a^2/d^2 = h^2+k^2+l^2$ if $h+k+l$ is even.

The inequality thus assumes the form

(i) $h^2+k^2+l^2 \leq \mathscr{S}^2/3+\frac{4}{3}$ if $h+k+l$ is odd,

(ii) $h^2+k^2+l^2 < 4\mathscr{S}^2/3+\frac{16}{3}$ if $h+k+l$ is even.

Setting $\mathscr{S} = 1$, the only possibilities to be considered are:

(i) 100; (ii) 101, 112.

Of these planes, (100) and (101) are symmetry planes, thus indicating (112) as the twinning plane. S and η_1 for this plane are then found by applying the projection technique, as already shown.

If the plane $\bar{1}$ has the equation $hx+ky+lz = 0$, then the plane 1 has the equation $hx+ky+lz = 2$, where $[x, y, z]$ are the co-ordinate parameters of a lattice point in the plane. Accordingly, regarding P as the origin, and writing $\boldsymbol{\mathscr{E}} = [\mathscr{E}_x, \mathscr{E}_y, \mathscr{E}_z]$, we have $h\mathscr{E}_x+k\mathscr{E}_y+l\mathscr{E}_z = 2$. Of all the possible solutions of $hx+ky+lz = 2$, the solution $[\mathscr{E}_x, \mathscr{E}_y, \mathscr{E}_z]$ defines the vector of shortest length, which property may be used as a means of identifying it. Once $\boldsymbol{\mathscr{E}}$ is known for a given set of planes (hkl), we may write

$$\mathscr{S}^2 = \mathscr{E}^2/d^2 - 4,\ \mathscr{T} = \boldsymbol{\mathscr{E}} - 2\mathbf{d}.$$

Alternatively, of course, $\mathscr{S}$ may be found directly by projecting plane 1 on to $\bar{1}$. In the case of the operative twinning plane K_1, we write $\boldsymbol{\mathscr{E}} = \boldsymbol{\mathscr{E}}_0$; also $\mathscr{T} \equiv \mathbf{T}$. Accordingly,

$$S^2 = \mathscr{E}_0^2/d^2 - 4,\ \mathbf{T} = \boldsymbol{\mathscr{E}}_0 - 2\mathbf{d}.$$

Our results show that $\boldsymbol{\mathscr{E}}_0$, $\mathbf{T}$ always have the directions of η_2, η_1 respectively. The vector $\boldsymbol{\mathscr{E}}_0$ does not

usually coincide with the shortest lattice vector **E**, but happens to do so for the b.c.c. $K_1 = (112)$. On setting $\boldsymbol{\mathscr{E}}_0 = \mathbf{E} = [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$, $\mathbf{d} = \frac{1}{6}[1, 1, 2]$, it may be readily verified that the preceding equations yield the correct S, η_1 for this lattice.

The indium lattice may be referred to a face-centred tetragonal unit cell, of axial ratio $q = c/a = 1{\cdot}078$. The inequality theorem indicates $K_1 = (101)$ for all f.c.t. lattices within the range $\frac{1}{3} < q^2 < 3$, and the projection method then gives

$$S = (q^2-1)/q, \quad \eta_1 = [10\bar{1}] .$$

These results are borne out by indium, and also include the b.c.c. results as a particular case: this lattice may be referred to a face-centred cell which is tetragonal, of axial ratio $q = 1/\sqrt{2}$, whence

$$(112)\ [11\bar{1}] \rightarrow (101)\ [10\bar{1}]$$

and $S = (q^2-1)/q = 1/\sqrt{2}$. The f.c.c. lattice corresponds to the case $q = 1$, for which $S = 0$, thus showing that twins of this mode are precluded from forming. The mercury lattice may be referred to a face-centred structure cell which is rhombohedral, of angle $\alpha = \cos^{-1} \bar{1}/7$, and it is interesting to note that with these axes K_1 has again the indices (101). From the inequality theorem, $K_1 = (101)$ or (010), but the latter plane is never found to be operative; this may be due to the fact that it possibly functions as a slip plane, as proposed by Andrade & Hutchings (1935). Projecting on (101) gives

$$S = 2w/\sqrt{\{\tfrac{1}{2}(1+w)-w^2\}}, \quad \eta_1 = [0\bar{1}0] ,$$

where $w = \cos\alpha$. The f.c.c. lattice corresponds with the case $\alpha = \frac{1}{2}\pi$, for which, as expected, $S = 0$.

Theory of multiple lattices

A multiple lattice, e.g. that defined by the c.p.h. structure, may be regarded as consisting of two interpenetrating lattices, so that all planes occur in pairs. Using an obvious adaptation of the preceding notation, successive parallel planes of the one lattice are denoted $\ldots\bar{2}a, \bar{1}a, 0a, 1a, 2a\ldots$, and the corresponding planes of the other lattice $\ldots\bar{2}b, \bar{1}b, 0b, 1b, 2b\ldots$, as depicted in Fig. 4. Given the plane $0a$, there are two possibilities for the associated plane $0b$, namely the neighbouring b plane separated by the narrow gap and the neighbouring b plane separated by the wide gap. This leads to four* distinct possibilities for the nature of K_1:

(1) K_1 coincides with $0a$.
(2) K_1 coincides with $0b$.
(3) K_1 is taken to be the plane of an imagined mirror midway between $0a$ and $0b$ (narrow gap). This hypothetical plane is denoted by the symbol D, and illustrated by the dotted line in Fig. 4(i).
(4) K_1 is taken to be the plane of an imagined mirror midway between $0a$ and $0b$ (wide gap). This hypothetical plane is denoted by the symbol D', and illustrated by the dotted line in Fig. 5(i).

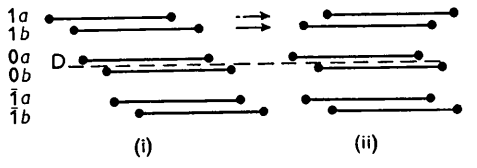

Fig. 4. Narrow gap possibility. The planes $0a$, $0b$ assume a compromise position between twin and matrix, but the stacking of $0a$, $0b$ is approximately maintained. (Schematic.)

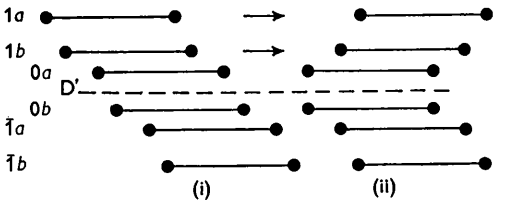

Fig. 5. Wide gap possibility. The planes $0a$, $0b$ alter their stacking to assume an ideal twin configuration. (Schematic.)

Of these possibilities, (3) is equivalent to (4) in the sense that any macroscopic results deduced with (3) may be reproduced with (4) using essentially the same criteria of calculation. However, (3) has the theoretical advantage of enabling us to form a simpler picture of the atomic movements. Any results deduced with (3) or (4) may also be deduced with (1) or (2), but more complicated atomic adjustments are required and are unlikely on physical grounds. For these reasons K_1 is identified with D in most of the following treatment, but it may be emphasized that the macroscopic significance of the work remains unaffected even should this choice turn out to be wrong in any particular case.

As regards the detailed structure of the composition plane, we note that in an ideal twin the planes $0a$, $0b$ should be mirror images with respect to D or D', depending on which is operative. Such a configuration, however, would generally require a drastic distortion of the equilibrium stacking of $0a$, $0b$, and which could hardly be tolerated if D were operative. In this case, it seems likely that the equilibrium stacking is largely maintained, but that $0a$, $0b$ move forward to a compromise position between twin and matrix (Fig. 4(ii)); the main contribution to the boundary energy then arises from the misfit between the widely spaced neighbouring planes $0b$, $\bar{1}a$ and $0a$, $1b$. If a drastic distortion of the equilibrium stacking could be tolerated, as seems likely if D' were operative, then an approximation to the ideal twin configuration may be realized

* There exists a fifth possibility, namely that $0a$, $0b$ coalesce into a single plane, thus enabling an ideal twin to be produced. An analysis based on this possibility would be identical with that based on (3).

(Fig. 5(ii)); in this case, the main contribution to the boundary energy arises from the stacking misfit of the widely spaced neighbouring planes $0a$, $0b$. Which kind of boundary involves the lower misfit energy cannot be decided from qualitative arguments. Diamond presents an interesting situation in that $0b$ is in any case stacked directly over $0a$, for the wide gap between (111) planes, thus enabling an ideal twin to be formed without any nearest-neighbour misfit whatever. In spite of this, no mechanical twinning has ever been substantiated for diamond, presumably because of the large activation energy required for the atomic movements. This illustrates a general principle implied by the results of the present investigation, namely the existence and choice of K_1 is determined primarily by the nature of the atomic twinning movements involved, and not by the misfit energy at the boundary.

From the foregoing paragraphs, it appears that the boundary distortion may be ignored in calculating the macroscopic twinning properties of a crystal. The problem thus reduces to that of determining the most likely twinning displacements of the succeeding crystal planes $1a$, $1b$, $2a$, $2b$, ... When a crystal undergoes a homogeneous macroscopic shear, the most natural assumption we can make about the microscopic shear is that of homogeneity on the scale of each crystal plane. Topologically, however, this is only possible for simple lattices. In multiple lattices, the analogous assumption is that of homogeneity on the scale of succeeding units of pairs of planes $1a$, $1b$; $2a$, $2b$; .... More precisely, the pair $1a$, $1b$ have a mean or average twinning translation $\mathbf{T}$, the pair $2a$, $2b$ have a mean twinning translation $2\mathbf{T}$, and so on. The successive mean translations $\mathbf{T}$, $2\mathbf{T}$, ..., $n\mathbf{T}$, ... constitute the homogeneous component of the microscopic shear, and produce the macroscopic shape deformation of the crystal, namely a twinning shear of amount $S = T/d$ in the direction of $\mathbf{T}$. Superimposed on the homogeneous component, there are inhomogeneous displacements of the crystal planes; these have no macroscopic effects, but are necessary in order to generate the twinned configuration. For a given homogeneous component, the inhomogeneous displacements cannot be uniquely defined mathematically. On physical grounds, however, we lay down the requirement that they be as small as possible. A microscopic shear, with homogeneous and inhomogeneous components thus defined, amounts as nearly as possible to a homogeneous shear compatible with producing a twinned configuration, and will therefore be referred to as a semi-homogeneous twinning shear. The properties of the semi-homogeneous shear in multiple lattices bear a close analogy to the properties of the homogeneous shear in simple lattices, in particular the former is effectively determined by the mean twinning displacement of the first pair of planes $1a$, $1b$ just as the latter is determined by the twinning displacement of the plane 1.

Our detailed analysis of the twinning displacements of the planes $1a$, $1b$ is as follows. Referring to Fig. 4, the plane $1a$ undergoes a twinning translation $\mathbf{T}_a$, parallel to D, to become the mirror image of plane $\bar{1}b$ with respect to D. This kind of translation is not unique, for if $\mathbf{L}$ is any lattice vector parallel to D then $\mathbf{T}_a+\mathbf{L}$ is also a twinning translation. To remove ambiguity, we define $\mathbf{T}_a$ to be the smallest possible twinning translation of plane $1a$, i.e. $T_a < |\mathbf{T}_a+\mathbf{L}|$; $\mathbf{T}_a$ can be picked out at sight by projecting plane $1a$ on to $\bar{1}b$. Similarly, the plane $1b$ undergoes the smallest possible twinning translation $\mathbf{T}_b$, parallel to D, to become the mirror image of $\bar{1}a$ with respect to D; $\mathbf{T}_b$ can be picked out at sight by projecting plane $1b$ on to $\bar{1}a$. The mean or average of $\mathbf{T}_a$, $\mathbf{T}_b$ is given by $\mathbf{T} = \frac{1}{2}(\mathbf{T}_a+\mathbf{T}_b)$. The relative translation of the two planes is given by $\mathbf{T}_a-\mathbf{T}_b$, defining the reshuffle vector $\mathbf{t} = \frac{1}{2}(\mathbf{T}_a-\mathbf{T}_b)$; it will be seen that $\mathbf{T}_a = \mathbf{T}+\mathbf{t}$, $\mathbf{T}_b = \mathbf{T}-\mathbf{t}$. We may thus regard the planes $1a$, $1b$ as undergoing a common translation $\mathbf{T}$ (homogeneous component), accompanied by a horizontal reshuffle $\mathbf{t}$, $-\mathbf{t}$ (inhomogeneous component) which carries them into the twinned configuration. The vector $\mathbf{T}$ formally serves to define a shear $S = T/d$, which may be expected to have macroscopic significance. For the c.p.h. $(10\bar{1}2)$ mode, the β-tin (331)* mode, and the α-uranium (112) mode, referred to hereafter as X_1-modes, S accords in both magnitude and direction with the experimentally determined macroscopic shear. This consideration, and the fact that $\mathbf{t}$ never amounts to more than an interatomic spacing along the most close-packed lattice direction of K_1, suggest that $\mathbf{T}_a$, $\mathbf{T}_b$ describe the actual net displacements of the planes $1a$, $1b$ when mechanical twinning takes place in X_1-modes.

So far we have completely ignored the possibility of an interchange of the levels of $1a$, $1b$ (Fig. 6). Thus, the plane $1a$ may undergo a translation $\mathbf{T}'$, parallel to D, till it projects directly over plane $\bar{1}a$. Such a translation is not unique, for $\mathbf{T}'+\mathbf{L}$ produces the same effect as $\mathbf{T}'$. To remove ambiguity, we define $\mathbf{T}'$ to be the smallest possible translation which carries plane $1a$ over plane $\bar{1}a$, i.e. $T' < |\mathbf{T}'+\mathbf{L}|$; $\mathbf{T}'$ can be picked out at sight by the projection method. The

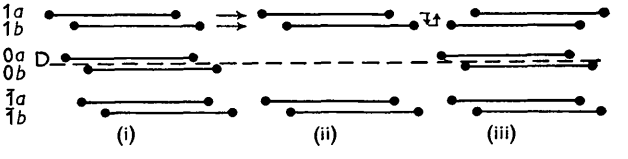

Fig. 6. Interchange mechanism. The planes $1a$, $1b$ move forward by a common translation (ii) and interchange levels (iii). These movements do not necessarily take place successively, so that the intermediate configuration (ii) has not necessarily any physical significance. The planes $0a$, $0b$ assume the same final position as in Fig. 4.

* These are the indices of the operative mode when the β-tin crystal is referred to a face-centred tetragonal unit cell. This choice of cell facilitates comparison with indium.

same translation, applied to plane $1b$, carries it directly over $\bar{1}b$. If these translations are combined with an interchange of the levels of the planes $1a$, $1b$ then a twinned configuration is achieved, i.e. $1a$, $1b$ become the mirror images of $\bar{1}a$, $\bar{1}b$ respectively, with respect to the mirror plane D. The homogeneous component of the twinning displacements is $\mathbf{T}'$, and the reshuffle vector is identified with the interplanar spacing vector between $1a$, $1b$. For the rhombohedral (110) mode, and the α-uranium (130) mode, referred to hereafter as Y_1-modes, the shear $S = T'/d$ accords, in both magnitude and direction, with the experimentally determined macroscopic shear. This consideration, and the fact that the stacking configuration of $1a$, $1b$ is favourable for interchange, suggest that the interchange mechanism describes the actual net displacements of $1a$, $1b$ when mechanical twinning takes place in Y_1-modes.

When the horizontal reshuffle mechanism is applied to Y_1-modes, it is found that $T > T'$. Conversely, when the vertical interchange mechanism is applied to X_1-modes, it is found that $T' > T$. Consequently, the nature of the mode defined by any given rational composition plane, i.e. whether an X_1-mode or a Y_1-mode, may be established at once by working out $\mathbf{T}$ and $\mathbf{T}'$ and comparing their magnitudes. In all cases, the vector of smaller magnitude predicts the magnitude and direction of the observed macroscopic shear. Bearing in mind that the smaller of the two vectors $\mathbf{T}$, $\mathbf{T}'$ defines the smallest possible semi-homogeneous parallel to K_1 that twins the crystal, we are led to the conclusion given in the introduction.

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The Crystal Structure of NbO_2F and TaO_2F

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Niobium dioxyfluoride and tantalum dioxyfluoride have the ReO_3 structure in which fluorine atoms and oxygen atoms are randomly distributed in octahedral positions about the metal atom. The simple cubic unit cell for NbO_2F has $a = 3{\cdot}902 \pm 0{\cdot}001$ Å; and for TaO_2F, $a = 3{\cdot}896 \pm 0{\cdot}003$ Å.

Preparation

A weighed quantity of 99·9% Ta metal was dissolved in 48% aq. HF (reagent grade) in a platinum crucible at ~ 80° C. The clear colorless solution was evaporated to dryness on a steam bath and then heated at 250° C. for 1 hr. Subsequent heating for 1 hr. at 250° C. resulted in 0·19% weight loss. The white powder was analyzed chemically: 76·1±0·5% Ta, 9·04±0·10% F, 0·15±0·01% H (oxygen was not determined directly). Tantalum dioxyfluoride was found to be stable in air at 300° C. but decomposed above 500° C. into Ta_2O_5. When heated in dry oxygen TaO_2F lost some tantalum, presumably by volatilization of TaF_5.

Niobium dioxyfluoride was prepared by digesting pseudohexagonal Nb_2O_5 (Frevel & Rinn, 1955) in 48% aq. HF, evaporating the solution to dryness, and heating the resultant white powder at 250° C. for 1 hr. A larger quantity of NbO_2F was prepared by dissolving niobium metal in 48% aq. HF and heating the solid from evaporation to 275° C. for 5 hr. A chemical analysis yielded 62·6±0·5% Nb, 15·61±0·10% F, 0·21±0·01% H.

X-ray data and structure identification

Powder diffraction patterns were obtained with filtered Cu $K\alpha$ radiation in a cylindrical G.E. camera (71.8 mm. radius) and with a Norelco diffractometer. Relative intensities measured photographically compared favorably with the integrated intensities from the diffractograms. No indication of preferred orientation of crystallites was observed between pressed powder samples and carefully loaded samples. The patterns obtained could be indexed on the basis of a primitive cubic cell. Prolonged exposures or slow scanning failed to reveal any additional lines requiring a larger unit cell. The powder of tantalum dioxyfluoride was found to be isotropic under a polarizing microscope. A comparison of the powder pattern of $TiOF_2$ (Voores & Donohue, 1955) with that of TaO_2F immediately suggested the correct structure; namely,