Acta Cryst. (1960). **13**, 232

The Crystallography of Deformation Twinning

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(*Received* 16 *March* 1959)

The crystallography of deformation twinning is formulated on a fresh mathematical basis. This leads to a simplified technique for calculating the reciprocal elements corresponding to a given pair of rational twinning elements. It is shown how the scale of homogeneity of the deformation may be deduced from macroscopically available data. A new analysis is presented of the atomic displacements involved in rotation twinning. Criteria are laid down for the selection of operative twinning modes out of all those mathematically admissible.

Introduction

Twinned crystals are usually characterised by four crystallographic elements symbolised K_1, K_2, η_1 and η_2, together with two subsidiary elements P and λ, as illustrated in Fig. 1 and enumerated in the following Table.

K_1: twin plane.
K_2: 'second undistorted' plane.
P: plane of shear (perpendicular to K_1, K_2, λ).
η_1: line of intersection of P, K_1.
η_2: line of intersection of P, K_2.
λ: line of intersection of K_1, K_2 (perpendicular to η_1, η_2, P).

Either K_1, η_2 must be rational (reflection twin, or twin of the first kind) or η_1, K_2 must be rational (rotation twin, or twin of the second kind). If K_1 is rational, it may be regarded as a mirror plane which reflects the structure of the twin into that of the matrix crystal.† If η_1 is rational, it may be regarded as an axis about which a rotation of 180° transforms the structure of the twin into that of the matrix crystal.† As regards metals, apart from certain twins in α-uranium and possibly in magnesium and titanium, all four elements are found to be rational and the distinction between the two kinds loses its significance (compound twin). Twinning of either kind may be produced by mechanical means. On the macroscopic scale, the deformation effectively consists of homogeneous simple shear displacements parallel to the plane K_1, in the direction η_1, of shear magnitude defined by

$$S=2\cot\widehat{\eta_1\eta_2}=2\tan\widehat{\eta_1K_2}=2\tan\widehat{\eta_2K_1}\,, \qquad (1)$$

where $\widehat{\eta_1\eta_2}$ denotes the acute angle between the two directions concerned, $\widehat{\eta_1K_2}$ denotes the acute angle between η_1 and the normal to the plane K_2, etc. (Fig. 1).

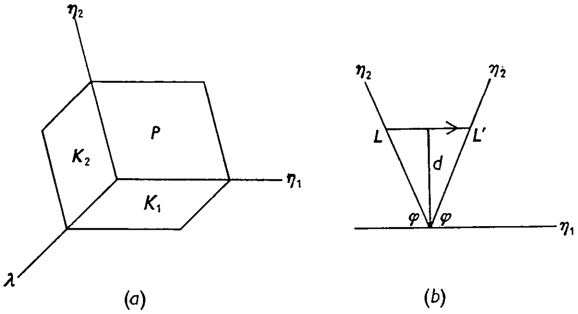

Fig. 1. (*a*) Relation between planes K_1, K_2, P and directions η_1, η_2, λ. (*b*) If atom at L is displaced to L', then $S=LL'/d=2\cot\varphi=2\cot\widehat{\eta_1\eta_2}$, etc.

To any given twin mode

$$K_1=(hkl),\ K_2=(h'k'l'),\ \eta_1=[uvw],\ \eta_2=[u'v'w']$$

there corresponds theoretically a conjugate or reciprocal mode

$$K_1=(h'k'l'),\ K_2=(hkl),\ \eta_1=[u'v'w'],\ \eta_2=[uvw]\,,$$

involving the same S. Accordingly, apart from compound twins, the reciprocal of a reflection twin is a rotation twin, and vice versa. From the macroscopic point of view, there should be nothing to choose between a mode and its reciprocal since both accomplish equivalent deformations. On the other hand, the two displacement systems involved have markedly different crystallographic characteristics, bringing into play different physical factors. It is not surprising to find, therefore, that in most cases one of the pair hardly ever becomes operative except, possibly, under special conditions of temperature and loading. Thus, as shown recently by Japanese investigators (Maruyama & Kiho, 1956), the theoretically expected β-tin $K_1=(101)$ mode makes an appearance

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† In conformity with metallurgical usage the two twin-related parts are here distinguished as 'twin' and 'matrix', respectively.

when the usual $K_1=(301)$ mode is prevented from becoming active by external constraints; it had never previously been reported operative. Mechanical twins in α-uranium polycrystals have been studied by Cahn (1953), and in single crystal specimens by Lloyd & Chiswick (1955). The compound twin

$$K_1=(130),\ K_2=(1\bar{1}0),\quad \eta_1=[3\bar{1}0],\ \eta_2=[110],\ S=0{\cdot}298 \qquad (2)$$

and the rotation twin

$$K_1=\text{‘}(1\bar{7}2)\text{’},\ K_2=(112),\quad \eta_1=[312],\ \eta_2=\text{‘}[3\bar{7}2]\text{’},\ S=0{\cdot}227 \qquad (3)$$

have been established by both investigations; the rotation twin

$$K_1=\text{‘}(\bar{1}\bar{7}6)\text{’},\ K_2=(111),\quad \eta_1=[512],\ \eta_2=\text{‘}[12\bar{3}]\text{’},\ S=0{\cdot}214\ , \qquad (4)$$

has been reported by Lloyd & Chiswick, and the reflection twin

$$K_1=(112),\ K_2=\text{‘}(1\bar{7}2)\text{’},\quad \eta_1=\text{‘}[3\bar{7}2]\text{’},\ \eta_2=[312],\ S=0{\cdot}227\ , \qquad (5)$$

i.e. the reciprocal of (3), has been reported by Cahn. Dashed brackets indicate a convenient rational approximation for an irrational element. The modes are here enumerated according to relative frequency of occurrence. It will be noted that the reciprocals of (2) and (4) do not seem to be operative, and that twins of the second kind are preferred to their reciprocals of the first kind.

Although the crystallography of twinning was first examined over fifty years ago, various important problems in this field still require attention. For instance, the scale of homogeneity of the deformation is indicated by the value of certain crystallographic invariants, but this correlation has never been systematically exploited. No satisfactory treatment exists of rotation twinning atomic displacements, partly because the conventional projection of the crystal on to P yields little, and sometimes misleading, information. Again, to be given a rational pair of twinning elements automatically implies, in principle, a knowledge of the reciprocal pair, but explicit formulae for calculating the latter pair have been lacking. Finally, although twinning phenomena are determined primarily by the crystal structure and not by the specific kind of atom involved, crystallographic criteria for understanding the selection of operative modes have only recently progressed beyond Mallard's law. Failure of an adequate attack on these problems stems from a fundamental limitation inherent in the usual approach to the subject: this first introduces deformations on the macroscopic scale, and only within that framework develops an atomic model. This approach is reversed in the present paper. Our procedure essentially consists of making plausible hypotheses about atomic net twinning displacements, and concentrating on those that lead to the correct macroscopic features. This enables the theory to be formulated on a fresh mathematical basis, in which its powers and limitations become more clearly revealed. Particular emphasis is placed here on rotation twinning displacements, as the less familiar case; this emphasis also facilitates comparison with the data on α-uranium. These displacements are related to their reciprocal reflection twinning displacements by a rigid-body rotation, so that an analysis of the former implies, in fact, a corresponding analysis of the latter.

It is convenient to distinguish between crystals of monatomic and of diatomic motif units. In the former, the atomic sites constitute a Bravais space lattice, as exemplified by b.c.c. metals, indium and mercury. The latter are characterized by a motif structure, as exemplified by c.p.h. metals, α-uranium, β-tin, diamond and bismuth. The text is divided accordingly, each section being supported by a mathematical appendix. These two sections provide an analysis of twins that occur in practice. The third section is concerned with the factors responsible for the selection of operative modes, out of all those mathematically admissible. The main conclusions of this and of previous work are embodied in the final section.

Rotation twinning: Monatomic motif units

A rational axis $\eta_1=[pqr]$ is introduced and a hypothetical crystal deformation $\mathscr{D}$ set up subject to three requirements: each atom undergoes a displacement in the direction η_1, by an amount linearly dependent on its position, to become twin-related to some matrix atom by virtue of a 180° rotation about η_1 (Fig. 2). Analysis (App. I) shows that these three requirements automatically imply an invariant plane strain, i.e. homogeneous simple shear displacements parallel to an invariant plane possibly combined with a uniaxial extension or compression normal to the plane. It will

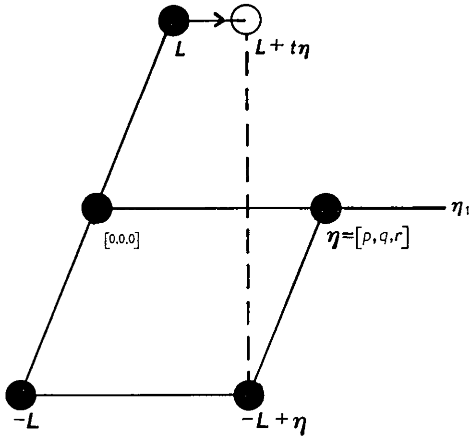

Fig. 2. Atom at $\mathbf{L}$ undergoes displacement $t\boldsymbol{\eta}$ to become twin-related to atom at $-\mathbf{L}+\boldsymbol{\eta}$. In Appendix I the latter point is taken more generally to be $-\mathbf{L}+n\boldsymbol{\eta}$.

be noted that η_1 does not lie within the invariant plane unless the latter component is absent. $\mathscr{D}$ is completely determined by any three assigned integers n_1, n_2, n_3; and it leaves the plane $(n_1n_2n_3)$ undistorted, i.e. related to its original configuration by a rigid-body rotation and translation. Depending on the choice of integers, three possibilities now arise:

(*a*) $\mathscr{D}$ consists of a shear plus a compression. This would not be acceptable since it requires atoms to interchange places, or even to coalesce.

(*b*) $\mathscr{D}$ consists of a shear plus an extension. This would not be acceptable, since the deformed crystal generates only a superlattice of the matrix crystal on rotating through 180° about η_1.

(*c*) $\mathscr{D}$ consists of a shear alone. In this case: the deformed crystal generates the complete matrix crystal on rotating by 180° about η_1; the direction η_1 lies within the invariant plane, which may evidently now be identified as the element K_1 of a possible twin; and the plane $(n_1n_2n_3)$ undergoes only a net rigid-body rotation, becoming identified as the element K_2 of the twin. Since the crystal can be built up from the set of parallel planes $(n_1n_2n_3)$, we may picture $\mathscr{D}$ as a net rigid-body rotation of each plane $(n_1n_2n_3)$ about its line of intersection λ with K_1 (Fig. 3).

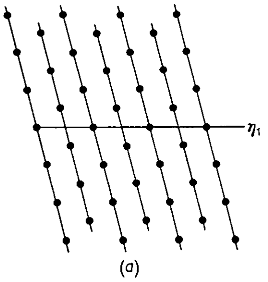

Fig. 3. (*a*) Untwinned lattice, indicating traces of K_2-planes (schematic). (*b*) Twinned lattice, case $\Sigma = 2$. Omitting alternate K_2-planes in (*a*) and (*b*) corresponds to case $\Sigma = 1$.

Subject to certain conventions in the labelling of η_1, the restriction (*c*) is achieved by choosing only integers which satisfy the fundamental relation

$$\Sigma = pn_1 + qn_2 + rn_3 = 2 \, . \qquad (6)$$

The same conventions ensure that $\Sigma < 2$ corresponds with the possibility (*a*) above and $\Sigma > 2$ with (*b*). These hypothetical interpretations are, of course, limited by the supposition of perfect homogeneity and could never be invoked in practice; relaxing the homogeneity requirement gives $\Sigma > 2$ a completely different significance, as discussed in the next paragraph. Relation (6) holds on the understanding that the integers p, q, r have no common factor, and that they refer to a primitive unit cell of the space lattice. Geometrically interpreted, (6) means that the join of $[o, o, o]$ to $[p, q, r]$ is bisected by an $(n_1n_2n_3)$ plane: these two points lie on the planes $n_1x + n_2y + n_3z = 0{,}2$ respectively, which are separated by the plane $n_1x + n_2y + n_3z = 1$. Discarding reference to any coordinate system, (6) means that the unit lattice vector in the direction η_1 is intersected by a K_2-plane. As a corollary, the number of such planes intersecting this vector provides the invariant value of Σ corresponding to a given η_1, K_2. For instance $\eta_1 = [111]$, $K_2 = (112)$, in the b.c.c. lattice. The relevant vector joins $[o, o, o]$ to $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$, which points lie on the planes $x + y + 2z = 0{,}2$ respectively; these are interleaved by the plane $x + y + 2z = 1$, and by no other (112) plane, whence $\Sigma = 2$. The integers n_1, n_2, n_3 satisfying (6) may have a common factor 2, usually cancelled out in defining the indices of K_2: this means that no K_2-plane intersects the unit lattice vector, as is the case with indium and mercury. However, by doubling the indices of K_2, we formally introduce an imagined K_2-plane between any two neighbouring actual K_2-planes and thus regain contact with (6).

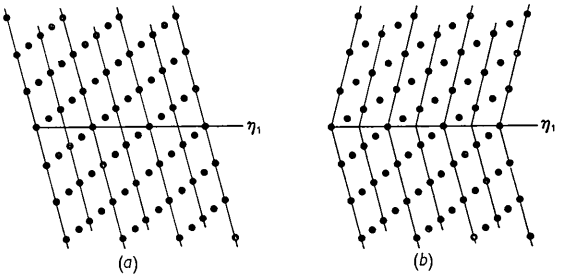

Fig. 4. (*a*) Untwinned lattice, indicating traces of successive K_2-planes, case $\Sigma = 4$. (*b*) Lattice as deformed by $\mathscr{S}$. Every second K_2-plane is twinned.

Since the crystal shear $\mathscr{D}$ is perfectly homogeneous, it may be identified with the macroscopic shear $\mathscr{S}$. From the point of view of $\mathscr{S}$, relation (6) hinges critically on the requirement that every atom arrives at its twin position by executing $\mathscr{S}$. If this requirement were relaxed, it being supposed that only a superlattice of the atoms twins in accordance with $\mathscr{S}$, (6) would be replaced by

$$\Sigma = 2N \, , \qquad (7)$$

where N stands for the number of atoms per unit cell of the superlattice. We may picture $\mathscr{S}$ as formally subjecting each K_2-plane to a net rigid-body rotation, but twinning only every Nth plane of the series (Fig. 4); atoms on the intervening planes undergo additional, inhomogeneous, displacements (which cannot be uniquely determined) before reaching their final positions. Conversely, a macroscopic twinning shear characterized by (7) could be homogeneous only on the scale of the relevant superlattice. The inference for b.c.c. metals, indium and mercury, where in each case $N = 1$, is obvious.

Given a pair of rational elements η_1 and K_2, the indices of K_1 may be readily calculated by a new method that emerges from the analysis (App. II). With K_1 and K_2 known, the remaining elements λ, P, η_2—in that order—are found by straightforward analytical geometry. Given only the rational element η_1, there exist an infinite number of mathematically admissible possibilities for K_2. Criteria for selecting the most likely operative K_2 are given in a later section. Reciprocal theorems can be formulated without difficulty.

Rotation twinning: Diatomic motif units

A crystal structure is characterized by two distinct features: the grouping of atoms, or motif, which provides the unit of repetition; and the reference lattice of the crystal, which defines how the unit is repeated. For nearly all metal structures the motif consists of not more than two atoms. We denote these by the symbols a, b and their mean-centre by the symbol r; the array of mean-centres constitutes a Bravais space lattice R. The equations of all planes and directions in the crystal formally refer to R, but the association of a motif unit with each lattice point will be understood. When the motif reduces to a single atom, R becomes identified as the array of atomic sites.

The stability of metals is governed mainly by long-range forces, e.g. the Fermi energy, with the result that the motif behaves much less as a physical unit than might appear from the crystallographic formalism. In particular there are no appreciable energy barriers to its undergoing disruption in the course of glide processes. This possibility stands in marked contrast to crystals such as calcite, where deformation properties are largely determined by the stability of the CO_2-radical. Analysis shows that the latter type of mechanism applies, in metals, to the α-uranium twin (2) and to the usual bismuth twin: two cases where twinning takes place with unusual facility. Formally it also applies to the α-uranium twin (4), but this twin has only been reported in one investigation and seems of infrequent occurrence. There are theoretical grounds for believing that a particularly high activation energy barrier opposes the reaction here, arising from the semi-covalent nature of the α-uranium structure (Dove, 1956). For all other established metal twins, disruption is found to play a key role in the mechanism of deformation.

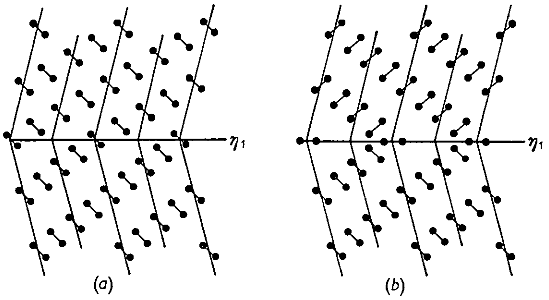

Fig. 6. (a) Crystal as deformed by $\mathscr{S}$, case $\Sigma=4$. (b) Final twinned crystal. Motif units on alternate planes have undergone rotational reshuffle, as in Fig. 7. Those on intervening planes have disrupted, as described in Fig. 8.

Following the treatment of the preceding section, we picture the macroscopic shear as formally subjecting each motif unit to a rigid-body translation in the direction η_1, by an amount depending linearly on the position of its mean-centre. The deformed array of mean-centres may be twin-related to R by a 180° rotation about η_1, as depicted in Fig. 5 (Y-mechanism); $\mathscr{S}$ is then characterized by $\Sigma=2$, exemplified by the modes of the preceding paragraph. More generally (X-mechanism), only a superlattice of mean-centres is twinned by $\mathscr{S}$ (Fig. 6) and the characteristic integers satisfy a relation of the form (7). For all X-modes that occur in practice, $N=2$ in (7), i.e.

$$\Sigma=4 \tag{8}$$

exemplified by the α-uranium twin (3), the usual c.p.h. twins, and the usual β-tin twin. As previously, the K_2-planes occupy a key role: each formally undergoes a rigid-body rotation with respect to $\mathscr{S}$, mean-centres on every plane being twinned if (6) is satisfied and on every Nth plane if (7) is satisfied.

The preceding displacements define only the homogeneous component of the deformation. This must be supplemented by an inhomogeneous component, i.e. additional displacements (termed 'reshuffles') which produce no macroscopic effects but serve to generate

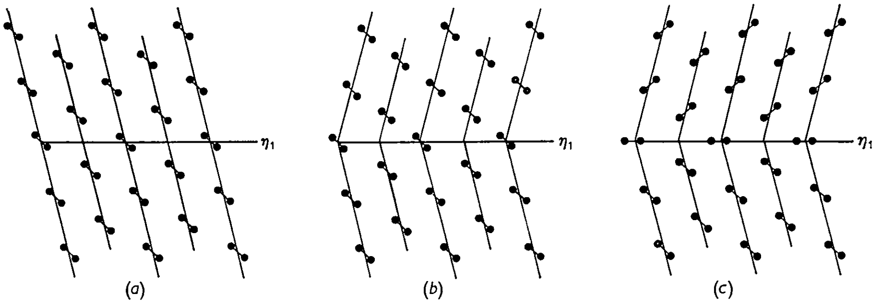

Fig. 5. (a) Untwinned crystal indicating traces of K_2-planes (schematic). (b) Crystal as deformed by $\mathscr{S}$, case $\Sigma=2$. (c) Final twinned crystal, after rotational reshuffle of each motif unit, as described in Fig. 7.

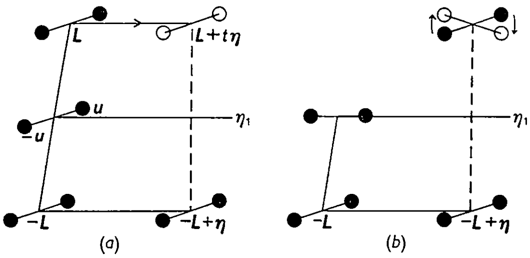

Fig. 7. Y-mechanism. (a) The motif unit at **L** undergoes rigid body displacement $t\boldsymbol{\eta}$ so that its mean centre becomes twin-related to mean centre at $-\mathbf{L}+\boldsymbol{\eta}$. ($b$) Completion of twin by rotational reshuffle (schematic).

the twin configuration. If the mean-centre r of a motif unit is twinned by $\mathscr{S}$, the most likely reshuffle consists of net rotation of the unit about an axis through r normal to η_1 (Fig. 7). According to the Y-mechanism, all the motif units behave in this way. According to the X-mechanism, those on every second K_2-plane behave thus when $N=2$, on every third plane when $N=3$, and so on. Mean-centres on the intervening planes are not twinned by $\mathscr{S}$: the corresponding motif units suffer disruption and reconstruction according to a specific pattern, depending on N, in the course of which they become organised into a new array bearing the correct twin relation to the matrix crystal. It can be proved (App. II), when $N=2$, that:

(a) the constituent atoms of a disrupting motif unit may achieve twin positions by undergoing equal and opposite displacements in the direction η_1 (Fig. 8);

(b) these displacements may be chosen so as not to exceed an interatomic spacing in the direction η_1.

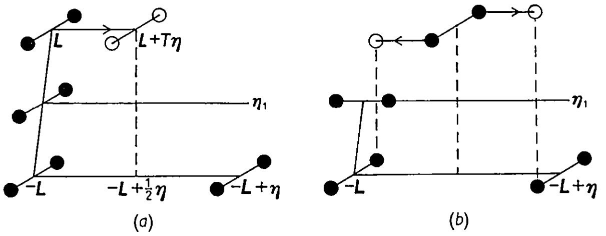

Fig. 8. X-mechanism, case $\Sigma=4$. (a) The motif unit at **L** undergoes rigid-body displacement $T\boldsymbol{\eta}$ so that its mean centre becomes twin-related to $-\mathbf{L}+\frac{1}{2}\boldsymbol{\eta}$. ($b$) Completion of twin by disruption through equal and opposite displacements parallel to η_1 (schematic).

When $N>2$ an increasing fraction of motif units suffer disruption; also the reshuffles follow a much more complex pattern than that just described. Evidently, therefore, $N=2$ defines the most energetically favourable disruption mechanism that can be envisaged. The restriction of operative X-modes to those satisfying (8) thus becomes readily understandable. The question of competition between Y-modes and X-modes will be taken up in the following section.

The selection of operative modes

We now enquire: what physical factors select the usually operative twins, for a given crystal, out of all the mathematically admissible possibilities? Aided by an invaluable inequality theorem, recent work (Jaswon & Dove, 1956; Kiho, 1954) has proved that the choice of operative rational elements $[pqr]$, $(n_1n_2n_3)$—interpreted indifferently as either η_1, K_2 or n_2, K_1—can be understood on the basis of three main criteria.

1. Reshuffles are as far as possible avoided, thereby reducing the activation energy barrier for the reaction. With monatomic motif units they may be completely eliminated, hence the restriction (6) found in practice. With polyatomic motif units (apart from an exceptional case mentioned later) they are topologically unavoidable, the most tolerable being those in accordance with the restrictions (6) or (8).

2. Subject to the preceding criterion being satisfied: the smaller the S of a possible mode, the greater its chance of being operative. More precisely, all the hypothetical modes satisfying (6) determine an infinite class of discrete shear values; denoting the minimum of the class (apart from a possible zero) by S_2, this defines the usual b.c.c., indium and mercury twins respectively. It also defines the usual bismuth twin and the α-uranium twin (4), whilst the next successive value of S defines the α-uranium twin (2). Similarly S_4, referring to the class satisfying (8), defines the usual c.p.h. and β-tin twins respectively, and the α-uranium twin (3). It is seen without difficulty that $S_4 \leq S_2$.

3. A Y-mode is generally preferred to an X-mode of equal or comparable S, since it affords a slightly more favourable reshuffle mechanism. Thus the α-uranium twin (2) occurs more frequently than (3) even though it has a somewhat higher S. The exceptional feature of the α-uranium twin (4) has already been noted. In the bismuth case, it turns out that $S_4=S_2$ with the result that only the Y-mode is found operative. If, however, S_4 is significantly lower than S_2, this factor outweighs the reshuffle factor and leads to the appearance of X-modes found in practice.

As a corollary from these criteria, we may infer the most likely operative K_2 corresponding to a given rational η_1, and, reciprocally, the most likely operative η_2 corresponding to a given rational K_1.

The 'least shear' criterion has an interesting geometrical interpretation. By virtue of (1) it implies that the angle $\widehat{\eta_1K_2}$ or $\widehat{\eta_2K_1}$, as the case may be, is preferably as small as possible, i.e. that the pair of rational elements satisfying (6) or (8) should be as nearly as possible perpendicular. From this point of view, the present theory makes contact with Mallard's law (Friedel, 1926), an early attempt at relating twinning elements to lattice planes and directions of pseudosymmetry. However, our analysis goes beyond Mallard's law in two respects. The latter is illuminating as regards indium or mercury, where the operative angle happens to be extremely small, but fails for b.c.c. twins, where $\widehat{\eta_1 K_2} = \widehat{\eta_2 K_1} = 19° \, 28'$; only detailed mathematical analysis can establish the latter angle as the minimum of its class. A further limitation appears with diatomic motif units: Mallard's law has relevance only to Y-modes and thus fails to disclose the existence of possible X-modes. By recognising the loss of symmetry in passing from zinc to α-uranium, Frank (1953) was able to anticipate the Y-mode (2) but not the Y-mode (4); the reciprocal X-modes (3), (5) were also anticipated by Frank, but on the basis of a straightforward comparison with the X-modes of zinc and not by virtue of Mallard's law.

As shown by the success of the selection criteria, the choice of operative modes is governed mainly by crystallographic factors and not by the misfit energy at the twin boundary. However, the influence of the latter factor most probably determines the preference for rotation twins as against their reciprocal reflection twins: an irrational habit plane passes through only one row of atoms, and therefore involves less boundary misfit energy than a rational habit plane. For similar reasons, with compound twins, the K_1 of higher indices is preferred, e.g. in α-uranium $K_1=(130)$ rather than $(1\bar{1}0)$ and in β-tin $K_1=(301)$ rather than (101). As regards the preference for $K_1=(110)$ to $K_2=(001)$ in bismuth, a reason has already been advanced on the basis of reaction-path analysis (Jaswon & Dove, 1956): this does not exclude the boundary energy as an additional factor working in the same direction. If the reaction-path factor is valid for bismuth, then $K_1=(001)$ should not be exhibited even when the usual mode is prevented from growing by external constraints.

The selection criteria indicate

$$K_1=(111),\ K_2=(11\bar{3}),\quad \eta_1=[\bar{1}\bar{1}2],\ \eta_2=[332],\ S=1/(2\sqrt{2}) \quad (9)$$

and its reciprocal, as the most likely operative X-modes for crystals based on the f.c.c. lattice, e.g. diamond and galena. According to Tertsch (1949), these modes are actually exhibited by the latter. Deformation twinning has never been substantiated in diamond, but has been reported in germanium and silicon under critical conditions of temperature and loading, apparently characterized by composition planes (111) and (123). Unfortunately no accompanying element η_2 has been determined, with the result that neither S nor Σ are available from the experimental data. It may be remarked, however, that $K_1=(123)$ has an exceptional property, invoked in an analysis by Bullough (1957): reshuffles are completely eliminated for twinning displacements parallel to this plane, since it passes through both atoms of the motif unit. This could well be a significant factor, bearing in mind the strong, directed bonds linking neighbouring atoms in diamond, and to a lesser extent in germanium and silicon. On the other hand, for the class of homogeneous twinning shears on the plane (123), calculation shows that $S_2=2\sqrt{6}$. This value is extraordinarily high, since $S<1$ for every other twin so far established. A tolerable S could be obtained by supposing every fifth or sixth plane to execute the macroscopic deformation, but this raises the problem of why such a mode should be preferred to (9). The composition plane (111) is consistent with (9) or with the most likely operative Y-mode

$$K_1=(111),\ K_2=(11\bar{1}),\quad \eta_1=[11\bar{2}],\ \eta_2=[112],\ S=1/\sqrt{2}\,. \quad (10)$$

Concluding remarks

From the work of this and previous papers, we draw the following general conclusions.

1. The limitations inherent in the conventional treatment of twinning, which proceeds by first setting up deformations in a continuous medium and then introducing an atomic model, may be obviated by a direct approach at the atomic level.
2. The invariant quantity $\Sigma=pn_1+qn_2+rn_2$ characterises the scale of homogeneity of the deformation. For all metal twins so far established, $\Sigma=2$ or 4, indicating homogeneity on the finest possible scale. Any reported twin for which $\Sigma>4$ should be treated with reserve.
3. Formal crystallographic criteria successfully select all the established operative twinning modes. Boundary misfit energy forms a minor factor in comparison, but—as between a mode and its reciprocal—governs the preference for the composition plane of higher indices.
4. The rule, suggested by Cahn (1953), that P and λ are always at least approximately rational, has little significance as regards the selection of operative modes. In particular, if a plane of symmetry is found to exist perpendicular to K_1, it should not be identified as P without closer examination.
5. The conventional, unsatisfactory, technique of projecting the crystal on to P in order to examine atomic twinning displacements, is unnecessary. If K_1 is rational, the displacements of planes parallel to K should be examined, as described elsewhere (Jaswon & Dove, 1956). If η_1 is rational, the displacements of planes parallel to K_2 should be examined, as described in the present text.

The work reported here is concerned primarily with net twinning displacements, and not with the reaction paths of the atoms in moving from initial to final positions. In this respect, the treatment is comparable with current formal treatments of the martensite transformation, which are successful in selecting the operative martensite habit planes (Bilby & Christian, 1955). Some differences between martensite and twinning may, however, be noted. Martensite atom displacements are never perfectly homogeneous, even in the simplest crystals. Nothing akin to rotation twinning is envisaged in martensite theory, even though most of the reported habit planes are irrational. The martensite transformation can only, in general, be accomplished by an invariant plane strain. The martensite habit plane generally bears little or no relation to the planes on which the main glide processes take place (Jaswon, 1958), whereas the twinning habit plane may be generally identified as the plane K_1 of the crystallographic analysis. Finally, by virtue of the inequality theorem, selection criteria for twinning planes have been established on a much more rigorous basis than the corresponding criteria for martensite habit planes.

APPENDIX I

Fig. 2 depicts three parallel lattice rows passing respectively through the atoms at $\mathbf{L}$, 0, $-\mathbf{L}$. The symbol $\mathbf{L}=[x, y, z]$ stands either for the lattice point of (integer) co-ordinates x, y, z or for the lattice vector joining the origin to this lattice point. The central row is identified as the twin axis $\eta_1=[pqr]$, and $\boldsymbol{\eta}=[p,q,r]$ stands for the unit lattice vector (or corresponding lattice point) in this direction. We now suppose the atom at $\mathbf{L}$ suffers a displacement $t\boldsymbol{\eta}$, thereby becoming twin-related to some atom in the row passing through $-\mathbf{L}$, i.e. an atom having a lattice position of the form $-\mathbf{L}+n\boldsymbol{\eta}$ where n is an integer. This relationship is compactly symbolized

$$\mathbf{L} \rightarrow \mathbf{L}+t\boldsymbol{\eta} \mathbin{/\!/} -\mathbf{L}+n\boldsymbol{\eta}\,, \tag{1}$$

twinning of the second kind being implied by the double solidus. Introducing the condition that the join of the twin-equivalent positions must be perpendicular to $\boldsymbol{\eta}$, we arrive at the equation

$$t=n-2\mathbf{L}\cdot\boldsymbol{\eta}/\eta^2;\quad \eta \equiv |\boldsymbol{\eta}|\,. \tag{2}$$

For any integer n, (2) determines a possible twinning displacement, $t\boldsymbol{\eta}$, of the atom at $\mathbf{L}$. On the other hand, given that the atom at $\mathbf{L}$ undergoes a certain displacement $t\boldsymbol{\eta}$, this will be a possible twinning displacement only if an integer n exists to satisfy (2).

Applying (2) to the three special lattice points [1, 0, 0], [0, 1, 0], [0, 0, 1] defining a primitive unit cell, we introduce the three displacement parameters

$$t_1=n_1-2[1,0,0]\cdot\boldsymbol{\eta}/\eta^2,\ t_2=n_2-2[0,1,0]\cdot\boldsymbol{\eta}/\eta^2,\ t_3=n_3-2[0,0,1]\cdot\boldsymbol{\eta}/\eta^2, \tag{3}$$

where n_1, n_2, n_3 are any three assigned integers. These displacements, together with the condition that the origin atom remains fixed, determine a homogeneous deformation $\mathscr{S}$ of the crystal on bearing in mind that

$$[x, y, z] \equiv x[1,0,0]+y[0,1,0]+z[0,0,1]\,.$$

With respect to $\mathscr{S}$, the atom at $[x, y, z]$ undergoes a displacement

$$(t_1x+t_2y+t_3z)\boldsymbol{\eta} \tag{4}$$

as can be seen directly, or more formally by setting up the linear transformation defined by

$$[0,0,0] \rightarrow [0,0,0],\quad [1,0,0] \rightarrow [t_1p, t_1q, t_1r]\,,\ \text{etc.}$$

The displacement (4) is a twinning displacement. For on multiplying the three equations (3) by x, y, z respectively and adding, it follows that

$$t_1x+t_2y+t_3z=n_1x+n_2y+n_3z-2[x,y,z]\cdot\boldsymbol{\eta}/\eta^2; \tag{5}$$

by comparison with (2), since $n_1x+n_2y+n_3z$ is an integer, we may assert

$$[x,y,z] \rightarrow [x,y,z]+(t_1x+t_2y+t_3z)\boldsymbol{\eta} \mathbin{/\!/} -[x,y,z] + (n_1x+n_2y+n_3z)\boldsymbol{\eta}\,, \tag{6}$$

utilising the symbolic scheme (1). Strictly speaking, the second of the twin-related positions in (6) should not be held, at this stage, as referring to an actual atom position but to a site occupied by an atom prior to deformation, for no distinction has yet been drawn between a strained and unstrained region of the crystal. Alternatively, we may think of a 'ghost' crystal superimposed on the actual crystal and unaffected by $\mathscr{S}$: the deformed actual crystal is then related to the 'ghost' by a rotation of 180° about η_1.

It follows, as an immediate corollary from (4), that the plane $t_1x+t_2y+t_3z=0$, here denoted K, remains invariant with respect to $\mathscr{S}$. Furthermore, the displacement of the atom at $[x, y, z]$ varies as its distance from K. The deformation must therefore consist of homogeneous simple shear displacements parallel to K, possibly combined with a uniaxial expansion or contraction normal to K. Only when the latter component is absent does the displacement direction $[pqr]$ lie within K, and conversely. This limitation is ensured by the mathematical condition

$$V=pt_1+qt_2+rt_3=0\,, \tag{7}$$

an equation which implies relation (6) of the text on bearing in mind that $V=\Sigma-2$ from (5). In these circumstances K becomes identified as the element K_1 of a possible twin, its indices being provided at once from (3). The existence of an invariant plane allows us to envisage $\mathscr{S}$ as applied to only one of the regions defined by this plane, i.e. the 'twinned crystal', the other region being the 'matrix crystal', so that the concept of a 'ghost' crystal becomes unnecessary. Equation (7) admits of a second interpretation, equivalent in effect to the preceding: it signifies that the atom at $[p, q, r]$ suffers no displacement, i.e. that the direction η_1 itself remains unstrained. Failing $V=0$, there arise the possibilities $V=\pm 1, \pm 2, \ldots$ depending on the choice of n_1, n_2, n_3. Positive values for V imply extensions of 100%, 200%, ... in the direction η_1, showing that only a superlattice of the twin is generated; negative values for V imply corresponding contractions, implying that the atoms coalesce ($V=-1$) or interchange places ($V<-1$). These possibilities have interesting topological consequences, but can have no physical significance in ordinary three-dimensional space.

The vector $[x, y, z]$ remains unchanged in length if

$$|[x, y, z]| = |[x, y, z] + (t_1x + t_2y + t_3z)\boldsymbol{\eta}|\,,$$

i.e. if

$$t_1x + t_2y + t_3z = -2[x, y, z]\cdot\boldsymbol{\eta}/\eta^2.$$

By comparison with (5), the locus of the point x, y, z is seen to be the plane $n_1x + n_2y + n_3z = 0$. This plane suffers no net distortion with respect to $\mathscr{S}$ and therefore effectively undergoes a rigid-body rotation Ω about its axis of intersection with K. When $V = 0$, all parallel planes behave in the same way, becoming identified as the K_2-planes of a possible twin. When $V = N$, however, the planes

$$n_1x + n_2y + n_3z = \pm 1,\ \pm 2,\ \dots$$

in addition to the rotation Ω, undergo rigid-body translations $\pm N\boldsymbol{\eta}$, $\pm 2N\boldsymbol{\eta}$, … respectively, in accordance with the concluding remarks of the preceding paragraph.

APPENDIX II

Fig. 7 depicts three diatomic motif units, centred on the reference lattice points $\mathbf{L}$, 0, $-\mathbf{L}$ respectively. The constituent pairs of atoms have co-ordinates $\mathbf{L} \pm \mathbf{u}$, $\pm \mathbf{u}$, $-\mathbf{L} \pm \mathbf{u}$ respectively, where $2\mathbf{u}$ denotes the 'basis' vector defining the structure of the motif. The twinning axis is identified as the direction of the unit reference lattice vector $\boldsymbol{\eta} = [p, q, r]$. We now suppose the motif unit at $\mathbf{L}$ undergoes a rigid-body translation according to the scheme (1) of Appendix I. Its mean-centre r is twinned by this translation, and twinning is completed by a reshuffle which effectively amounts to a rotation of the unit about an axis through r perpendicular to $\boldsymbol{\eta}$, $\mathbf{u}$. On applying to each unit an appropriate translation, i.e. of amount (4) for the unit centred at $[x, y, z]$, we thereby set up a homogeneous deformation $\mathscr{S}$ which twins all the mean-centres. If so, each motif unit without exception completes its twinning by means of the rotational reshuffle. $\mathscr{S}$ has formally the same properties as the simple crystal deformation characterized by $\Sigma = 2$. This completes the description of the Y-mechanism, the simplest twinning mechanism that can be envisaged for a diatomic motif.

We now extend the analysis to embrace the possibility of the motif unit suffering disruption. This is effected by writing, in place of (1) and (2),

$$\mathbf{L} \rightarrow \mathbf{L} + T\boldsymbol{\eta} \;//\; -\mathbf{L} + \tfrac{1}{2}n\boldsymbol{\eta};\quad T = \tfrac{1}{2}n - 2\mathbf{L}\cdot\boldsymbol{\eta}/\eta^2, \qquad (8)$$

where n is any integer: in words, the unit at $\mathbf{L}$ undergoes a translation $T\boldsymbol{\eta}$ whereby its mean-centre becomes twin-related to the point $-\mathbf{L} + \frac{1}{2}n\boldsymbol{\eta}$. If n is even, the latter qualifies as a lattice point of R and twinning is completed as above. If n is odd, the latter falls halfway between two lattice points of R and the preceding mechanism cannot apply. The only feasible alternative is for the constituent atoms to separate, preferably by means of equal and opposite displacements in the direction η_1. That the required reshuffles exist for the case $\Sigma = 4$ is evident from Fig. 8. This may also be proved formally, as well as the fact that the constituent atoms need never separate by more than an interatomic spacing in the direction η_1.

Identifying $\mathbf{L}$ successively with the reference lattice points $[1, 0, 0]$, etc., we introduce the translation parameters

$$T_1 = \tfrac{1}{2}n_1 - 2[1, 0, 0]\cdot\boldsymbol{\eta}/\eta^2,$$
$$T_2 = \tfrac{1}{2}n_2 - 2[0, 1, 0]\cdot\boldsymbol{\eta}/\eta^2, \text{ etc.}, \qquad (9)$$

where at least one of the assigned integers n_1, n_2, n_3 is odd. These determine a homogeneous deformation $\mathscr{S}$, with respect to which the motif unit at $[x, y, z]$ undergoes a rigid-body translation $(T_1x + T_2y + T_3z)\boldsymbol{\eta}$ given by

$$T_1x + T_2y + T_3z = \tfrac{1}{2}(n_1x + n_2y + n_3z) - 2[x, y, z]\cdot\boldsymbol{\eta}/\eta^2. \qquad (10)$$

It will be noted that the integer $n_1x + n_2y + n_3z$ may be even or odd. From (10) it follows that

$$0 = T_1p + T_2q + T_3r = \tfrac{1}{2}(n_1p + n_2q + n_3r) - 2$$

expresses the condition for $\mathscr{S}$ to be a simple shear, as already formulated in relation (7) of the text. From (10) it also follows, as in the preceding Appendix, that the plane $(n_1n_2n_3)$ undergoes a net rigid-body rotation with respect to $\mathscr{S}$.

Mean-centres on the even planes $n_1x + n_2y + n_3z = 0$, ± 2, … are twinned by $\mathscr{S}$, thereby enabling the corresponding motif units to undertake the rotational reshuffle. Mean-centres on the odd planes $n_1x + n_2y + n_3z = \pm 1$, ± 3, … are not twinned by $\mathscr{S}$, and the corresponding motif units must suffer disruption: half the atoms on plane $2N + 1$ move into plane $2N + 3$ and the other half move into plane $2N - 1$; in return, plane $2N + 1$ is reconstituted in the correct twin configuration by atoms from planes $2N - 1$ and $2N + 3$. This completes the description of the X-mechanism for the case $\Sigma = 4$, the simplest case that can be envisaged. The analysis may be readily extended to the case $\Sigma = 2N$ by writing

$$T_1x + T_2y + T_3z = 1/N(n_1x + n_2y + n_3z) - 2[x, y, z]\cdot\boldsymbol{\eta}/\eta^2$$

in place of (10).

Given a pair of rational twinning elements η_1 and K_2, the indices of K_1 are provided either by (3) or (9) according as $\Sigma = 2$ or 4 respectively. These formulae are, however, limited to co-ordinate systems based on a primitive unit cell of the space lattice. A more general formula for $K_1 = (h'k'l')$, which holds for any choice of unit cell, is

$$
\begin{aligned}
h' &= h - N[1,0,0]\cdot[p,q,r]/[p,q,r]^2,\\
k' &= k - N[0,1,0]\cdot[p,q,r]/[p,q,r]^2,\\
l' &= l - N[0,0,1]\cdot[p,q,r]/[p,q,r]^2,
\end{aligned} \qquad (11)
$$

where

$$[pqr] \equiv \eta_1,\ (hkl) \equiv K_2,\ hp+kq+lr=N\ .$$

This obviously embraces (3) and (9) as special cases. The formula may be proved by a slight re-adaptation of the analysis, or directly by noting that the plane $(h'k'l')$ has two properties which identify it as K_1: it contains η_1, and its intersection with K_2 is perpendicular to η_1.

As an exercise on the use of (11), we find the α-uranium K_1 corresponding to $\eta_1=[312]$, $K_2=(112)$:

$$
\begin{aligned}
h' &= 1 - \frac{8[1,0,0]\cdot[3,1,2]}{9a^2+b^2+4c^2} = 1 - \frac{8\cdot 3a^2}{9a^2+b^2+4c^2}\\
&= \frac{-15a^2+b^2+4c^2}{9a^2+b^2+4c^2}\,,\\
k' &= 1 - \frac{8[0,1,0]\cdot[3,1,2]}{9a^2+b^2+4c^2} = 1 - \frac{8\cdot b^2}{9a^2+b^2+4c^2}\\
&= \frac{9a^2-7b^2+4c^2}{9a^2+b^2+4c^2}\,,\\
l' &= 2 - \frac{8[0,0,1]\cdot[3,1,2]}{9a^2+b^2+4c^2} = 2 - \frac{8\cdot 2c^2}{9a^2+b^2+4c^2}\\
&= \frac{18a^2+2b^2-8c^2}{9a^2+b^2+4c^2}\,,
\end{aligned}
$$

whence $(h'k'l')=$ '$(1\bar{7}2)$' on eliminating the denominator and inserting numerical values for the lattice parameters a, b, c. It need hardly be stated that the corresponding reciprocal problem is also solved by (11).

Thanks are due to Dr J. D. H. Donnay for helpful advice on crystallographic terminology, and to Dr B. A. Bilby for reading the manuscript.

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An Axial Retigraph

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(*Received* 14 *August* 1959)

A retigraph, an X-ray diffraction camera recording on film an undistorted projection of one plane of the reciprocal lattice of a crystal, has been constructed with some novel features. The mapping of the remainder of the reciprocal lattice on to the film plane is analysed together with other aspects of the camera geometry which also applies to the precession camera. The Lorentz and polarization corrections, both for polarized and for unpolarized incident radiation, are calculated. Methods of setting such instruments employ characteristic spots or Laue streaks.

1. Introduction

The precession camera (Buerger, 1944), which is being increasingly used for all types of crystallographic examinations, has certain drawbacks which restrict its application. The chief of these are the non-uniformity of the speed of precession (Waser, 1951), which requires the use of complicated charts for applying the Lorentz velocity-factor correction, and the long minimum specimen-to-film distance (about 50 mm.), which is much greater than the optimum for small crystals (Huxley, 1953).

An axial retigraph has been designed and constructed with the limited objective of eliminating these deficiencies. In mechanism it differs from most other retigraphs (de Jong & Bouman, 1938; Bagaryatskii & Umanskii, 1949; Kvitka & Umanskii, 1951; Torroja, Pajares & Amorós, 1951; Gay & Clastre, 1953; Rimsky, 1952) in permitting μ, the angle of precession,