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Twinning modes in lattices

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Deformation twinning is an important contributory factor in the plastic deformation of crystalline materials. The macroscopic shape deformation associated with deformation twinning is a simple shear, and in this paper the generalized theory of twinning shears developed in an earlier paper (Bevis & Crocker 1968), is applied to specific lattices and the resulting twinning modes described. Examples of all seven different classes of twinning mode, five of which do not satisfy the classical orientation relations of deformation twinning are first examined for the special case of cubic lattices. Relations between modes in the seven crystal systems which arise from variants of the unit correspondence matrix are then investigated. These modes are all conventional in character, but, when this procedure is repeated for a more complex correspondence matrix, most of the resulting modes are non-conventional, having four irrational twinning elements. The orientation relations associated with several of these modes are discussed in detail. Although the modes presented have been chosen specifically to illustrate pertinent features of the theory, many of them are shown to be the operative deformation twinning modes in metals and other crystalline materials. Finally the physical significance of the component correspondence and rotation matrices, into which a twinning shear is formally resolved in the theory, is discussed and extensions of the analysis, which enable transformation shears in lattices to be studied, are briefly considered.

1. INTRODUCTION

In a previous paper (Bevis & Crocker 1968; to be referred to as I) a generalized theory of twinning shears in lattices was developed. The analysis was based on the definition (Bilby & Crocker 1965) that a twinning shear restores a lattice in a new orientation, and it was shown that all shears of this kind may be derived from unimodular correspondence matrices satisfying certain simple restrictions. By examining the properties of these matrices it was then deduced that twinning modes may be divided into seven different classes. The general features of modes belonging to these classes were also summarized but no specific examples were reported. The present paper contains several applications of the theory and discusses in detail important examples of all seven classes of twinning modes for all fourteen Bravais lattices.

Following the usual procedure (Bilby & Crocker 1965) the four twinning elements $K_1 K_2 \eta_1 \eta_2$ and the magnitude g of the shear strain will be quoted for all the twinning modes discussed. Here, K_1 is the shear or twinning plane, K_2 is the conjugate twinning plane, which is the second undistorted but rotated plane of the shear, and η_1 and η_2 are the shear or twinning direction and the conjugate twinning direction respectively. The plane of shear S, which is perpendicular to K_1 and K_2 and contains η_1 and η_2, will also be used. The conjugate twinning mode corresponding to

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$K_1 K_2 \eta_1 \eta_2; g$ is obtained by permuting the elements to give $K_2 K_1 \eta_2 \eta_1; g$. When the elements $K_1 K_2 \eta_1 \eta_2$ are represented by the vector components h_i, k_i, p^i, q^i the relative signs are chosen such that on twinning, the positive side of the K_1 plane shears in the positive η_1 direction and similarly for the conjugate shear. In addition the angle between η_1 and η_2 is chosen to be obtuse.

For lattices the classical types I and II orientation relations now reduce to reflexion in K_1 and rotation of π about η_1 respectively. The corresponding restrictions on the twinning elements are that K_1 and η_2 must have rational indices for type I twinning modes and that K_2 and η_1 must be rational for type II modes. In general the remaining two elements are irrational, but degenerate cases in which either three or four elements are rational do arise, modes of the latter kind being known as compound. These twinning modes are all conventional but, as explained in §I 6 (§6 of paper I), many twinning modes with four irrational elements which do not satisfy the classical orientation relations also arise. Indeed, the main purpose of the present paper is to discuss examples of this type of twinning mode. Thus in §2 the correspondence matrices contained in table I 2 (table 2 of paper I) are used to obtain examples of all seven classes of twinning modes for cubic lattices, and these are discussed in detail. Five of the classes involve non-conventional twinning modes. Then, in §3, we examine the twinning modes predicted by the unit correspondence matrix and its variants for the seven crystal systems. This procedure is repeated in §4 for a more complicated correspondence matrix which illustrates several unusual characteristics of twinning modes which are absent in §3. Then in §5 the twinning modes presented in this paper are compared with the operative modes in crystalline materials in general and metals in particular. Finally some examples of the physical significance of the component correspondences and rotations into which the twinning shears are formally resolved are discussed and some extensions of the theory considered.

2. Twinning modes in cubic lattices

2.1. *The seven twin classes*

The sixty unimodular correspondence matrices given in table I 2 have been used as data in the general analysis of twinning shears, presented in §I 2, for the special case of cubic lattices. A selection of the resulting twinning modes is given in table 1, the notation employed being the same as that in I. Thus, correspondence matrices are labelled by two integers m and n. The former is the reciprocal of the fraction of lattice points sheared directly to correct twin positions in a primitive lattice, the remaining points having to shuffle. Thus, when the simple cubic lattice is being considered, no lattice points shuffle in the first six modes of table 1, one-half must shuffle in the next fifteen modes, and three-quarters in the final five modes. The second integer n is the position of the matrix in table I 2. For each value of m it increases with the magnitude g of the twinning shear which is given by equation (I 22) and is represented in table 1 by the integer m^2g^2. In some cases a bar is placed above the two integers m and n indicating that the matrix is the inverse of the

TABLE 1. TWINNING MODES IN CUBIC LATTICES

$m.n$	class	K_1	K_2	η_1	η_2	S	m^2g^2	m_{I}	m_{F}
1.2	$7a$	100	$1\bar{2}0$	$0\bar{1}0$	210	001	1	2	2
1.3	2	100	111	011	$2\bar{1}\bar{1}$	$01\bar{1}$	2	2	1
1.4	$6b$	a^+11	a^-11	$\bar{a}^-11$	$a^+\bar{1}\bar{1}$	$01\bar{1}$	4	2	2
1.5	$7a$	100	$1\bar{1}0$	$0\bar{1}0$	110	001	4	1	1
1.6	2	100	524	012	$2\bar{1}\bar{2}$	$02\bar{1}$	5	2	2
1.7	$6a$	$0b^+1$	$0b^-1$	$0\bar{1}b^+$	$01\bar{b}^-$	100	5	2	2
2.1	$7a$	100	$1\bar{4}0$	$0\bar{1}0$	410	001	1	4	4
2.2	2*	111	$\bar{1}11$	$\bar{2}11$	211	$01\bar{1}$	2	4	1
2.3	2	100	$1\bar{2}\bar{2}$	$0\bar{1}\bar{1}$	411	$01\bar{1}$	2	4	2
2.4	$4a$	$01c^+$	$01c^-$	$0c^+\bar{1}$	$0\bar{c}^-1$	100	2	4	4
$\bar{2}.\bar{4}$	4*	$01d$	$0\bar{1}d$	$0\bar{d}1$	$0d1$	100	2	4	4
2.5	$7a$	110	$\bar{1}30$	$\bar{1}10$	310	001	4	2	2
2.6	2	100	$5\bar{4}\bar{8}$	$01\bar{2}$	412	$02\bar{1}$	5	4	4
2.7	1	$1e^+1$	$1e^-1$	$2\bar{e}^-2$	$\bar{2}e^+\bar{e}$	$10\bar{1}$	6	2	4
$\bar{2}.\bar{7}$	1	$11f^+$	$\bar{1}\bar{1}f^-$	$\overline{44}f^-$	$44f^+$	$1\bar{1}0$	6	2	4
2.8	2	110	$\bar{1}7\bar{4}$	$\bar{1}1\bar{1}$	311	$\bar{1}12$	6	1	4
2.9	7*	120	$\bar{1}20$	$\bar{2}10$	210	001	9	4	4
2.10	$7a$	100	$3\bar{4}0$	$0\bar{1}0$	430	001	9	4	4
2.11	$7b$	210	$25\bar{4}$	$\bar{2}4\bar{5}$	201	$\bar{1}22$	9	4	4
2.12	$4a$	$0g^+\bar{1}$	$0g^-1$	$01g^+$	$01\bar{g}^-$	100	10	4	4
$\bar{2}.\overline{12}$	$4a$	$03h^+$	$0\bar{3}h^-$	$0\bar{h}^+3$	$0h^-3$	100	10	4	4
4.4	$5b$	$2i^-2$	$2\bar{i}^+2$	$1\bar{i}^+1$	$1i^-1$	$10\bar{1}$	4	4	4
4.14	1	$11\bar{1}$	$11, \bar{1}, 1$	$2\bar{1}1$	$2, 11, \overline{11}$	011	18	8	2
$\bar{4}.\overline{14}$	1	$11\bar{1}$	$\bar{5}7\bar{7}$	$\bar{2}1\bar{1}$	$14, 5, \bar{5}$	011	18	8	2
4.23	3	$2j^+\bar{1}$	$\bar{2}j^-1$	$\bar{8}j^-4$	$8j^+\bar{4}$	102	34	8	4
4.28	5*	$\bar{k}^-2k^+$	$\bar{k}^+\bar{2}k^-$	$l^+\bar{4}l^-$	l^-4l^+	$1\bar{1}1$	36	4	4

$a^\pm = 2 \pm 2^{\frac12}$; $b^\pm = 3 \pm 5^{\frac12}$; $c^\pm = 3 \pm 8^{\frac12}$; $d = 2^{\frac12}$; $e^\pm = 4 \pm 12^{\frac12}$; $f^\pm = 12^{\frac12} \pm 2$;
$g^\pm = 10^{\frac12} \pm 2$; $h^\pm = 40^{\frac12} \pm 1$; $i^\pm = 8^{\frac12} \pm 2$; $j^\pm = 24^{\frac12} \pm 2$; $k^\pm = 12^{\frac12} + 1$; $l^\pm = 2 \pm 3^{\frac12}$.

preceding one. Note that the unit matrix, a variant of which is labelled 1.1 in table I 2 and for which g is zero for cubic lattices, has been omitted. This correspondence matrix, and all its variants, are considered in detail for all seven crystal systems in §3.

As described in I, the most general class of twinning mode arises when the correspondence matrix or one of its variants is equal to neither its own inverse nor its own transpose. In such a case the indices of the twinning elements $K_1 K_2 \eta_1 \eta_2$ associated with the matrix and its inverse will all be distinct. However, as summarized in table I 3, various relations between twinning elements occur when the correspondence matrix becomes degenerate. In all, seven classes of matrix were shown to arise and examples of all these have been included in table 1. In principle, classes 4 to 7 each subdivide to give two different relations between the twinning elements and these have here been labelled a and b. No direct examples of classes $4b$ and $5a$ arise from table I 2, but degenerate cases in which the subdivisions are indistinguishable do occur for classes 4, 5 and 7. These and another degeneracy arising for a class 2 correspondence matrix are indicated by asterisks in table 1. Degeneracies of this kind and also modes of class 7*b* were not discussed in I.

2.2 *The twinning modes*

The twinning elements $K_1 K_2 \eta_1 \eta_2$ presented in table 1 were determined using the general equations of §I 2 for the special case of cubic lattices when the metric tensors c_{ij} and c^{ij} may be replaced by the Kronecker deltas δ_{ij} and δ^{ij}, the crystallographic variants given arising directly from the correspondence matrices presented in table I 2. As described in §I 4.1, and summarized in table I 1, 576 variants of a given unimodular matrix may in general be obtained by interchanging rows, interchanging columns and changing the signs of rows and columns, but for cubic lattices, these variants all predict crystallographically equivalent twinning modes and thus only the matrices quoted in table 1 need be considered here. Thirteen of these twenty-six matrices, those of classes 2 and 7, are found to predict conventional twinning modes. Furthermore, as types I and II twins cannot occur in cubic lattices (Crocker & Bevis 1963), these modes are in fact all compound, the shear plane with smaller indices having been arbitrarily labelled K_1. Apart from two important exceptions, which will be discussed in detail later, the remaining modes all have four irrational twinning elements and thus have different crystallographic characteristics from all classical twinning modes. The irrational indices are all algebraic, having the form $\alpha \pm \beta^{\frac{1}{2}}$ where α and β are integers, and wherever possible the shear plane with indices involving positive roots has been labelled K_1. Although the four twinning elements of these modes are irrational, the plane of shear S, also given in table 1, is in each case rational. This is in fact a general feature of all twinning modes in cubic lattices as may be deduced by considering the pairs of solutions of equations (I 10) and (I 17).

The non-conventional twinning modes all have a different crystallographic description when referred to the twin rather than the parent basis and, as shown in §I 4.3, the alternative twinning elements may be derived from the inverse of the correspondence matrix. However, as summarized in table I 3, for matrices in classes 3, 5*a*, 5*b*, 6*a* and 6*b* the new modes can be obtained by simply permuting the elements $K_1 K_2 \eta_1 \eta_2$ predicted by the matrix itself so that they become $K_2 K_1 \eta_2 \eta_1$, $\eta_2 \bar{\eta}_1 \bar{K}_2 K_1$, $\eta_1 \bar{\eta}_2 \bar{K}_1 K_2$, $K_2 K_1 \eta_2 \eta_1$ and $K_2 K_1 \eta_1 \eta_2$ respectively. Here bars, indicating a change in sign of the indices of a twinning element, have been introduced in order to retain the correct relative signs of the four elements of a mode. Thus for the examples of these types in table 1 it is not necessary to consider the inverse of the correspondence matrices. For the remaining classes 1 and 4 the twinning elements arising from a matrix and its inverse are distinct and thus in these cases both modes are included in table 1. Note that for all non-conventional modes the K_1 planes quoted for the matrix and its inverse define the same twinning plane but referred to parent and twin lattice bases respectively.

By interchanging K_1 and K_2, and η_1 and η_2 in the modes given in table 1 we obtain the associated conjugate twinning modes. In general these are distinct from the original modes, although for the degenerate cases marked with asterisks the modes and their conjugates are crystallographically equivalent. Note that many of the K_1 planes of the compound modes in table 1 are mirror planes so that the parent and twin lattices have the same orientation. Thus, these modes represent homogeneous shears to the identity and are not strictly twinning modes. However, the associated conjugate modes do in general describe twinning shears resulting in a change of orientation of the lattice and are thus genuine twinning modes.

Additional twinning modes may also be obtained from those in table 1 by interchanging K_1 and η_1, and K_2 and η_2 and, to preserve the correct relative signs of the four elements, reversing the signs to either the old or the new K_2 and η_1. As explained in §I 4.2 the resulting modes are those arising from the transposes of the inverses of the original correspondence matrices. In general such a procedure would have to be accompanied by a change from direct to reciprocal lattice parameters but for the primitive cubic system being considered here the two lattices are identical. The new modes are in general distinct from the original ones, but because of the particular degeneracies involved, the modes or their conjugates are crystallographically equivalent for correspondence matrices belonging to classes 4, 6 and 7. Further modes can be obtained by applying this same operation to the twinning elements associated with the inverses of the correspondence matrices and in all cases the conjugate modes are possible. Thus for the most general case of a class 1 correspondence matrix we obtain in all eight different modes.

2.3. *Centred lattices*

The twinning modes presented in table 1, together with the associated modes obtained by interchanging the elements in the ways described above, may be applied to the centred cubic lattices in addition to the primitive cubic lattice for which they were developed. However, for centred lattices the fraction of lattice points shearing direct to twin positions will in general be different from the corresponding fraction for primitive lattices. For body-centred and face-centred cubic lattices the reciprocals of these fractions are given in table 1 by the integers m_{I} and m_{F} respectively. These values apply to the correspondence matrices quoted in table I 2 and hence the twinning modes given in table 1 together with their conjugates. They also apply to the inverses of these matrices and their associated twinning modes and conjugate modes. The remaining modes, those associated with the transposes and inverses of the transposes of the original correspondence matrices are referred to the reciprocal bases. Thus, as face-centred and body-centred cubic lattices are reciprocal to each other, the integers m_{I} and m_{F} have to be interchanged for these modes.

As there are only two lattice points associated with a body-centred cell the maximum permitted value of m_{I} is $2m$. This also applies to m_{F} as, although there are four lattice points in a face-centred cell, when the reciprocal basis is being considered this integer describes the type of shuffling in a body-centred cubic cell. The cases of particular interest are, however, those with values of m_{I} or m_{F} equalling unity and several examples of these arise in table 1. It is interesting that these are all conventional compound modes, belonging to classes 2 or 7 although, when larger shears are considered, some non-conventional modes involving no shuffles are obtained. Twinning modes with more than one-half of the lattice points shuffling, corresponding to m, m_{I} or m_{F} greater than 2, are unlikely to describe operative twinning mechanisms in crystalline materials. Thus three of the matrices for which m equals 4, also have m_{I} and m_{F} at least 4 and are consequently of little interest when applied to cubic structures. However, if base-centred cells are considered, and this of course is not appropriate for cubic lattices, at least one of the variants of the corresponding twinning modes would in each case involve only one-half of the lattice points shuffling.

2.4. *Some illustrative examples*

We shall now examine in detail the features of some specific modes contained in table 1. First, the relations between the eight different twinning modes associated with a given class 1 correspondence matrix are considered for matrix 2.7, the three rows of which are 110, 011 and $\frac{1}{2}\,0\,\frac{1}{2}$ respectively. The modes and their conjugates for the correspondence matrix, the transpose of its inverse, its inverse and its transpose have elements $K_1 K_2 \eta_1 \eta_2;\, g$ given by

$$\{1\,e^{+}\,1\}\quad \{1\,e^{-}1\}\quad \langle 2\,\bar{e}^{-}\,2\rangle\quad \langle \bar{2}\,e^{+}\,\bar{2}\rangle;\quad (\tfrac{3}{2})^{\frac{1}{2}}, \tag{1}$$

$$\{1\,e^{-}\,1\}\quad \{1\,e^{+}\,1\}\quad \langle \bar{2}\,e^{+}\,\bar{2}\rangle\quad \langle 2\,\bar{e}^{-}\,2\rangle;\quad (\tfrac{3}{2})^{\frac{1}{2}}, \tag{2}$$

$$\{2\,\bar{e}^{-}\,2\}\quad \{2\,\bar{e}^{+}\,2\}\quad \langle \bar{1}\,\bar{e}^{+}\,\bar{1}\rangle\quad \langle 1\,e^{-}\,1\rangle;\quad (\tfrac{3}{2})^{\frac{1}{2}}, \tag{3}$$

$$\{2\,e^{+}\,2\}\quad \{\bar{2}\,e^{-}\,\bar{2}\}\quad \langle \bar{1}\,\bar{e}^{-}\,\bar{1}\rangle\quad \langle 1\,e^{+}\,1\rangle;\quad (\tfrac{3}{2})^{\frac{1}{2}}, \tag{4}$$

$$\{\bar{1}\,\bar{1}\,f^{-}\}\quad \{1\,1\,f^{+}\}\quad \langle 4\,4\,\bar{f}^{+}\rangle\quad \langle \bar{4}\,\bar{4}\,f^{-}\rangle;\quad (\tfrac{3}{2})^{\frac{1}{2}}, \tag{5}$$

$$\{1\,1\,f^{+}\}\quad \{1\,1\,f^{-}\}\quad \langle 4\,4\,f^{-}\rangle\quad \langle 4\,4\,f^{+}\rangle;\quad (\tfrac{3}{2})^{\frac{1}{2}}, \tag{6}$$

$$\{4\,4\,f^{+}\}\quad \{4\,4\,\bar{f}^{-}\}\quad \langle 1\,1\,\bar{f}^{-}\rangle\quad \langle 1\,1\,f^{+}\rangle;\quad (\tfrac{3}{2})^{\frac{1}{2}}; \tag{7}$$

$$\{4\,4\,\bar{f}^{-}\}\quad \{4\,4\,f^{+}\}\quad \langle 1\,1\,f^{+}\rangle\quad \langle 1\,1\,\bar{f}^{-}\rangle;\quad (\tfrac{3}{2})^{\frac{1}{2}}, \tag{8}$$

respectively, where $e^{\pm} = 4 \pm 12^{\frac{1}{2}}$; $f^{\pm} = 12^{\frac{1}{2}} \pm 2$. The orientation relations for these eight distinct twinning modes are illustrated in figure 1, where the parent and twin simple cubic lattices are projected on to the plane of shear, which has indices belonging to the form $\{110\}$. In each case one-half of the parent lattice points are sheared direct to correct twin positions and the remainder have to shuffle. Note that the conventional orientation relations of reflexion in K_1 and rotation of π about η_1 are not obeyed by any of these twins. However, in all cases the twin lattice may be obtained from the parent by rotations about the normal to the plane of shear. This is also true of all of the other non-conventional twinning modes derived from correspondence matrices of classes 3 to 6, but in these cases fewer than eight independent modes arise.

Secondly, we shall consider the modes associated with correspondence matrix 2.2 of table 1, the three rows of which are 011, $\frac{1}{2}\bar{\frac{1}{2}}\frac{1}{2}$ and $\frac{1}{2}\frac{1}{2}\bar{\frac{1}{2}}$ respectively. This matrix is a degenerate form of class 2, giving rise to compound modes in which K_1 and η_1 are crystallographically equivalent to K_2 and η_2 respectively. Thus only two basically different modes arise and these may be conventionally represented by $K_1 K_2 \eta_1 \eta_2; g$ and $\bar{\eta}_1 \eta_2 K_1 \bar{K}_2; g$ or more specifically by

$$\{111\} \quad \{\bar{1}11\} \quad \langle\bar{2}11\rangle \quad \langle 211\rangle; \quad 2^{-\frac{1}{2}}, \tag{9}$$

$$\{2\bar{1}\bar{1}\} \quad \{211\} \quad \langle 111\rangle \quad \langle\bar{1}11\rangle; \quad 2^{-\frac{1}{2}}, \tag{10}$$

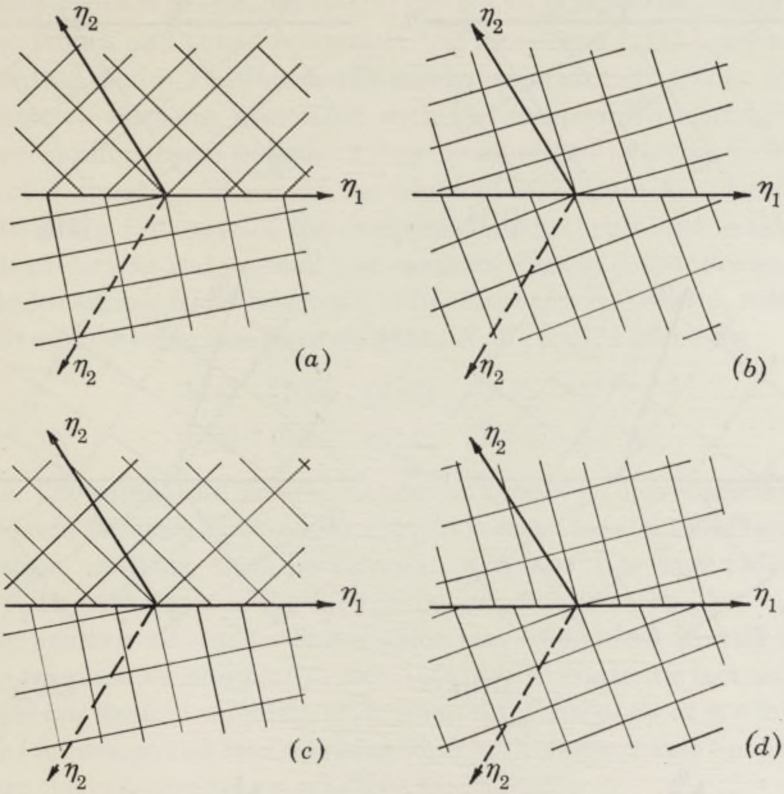


FIGURE 1. The orientation relations of the eight related but distinct simple cubic twinning modes (1) to (8) arising from correspondence matrix 2.7, illustrated by projecting the parent and twin lattices on to the plane of shear {110}. If the lower parts of the figures are considered to be the parent lattices and the upper parts the twins, diagrams (*a*), (*b*), (*c*) and (*d*) represent modes (1 to 4) respectively. In all four cases, the η_1 and η_2 directions, referred to the parent lattices are shown by bold continuous arrows. Alternatively if the roles of parent and twin are interchanged the diagrams represent modes (5 to 8) respectively. The twinning directions η_1 are then unchanged, but the η_2 directions referred to the new parent lattice are given by the bold broken arrows. In all eight modes only one-half of the lattice points are sheared to correct twin positions, but this is exemplified by the diagrams in two different ways. Thus, considering the {110} planes to be stacked –ABABAB–, all lattice points are sheared correctly in the A planes of (*a*) and (*b*), but none in the B planes. Alternatively in (*c*) and (*d*) one-half of the points are sheared directly to twin positions in both A and B planes.

respectively. It is particularly instructive to examine the shuffles associated with these modes in both the primitive and centred cubic lattices. The fractions of parent lattice points which shear direct to correct twin lattice points for the cases of simple cubic, body-centred cubic and face-centred cubic lattices are defined by the inverses of the integers m, m_{I} and m_{F}, given in table 1. For correspondence matrix 2.2

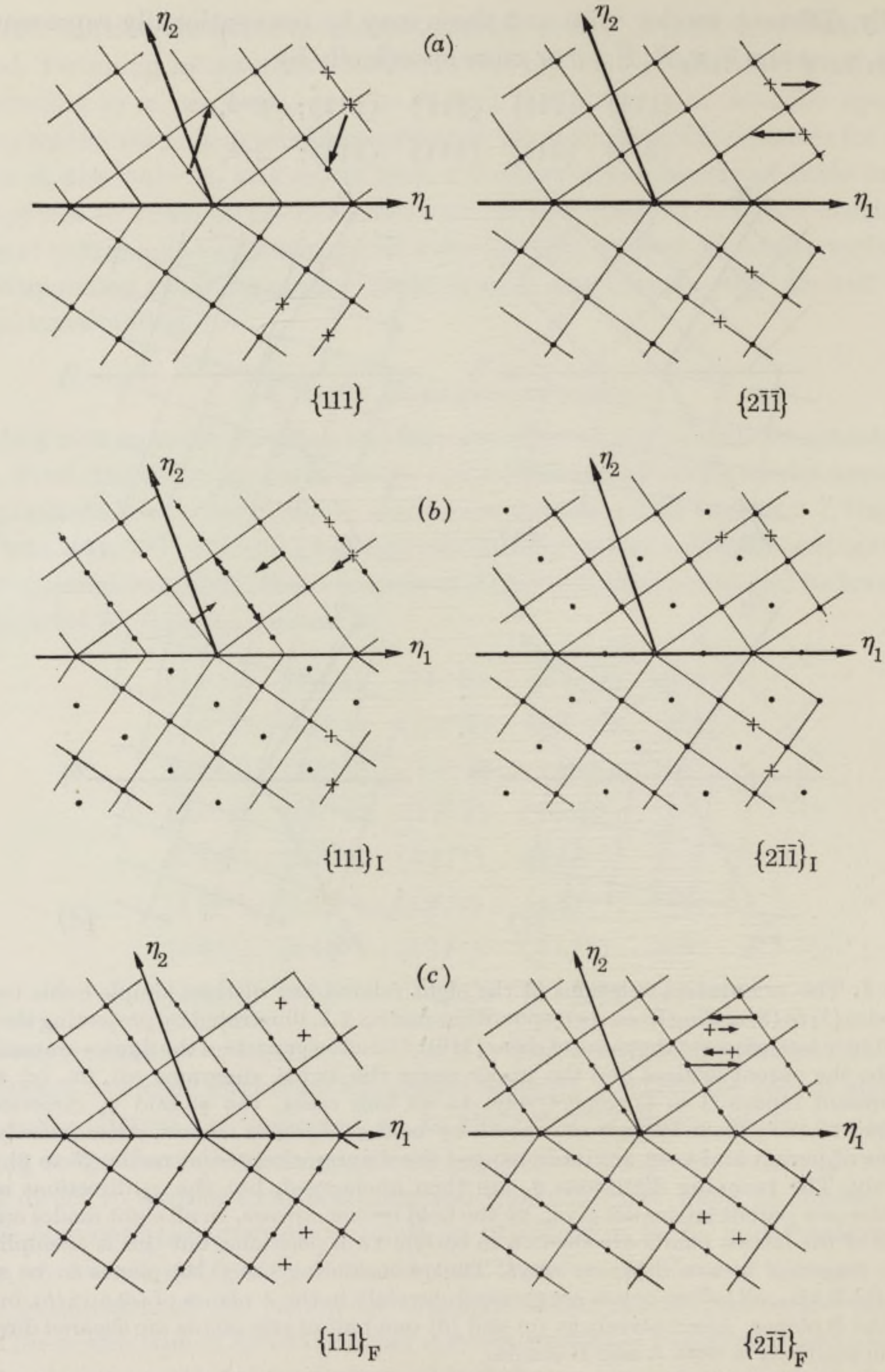


FIGURE 2. The parent and sheared lattices associated with twinning modes (9) and (10) arising from correspondence matrix 2.2 and its transpose. Diagrams, $\{111\}$, $\{111\}_{\mathrm{I}}$ and $\{111\}_{\mathrm{F}}$ illustrate the mode with $K_1\,K_2\,\eta_1\,\eta_2$ elements given by $\{111\}\,\{\bar{1}11\}\,\langle\bar{2}11\rangle\,\langle 211\rangle$ for the cases of simple cubic, body-centred cubic and face-centred cubic lattices respectively; diagrams $\{2\bar{1}\bar{1}\}$, $\{2\bar{1}\bar{1}\}_{\mathrm{I}}$, $\{2\bar{1}\bar{1}\}_{\mathrm{F}}$ show the related mode with elements $\{2\bar{1}\bar{1}\}\,\{211\}\,\langle 111\rangle\,\langle\bar{1}11\rangle$ for these three cases. The lattices are projected on to the common $\{01\bar{1}\}$ plane of shear which is stacked –ABABAB–. Lattice points in the A planes are indicated by dots and a few specimen points in the B planes by crosses. The sheared lattices are identical to the parent lattice in $\{111\}_{\mathrm{F}}$ and $\{211\}_{\mathrm{I}}$, so that no additional shuffling is necessary to create the twinned lattice. However, in order to obtain the correct twin in $\{111\}$ and $\{2\bar{1}\bar{1}\}$ one-half of the points must shuffle following the shear and in $\{111\}_{\mathrm{I}}$ and $\{2\bar{1}\bar{1}\}_{\mathrm{F}}$ the fraction is three-quarters. Possible shuffle mechanisms are indicated by short arrows for typical lattice points.

itself, which gives rise to mode (9) these integers are 2, 4 and 1 respectively and for the transpose of this matrix, which gives rise to mode (10), they become 2, 1, and 4. The six cases are illustrated in figure 2 by projecting the parent and sheared lattices on to the $\{01\bar{1}\}$ plane of shear. No shuffling is necessary in the $\{111\}$ face-centred and $\{2\bar{1}\bar{1}\}$ body-centred modes, one-half of the lattice points must shuffle in the two simple cubic modes and three-quarters in the remaining $\{111\}$ body-centred and $\{2\bar{1}\bar{1}\}$ face-centred modes. Possible shuffle mechanisms are indicated in the figure.

The orientation relations associated with the compound twinning modes discussed above and illustrated in figure 2 may be described as either reflexion in K_1 or rotation of π about η_1. These are the conventional orientation relations of deformation twinning but some of the compound modes contained in table 1 satisfy more complex relations and we shall now examine these in detail. For example, two twinning modes arising from the class 2 correspondence matrix 1.6, with rows 100, $2\bar{1}0$ and $10\bar{1}$, and its transpose have elements $K_1 K_2 \eta_1 \eta_2; g$ given by

$$\{524\} \quad \{100\} \quad \langle 2\bar{1}\bar{2} \rangle \quad \langle 012 \rangle; \quad 5^{\frac{1}{2}}, \tag{11}$$

$$\{\bar{2}12\} \quad \{012\} \quad \langle 524\} \quad \langle \bar{1}00 \rangle; \quad 5^{\frac{1}{2}}, \tag{12}$$

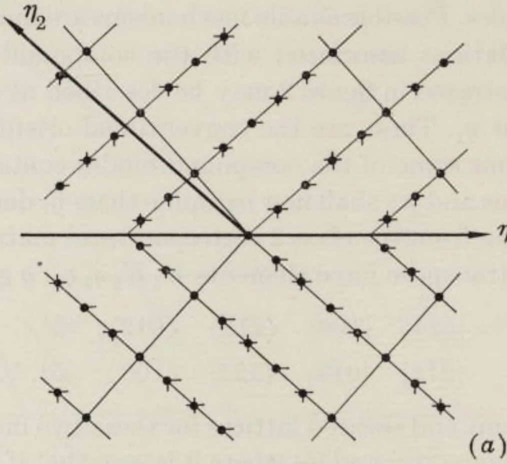
respectively. The parent and sheared lattices for these two modes are shown for the simple cubic case in figure 3 (a) and (b) where it is seen that if no shuffling is allowed the orientation relations must be rotation of π about η_1 and reflexion in K_1 respectively. In both cases if the alternative relation is to be obeyed four-fifths of the lattice points must shuffle. This fraction may be deduced directly from standard expressions given by Bilby & Crocker (1965) and is due to the fact that the plane of shear $\{02\bar{1}\}$ has fivefold stacking. Only when the plane of shear is a mirror plane, and it can be for compound modes arising from both classes 2 and 7 correspondence matrices, are the two orientation relations equivalent.

Finally we shall consider the two related compound modes associated with the class 1 correspondence matrix 4.14 with rows $\frac{3}{2}\,\bar{\frac{1}{2}}\,\bar{\frac{1}{2}}$, $\bar{\frac{1}{4}}\,\frac{3}{4}\,\frac{1}{4}$ and $\frac{1}{4}\,\frac{1}{4}\,\frac{3}{4}$ and its inverse. As quoted in table 1 these modes have the same K_1 plane and equal and opposite η_1 directions. These shears restore the lattice identically and are thus not genuine twinning shears. However, the two conjugate modes with elements $K_1 K_2 \eta_1 \eta_2$; g given by

$$\{11, 1, \bar{1}\} \quad \{11\bar{1}\} \quad \langle 2, 11, \overline{11} \rangle \quad \langle 2\bar{1}1 \rangle; \quad (\tfrac{9}{8})^{\frac{1}{2}}, \tag{13}$$

$$\{\bar{5}7\bar{7}\} \quad \{11\bar{1}\} \quad \langle 14, 5, \bar{5} \rangle \quad \langle \bar{2}1\bar{1} \rangle; \quad (\tfrac{9}{8})^{\frac{1}{2}}, \tag{14}$$

respectively, produce the same lattice in new orientations and are thus satisfactory twinning modes. The orientation relations for these two modes are illustrated for the simple cubic lattice in a single diagram in figure 4, where it is seen that only one-twelfth of the sheared lattice points are located at correct twin positions, if conventional orientation relations are adopted. This ratio is increased to one-quarter for the non-conventional relation shown in figure 4 and, as indicated in table 1, becomes one-half for the face-centred cubic lattice. Thus, these compound modes are associated with very complicated shuffle mechanisms if the traditional orientation relations are assumed, but most of the shuffling is eliminated if more general relations are accepted. As these modes are degenerate cases of those with four irrational elements it is to be expected that the parent and twin lattices are related by a rotation about the normal to the plane of shear and this is confirmed by figure 4.



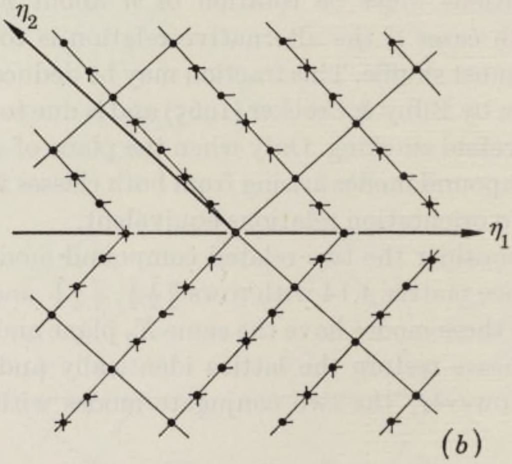


FIGURE 3. The orientation relations of the two related simple cubic twinning modes (11) and (12) with {524} and {$\bar{2}$12} composition planes, arising from correspondence matrix 1.6 and its transpose. The parent and sheared lattices are projected on to the {02$\bar{1}$} plane of shear, which has fivefold stacking. Lattice points in these planes are indicated by dots with 0, 1, 2, 3 and 4 bars respectively. In (a) and (b) the orientation relations are rotation of π about the η_1 direction [2$\bar{1}\bar{2}$] and reflexion in the K_1 plane ($\bar{2}$12) respectively. No shuffling is necessary if these relationships are obeyed but in both cases four-fifths of the lattice points must shuffle if the alternative orientation relations are imposed.

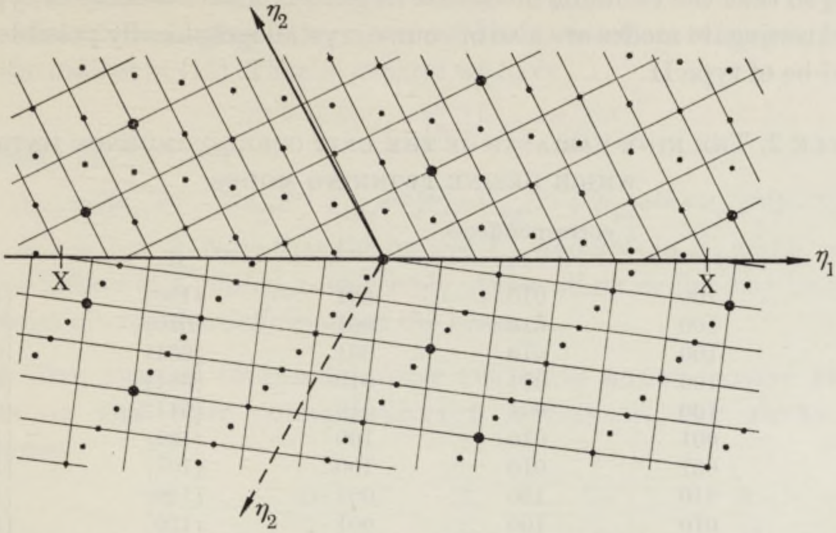


FIGURE 4. The orientation relations of the related simple cubic twinning modes (13) and (14), with $\{11, 1, \bar{1}\}$ and $\{\bar{5}\ 7\ \bar{7}\}$ composition planes, arising from correspondence matrix 4.14 and its inverse. The parent and product lattices are projected on to the $\{011\}$ plane of shear, the repeat distance in the rational interface being indicated by X–X. Considering first the lower part of the diagram to be the parent lattice the continuous arrows represent the appropriate η_1 and η_2 directions for the $\{11, 1, \bar{1}\}$ composition plane. The dots above the interface are then the sheared lattice points. For the non-conventional twin lattice orientation shown one-quarter of these dots coincide with lattice points. If a conventional orientation relation were chosen only one-twelfth of the sheared lattice points, those represented by large dots, would be in correct twin positions. The same ratios are obtained when neighbouring planes of shear are included. These conclusions are also reached when the upper part of the diagram is considered to be the parent lattice. The η_2 direction is then given by the broken arrow and the composition plane becomes $\{\bar{5}\ 7\ \bar{7}\}$.

3. The unit correspondence matrix

When used as a correspondence matrix in the general analysis of twinning shears presented in §I 2 the unit matrix results in shears of zero magnitude for all lattices and thus does not produce any twinning modes. However, variants of the unit matrix, obtained by interchanging rows, interchanging columns, and changing the signs of rows and columns, may predict possible twinning modes. In all, twenty-four unimodular variants of the unit matrix arise. However, of these, only the ten symmetric matrices satisfy the restriction (I 16) that the shear magnitude predicted by a correspondence matrix must be identical to that predicted by its inverse. We exclude now the unit matrix itself and the remaining nine matrices, three of which are diagonal, are given in table 2. These nine matrices have the additional property that they are identical to their own inverses and hence as shown in §I 6 each one must result in a conventional twinning mode with at least two rational elements. These pairs of elements, which are sufficient to define the twinning modes uniquely are independent of the metric tensors c_{ij} and c^{ij} and are thus the same for all lattices. They are given for all nine correspondence matrices in table 2, where they are labelled

K_1 and η_2 so that the twinning modes are in general conventionally of type I. The associated conjugate modes are also of course crystallographically possible and will in general be of type II.

Table 2. The nine variants of the unit correspondence matrix which define twinning modes

	correspondence			K_1	η_2
1	100	0$\bar{1}$0	00$\bar{1}$	(100)	[100]
2	$\bar{1}$00	010	00$\bar{1}$	(010)	[010]
3	$\bar{1}$00	0$\bar{1}$0	001	(001)	[001]
4	$\bar{1}$00	001	010	(011)	[011]
5	$\bar{1}$00	00$\bar{1}$	0$\bar{1}$0	(01$\bar{1}$)	[01$\bar{1}$]
6	001	0$\bar{1}$0	100	(101)	[101]
7	00$\bar{1}$	0$\bar{1}$0	$\bar{1}$00	(10$\bar{1}$)	[10$\bar{1}$]
8	010	100	00$\bar{1}$	(110)	[110]
9	0$\bar{1}$0	$\bar{1}$00	00$\bar{1}$	(1$\bar{1}$0)	[1$\bar{1}$0]

The three rows of each matrix are given as a single row in the table, bars indicating negative elements.

A significant feature of table 2 is that corresponding K_1 and η_2 elements have the same indices. In addition, the three diagonal matrices predict closely related twinning modes, as do the other six matrixes. The remaining twinning elements K_2, η_1 and g do depend on the metric tensors and thus the lattice parameters. They may be obtained using the general analysis given in I or in terms of the K_1 and η_2 elements in table 2 by making use of equations given by Bilby & Crocker (1965).

In the triclinic lattice all nine modes in table 2 are independent. The full twinning elements $K_1 K_2 \eta_1 \eta_2$; g arising from matrix 1 are

$$(100) \quad (0\,\overline{c_{12}}\,\overline{c_{31}}) \quad [0\,c^{12}\,c^{31}] \quad [100]; \quad 2(c_{11}c^{11}-1)^{\frac{1}{2}}. \tag{15}$$

Matrices 2 and 3 give rise to similar but distinct modes and all three modes can be written in the general form

$$(\delta_{\alpha i}) \quad (-c_{\alpha i}+c_{\alpha\alpha}\delta_{\alpha i}) \quad [c^{\alpha i}-c^{\alpha\alpha}\delta^{\alpha i}] \quad [\delta^{\alpha i}]; \quad 2(c_{\alpha\alpha}c^{\alpha\alpha}-1)^{\frac{1}{2}}, \tag{16}$$

where α, $i = 1, 2, 3$ and no summation is implied when Greek letters are repeated. The form of the twinning elements in (16) clearly indicates that the three different modes may be considered to arise through labelling the basic vectors in different ways which is of course permissible for a triclinic lattice. However, for a given lattice with this symmetry all these modes are independent.

The full twinning elements arising from matrix 4 may be written

$$(011^*) \quad (T_{123}, 1, \bar{1}^*) \quad [T^{123}, 1, \bar{1}^*] \quad [011^*]; \quad g_{123}, \tag{17}$$

where

$$T_{123} = 2(c_{12}+c_{13}^*)\,(c_{22}-c_{33})^{-1}, \quad T^{123} = 2(c^{12}+c^{13*})\,(c^{22}-c^{33})^{-1},$$

and

$$g_{123} = \{[c_{11}c^{11}-2(c_{12}c^{31}+c_{13}c^{21})^*]+[c_{22}c^{33}+2c_{23}c^{23}+c_{33}c^{22}]-3\}^{\frac{1}{2}}.$$

The corresponding elements for matrix 5 may be obtained from (17) by changing the signs of the terms indicated by asterisks. Modes 6 to 9 are now obtained by permuting the indices in (17). Thus in general we have

$$T^{\alpha\beta\gamma} = 2(c_{\alpha\beta}+c^{*}_{\alpha\gamma})\,(c_{\beta\beta}-c_{\gamma\gamma})^{-1}$$

and similarly for $T^{\alpha\beta\gamma}$ and

$$g_{\alpha\beta\gamma} = \{[c_{\alpha\alpha}c^{\alpha\alpha}-2(c_{\alpha\beta}c^{\gamma\alpha}+c_{\alpha\gamma}c^{\beta\alpha})^{*}]+[c_{\beta\beta}c^{\gamma\gamma}+2c_{\beta\gamma}c^{\beta\gamma}+c_{\gamma\gamma}c^{\beta\beta}]-3\}^{\frac{1}{2}},$$

where $\alpha, \beta, \gamma = 1, 2, 3$. Note that the indices $T_{\alpha\beta\gamma}$ and $T^{\alpha\beta\gamma}$ in K_2 and η_1 correspond to the zero indices in K_1 and η_2 respectively. Again all six modes may be considered to arise from alternative definitions of the bases.

Table 3. The number of independent twinning modes arising from variants of the unit correspondence matrix in the seven crystal systems

Tr	*M*	O	H	Te	R	C
1	1*	0	(1*)	0	1*	0
2	0	0	(1*)	0	1*	0
3	1*†	0	(1*)	0	1*	0
4	4	4*	4	4*	1*†	0
5	4	4*	4	4*	0	0
6	6*	6*	0	4*	1*†	0
7	6*†	6*	0	4*	0	0
8	8	8*	4	0	1*†	0
9	8	8*	4	0	0	0

The crystal systems are specified at the head of the table by means of their initial letters. The symbols * and † indicate compound and conjugate modes and ( ) and 0 shears to the identity and shears of zero magnitude respectively.

We shall now consider the way in which the nine independent twinning modes of table 2 degenerate as the symmetry increases from triclinic to cubic. This is summarized in table 3 for the seven crystal systems. In this table the nine triclinic modes discussed above are labelled 1 to 9 and corresponding modes in the other systems for which the shear magnitude is zero, and thus the modes non-existent, are indicated by 0. Crystallographically equivalent modes in a given system are indicated by repetition of the mode number, compound modes by asterisks and conjugate modes by obeli. Finally numbers in brackets indicate that the shear restores the lattice in the same orientation and is thus not strictly a twinning shear.

In monoclinic lattices we obtain four independent modes. These arise directly from matrices 1, 4, 6 and 8 on letting the metric elements c_{12}, c_{23}, c^{12}, c^{23} equal zero in the expressions for the triclinic twinning elements given above. They have elements $K_1 K_2 \eta_1 \eta_2$; g given by

$$(100)\quad (001)\quad [001]\quad [100];\quad 2c_{13}[c_{11}c_{33}-(c_{13})^2]^{-\frac{1}{2}}, \tag{18}$$

$$(011)\quad (M_{23}\,1\,\bar{1})\quad [M^{23}\,1\,\bar{1}]\quad [011];\quad [c_{11}c^{11}+c_{22}c^{33}+c_{33}c^{22}-3]^{\frac{1}{2}}, \tag{19}$$

$$(101)\quad (\bar{1}\,0\,1)\quad [\bar{1}\,0\,1]\quad [101];\quad (c_{33}-c_{11})\,[c_{11}c_{33}-(c_{13})^2]^{-\frac{1}{2}}, \tag{20}$$

$$(110)\quad (1\,\bar{1}\,M_{12})\quad [1\,\bar{1}\,M^{12}]\,[110];\quad [c_{33}c^{33}+c_{11}c^{22}+c_{22}c^{11}-3]^{\frac{1}{2}}, \tag{21}$$

respectively, where $M_{12} = 2c_{13}(c_{11}-c_{22})^{-1}$, $M_{23} = 2c_{13}(c_{22}-c_{33})^{-1}$, and similarly for M^{12} and M^{23}. In addition to the large reduction in the number of independent modes for monoclinic lattices the twinning elements K_2 and η_1 of modes (18) and (20) simplify to rational forms so that these modes become compound. The expressions for the shear magnitudes also simplify considerably, but in the case of modes (19) and (21) it has still been found convenient to use the components of both the direct and reciprocal lattice metrics.

The orthorhombic modes may be readily obtained by letting c_{13} and c^{13} and hence M_{12}, M_{23}, M^{12} and M^{23} be zero in modes (18) to (21). Mode (18) then has a zero shear but the remaining three modes have shears given by $(c_{22}-c_{33})(c_{22}c_{33})^{-\frac{1}{2}}$, $(c_{33}-c_{11})(c_{33}c_{11})^{-\frac{1}{2}}$ and $(c_{11}-c_{22})(c_{11}c_{22})^{-\frac{1}{2}}$ respectively. Thus we obtain three compound modes corresponding to the three alternative ways of labelling the axes. These three modes also define hexagonal modes referred to the orthohexagonal basis (Otte & Crocker 1965). However, in this case we have $c_{22} = 3c_{11}$ so that the shear magnitudes become $3^{-\frac{1}{2}}\gamma - 3^{\frac{1}{2}}\gamma^{-1}$, $\gamma-\gamma^{-1}$ and $(\frac{4}{3})^{\frac{1}{2}}$ for modes (19), (20) and (21) respectively, where $\gamma = (c_{33}/c_{11})^{\frac{1}{2}}$ is the axial ratio. This last mode is in fact a shear to the identity and not strictly a twinning shear. For the more commonly used primitive hexagonal basis we let

$$c_{11} = c_{33} = -2c_{13};\quad c^{11} = c^{33} = 2c^{13};\quad c_{11}c^{11} = \tfrac{4}{3};\quad c_{22}c^{22} = 1,$$

and $\gamma = (c_{22}/c_{11})^{\frac{1}{2}}$ in modes (18) to (21) so that M_{12}, M_{23}, M^{12} and M^{23} reduce to

$$H_{12} = -H_{23} = (\gamma^2-1)^{-1} \quad\text{and}\quad H^{12} = -H^{23} = [1-(\tfrac{3}{4})\gamma^{-2}]^{-1}.$$

The twinning shear of mode (20) is then zero and on interchanging the second and third indices to obtain the conventional hexagonal basis modes (19) and (21) become crystallographically equivalent with a shear magnitude of $[(4\gamma^2+3\gamma^{-2}-5)/3]^{\frac{1}{2}}$. This is the only true twinning mode for this basis as the twinning shear of $(\frac{4}{3})^{\frac{1}{2}}$ arising from mode (18) restores the lattice in its original orientation. This last mode is in fact crystallographically equivalent to the mode with the same shear strain deduced above from mode (20) using the orthohexagonal basis. This is demonstrated when the hexagonal modes are written using the Miller–Bravais system of indices (Otte & Crocker 1965), the elements $K_1 K_2 \eta_1 \eta_2;\, g$ becoming

$$\{10\bar{1}2\}\quad \{10\bar{1}\bar{2}\}\quad \langle 10\bar{1}\bar{1}\rangle\quad \langle 10\bar{1}1\rangle;\quad 3^{-\frac{1}{2}}\gamma - 3^{\frac{1}{2}}\gamma^{-1}, \tag{22}$$

$$\{1\bar{2}12\}\quad \{\bar{1}2\bar{1}2\}\quad \langle \bar{1}2\bar{1}3\rangle\quad \langle 1\bar{2}13\rangle;\quad \gamma-\gamma^{-1}, \tag{23}$$

$$\{1\bar{1}00\}\quad \{01\bar{1}0\}\quad \langle 11\bar{2}0\rangle\quad \langle 2\bar{1}\bar{1}0\rangle;\quad (\tfrac{4}{3})^{\frac{1}{2}}, \tag{24}$$

$$\{0\bar{1}11\}\quad H_1\quad H^1\quad \langle \bar{1}2\bar{1}3\rangle;\quad [(4\gamma^2+3\gamma^{-2}-5)/3]^{\frac{1}{2}}, \tag{25}$$

where

$$H_1 = [(\gamma^2-1)^{-1}, 1, -\gamma^2(\gamma^2-1)^{-1}, \bar{1}],$$

and

$$H^1 = [4+3\gamma^{-2}, 4-6\gamma^{-2}, -8+3\gamma^{-2}, -12+9\gamma^{-2}].$$

Increasing the symmetry to tetragonal by letting $c_{11} = c_{22}$ in the orthorhombic modes results in the single mode with elements $K_1 K_2 \eta_1 \eta_2;\, g$ given by

$$\{101\}\quad \{\bar{1}01\}\quad \langle \bar{1}01\rangle\quad \langle 101\rangle;\quad \gamma^{-1}(\gamma^2-1), \tag{26}$$

where $\gamma = (c_{33}/c_{11})^{\frac{1}{2}}$ is the axial ratio. Similarly, in the rhombohedral lattices only one mode

$$\{100\} \quad \{011\} \quad \langle 011\rangle \quad \langle 100\rangle; \quad 8^{\frac{1}{2}}c(1+c-2c^2)^{-\frac{1}{2}} \tag{27}$$

arises, where c is the cosine of the rhombohedral angle. Finally on letting γ and c equal unity and zero respectively in modes (26) and (27) the corresponding cubic modes are found to have zero shears. Thus none of the nine triclinic twinning modes arising from variants of the unit correspondence matrix degenerate to possible modes in the cubic lattice. This result may of course be deduced directly from table 2 where it is seen that all nine η_2 directions will be perpendicular to the corresponding K_2 planes in the cubic system and hence predict zero shears.

4. A class 4 correspondence matrix

In order to illustrate the relations between non-conventional twinning modes in different crystal systems, correspondence matrix 2.4 of table 1, with rows given by 100, 011 and $0\,\overline{\tfrac{1}{2}}\,\tfrac{1}{2}$ will now be considered. This matrix is of class 4, being equal to a variant of its own inverse transposed. It has a simple form which results in the total number of possible crystallographically distinct variants for all seven crystal systems being reduced from 818, as indicated in table I 1 for the most general correspondence matrix, to 227. On using these matrices in the general analysis of twinning shears presented in §I 2 it is found that only 20 variants define twinning modes. In particular for the cubic, hexagonal, tetragonal, orthorhombic and monoclinic systems there are one, two, three, six and eight modes respectively. The actual variants involved are summarized in table 4, in all cases the four elements of zero magnitude being symmetrically disposed about the principal diagonal. When these elements are contained in the first row and column the plane of shear of the resulting twinning mode

Table 4. The variants of correspondence matrix 2.4 which result in twinning modes

	Tr	M	O	H	Te	R	C
1	—	2121	1212	2323	1212	—	1212
2	—	$21\bar{2}\bar{1}$	2121	$232\bar{3}$	2323	—	—
3	—	2131	2323	—	3131	—	—
4	—	$21\bar{3}\bar{1}$	3232	—	—	—	—
5	—	3131	3131	—	—	—	—
6	—	$31\bar{3}\bar{1}$	1313	—	—	—	—
7	—	3121	—	—	—	—	—
8	—	$31\bar{2}\bar{1}$	—	—	—	—	—

The crystal systems are specified at the head of the table by means of their initial letters. The notation defined in §I 4.1 has been adopted. Thus the first two integers give the first two rows of the variant, using the convention that 1, 2, 3 represent the rows 100, 011 and $0\,\overline{\tfrac{1}{2}}\,\tfrac{1}{2}$ respectively of the parent matrix. Similarly, the second two integers specify the first two columns, 1, 2, 3 representing the columns 100, $0\,1\,\overline{\tfrac{1}{2}}$ and $0\,1\,\tfrac{1}{2}$. Negative rows and columns are indicated by bars and the last row and last column are defined by the two unused integers, which are chosen to be positive. If this results in a matrix with determinant equalling -1, the signs of all the elements have to be changed. Thus, for example, $21\bar{3}\bar{1}$ has rows $10\bar{1}$, 010 and $\tfrac{1}{2}\,0\,\tfrac{1}{2}$.

is (100). Similarly, when they are in the second or third rows and columns the plane of shear is (010) or (001) respectively. The theory also restricts these planes to be mirror planes, which explains why no modes arise in the rhombohedral and triclinic systems in which no such planes exist. This point is emphasized by the two vacant columns in table 4.

We consider first the eight monoclinic modes all of which have the unique (010) mirror plane as plane of shear and elements $K_1\, K_2\, \eta_1\, \eta_2$; g given by

$$(m^+, 0, 1) \quad (m^-, 0, 1) \quad [1, 0, \overline{m}^+] \quad [1, 0, \overline{m}^-]; \quad g_M. \tag{28}$$

Here m^+ and m^- are the roots of the quadratic equation

$$M_2 m^2 + 2M_1 m + M_0 = 0,$$

and

$$g_M = (M_2 c_{11} + 2M_1 c_{13} + M_0 c_{33})^{\frac{1}{2}} \quad [c_{11} c_{33} - (c_{13})^2]^{-\frac{1}{2}},$$

where M_2, M_1 and M_0 are functions of the direct metric elements c_{11}, c_{13} and c_{33}. In particular for matrix 1 of table 4 we have

$$M_2 = c_{11} + c_{13}^{\dagger} - \tfrac{3}{4}c_{33}, \quad M_1 = c_{11}^{*} + c_{13} + \tfrac{1}{4}c_{33}^{*}, \quad M_0 = -c_{13}^{\dagger} + \tfrac{1}{4}c_{33}.$$

The corresponding expressions for matrices 2 and 3 are obtained by changing the signs of the terms marked with asterisks and obeli respectively and for matrix 4 the signs of both sets of terms are changed. The modes arising from matrices 5 to 8 are now obtained by interchanging the subscripts 1 and 3 of the metric elements and the expressions M_2 and M_0 for matrices 1 to 4 respectively. Thus all four twinning elements of all eight modes are functions of the lattice parameters and are therefore irrational. Hence these modes are all non-conventional.

In the orthorhombic system changing the sign of an index does not produce a distinct crystallographic variant. This is also true for rows and columns of correspondence matrices so that the eight monoclinic modes arising from table 4 immediately degenerate to four orthorhombic modes. This number is further reduced to two, due to the fact that, for this particular correspondence matrix, interchanging the positions of the columns labelled 2 and 3 in table 4 leaves the resulting mode unaltered. However, in the orthorhombic system two additional mirror planes, (100) and (001) may act as the plane of shear so that, in all, six twinning modes arise. In each of these all four elements have zero indices in the location corresponding to the non-zero index of the plane of shear. Thus, for example, orthorhombic mode 1 in table 4 has a (100) plane of shear and twinning elements $K_1\, K_2\, \eta_1\, \eta_2$; g given by

$$(0, 0_{23}^{+}, 1) \quad (0, 0_{23}^{-}, 1) \quad [0, 1, \overline{0}_{23}^{+}] \quad [0, 1, \overline{0}_{23}^{-}]; \quad g_{23}. \tag{29}$$

Here $0_{23}^{\pm}$ and g_{23} satisfy

$$0_{\beta\gamma}^{\pm} = \{-4c_{\beta\beta} + c_{\gamma\gamma} \pm 2[4(c_{\beta\beta})^2 + (c_{\gamma\gamma})^2 - 3c_{\beta\beta} c_{\gamma\gamma}]^{\frac{1}{2}}\}(3c_{\gamma\gamma} - 4c_{\beta\beta})^{-1},$$
$$g_{\beta\gamma} = \tfrac{1}{2}[4(c_{\beta\beta}/c_{\gamma\gamma}) + (c_{\gamma\gamma}/c_{\beta\beta}) - 3]^{\frac{1}{2}},$$

where β and γ are 2 and 3 respectively. In general β and γ are unequal and take on the values 1, 2, 3, β and γ indicating the location of the indices $0_{\beta\gamma}^{\pm}$ in K_1 and K_2 and of

$\bar{0}^{\pm}_{\beta\gamma}$ in η_1 and η_2 respectively. The missing integer then locates the zero indices and the remaining indices are unity. On this convention orthorhombic modes 1 to 6 of table 4 are associated with values of β and γ given by 23, 13, 12, 21, 31 and 32 respectively.

On letting $c_{22} = 3c_{11}$, the six orthorhombic modes reduce to six hexagonal modes referred to the orthohexagonal basis. In particular the mode corresponding to orthorhombic mode 3 then becomes the conventional compound mode.

$$(350) \quad (1\bar{1}0) \quad [5\bar{3}0] \quad [110]; \quad 3^{-\frac{1}{2}}. \tag{30}$$

The remaining five modes have irrational elements, all of which are functions of the axial ratio except those corresponding to orthorhombic mode 4 which becomes

$$(1, H^{+}_{\bar{2}\bar{1}}, 0) \quad (1, H^{-}_{\bar{2}\bar{1}}, 0) \quad [\bar{H}^{+}_{\bar{2}\bar{1}}, 1, 0] \quad [\bar{H}^{-}_{\bar{2}\bar{1}}, 1, 0]; \quad (\tfrac{7}{3})^{\frac{1}{2}}, \tag{31}$$

where $H^{\pm}_{\bar{2}\bar{1}} = (11 \mp 112^{\frac{1}{2}})/9$. Alternatively, on the primitive hexagonal basis, the two variants of the correspondence matrix noted in table 4 produce the following twinning modes:

$$(H^{+}_{\bar{1}}, \bar{1}, 0) \quad (H^{-}_{\bar{1}}, 1, 0) \quad [1, \bar{H}^{-}_{\bar{1}}, 0] \quad [1, H^{-}_{\bar{1}}, 0]; \quad (\tfrac{7}{3})^{\frac{1}{2}}, \tag{32}$$

$$(310) \quad (1\bar{1}0) \quad [1\bar{3}0] \quad [110]; \quad 3^{-\frac{1}{2}}, \tag{33}$$

where $H^{\pm}_{\bar{1}} = 28^{\frac{1}{2}} \pm 5$. These two modes may be deduced from the variants of mode (28) associated with monoclinic matrices 1 and 2 by letting $c_{11} = c_{33} = -2c_{13}$ and interchanging the second and third indices to obtain the conventional hexagonal basis. Modes (30) and (33) are in fact equivalent, both being variants of

$$\{13\bar{4}0\} \quad \{\bar{1}100\} \quad \langle 5\bar{7}20\rangle \quad \langle 11\bar{2}0\rangle; \quad 3^{-\frac{1}{2}}, \tag{34}$$

when the Miller–Bravais system is used. However, modes (31) and (32) are distinct, despite the fact that they have the same shear magnitude.

The six orthorhombic modes also reduce to three crystallographically distinct tetragonal modes on letting $c_{11} = c_{22}$. Thus tetragonal modes 1, 2 and 3 of table 4 have twinning elements

$$(T^{+}_{\bar{1}\bar{1}}, 1, 0) \quad (T^{-}_{\bar{1}\bar{1}}, 1, 0) \quad [1, \bar{T}^{+}_{\bar{1}\bar{1}}, 0] \quad [1, \bar{T}^{-}_{\bar{1}\bar{1}}, 0]; \quad 2^{-\frac{1}{2}}, \tag{35}$$

$$(0, T^{+}_{\bar{1}\bar{3}}, 1) \quad (0, T^{-}_{\bar{1}\bar{3}}, 1) \quad [0, 1, T^{+}_{\bar{1}\bar{3}}] \quad [0, 1, T^{-}_{\bar{1}\bar{3}}]; \quad \tfrac{1}{2}(\gamma + 4\gamma^{-1} - 3)^{\frac{1}{2}}, \tag{36}$$

$$(1, 0, T^{+}_{\bar{3}\bar{1}}) \quad (1, 0, T^{-}_{\bar{3}\bar{1}}) \quad [\bar{T}^{+}_{\bar{3}\bar{1}}, 0, 1] \quad [\bar{T}^{-}_{\bar{3}\bar{1}}, 0, 1]; \quad \tfrac{1}{2}(4\gamma + \gamma^{-1} - 3)^{\frac{1}{2}}, \tag{37}$$

where $T^{\pm}_{\bar{1}\bar{1}} = 3 \pm 8^{\frac{1}{2}}$, $T^{\pm}_{\bar{1}\bar{3}} = \{-4 + \gamma \pm 2[4 - 3\gamma + \gamma^2]^{\frac{1}{2}}\}(3\gamma - 4)^{-1}$, and $T^{\pm}_{\bar{3}\bar{1}}$ is obtained by changing γ, the axial ratio, to γ^{-1} in the expression for $T^{\pm}_{\bar{1}\bar{3}}$. Finally when we let $\gamma = 1$ these three modes reduce to a single cubic mode with elements identical to those of mode (35).

Of the modes discussed here, only (34) has a conventional orientation relation. The others all involve four irrational twinning elements which must therefore have different indices when referred to parent and twin bases. The indices h_i, k_i, p^i, q^i

quoted here and defined in §1 are of course relative to the parent basis, the corresponding indices relative to the twin basis being given by the theory when, as explained in §I 4.3, the inverse of the correspondence matrix is used. However, they are also given more conveniently by $U^{-1j}{}_i h_j$, $U^{-1j}{}_i k_j$, $U^i_j p^j$, $U^i_j q^j$, where U^i_j is the correspondence matrix. Thus the data given in the present section are sufficient to describe all the modes associated with correspondence 2.4 and its inverse.

5. Discussion

The examples of twinning modes discussed in the present paper have been chosen primarily to illustrate the characteristic features of the seven classes of mode which arise when the generalized theory of twinning shears (Bevis & Crocker 1968) is applied to specific lattices. However, many of the modes presented, particularly the conventional modes belonging to classes 2 and 7, are operative deformation twinning modes in crystalline materials. Thus, for example, modes (9) and (10) are the observed modes in metals with the face-centred cubic and body-centred cubic structures respectively (Christian 1965). These modes involve the smallest possible twinning shear strains in these structures which are consistent with the absence of atomic shuffling. Again mode (22) is the most frequently observed twinning mode in metals with the hexagonal close packed structure, although as discussed in detail by Crocker & Bevis (1969) for the particular case of titanium, many conventional modes are possible and are indeed observed in hexagonal structures. This is essentially due to the fact that these structures consist of atoms at the lattice points of two or more interpenetrating lattices so that atomic shuffling must in general accompany any twinning shear (Bilby & Crocker 1965). Whether or not a particular mode operates, then depends on the complexity of the shuffle mechanism in addition to the magnitude of the twinning shear. Thus mode (23) (Hall 1954) which has a large shear but a simple shuffle mechanism does not describe the crystallography of twins on $\{11\bar{2}2\}$ planes in titanium, the operative mode (Crocker & Bevis 1969) having a smaller shear but more complex shuffles. The rhombohedral metals bismuth, antimony and arsenic also have double lattice structures, the operative twinning mode (Hall 1954) being the conjugate of the compound mode (27). However, in mercury, which has a single lattice rhombohedral structure, the observed mode (Guyoncourt & Crocker 1968) is of type II, with a habit plane near $\{\bar{1}\bar{3}5\}$, which like modes (9) and (10) is predicted by correspondence matrix 2.2. Mode (26) is observed in the tetragonal metal indium (Hall 1954), which has an axial ratio near unity, and also as the lattice invariant shear in several martensitic transformations (Crocker 1964). Modes (19 to 21) are not operative in the orthorhombic α-phase of uranium because for this metal, as shown by Crocker (1965a), several other modes with smaller shears are possible and are indeed observed.

For examples of twinning modes in triclinic and monoclinic structures it is necessary to consider non-metallic crystals (Tertsch 1949; Klassen-Neklyudova 1964). Mode (16) and its conjugate is then found to describe an operative twin in the plagioclase felspars which comprise a group of minerals with triclinic symmetry. Mode (13) occurs in the monoclinic minerals jordanite and diopside and the salt barium bromide and the conjugate of mode (21) is observed in cryolite, which is also monoclinic. Again the degenerate orthorhombic form of mode (20) occurs in anhydrite and of mode (21) in baryte and bournonite. However, in these complex materials operative twinning modes are likely to be controlled by the structure of the unit cells rather than by lattice geometry, which is the basis of the present analysis. Detailed consideration of these non-metallic crystals is therefore unlikely to be worthwhile at this stage.

The observed deformation twinning modes discussed above have all been conventional in character. However, our main purpose in developing a generalized theory of twinning shears in lattices was to consider non-conventional modes in which all four twinning elements may be irrational. Particular examples of modes of this kind were first discussed by Crocker (1962) as a possible explanation of the habits of doubly twinned bands in the hexagonal close-packed metal magnesium and its alloys. Other specific examples for cubic, rhombohedral and orthorhombic lattices have also been reported and compared with observed twinning modes in steels, crystalline mercury and α-uranium (Crocker & Bevis 1963; Bevis, Rowlands & Acton 1968; Crocker, Heckscher, Bevis & Guyoncourt 1966; Bevis 1968). However, there is as yet no conclusive evidence that any of these non-conventional modes describe the crystallographic features of operative deformation twinning mechanisms; this is also true of modes (1 to 8), and the non-conventional modes of §4. Nevertheless many deformation twins with crystallographic features which cannot be adequately described using classical twinning modes have been reported and it is probable that at least some of these have the unusual characteristics of the non-conventional modes discussed in the present paper.

An important aspect of the generalized theory of twinning shears is that it lays emphasis on the correspondences relating unit cells in parent and twin lattices. These correspondences have recently proved very valuable in analyses of interactions between slip dislocations and twin boundaries in various metals (Sleeswyk & Verbraak 1961; Ishii & Kiho 1963; Yoo & Wei 1966; Tomsett & Bevis 1969*a*, *b*) and it thus seems particularly appropriate that they should form the basis of the new theory. A general analysis of these interactions has also been developed (Saxl 1968) and makes extensive use of the notation introduced by Bilby & Crocker (1965). In addition to the correspondence, the twinning shear of the theory involves a rotation and this also has an immediate physical significance in, for example, the interpretation of diffraction patterns taken from twinned crystals. The detailed relations between the superimposed parent and twin patterns have been the subject of several recent studies (Meieran & Richman 1963; Johari & Thomas 1964; Crocker 1965*b*; Bullough & Wayman 1966; Calbick & Marcus 1967) and are directly related to this rotation.

Finally possible extensions of the present analysis to more involved situations may be considered. For example, the phenomenon of double twinning (Crocker

1962) may be treated very simply by considering the combined effect of two correspondences together with a rotation. Again either single or multiple transformation shears involving parent and product lattices of different symmetry can be examined by introducing the metric tensors of both lattice bases. Such an analysis could be developed into a new theory of martensite crystallography and indeed it is interesting that the well-established crystallographic theories of this phenomenon (Christian 1965) can be formulated more simply using the present notation. In order that the interface between parent and product lattices may be invariant these theories involve a single lattice invariant shear but in practice (Oka & Wayman 1968; Rowlands, Fearon & Bevis 1969) two or more shears of this kind are often observed in individual martensite plates. The generalized theory necessary to analyse these results can again be obtained in the most elegant manner by extending the basic analysis of twinning shears in lattices developed earlier and applied in the present paper to study the different classes of twinning modes in the different crystal classes. These extensions of the theory to the case of transformation shears in lattices will be described in a subsequent paper.

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