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Application of the Twinning Transformation Matrix to Derivation of the Generalized Reciprocal Lattice with Multiple Diffraction

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A general twinning matrix applicable to any crystal system is developed in tensor notation. The symmetry of the cubic system results (1) in the equivalence for twinning of orthogonal planar groups, (2) in successive twinning yielding the same lattice as twinning on certain higher order planes. Selection rules for the calculation of interstitial points in cubic systems show that the generalized reciprocal lattice has a periodicity which is the product of $(h)^2=(h_1)^2+(h_2)^2+(h_3)^2$ and of the periodicity of the host lattice. Double diffraction produces, in the generalized lattice of all possible relpoints, a large number of points additional to the twin points. In general, the periodicity of noncubic systems is infinite. The hexagonal system, both close-packed and rhombohedral, is treated. Lattice transformations may permit a pseudo-cubic approximation to the generalized lattice.

Introduction

When a crystal is twinned, it is well known that additional spots due to the twin structure may appear in the diffraction pattern. If a twin spot is sufficiently intense, the beam producing it acts as an additional primary beam and may produce a complete additional pattern, a process called double diffraction (Burbank & Heidenreich, 1960; Pashley & Stowell, 1963). The generalized reciprocal lattice with twinning and double diffraction is the array of all possible reciprocal lattice points so occurring for twinning on all planes of a particular form. Still more points must be added if possible multiple diffraction is considered.

Formulae for twinning in any of the seven crystal systems have been given by Andrews & Johnson (1955) using conventional crystallographic notation. Crocker (1965) has developed formulae using tensor notation and applied them to the rhombohedral system. Kelly (1965) has presented an extension of the calculations of Meireran & Richman (1963) for the cubic system, exhibiting the twin points in stereographic projection. This projection becomes quite complicated for the generalized lattice with double or multiple diffraction. Johari & Thomas (1964) used Buerger's method to obtain the matrix for twinning on the cubic system.

In the present paper, the twinning matrix in tensor notation is simply derived. Orthogonal planar groups in the cubic system are shown to be equivalent for twinning and general selection rules for the twin reciprocal lattice points are developed. The size of the repeating unit is $(h)^2$ times that of the basic reciprocal lattice; in noncubic systems $(h)^2$ is commonly not an integer, and the size is an integral multiple of $(h)^2$ which may be very large or infinite. Successive twinning on {111} or the equivalent {211} planes is shown to be equivalent to single twinning on the orthogonal pair {221}, {411} in second generation twinning, and may or may not be equivalent in third and fourth generation twinning to {511}, {552} and {744}, {877} twinning.

Tensor notation

For use of this notation in crystallography, the covariant system of unitary vectors $(\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3)$ is taken as the sides of the unit cell. The contravariant or reciprocal unitary system $[\mathbf{a}^1\mathbf{a}^2\mathbf{a}^3]$ is defined by $\mathbf{a}_i \cdot \mathbf{a}^j=\delta_i^j=\begin{cases}1, & i=j\\0, & i\neq j\end{cases}$. Subscripts and superscripts denote co- and contravariancy. A vector, or in fact any physical quantity, is invariant to changes in the frame of reference (unless, as in relativity theory, one is moving with respect to the other) and is denoted by the product of co- and contravariant quantities, such that the number of subscripts equals the number of superscripts. The metrical and reciprocal metrical tensors and matrices denoted by

$$\|m_{ij}\|=\|\mathbf{a}_i \cdot \mathbf{a}_j\| \text{ and } \|m^{ij}\|=\|\mathbf{a}^i \cdot \mathbf{a}^j\|,\ i,j=1,2,3 \quad (1)$$

are respectively doubly co- and doubly contravariant. The summation convention due to Einstein is that whenever a letter symbol appears twice in a product, summation from 1 to 3 is directed. Thus an atomic lattice vector $\mathbf{r}=r^1\mathbf{a}_1+r^2\mathbf{a}_2+r^3\mathbf{a}_3=r^i\mathbf{a}_i$ is the sum of the products of contravariant coefficients r^i and the covariant unitary vectors $\mathbf{a}_i$. Similarly a reciprocal lattice vector $\mathbf{h}=h_i\mathbf{a}^i$; the covariant coefficients h_i are the Miller indices. Either vector could be expressed on the other system, but the coefficients would not in general be integers. Parentheses around a letter indicate that the following superscript denotes a power. Thus $\mathbf{r} \cdot \mathbf{r}=(r)^2=m_{ij}r^ir^j$ and $\mathbf{h} \cdot \mathbf{h}=(h)^2=m^{ij}h_ih_j$.

1. The twinning transformation

Reflection in a plane whose normal is the relvector $\mathbf{h}=h_1\mathbf{a}^1+h_2\mathbf{a}^2+h_3\mathbf{a}^3$ changes the vector $\mathbf{r}$ to the twin vector

$$\tilde{\mathbf{r}}=\mathbf{r}-2(\mathbf{r} \cdot \mathbf{h})\mathbf{h}/(h)^2 \quad (2)$$

which can be represented by the matrix T operating on the coefficients $[r^1r^2r^3]$ of $\mathbf{r}$, with

$$T = I - \frac{2}{(h)^2} \|m^{ij}\| \times \|h_i h_j\| \, . \qquad (3)$$

I is the idemfactor. Rotation, equivalent to reflection in all systems with a center of symmetry, is given by the negative of T. T is invariant, and $|T| = -1$. By writing the invariant vector $\mathbf{r}$

$$\mathbf{r} = r^i \mathbf{a}_i = \mathbf{a}_i r^i = (\mathbf{a}_i T^{-1})(T r^i) \qquad (4a)$$

it is evident that the unitary vectors $(\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3)$ transform by T^{-1} operating in reverse order; *i.e.*, by the transpose of T^{-1} operating on $(\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3)$ in the normal order. Similarly

$$\mathbf{h} = h_i \mathbf{a}^i = (h_i T^{-1})(T\mathbf{a}^i) = (T_{\mathrm{tr}}^{-1} h_i)(T\mathbf{a}^i) \qquad (4b)$$

No restriction has been imposed on the unitary system.

2. The cubic system

The T-matrix simplifies to

$$T = \frac{1}{(h)^2} \left\| \begin{matrix} (h_2)^2+(h_3)^2-(h_1)^2 & -2h_1h_2 & -2h_1h_3 \\ -2h_2h_1 & (h_3)^2+(h_1)^2-(h_2)^2 & -2h_2h_3 \\ -2h_3h_1 & -2h_3h_2 & (h_1)^2+(h_2)^2-(h_3)^2 \end{matrix} \right\| \qquad (5)$$

The high symmetry of the cubic system is reflected in the fact that $T = T_{\mathrm{tr}} = T^{-1} = T_{\mathrm{tr}}^{-1}$.*

2.1 *Equivalence of planar groups*

Because the cubic system is isometric and orthogonal with a center of symmetry, axes can be interchanged or reversed. Matrices belonging to two orthogonal planes such as (111), $(\bar{2}11)$ can be made identical by interchange and change of sign of columns. Thus

$$T_{(111)} = \tfrac{1}{3} \left\| \begin{matrix} 1 & \bar{2} & \bar{2} \\ \bar{2} & 1 & \bar{2} \\ \bar{2} & \bar{2} & 1 \end{matrix} \right\| \quad T_{(\bar{2}11)} = \tfrac{1}{3} \left\| \begin{matrix} \bar{1} & 2 & 2 \\ 2 & 2 & \bar{1} \\ 2 & \bar{1} & 2 \end{matrix} \right\| \, .$$

The matrix $T_{(111)}$ operating on $(g_1g_2g_3)$ yields the same vector as $T_{(\bar{2}11)}$ operating on $-(g_1g_3g_2)$. Since both vectors $\mathbf{g}$ are in the group $\{g_1g_2g_3\}$, the matrices are equivalent. The three $\{211\}$ planes normal to (111) all yield such equivalent matrices. Reflection in planes $(\bar{2}11)$, $(1\bar{2}1)$, $(11\bar{2})$ thus yields a twin reciprocal lattice *identical* with that produced by reflection in the (111) plane. The *composition* planes, on which the reflections actually occur, are of course different and yield different traces in micrography of the crystal. But no such distinction occurs in the reciprocal lattice, which occupies all space. It follows that the generalized reciprocal lattices produced by $\{111\}$ and $\{211\}$ twinning are identical. Other pairs of groups have the same property: if $\mathbf{h}_{(1)}$, $\mathbf{h}_{(2)}$ represent vectors respectively in the lower and higher index group, orthogonality between individual planes, one in each group, may be designated by the form $\{\mathbf{h}_{(1)} \cdot \mathbf{h}_{(2)}\} = 0$. Except for the $\{111\}$, $\{211\}$ pair, a one-to-one correspondence exists. A second property is that the square of the magnitude of $\mathbf{h}_{(2)}$ is double that of $\mathbf{h}_{(1)}$, *i.e.*, $(h_{(2)})^2 = 2(h_{(1)})^2$. In certain cases, one or both of these properties may be shared by another $\mathbf{h}_{(2)}$ group, *e.g.*, $\mathbf{h}_{(1)} = \{511\}$, $\mathbf{h}_{(2)} = \{552\}$, $\{721\}$. Calculation of the matrices shows that only one, $\{552\}$, is equivalent to $\{511\}$. It is characteristic of orthogonal pairs of groups that the vectors in each group are not orthogonal among themselves. Pairs of groups such as $\{210\}$, $\{310\}$, each of which has orthogonal vector pairs, do not have the property $\{\mathbf{h}_{(1)} \cdot \mathbf{h}_{(2)}\} = 0$, although the condition $(h_{(2)})^2 = 2(h_{(1)})^2$ is satisfied.

2.2 *Selection rules for twin relpoints interstitial in the host lattice*

The vector $\mathbf{p} = T\mathbf{g}$ is

$$\mathbf{p} = (g_1g_2g_3) - \frac{2}{h^2}(h_1g_1 + h_2g_2 + h_3g_3)(h_1h_2h_3) \, . \quad (6)$$

$(h_1h_2h_3)$ are mutually prime, but $(h)^2$ may be odd or even. When it is odd, let $2(h_1g_1 + h_2g_2 + h_3g_3) = l(h)^2 - n$. Then

$$\mathbf{p} = [(g_1 - lh_1)(g_2 - lh_2)(g_3 - lh_3)] + \frac{n}{(h)^2}(h_1h_2h_3) \, .$$

Or in group form

$$\{p_1p_2p_3\} = \{q_1q_2q_3\} + \frac{n}{(h)^2}\{h_1h_2h_3\} \, . \qquad (7)$$

$\{q_1q_2q_3\}$ is a group of host lattice points from which fractional vectors $\frac{n}{(h)^2}\{h_1h_2h_3\}$ proceed to twin points interstitial in the host lattice. The integer l can be chosen so that n takes on only the values $0, \pm 1, \pm 2, \ldots \pm \frac{(h)^2 - 1}{2}$. When $(h)^2$ is even, it is replaced by the odd quantity $(h)^2/2$, but $\{h_1h_2h_3\}$ are left unchanged. The value $n = 0$ is eliminated because it corresponds to a twin point coinciding with a host relpoint.

The general selection equation is obtained by squaring equation (7).

$$2\Sigma\, h_i q_i = \frac{(h)^2}{n}[(p)^2 - (q)^2] - n \, . \qquad (8)$$

This is a generalization of the Pashley & Stowell (1963) calculation for (111) twinning. In the important case of $\{111\}$ twinning n has only the value ± 1 and hence $(p)^2 - (q)^2$ must be odd. Hence, if N is any integer,

$$\pm q_1 \pm q_2 \pm q_3 = 3N + 1 \qquad (8.1)$$

for a simple cubic lattice where $(g_1g_2g_3)$ are unrestricted.

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* The matrix terms appear to be doubly covariant only because $\|m^{ij}\| = I$ in the cubic system.

When $(g_1g_2g_3)$ are restricted, as for centered and diamond lattices, it may be noted that the matrices $T_{(111)}$ have rows composed of one odd and two even integers and hence that $(h)^2\{p_1p_2p_3\}$ has the same restriction as $(g_1g_2g_3)$. Since $\{h_1h_2h_3\}=\{111\}$ are all odd, $(q_1q_2q_3)$ are all odd when $(g_1g_2g_3)$ are all even and *vice versa*, and one odd when $(g_1g_2g_3)$ is one even. The selection equations become:

$$\Sigma\, h_iq_i = 2(h)^2N + \frac{(h)^2-1}{2} \quad [(g)^2 \text{ even}] \qquad (8.2)$$

$$\Sigma\, h_iq_i = 2(h)^2N + \frac{3(h)^2-1}{2} \quad [(g)^2 \text{ odd}] \qquad (8.3)$$

in which $(h)^2$ is replaced by $(h)^2/2$ if $(h)^2$ is even. For $\{111\}$ twinning

$$\pm q_1 \pm q_2 \pm q_3 = 6N+1 \quad [(g)^2 \text{ even}]$$
$$6N+4 \quad [(g)^2 \text{ odd}]\,. \qquad (8.4)$$

The factor multiplying N may be called the periodicity of the generalized lattice. It is the product of the periodicity $(h)^2$ of the twinning lattice and that of the host lattice. The latter is 2 for centered lattices, and 4 for the diamond lattice, for which $\pm q_1 \pm q_2 \pm q_3 = 12N+1$ when $g_1g_2g_3$ are all even. Table 1 lists $(q_1q_2q_3)$ and the specific directions of type $\{111\}$ along which interstitial twinning points occur at displacements $\frac{1}{3}\{111\}$, for the generalized reciprocal lattice cell given by allowing q_1, q_2, q_3 to assume positive values less than 6. The combinations $(q_1q_2q_3)$ should be permuted, with corresponding permutations of $\{111\}$ to obtain all the points within the repeating unit.* The first and second sections of the table give the b.c.c. twinning lattice, the first and third the f.c.c.

When $(h)^2 > 3$, n also assumes values greater than 1; $(h)^2$ may be taken as odd (if it is even, it is divided by two to give an odd integer) in equation (8); it is either a prime number or a product of prime numbers. Selection equations similar to (8.1) must be derived

* The essential information is actually comprised within a portion of the table, $q_1, q_2, q_3 \leq 3$, which can be reflected successively in the three coordinate planes to give the complete twinning lattice.

Table 1. *Displacement vectors in* $\{111\}$ $\{211\}$ *twinning*

	Host lattice point $(q_1q_2q_3)$	Selection rule $\pm q_1 \pm q_2 \pm q_3 = 6N+1$				$\frac{1}{3}\{111\}$ Displacement vectors $\{111\}$			
$(g_1g_2g_3)$ all even	(111)	+1	+1	+1		$(11\bar{1})$	$(1\bar{1}1)$	$(\bar{1}11)$	
	(311)	1	−5			$(1\bar{1}\bar{1})$	$(\bar{1}\bar{1}\bar{1})$		
	(511)	7	−5	−5		(111)	$(\bar{1}1\bar{1})$	$(\bar{1}\bar{1}1)$	
	(331)	7	1	1		(111)	$(1\bar{1}1)$	$(\bar{1}11)$	
	(531)	7	1			$(11\bar{1})$	$(1\bar{1}\bar{1})$		
	(333)								
	(533)	11	1	−5	−5	(111)	$(\bar{1}11)$	$(\bar{1}1\bar{1})$	$(\bar{1}\bar{1}1)$
	(551)	1	1	−11		$(1\bar{1}1)$	$(\bar{1}11)$	$(\bar{1}\bar{1}\bar{1})$	
	(553)	13	7			(111)	$(11\bar{1})$		
	(555)	−5	−5	−5		$(1\bar{1}\bar{1})$	$(\bar{1}1\bar{1})$	$(\bar{1}\bar{1}1)$	
$(g_1g_2g_3)$ one even	(100)	1	1	1	1	(111)	$(11\bar{1})$	$(1\bar{1}1)$	$(1\bar{1}\bar{1})$
	(300)								
	(500)	−5	−5	−5	−5	$(\bar{1}11)$	$(\bar{1}\bar{1}1)$	$(\bar{1}1\bar{1})$	$(\bar{1}\bar{1}\bar{1})$
	(120)	1	1			$(\bar{1}11)$	$(\bar{1}1\bar{1})$		
	(320)	1	1	−5	−5	$(1\bar{1}1)$	$(1\bar{1}\bar{1})$	$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}\bar{1})$
	(520)	7	7			(111)	$(11\bar{1})$		
	(122)	1	1	−5		$(11\bar{1})$	$(1\bar{1}1)$	$(\bar{1}\bar{1}\bar{1})$	
	(322)	7	1			(111)	$(\bar{1}11)$		
	(522)	1	−5	−5		$(1\bar{1}\bar{1})$	$(\bar{1}1\bar{1})$	$(\bar{1}\bar{1}1)$	
	(140)	−5	−5			$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}\bar{1})$		
	(340)	7	7	1	1	(111)	$(11\bar{1})$	$(\bar{1}11)$	$(\bar{1}1\bar{1})$
	(540)	1	1			$(1\bar{1}1)$	$(1\bar{1}\bar{1})$		
	(142)	7	1	−5		(111)	$(\bar{1}1\bar{1})$		
	(342)	1	−5			$(1\bar{1}1)$	$(\bar{1}\bar{1}1)$		
	(542)	7	1	−11		$(11\bar{1})$	$(\bar{1}11)$	$(\bar{1}\bar{1}\bar{1})$	
	(144)	7	1	1		$(\bar{1}11)$	$(11\bar{1})$	$(1\bar{1}1)$	
	(344)	−5	−11			$(1\bar{1}\bar{1})$	$(\bar{1}\bar{1}1)$		
	(544)	13	−5	−5		$(\bar{1}\bar{1}\bar{1})$	$(\bar{1}1\bar{1})$	$(\bar{1}\bar{1}1)$	
		$\pm q_1 \pm q_2 \pm q_3 = 6N+4$							
$(g_1g_2g_3)$ all odd	(200)	−2	−2	−2	−2	$(\bar{1}\bar{1}\bar{1})$	$(\bar{1}1\bar{1})$	$(\bar{1}\bar{1}1)$	$(\bar{1}11)$
	(220)	4	4			(111)	$(11\bar{1})$		
	(222)	−2	−2	−2		$(\bar{1}1\bar{1})$	$(1\bar{1}\bar{1})$	$(\bar{1}\bar{1}1)$	
	(400)	−2	−2	−2	−2	(111)	$(11\bar{1})$	$(1\bar{1}1)$	$(1\bar{1}\bar{1})$
	(420)	−2	−2			$(\bar{1}11)$	$(\bar{1}1\bar{1})$		
	(422)	4	4	−8		$(11\bar{1})$	$(1\bar{1}1)$	$(\bar{1}\bar{1}\bar{1})$	
	(440)	−8	−8			$(\bar{1}\bar{1}1)$	$(\bar{1}\bar{1}\bar{1})$		
	(442)	−2	−2			$(1\bar{1}\bar{1})$	$(\bar{1}1\bar{1})$		
	(444)	4	4	4		$(11\bar{1})$	$(1\bar{1}1)$	$(\bar{1}11)$	

specifically for each value of $(h)^2$ [or $(h)^2/2$]. As examples, let $\{h_1h_2h_3\}=\{221\}$ and $\{123\}$ for which $(h)^2=9$ and $(h)^2/2=7$; n assumes values 1,2,3,4, and 1,2,3, respectively. Since all terms in equation (8) are integers and $(h)^2$ is odd, for $n=2$ $[(p)^2-(q)^2]$ must be a multiple of 4. When $n=3$, the two examples diverge, because $(h)^2/3=3$ for $\{221\}$, and 7/3 for $\{123\}$. In the latter case, $[(p)^2-(q)^2]$ must be a multiple of 3; for [221] it must simply be odd as for $n=1$. The value $n=4$ does not occur for [123] for $\{221\}$, $[(p)^2-(q)^2]$ must be a multiple of 8. Such rules can easily be formulated in equations similar to equation (8.1). If $(g_1g_2g_3)$ are subject to restrictions as in centered lattices, these equations may be modified to other equations similar to equations (8.2) and (8.3) for $n=1$.

2.3 *Twinning with double diffraction*

It has been pointed out (Burbank & Heidenreich, 1960; Pashley & Stowell, 1963) that each interstitial point, if it is sufficiently close to the surface of the Ewald sphere, yields a new source beam and may be diffracted to produce a complete lattice. Since all values $\{h_1h_2h_3\}=(\pm1,\pm1,\pm1)$ occur for either f.c.c. or b.c.c., the generalized twinning plus double diffraction reciprocal lattice is composed of a total of 9 lattices similar to the host lattice, including the latter. This lattice includes all possible first generation twins. A portion $1/a_0(2\times6\times6)$ is shown in Fig. 1.

2.4 *Successive or multiple* {111} *twinning*

W. L. Bond (private communication) pointed out some years ago that successive twinning on two different {111} planes is equivalent to single {221} (or {411}) twinning. Thus, twinning on (111) followed by twinning on $(\bar111)$ gives

$$T=T_{(111)}T_{(\bar111)}=\tfrac{1}{3}\begin{Vmatrix}1&\bar2&\bar2\\ \bar2&1&\bar2\\ \bar2&\bar2&1\end{Vmatrix}\times\tfrac{1}{3}\begin{Vmatrix}1&2&2\\ 2&1&\bar2\\ 2&\bar2&1\end{Vmatrix}=\tfrac{1}{9}\begin{Vmatrix}\bar7&4&4\\ \bar4&1&\bar8\\ \bar4&\bar8&1\end{Vmatrix}.$$

Changing the signs in the first column, this becomes

$$\tfrac{1}{9}\begin{Vmatrix}7&4&4\\ 4&1&\bar8\\ 4&\bar8&1\end{Vmatrix}\ \text{which is } T_{(\bar122)}.$$

Bond expanded this concept to third and fourth generation twinning. If all three planes in third generation twinning are different, the product matrix is that of a {721} plane. If the third twinning vector is the same as the first, the product matrix is equivalent to that of a {511} (or {552}) plane. $T_{\{721\}}$ is not equivalent to $T_{\{511\}}$ even though the groups are orthogonal. Bond showed that the {721} planes produced by such triple twinning are not composition planes. Fourth generation twinning can yield matrices equivalent to {744}, {877}, and {1154}. The last of these is a group not orthogonal with {744}.

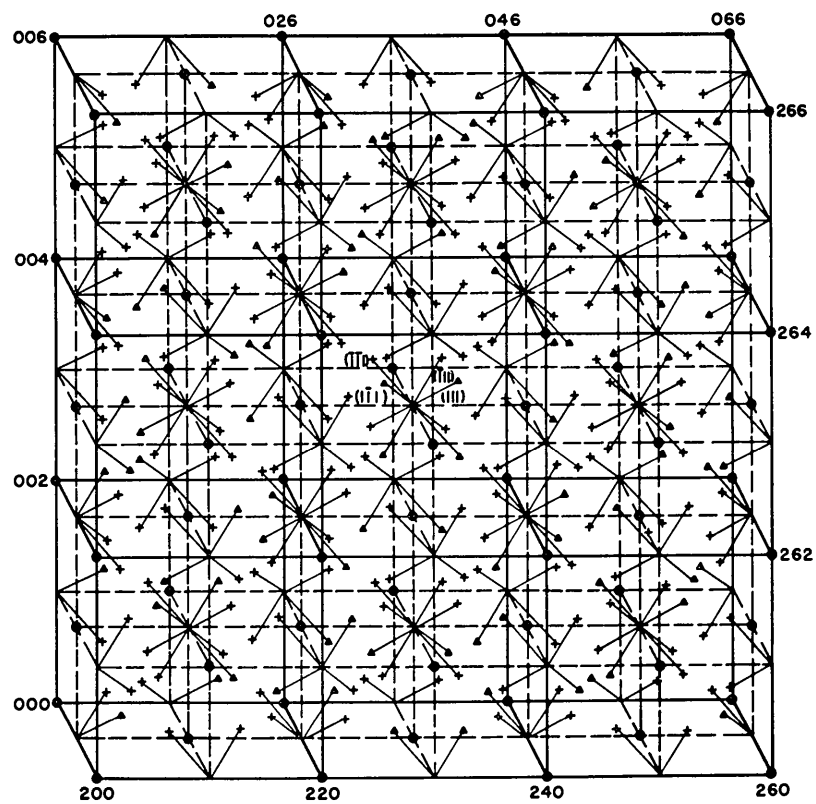

Fig. 1. Portion $(2\times6\times6)$ of generalized lattice; complete unit is $(6\times6\times6)$ for centered lattices. Solid circles: f.c. host lattice points; solid triangles: {111}{211} twin points; +: double diffraction points.

Cubic symmetry requires that the matrices for {100} and {110} twinning be equivalent to 1. Any number of successive twinnings yields simply the host lattice. Successive {111} twinning results in additional relpoints in the lattice. Considered as single {221} twinning, it permits values of $n = \pm 1, \pm 2, \pm 3, \pm 4$. The second generation lattice with double diffraction includes the first, which corresponds to $n = 3$. This process is iterative for each generation. The final resulting reciprocal lattice is large and complex even when only second generation twins are admitted. Since there are 24 [221] directions if both positive and negative are counted separately, each q-vector terminus is surrounded by 24 twinning or multiple diffraction points at fractional distances $1/3a_0$ plus others at greater distances. For centered lattices, the periodicity is 18; *i.e.*, the size of the repeating unit is $18/a_0$.

Twinning on more complex planes such as {123}, with double diffraction, also results in a very complex lattice. Each host-lattice point is surrounded by 48 points at distances $1/\sqrt{3 \cdot 5}\, a_0$ along {123} directions plus others at greater distances. The complexity is comparable with that of first and second generation {111} twinning. The repeating unit has size $14/a_0$.

2.5 *Diffraction patterns for twinned crystals*

A section through the generalized reciprocal lattice gives the planar array of spots which may be found in an electron diffraction pattern formed by transmission through a thin crystal. Unless the crystal is *very* thin the heights of the diffraction spikes are inadequate to reach the surface of the Ewald sphere and 'film buckling' is postulated to account for the host lattice spikes observed. This amounts to permitting replacement of the planar section by a slice of finite thickness. Figs. 2 and 3, for [110] and [111] directions of incidence, show the relpoints within slices of thickness $\pm 1/3a_0$ and $\pm 2/3\sqrt{3}a_0$, respectively. In the {111} case, still more points would occur if the slice were thicker. (Parenthetically, it should be noted that double diffraction spots *within* the slice may be associated with twin spots *outside* it; since the latter do not yield spots (*i.e.*, additional 'primary' beams), such double diffraction spots have been eliminated.)

3. Noncubic systems

The matrix (3) is general, and can be used for twinning calculations in any crystal system. The resultant generalized reciprocal lattice is nonperiodic and of infinite

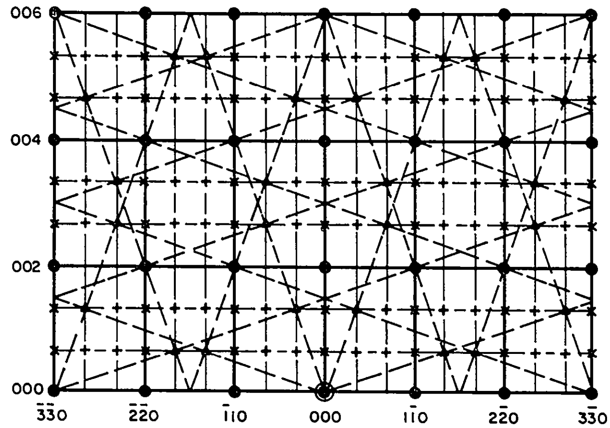

Fig. 2. Array of generalized reciprocal lattice points in (110) plane; solid circles: f.c. host lattice points; solid triangles: {111} or {211} twin points; +: double diffraction points. Short lines through $(3\bar{3}1)$ are lattice vectors $\pm\frac{1}{3}(\bar{1}11)$, $\pm\frac{1}{3}(1\bar{1}1)$. Vectors $\pm\frac{1}{3}(111)$, $\pm\frac{1}{3}(11\bar{1})$ terminate at projected positions $(g_1g_2[g_3\pm\frac{1}{3}])$, $g_1g_2g_3$ all odd (×). Vertical components of these vectors are $\pm\frac{1}{3}$, compared with interplanar spacing $\sqrt{2}$. Dashed lines show the rotated lattices on which twin points appear. Thin lines show 4 host lattices on which twin and double diffraction points are located.

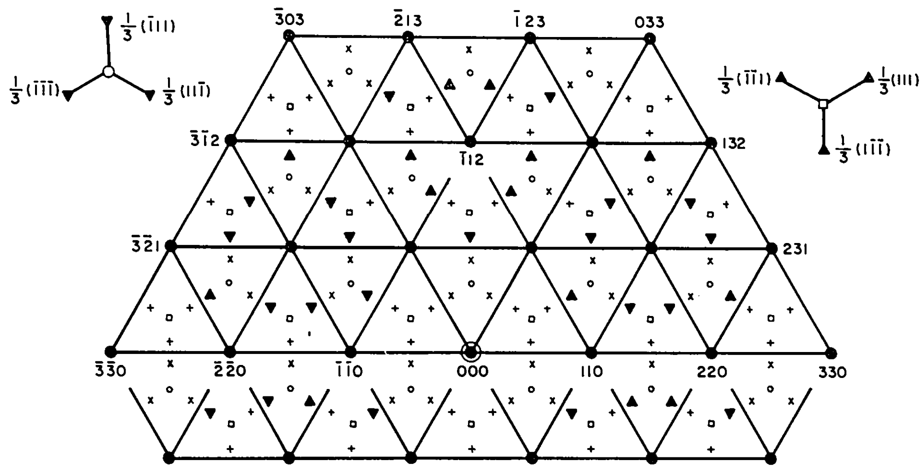

Fig. 3. Generalized reciprocal lattice points in and near a $(1\bar{1}1)$ plane. Host lattice points (solid circles) define reference plane; interplanar spacing is $2/\sqrt{3}$. Unoccupied sites (open circles and squares) are in planes displaced vertically $\pm 1/\sqrt{3}$. Twin points (solid triangles) are in planes at $\pm 2/3\sqrt{3}$. Associated displacement vectors $\frac{1}{3}\{111\}$ are shown in projection in small diagrams. Double diffraction points (+, ×) are also in these planes. Pattern has threefold symmetry around the (vertical) direction $(1\bar{1}1)$ and also centrosymmetry, so it is symmetrical across the $(\bar{1}12)$ line, and across a {110} line with interchange of above and below positions.

size unless special relations exist between the metrical coefficients m^{ij} and the twinning planes $\{h_1h_2h_3\}$ so that the T-matrix components are ratios of integers. The symmetry of the crystal may lead to certain equivalences, as in the cubic system. In general, each crystal must be considered separately but some crystals in the hexagonal system have axial ratios close enough to the theoretical close-packed value $\sqrt{8/3}$ so they can be treated as a group.

3.1 *The hexagonal matrix*

The direct and reciprocal metrical matrices for the hexagonal system are:

$$m_{ij}=\left\|\begin{matrix} 1 & \frac{\bar{1}}{2} & 0 \\ \frac{\bar{1}}{2} & 1 & 0 \\ 0 & 0 & \left(\frac{a_3}{a_1}\right)^2 \end{matrix}\right\| \quad m^{ij}=\left\|\begin{matrix} \frac{4}{3} & \frac{2}{3} & 0 \\ \frac{2}{3} & \frac{4}{3} & 0 \\ 0 & 0 & \left(\frac{a_1}{a_3}\right)^2 \end{matrix}\right\|. \tag{9}$$

The twinning matrix is

$$T=-\frac{4}{3(h)^2}\left\|\begin{matrix} h_1^2-h_2^2-\frac{3}{4}\left(\frac{a_1}{a_3}\right)^2 h_3^2 & (2h_1+h_2)h_2 & (2h_1+h_2)h_3 \\ (h_1+2h_2)h_1 & h_2^2-h_1^2-\frac{3}{4}\left(\frac{a_1}{a_3}\right)^2 h_3^2 & (h_1+2h_2)h_3 \\ \frac{3}{2}\left(\frac{a_1}{a_3}\right)^2 h_3h_1 & \frac{3}{2}\left(\frac{a_1}{a_3}\right)^2 h_3h_2 & -\frac{3(h)^2}{4}+\frac{3}{2}\left(\frac{a_1}{a_3}\right)^2 h_3^2 \end{matrix}\right\| \tag{10}$$

with

$$\frac{3(h)^2}{4}=(h_1)^2+(h_2)^2+h_1h_2+\frac{3}{4}\left(\frac{a_1}{a_3}\right)^2(h_3)^2. \tag{11}$$

T is not symmetrical as in the cubic case, but $T^{-1}=T$ so T_{tr} *operates on the coefficients of relvectors.*

3.11 *The close-packed hexagonal system* ($a_3/a_1=\sqrt{8/3}$)

In general, the terms inside the matrix signs must be multiplied by 32 to become integral. The scalar multiplier becomes $1/24(h)^2$; the periodicity (and size of repeating unit) is $24(h)^2$.

The h.c.p. system is composed of two simple hexagonal structures with one fiducial atom at [000], and the other at either $[\frac{1}{3}\frac{2}{3}\frac{1}{2}]$ or $[\frac{2}{3}\frac{1}{3}\frac{1}{2}]$. Neither can be transformed to a simple primitive lattice; but one is the mirror image of the other in the basal plane. The host reciprocal lattice has unoccupied sites when g_3 is odd and (g_1+2g_2), and hence also $(2g_1+g_2)$, is a multiple of three. Either lattice has periodicity 3 in the basal plane and 2 along the hexagonal axis. With (001) twinning, both lattices are present and the only unoccupied sites are those for which both g_1+2g_2 and $2g_1+g_2$ are multiples of 3, and g_3 is odd. For (h_1h_20) twinning, no fractional relvectors occur when $(h_1)^2+h_1h_2+(h_2)^2=1$, *i.e.*, for (100), (010), $(\bar{1}\bar{1}0)$; if $(2h_1+h_2)$ and (h_1+2h_2) are both multiples of 3, each term in the matrix has a factor 3, and no fractional relvectors occur for (110), $(\bar{1}20)$. The planes discussed are the most probable twinning planes, but twinning on many other planes does yield fractional relpoints.

3.2 *Rhombohedral crystals*

Rhombohedral axes, here designated $(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3)$, are isometric. The matrix A and its inverse A^{-1}

$$A=\left\|\begin{matrix} 1 & \bar{1} & 1 \\ 1 & 1 & 1 \\ \bar{1} & 1 & 1 \end{matrix}\right\| \quad A^{-1}=\tfrac{1}{2}\left\|\begin{matrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{matrix}\right\|$$

transform $(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3)$ to face-centered axes $(\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3)$ and *vice versa*. The axes $(\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3)$ are isometric; they are orthogonal and hence cubic if the rhombohedral angle $\alpha=60°$. The transformation $2A^{-1}$ applied to $(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3)$ yields body-centered axes, cubic if $\alpha=109{\cdot}5°$. If A is applied to a crystal with α near 60°, the result is a pseudo-cubic face-centered structure, for which twinning on cubic planes can be assumed as a first approximation. The displacements of the interstitial twinning points from their cubic positions can then be calculated. A similar procedure using $2A^{-1}$ would apply if α were near 109·5°.

The periodicity of the generalized lattice is not 6, as in the cubic case, but is large and probably infinite. This means that the displacement from the cubic position increases as the point under consideration goes farther from the origin. Double diffraction then results in groups of points close together, near each cubic interstitial relpoint in the generalized lattice.

The lattice $(\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3)$ is also rhombohedral, though face-centered. The transformation A could be applied to it, which is the same as applying the transformation

$$A^2=\left\|\begin{matrix} \bar{1} & 1 & 3 \\ 3 & \bar{1} & \bar{1} \\ \bar{1} & 3 & \bar{1} \end{matrix}\right\|$$

to $(\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3)$. If $\alpha=\cos^{-1}\frac{5}{6}=33°35'$, the transformed lattice is cubic. Similarly, if A^3 is applied, the transformed lattice is cubic if $\alpha=\cos^{-1}\frac{21}{22}=17°21'$. Rhombohedral crystals with such a small angle are very rare; however the transformation A^2 may in some cases be useful in producing a pseudo-cubic structure.

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