Acta Cryst. (1971). A27, 175

The Geometry of Coincidence-Site Lattices

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(*Received* 19 *February* 1970 *and in revised form* 29 *June* 1970)

The density of coincidence sites in cubic crystal lattice planes in coincidence-site-related crystals with a multiplicity less than or equal to 31 has been investigated. A comprehensive table of lattice planes with a high density of coincidence sites for each of the twenty-two coincidence-site relationships is presented. In addition a complete list of the alternative ways of describing the twenty-two coincidence-site relationships as defined by Friedel in 1926 is presented.

1. Introduction

There is now considerable evidence that the coincidence-site lattice defined by the common sites of two interpenetrating lattices is important in relation to the structure of grain boundaries in cubic crystals (Brandon, 1966). In particular, field-ion microscopy studies of the refractory metals (Brandon, Ralph, Ranganathan & Wald, 1964; Morgan & Ralph, 1967) have shown that the two crystals adjacent to a grain boundary often possess lattice sites defining a superlattice (the coincidence-site lattice) common to both crystal lattices. These experiments also indicate that such grain boundaries consist of a series of steps, and that the steps are planes that contain a high density of coincidence sites. The importance of the coincidence-site lattice concept is also evident from the results of recent electron-microscopy studies. Sargent (1968) has shown that steps in annealing twin boundaries in aluminum crystals define planes of the matrix and twin crystals for which all lattice sites are sites of the coincidence site lattice defined by the matrix twin crystal orientation relationship. Similar observations in austenitic stainless steel have been reported more recently by Vaughan (1969). Schober & Balluffi (1970) have made quantitative observations of orthogonal grids of grain boundary misfit screw dislocations in (001) twist boundaries in gold. These authors have shown that in the vicinity of coincidence site relationships the geometrical properties of the grids are consistent with those predicted for a boundary structure consisting of a suitable misfit dislocation grid embedded in the appropriate high density coincidence site interface.

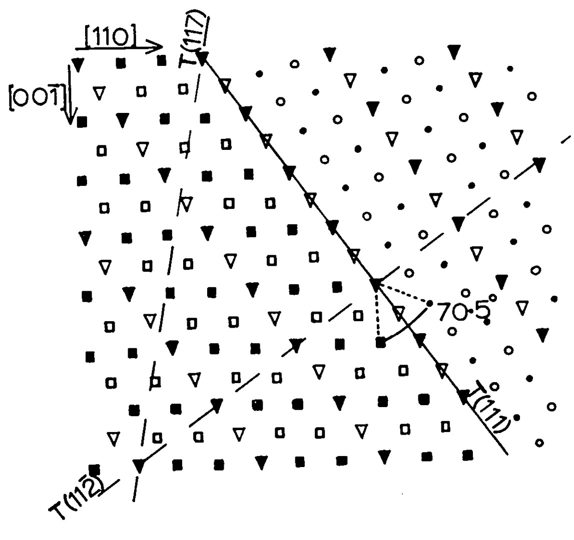

Fig. 1. The (1$\bar{1}$0) plane of projection of the matrix and annealing twin lattices of a face-centred cubic crystal. The matrix, twin and coincidence-site lattice sites in the plane of the paper are represented by closed squares, circles and triangles respectively, and the matrix, twin and coincidence-site lattice sites in the next parallel (1$\bar{1}$0) plane above and below the plane of the diagram are represented by open squares, circles and triangles respectively. The traces of the (111), (11$\bar{2}$) and (117) planes are indicated by $T(111)$, $T(11\bar{2})$ and $T(117)$ respectively. The directions [11$\bar{2}$], [111] and [77$\bar{2}$] are parallel to $T(111)$, $T(11\bar{2})$ and $T(117)$ respectively.

As an aid to the interpretation of experimental results, there is a requirement in the case of cubic crystals for a comprehensive set of tables of coincidence-site relationships and a table of planes possessing a high density of coincidence sites for each of the possible coincidence site relationships. Both of these tables are presented in this paper and apply to primitive, body-centred and face-centred cubic crystals.

When a rotational symmetry operation is applied to a point lattice, a lattice is produced which is completely coincident with the original lattice. However, the application of a rotation other than a rotation associated with a symmetry element of the lattice may result in partial coincidence of the two lattices. The lattices related by such a rotation have certain lattice sites in common, which in themselves define a lattice termed the coincidence-site lattice.

Friedel (1926) has shown that two identical cubic lattices that are related by a coincidence site lattice may be considered to be related by a rotation of 180° about the normal $[h_1h_2h_3]$ to a rational plane. The fraction of sites of each of the two interpenetrating lattices which are coincidence sites – that is sites which are common to both lattices – is equal to Σ^{-1}, where the multiplicity Σ is given by $\Sigma=(h_1^2+h_2^2+h_3^2)$, or

$\Sigma=(h_1^2+h_2^2+h_3^2)/2$ for $(h_1^2+h_2^2+h_3^2)$ odd or even respectively.

Annealing twins in the face-centred cubic metals for example possess a coincidence-site lattice of multiplicity $\Sigma=3$. The parent crystal and annealing twin lattices are related by a rotation of 180° about a $\langle 111\rangle$ direction, and the interface between the two crystals is usually the $\{111\}$ plane normal to the axis of rotation. The coincidence-site lattice associated with the twin related crystals is illustrated in Fig. 1, which shows the $(1\bar{1}0)$ plane of projection plot of both parent and twin lattices. The $(1\bar{1}0)$ face-centred cubic planes have a two-fold stacking sequence, the parent, twin and coincidence site lattice points in the plane of the diagram are represented by closed squares, circles and triangles respectively, whereas the lattice points in the next parallel $(1\bar{1}0)$ plane above and below the plane of the diagram are represented by open squares, circles and triangles respectively. The trace of the interface plane between the twin and parent crystals is represented by a bold continuous line. It is to be noted that the interface plane may be chosen so that all lattice points in this plane are coincidence sites. Planes which consist only of coincidence sites are expected to have the lowest energy and therefore are the most likely to form the boundary between two crystals. Examples of planes in addition to the (111) plane in which all sites may be coincidence sites are the $(11\bar{2})$ and (117) planes whose traces are represented by bold broken lines in Fig. 1. These planes have also been shown to be interface planes between parent and annealing twin crystals in aluminum (Sargent, 1968). The maximum fraction of sites in the lattice plane of particular Miller indices which can be coincidence sites will be represented by

Table 1. *Planes with a high density of coincidence sites for the twenty-two coincidence-site relationships with a multiplicity less than or equal to* 31

The twenty-two coincidence-site relationships are described by a rotation of 180° about the direction with indices given in column 2 of the Table. A detailed description of the remainder of the Table is given in the text.

Multiplicity	Axis of rotation			w^i_j													
3	111	$(11\bar{2})$	101	$\bar{1}11$	$0\bar{1}1$	111 $\bar{2}41$ $\bar{1}25$ $14\bar{5}$ $\bar{1}55$ $22\bar{7}$	$\bar{2}11$ $\bar{2}14$ 522 $5\bar{4}2_{\bullet}$ $7\bar{2}1_{\bullet}$ $\bar{5}44$	$1\bar{2}1$ $14\bar{2}$ 252 $52\bar{4}_{\bullet}$ $71\bar{2}_{\bullet}$ $4\bar{5}4$	$11\bar{2}$ $1\bar{2}4$ 225 $\bar{4}52_{\bullet}$ $\bar{2}71_{\bullet}$ $44\bar{5}$	$22\bar{1}_{\bullet}$ $\bar{5}11_{\bullet}$ 441 $\bar{4}25_{\bullet}$ $\bar{2}17_{\bullet}$	$2\bar{1}2_{\bullet}$ $1\bar{5}1_{\bullet}$ 414 $25\bar{4}_{\bullet}$ $17\bar{2}_{\bullet}$	$\bar{1}22_{\bullet}$ $11\bar{5}_{\bullet}$ 144 $2\bar{4}5_{\bullet}$ $1\bar{2}7_{\bullet}$	$411_{\bullet}$ $52\bar{1}$ $\bar{5}41$ 711 $552_{\bullet}$	$141_{\bullet}$ $5\bar{1}2$ $\bar{5}14$ 171 $525_{\bullet}$	$114_{\bullet}$ $25\bar{1}$ $4\bar{5}1$ 117 $255_{\bullet}$	$4\bar{2}1$ $2\bar{1}5$ $41\bar{5}$ $55\bar{1}$ $\bar{7}22$	$41\bar{2}$ $\bar{1}52$ $1\bar{5}4$ $5\bar{1}5$ $2\bar{7}2$
5	012	(031)	100	021	$0\bar{1}2$	012 $\pm 543_{\bullet}$	$02\bar{1}$ $\pm 53\bar{4}_{\bullet}$	031 $\pm 54\bar{2}$	$01\bar{3}$ ± 524	$043_{\bullet}$	$03\bar{4}_{\bullet}$	$07\bar{1}_{\bullet}$	$017_{\bullet}$	± 512	$\pm 52\bar{1}$	± 531	$\pm 51\bar{3}$
7	123		$1\bar{2}0$	112	$\bar{1}01$	123 $\bar{6}23_{\bullet}$	$3\bar{1}2$ $362_{\bullet}$	$\bar{2}31$ $2\bar{3}6_{\bullet}$	$41\bar{2}$	$24\bar{1}$	$12\bar{4}$	531	$\bar{3}15$	$1\bar{5}3$	$5\bar{4}1$	415	$\bar{1}54$
9	122	$(\bar{4}11)$	$0\bar{2}1$	112	$\bar{1}02$	122 $1\bar{1}2_b$	$\bar{4}11$ $2\bar{2}1$	511_a $21\bar{2}$	$2\bar{5}4$ $\bar{1}41_{\bullet}$	$24\bar{5}$ $\bar{1}14_{\bullet}$	$1\bar{7}2_b$ $15\bar{1}$	$12\bar{7}_c$ $1\bar{1}5$	$\bar{2}55_d$	:3:	$\bar{1}11_a$	211_d	$12\bar{1}_c$
11	113	$(33\bar{2})$	101	$\bar{1}31$	$0\bar{1}3$	113	$33\bar{2}$	$22\bar{5}$	441								
13a	023	(051)	100	032	$0\bar{2}3$	023	$03\bar{2}$	051	$01\bar{5}$								
13b	134		$1\bar{3}\bar{1}$	112	$\bar{1}02$	134	$4\bar{1}3$	$\bar{3}41$									
15	125		$1\bar{2}1$	212	$\bar{1}02$	125 :5: $15\bar{1}_3$	$24\bar{5}_e$ $\bar{1}11_1$ $1\bar{1}5_3$	:3: 211_1	$\bar{2}10$ $12\bar{1}$	120_e $1\bar{1}2_1$	310_1 $2\bar{2}1_3$	$\bar{1}30_1$ $21\bar{2}_3$	315 $122_{\bullet}$	$31\bar{5}_1$ $\bar{4}11_3$	$1\bar{3}5_1$ $\bar{1}41_3$	$\bar{1}35$ $\bar{1}14_1$	511_3
17a	014	(053)	100	041	$0\bar{1}4$	014	$04\bar{1}$	053	$03\bar{5}$								
17b	223	$(33\bar{4})$	102	$\bar{1}32$	$0\bar{2}3$	223	$33\bar{4}$	$11\bar{7}$	$55\bar{1}$								
19	133	$(\bar{6}11)$	$0\bar{3}1$	113	$\bar{1}03$	133	$\bar{6}11$	722	$\bar{5}44$								
21a	145		$1\bar{1}0$	144	$\bar{1}\bar{3}1$	145 $2\bar{1}1_1$	$5\bar{1}4$ $\bar{1}21_1$	$\bar{4}51$ 112_1	:3: 221_3	$3\bar{2}1$ $\bar{2}12_3$	213 $1\bar{2}2_3$	$\bar{1}32$ $41\bar{1}_3$	$\bar{5}13_1$ $14\bar{1}_3$	351_1 $11\bar{4}_3$	$1\bar{3}5_1$ $5\bar{1}1_3$	:7: $\bar{1}51_3$	$11\bar{1}$ 115_3
21b	124		$0\bar{2}1$	212	$\bar{1}04$	124 $\bar{1}12_1$	:3: $\bar{2}21_3$	$\bar{3}12_1$ 212_3	$2\bar{3}1$ $12\bar{2}_3$	$12\bar{3}_1$ $4\bar{1}1_3$	$53\bar{1}_1$ $1\bar{4}1_3$	$3\bar{1}5$ $1\bar{1}4_3$	$\bar{1}53$ $51\bar{1}_3$	:7: 151_3	$\bar{1}\bar{1}1_1$ $\bar{1}15_1$	$21\bar{1}$	121_1
23	136		$0\bar{3}\bar{1}$	212	$\bar{1}03$	136											
25a	034	(071)	100	043	$0\bar{3}4$	034	$04\bar{3}$	07 1	$01\bar{7}$	:5:	021_1	$01\bar{2}_1$	$03\bar{1}_1$	013_1	$\pm 53\bar{1}_1$	$\pm 513_1$	
25b	345		$25\bar{1}$	102	$\bar{2}34$	345	:5:	210_1	$\bar{1}20_1$	$\bar{3}10_1$	130_1	$3\bar{1}5_1$	$\bar{3}15_1$	$13\bar{5}_1$	135_1		
27a	127		274	$\bar{1}01$	$0\bar{1}3$	127 $1\bar{1}4_{\bullet}$	:3: 151	$12\bar{2}_1$ $\bar{1}15$	$4\bar{1}1_1$	$51\bar{1}$	:9:	$21\bar{1}_1$	121_1	$\bar{1}12_1$	$\bar{2}21_3$	212_3	$1\bar{4}1$
27b	115	$(55\bar{2})$	111	$\bar{1}41$	$0\bar{1}5$	115 $14\bar{1}$	$55\bar{2}$ $5\bar{1}1_3$	:3: $\bar{1}51_3$	221_1	$11\bar{4}_1$	:9:	$2\bar{1}1_1$	$\bar{1}21_1$	112_1	$\bar{2}12_3$	$1\bar{2}2_3$	$41\bar{1}$
29a	234		132	$\bar{2}\bar{2}3$	104	234											
29b	027	(073)	100	052	$0\bar{2}5$	025	$05\bar{2}$	073	$03\bar{7}$								
31a	156		$1\bar{5}\bar{2}$	113	$\bar{1}03$	156	$\bar{5}61$	$6\bar{1}5$									
31b	237		$\bar{3}\bar{2}0$	$2\bar{1}1$	014	237											

σ^{-1}, where σ is a rational factor of Σ being equal to one when all sites in a lattice plane are coincidence sites. In § 2 of this paper a procedure for determining the value of σ for a particular lattice plane is described, and the planes with σ values less than $\sigma = \Sigma$ are tabulated for a wide range of Miller indices for all coincidence site relationships with $\Sigma \leq 31$.

The orientation relationship between the parent and twin crystals illustrated in Fig. 1 may, for example, also be described by rotation of 180° about $[11\bar{2}]$ or 70·5° about $[1\bar{1}0]$. In general there are twenty-four different ways of describing the orientation relationship between two cubic crystals and hence twenty-four ways of describing the orientation relationship between two coincidence-site-related crystals. In § 3 of this paper the different ways of describing the orientation relationship between the coincidence-site-related crystals are tabulated for the coincidence-site relationship with $\Sigma \leq 31$. The ways in which the table may be used to aid the interpretation of experimental results is also described.

2. The density of coincidence sites in a crystal lattice plane

All coincidence-site lattices with a multiplicity Σ less than or equal to 31 have been considered, and the coincidence-site lattice relationships which arise in the range $\Sigma \leq 31$ are listed in Table 1 where Σ is given in column 1 and the corresponding axis of rotation $[h_1\, h_2\, h_3]$ is given in column 2. For some values of Σ two coincidence-site relationships which are not crystallographically equivalent arise; they are represented by Σ_a and Σ_b. In some cases a rotation of 180° about axes of a different form give rise to crystallographically equivalent relationships, as for example when the two axes are orthogonal and together define a symmetry plane. These alternative descriptions are given in column 3 of Table 1.

The following procedure was used for determining the Miller indices of planes parallel to a plane in the crystal lattice in which all sites can be sites of the coincidence-site lattice, or in which σ^{-1} of the crystal

Table 2. *The alternative ways of describing the twenty-two coincidence-site relationships with a multiplicity less than or equal to* 31

An asterisk indicates the description associated with the smallest angle of rotation for a particular multiplicity.

Axis of rotation	Multiplicity	Angle of rotation																		
100	5 *	36.9	310	5	180	411	9	180	511	7	158.2	610	19a	161.3	551	13a	164.1	733	17b	166.1
	13a*	22.6		7	115.4		11	129.5		9	120.0		23	127.5		15	134.4		19b	139.7
	17a*	28.1		11	144.9		17a	93.4		13a	92.2		31a	101.2		19b	110.0		23	117.2
	25a*	16.3		13b	76.7		19b	153.5		19a	73.2					25b	91.2		29b	98.9
	29b*	43.6		19a	93.0		27a	109.5		27a	60.0	532	19b	180.0						
				23	55.6		27b	70.5		27b	180.0		21b	144.1	711	13b	164.1	751	19a	166.8
110	3	70.5								31b	137.9		27a	114.0		15	134.4		21b	141.8
	9 *	38.9	311	3	146.4	331	5	154.2								19a	110.0		25b	120.0
	11 *	50.5		5	95.7		7	110.9	432	15	159.0	611	19a	180.0		25a	91.2		31b	102.1
	17b	86.6		9	67.1		11	82.2		19a	121.8		21b	144.1						
	19a*	26.5		11	180		17b	63.8		27a	94.3		27b	114.0	641	27b	164.4	753	21b	167.5
	27b*	31.6		15	50.7		19a	180		29a	180.0					31b	135.2		23	143.6
				15	117.8		23	130.7				443	21b	162.3					27b	122.5
111	3 *	60		23*	40.5		25b*	51.7	520	15	159.0		25a	129.8	720	27a	164.4			
	7 *	38.2		25b	168.3					19b	121.8					31b	135.2	911	21a	167.5
	13b*	27.8		27a	79.3	421	11	155.4		27b	94.3	540	21a	162.3					23	143.6
	19b*	46.8		31b	126.6		15	113.6		29b	180.0		25b	129.8	552	27b	180.0		27a	122.5
	21a*	21.8					21b	180								29b	149.6			
	31a*	17.9	320	7	149.0		23	85.0	521	15	180.0	621	21b	162.3				931	23	168.0
				11	100.5		25b	132.8		17b	139.9		25b	129.8	721	27a	180.0		25b	145.1
210	3	131.8		13a	180					23	107.7					29a	149.6		29a	124.7
	5	180		17b	122.0	332	11	180		31b	159,3	541	21a	180.0						
	7	73.4		19b	71.6		13a	133.8					23	145.7	544	29a	164.9	755	25b	168.5
	9	96.4		29a	84.1		19a	99.1	441	17a	160.3		29a	116.6					27b	146.4
	15*	48.2		31b	54.5		23	155.9		21b	124.9				722	29a	164.9		31a	126.6
	21b	58.4					29a	76.0		29a	97.9	533	11	162.7						
	23	163.0	321	7	180		31a	114.8					13b	130.8	730	29b	180.0	771	25a	168.5
	27a*	35.4		9	123.8				522	17b	160.3		17a	105.3		31b	150.6		27a	146.4
	29a	112.3		15	86.2	430	13b	157.4		21b	124.9		23	86.3					31b	126.6
				15	150.1		17b	118.1		29b	97.9		31b	72.2	553	15	165.2			
211	3	180		23	102.6		25a	180								17a	137.3	773	27a	169.0
	5	101.5		25b	63.9		25b	90	433	17b	180.0	542	23	163.0		21a	113.9		29b	147.7
	7	135.6					29a	136.4		19a	142.1		27a	131.8		27b	95.3			
	11	63.0	322	9	152.7					25a	111.1							951	27a	169.0
	15	78.5		13a	107.9	431	13b	180				631	23	180	731	15	165.2		29a	147.7
	21b*	44.4		17b	180		15	137.2	530	17a	180.0		25b	147.1		17b	137.3			
	25b	156.9		21a	128.3		21b	103.8		19b	142.1		31b	118.9		21b	113.9	953	29a	169.4
	29a	149.6		21b	79.0		27a	157.8		25b	111.1					27a	95.3		31b	148.7
	31b*	52.2					31b	80.7				632	25b	163.7						
			410	9	152.7				531	9	160.8		29a	133.6	645	31b	165.4	775	31b	169.7
221	5	143.1		13b	107.9	510	13a	180		11	126.2									
	9	90		17a	180		15	137.2		15	99.6	543	25b	180.0	650	31a	165.4	11,1,1	31a	169.7
	9	180		21a	79.0		21a	103.8		21b	80.4		27a	148.4						
	13b	112.6		21b	128.3		27b	157.8		29a	66.6				732	31b	180.0			
	17b*	61.9					31a	80.7				710	25a	180.0						
	25b	73.7											27a	148.4	651	31a	180.0			
	29a*	46.4																		

lattice sites can be coincidence sites for σ a rational factor of Σ not equal to Σ. For a particular coincidence site relationship the value of σ is the same for a particular plane in all three cubic Bravais lattices. For convenience the primitive cubic lattice will be considered.

The Miller indices of planes and directions in one of the crystal lattices (lattice 1) of the coincidence-site-related lattices will be referred to the orthonormal cubic lattice basis $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$. For convenience the two basis vectors $\mathbf{d}_1$ and $\mathbf{d}_2$ of the basis $\mathbf{d}_1$, $\mathbf{d}_2$, $\mathbf{d}_3$ defining a primitive cell of the coincidence lattice are chosen to be in the plane with normal $[h_1\, h_2\, h_3]$, and hence in cubic crystals the plane with Miller indices $(h_1\, h_2\, h_3)$. This plane is a lattice plane of the two crystal lattices and of the coincidence-site lattice. Procedures for determining the two vectors $\mathbf{d}_1 = l_i\mathbf{c}_i$ and $\mathbf{d}_2 = m_i\mathbf{c}_i$ which must define a primitive cell in the $(h_1\, h_2\, h_3)$ plane have been described by Jaswon (1965) and Bevis (1969). When the lattice planes $(h_1\, h_2\, h_3)$ have an odd stacking sequence (Jaswon & Dove, 1955) the vector $\mathbf{d}_3$ is chosen to be normal to this plane, so that $\mathbf{d}_3 = h_i\mathbf{c}_i$. In the case of a plane with an even stacking sequence the vector $\mathbf{d}_3$ may be taken to be any primitive vector of the vectors $\frac{1}{2}(l_i + m_i + h_i)\mathbf{c}_i$, $\frac{1}{2}(l_i + m_i)\mathbf{c}_i$, $\frac{1}{2}(l_i + h_i)\mathbf{c}_i$ or $\frac{1}{2}(m_i + h_i)\mathbf{c}_i$, and in general will be represented by $\mathbf{d}_3 = n_i\mathbf{c}_i$. The relationship between components of a vector referred to the orthonormal crystal lattice basis and the coincidence site lattice basis, represented by $\mathbf{x} = u_i\mathbf{c}_i$ and $\mathbf{x} = v_i\mathbf{d}_i$ respectively is given by $v_i = w_{ij}u_j$ where

$$w_{ij} = \begin{pmatrix} l_1 & m_1 & n_1 \\ l_2 & m_2 & n_2 \\ l_3 & m_3 & n_3 \end{pmatrix}.$$

The corresponding transformation of Miller indices is given by

$$b_i = w_{ji}a_i\,, \qquad (1)$$

where (a_i) and (b_i) are the Miller indices of a plane referred to the crystal lattice and coincidence site lattice bases respectively. If the vector $b_i\mathbf{d}_i$ is a primitive lattice vector, then the interplanar spacing of the planes $(b_1\, b_2\, b_3)$ is equal to the interplanar spacing of the parallel planes $(a_1\, a_2\, a_3)$, so that only $1/\Sigma$ sites in the plane $(a_1\, a_2\, a_3)$ are coincidence sites. If however $b_i\mathbf{d}_i$ is not a primitive reciprocal lattice vector, and is equal to $b_i\mathbf{d}_i = pb'_i\mathbf{d}_i$ where p is an integer and $b'_i\mathbf{d}_i$ is a primitive reciprocal lattice vector, then the interplanar spacing of the planes $(a_1\, a_2\, a_3)$ is then $1/p$ that of the planes $(b'_1\, b'_2\, b'_3)$. In this case a fraction $p/\Sigma = 1/\sigma$ sites in the plane $(a_1\, a_2\, a_3)$ are coincidence sites. When $p = \Sigma$ then all sites are coincidence sites.

The densities of coincidence sites in parallel lattice 1 and lattice 2 planes are in general not equal. The density of coincidence sites in a lattice 2 plane can be determined in exactly the same way as for lattice 1 planes. The Miller indices of the plane in lattice 2 parallel to the $(a_1\, a_2\, a_3)$ plane in lattice 1 has the Miller indices $(e_1\, e_2\, e_3)$ with respect to the lattice 2 basis given by $e^i = r_{ji}a_j$ where $r_{ij} = -\delta_{ij} + 2h_ih_j(h_kh_k)^{-1}$. The same matrix w_{ij} applies for lattice 2 and lattice 1.

With the aid of a digital computer the authors have used equation (1) to determine the density of coincidence sites in crystal lattice planes for the coincidence site relationships given in column 2 of Table 1. The three rows of the matrices w_{ij} for the twenty-two coincidence site relationships are given in columns 4, 5 and 6 of Table 1. For each coincidence-site relationship the Miller indices of the following crystal lattice planes are given:

(*a*) planes $(a_1 a_2 a_3)$ in which all sites can be coincidence sites, but with the limitation that only the fifty-four most densely packed primitive cubic lattice planes are considered, (*b*) planes $(a_1\, a_2\, a_3)$ in which a fraction $1/\sigma$ sites can be coincidence sites, but with the limitation that only the first nine most closely packed primitive, body-centred and face-centred cubic lattice planes are considered. The variants of planes given in Table 1 apply for the description of the coincidence-site relationship given in column 2 of the Table. The planes are given in columns 7–18 of Table 1 and are listed across the page, the planes with a fraction $1/\sigma$ of coincidence sites are preceded by $:\sigma:$. A difference in the density of coincidence sites in parallel lattice 1 and lattice 2 planes is indicated in the following way. If the density of coincidence sites in the lattice 2 plane parallel to the lattice 1 plane given in Table 1 is equal to $1/\Sigma$, then the indices of the lattice 1 plane are followed by a dot. If the Miller indices of a lattice 1 plane are followed by a number, then the reciprocal of the number is the density of coincidence sites in the parallel lattice 2 plane. In general the indices of the parallel lattice 2 planes do not fall within the range of planes investigated. However in cases where both planes fall within the range investigated the pairs of planes are followed by the same letter.

3. Alternative descriptions of coincidence-site relationships

In an experimental determination of the orientation relationship between two crystals of interest, for example in the case of two coincidence-site related crystals, the orientation relationship could be that described by column 2 of Table 1 or in twenty-three other ways which describe the same orientation relationship (Lange, 1967), and which result when any particular original rotation is combined with the twenty-four proper symmetry rotations associated with a cube having identical faces. Thus, unless the twenty-four ways of describing the orientation relationship determined experimentally are deduced, and then compared with the relationships of column 2 of Table 1, it is not possible to establish readily that a coincidence site relationship is operative. Only a limited number of the alternative ways of describing the orientation relationships of column 2 of Table 1 have been given previously. The most comprehensive list, which is, however, limited in extent, has been given by Ranganathan (1967), and are the results of an application of a procedure (Ranganathan, 1966) for determining the possible Σ values and corresponding angles of rotation associated with a particular axis of rotation. The authors have determined the axes of rotation and the corresponding angles of rotation (ω) for all twenty-four ways of describing each of the twenty-two coincidence-site relationships given in column 2 of Table 1. These results are presented in Table 2 with the limitation that only the form of the axes of rotation are given. However, an experimentally determined orientation relationship may be compared with the relationships presented in Table 2, thus allowing the operative coincidence-site relationship to be determined readily. The more convenient orientation relationship given in column 2 of Table 1 may then be adopted, and the further crystallographic information contained in Table 1 utilized directly.

In Table 2 the results are presented in multiples of three colums, the first, second and third column in every three gives the axis of rotation, the multiplicity and the angle of rotation (ω) respectively. For the [100], [110] and [111] symmetry axes the angles of rotation ($90-\omega$, $90+\omega$, $180-\omega$), ($180-\omega$) and ($120-\omega$, $120+\omega$) respectively also give rise to the coincidence-site relationships indicated in column 2. The relationship which gives the smallest value of ω for a particular value of Σ is indicated by an asterisk. Table 2 effectively gives the results of an application of the procedure described by Ranganathan (1966) for all possible rotations about axes with indices $[l_1\ l_2\ l_3]$ for $\{(l_1)^2+(l_2)^2+(l_3)^2\}<123$ which give rise to the coincidence site relationships with $\sum\leq 31$.

The authors are indebted to Mr E. B. Crellin for valuable discussions. The award of an S. R. C. studentship is acknowledged by one of us (AFA).

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The Effect of Refraction in the Small-Angle Diffraction of X-rays from Stacked Lamellae

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(*Received* 25 *May* 1969 *and in revised form* 13 *April* 1970)

An expression for the scattering of X-rays from a regular stack of lamellae is developed, releasing the prior restraint that no refraction may occur. The effect of refraction is to cause deviations from the classical Bragg condition. Further, a condition of total reflection is shown to occur within systems whose lamellar spacings are greater than a critical value.

Statement of the problem

The analysis of X-ray scattering data generally proceeds through a consideration of the amplitude of scattering $A(\mathrm{S})$ as given by

$$A(\mathrm{S})=A_e(\mathrm{S})\int\varrho(\mathrm{X})\exp\{2\pi i\mathrm{S}\,.\,\mathrm{X}\}dv_{\mathrm{x}}\,. \qquad (1)$$

Here, $A_e(\mathrm{S})$, ϱ, X, S, and v_{x} have their usual meanings: amplitude of scattering by an isolated electron, electron density, real space vector, reciprocal space vector, and real space volume. This expression is rigorously correct (in the kinematic approximation) only if (*a*) the medium is non-absorbing and (*b*) the vector S is permitted to vary as the X-ray beam traverses regions of differing refractive index. Indeed, absorptive and refractive corrections are not needed in the analysis of diffraction line breadths and peak positions; *e.g.*, the relative errors in atomic positional analysis are of the order of 10^{-5} and can safely be ignored. However, for the particular case of diffraction from a lamellar system whose elements are 100 Å or more in thickness both absorptive and refractive effects can become large. The under-

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