THE COINCIDENCE SITE LATTICE (CSL) AND GRAIN BOUNDARY (DSC) DISLOCATIONS FOR THE HEXAGONAL LATTICE

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Résumé. — On présente une nouvelle technique pour calculer les vecteurs de Burgers des dislocations (DSC) des joints intergranulaires et cette technique est appliquée au cas des réseaux cubiques et hexagonaux.

On peut toujours exprimer une rotation quelconque entre deux réseaux hexagonaux comme une *désorientation*, en indexant convenablement les deux réseaux.

On présente la méthode pour trouver la désorientation correspondant à une valeur donnée de Σ, quelconque, avec une valeur de $(c/a)^2$ rationnelle. Les résultats sont donnés pour quelques cas intéressants et on montre que le nombre des valeurs possibles de Σ est voisin de celui du cas cubique. On évalue par une méthode simple les probabilités qu'ont les joints de grains des métaux hexagonaux d'être proches d'un joint de coïncidence. On montre que, dans chaque cas, le réseau de Bravais donne une base convenable pour le système de coordonnées.

Abstract. — A new, general and convenient technique is presented for determining the burgers vectors of (DSC) grain boundary dislocations and it is applied to hexagonal lattices.

A general rotation between two hexagonal lattices may be expressed as a disorientation by a suitable reindexing of the two lattices, and it is shown how the disorientation giving rise to any desired possible value of Σ and any rational value of $(c/a)^2$ may be determined. The results are given for several interesting values and it is seen that the number of possible values of Σ is similar to that for the cubic case. A simple assessment is made of the possibilities of ordered structures within hexagonal metal grain boundaries. The unit cell of the Bravais lattice is shown to provide a convenient basis of the coordinate system in every case.

1. **Introduction.** — When two metal grains are in a relative orientation corresponding to a *CSL*, the structure of a (planar) grain boundary possesses periodic repeat units related to the (three dimensional) repeat distances of the *CSL*. For any given boundary plane and initial arbitrary relative displacement of the grains the structure will be preserved on additional displacement by a unique set of displacement vectors (*DSC* vectors). These vectors therefore are allowed burgers vectors for dislocations lying in the grain boundary [1]. Together they form what may be termed the *DSC* lattice. Networks of *DSC* dislocations will preserve the periodic pattern when the relative orientation deviates from a *CSL* ideal orientation. A non planar grain boundary may find it energetically favourable to preserve elements of a three dimensional unit, or it may facet and preserve alternately two two dimensional units (both drawn from the three dimensional *CSL*). In the former case only *DSC* dislocations will be necessary to maintain the structure on deviation from an ideal orientation ; in the latter case *partial DSC* displacements may be required to maintain continuity at arbitrary faceting positions. (Such displacements have apparently been detected at faceted twin boundaries in aluminium [2] and calculations for body centred cubic materials indicate that two alternative structures arising from the presence of a partial *DSC* displacement have closely similar energies [3].)

O lattice theory has been used to derive the possible *CSL* and *DSC* lattices, for cubic crystals, and although one must not expect a geometrical theory to explain all structural effects within grain boundaries many predictions of the O lattice theory have been verified both qualitatively and quantitatively.

Attention is now beginning to turn to more complex boundaries than between two cubic crystals and it is apparent that order does exist in such boundaries [5-8]. Ordered boundaries do appear to have lower energies and be preferred and they may well govern precipitation behaviour in the solid state. Studies of interphase boundaries have already been initiated and it seems opportune to examine, from the viewpoint of the *CSL* and *DSC* lattices, possible structures in grain boundaries between hexagonal lattices.

This paper shows how the O lattice approach to the determination of *CSL* and *DSC* lattices may be simplified by numerical techniques and derives such lattices for hexagonal materials. In addition the symmetries available in the hexagonal lattice are compared with those of cubic lattices and estimates made of the relative number of boundaries of random rotation that may be expected to

demonstrate the effects of geometrical periodicity. Only situations where three dimensional *CSL*'s exist will be treated.

2. **Determination of rotations leading to a CSL.** — The technique used follows from that Warrington and Bufalini [9] used for cubic crystals. A coincidence site lattice will occur for a cubic crystal for any rotation given by a rotation matrix $R = (r_{ij})/\Sigma$ where Σ is the ratio of *CSL* and crystal unit cell volumes, and the matrix elements r_{ij} are all integers and have no common divisor. In this way the three column vectors (all of unit length) represent the new rotated positions of unit vectors along the crystal axes.

The most convenient system for hexagonal crystals is to use a crystal coordinate system to describe a rotation matrix. It is helpful to choose a system in which *vectors* are conveniently manipulated. Of the possible system the most convenient is the three axis hexagonal system [10]. Let S be a matrix which transforms the crystal coordinates of a vector into orthogonal coordinate (for example, the x and z axes of the two coordinate systems being respectively parallel) S^{-1} be its inverse. G, the metric tensor, is then $S^{\mathrm{T}} S$ where S^{T} is the transpose of S.

S may be written as $a\begin{pmatrix} 1 & -1/2 & 0 \\ 0 & \sqrt{3/2} & 0 \\ 0 & 0 & c/a \end{pmatrix}$ where c and a are the hexagonal repeat units along the z and x axes. The length of a vector is given as

$$(uvw)\, G \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \left\{ u^2 + v^2 - uv + \left(\frac{c}{a}\right)^2 w^2 \right\}^{1/2}$$

and the angle between two vectors is given by

$$\cos^{-1} \frac{(u_1\, v_1\, w_1)\, G \begin{pmatrix} u_2 \\ v_2 \\ w_2 \end{pmatrix}}{(u_1\, v_1\, w_1)\, G \begin{pmatrix} u_1 \\ v_1 \\ w_1 \end{pmatrix} \times (u_2\, v_2\, w_2)\, G \begin{pmatrix} u_2 \\ v_1 \\ w_2 \end{pmatrix}}.$$

A matrix $R = (r_{ij})/\Sigma$ will lead to a *CSL* in the hexagonal system, provided the following conditions are satisfied :

a) the lengths of the three column vectors are respectively a, a and c

b) the angle between the first two column vectors is 120° and the angles these make with the third column vector are 90°

c) Σ and r_{ij} are integers with no common divisor.

Two solutions are therefore required of the equation

$$\Sigma^2 = u^2 + v^2 - uv + \left(\frac{c}{a}\right)^2 w^2, \qquad (1)$$

and one solution of the equation

$$\left(\frac{c}{a}\right)^2 \Sigma^2 = u^2 + v^2 - uv + \left(\frac{c}{a}\right)^2 w^2 \qquad (2)$$

for the columns of the rotation matrix that satisfy conditions *b*) and *c*).

In practice it is convenient to find solutions to eq. (1), check their correct angular relationship and treating them as zone axes to find the plane normal common to the two zones. This normal may be converted (for rational $(c/a)^2$) to a parallel unit vector to form the third solution (eq. (2)).

We note that since any (rational) hexagonal cell may be chosen from a sub lattice of a cubic lattice all rotations leading to any cubic *CSL* will give rise to a *CSL* of the hexagonal lattice. The latter however will often be of a higher value of Σ. Choose for example a hexagonal cell such that

100 hex. = 033 cubic
010 hex. = $3\bar{3}0$ cubic
001 hex. = $44\bar{4}$ cubic

Then

$$S = \begin{bmatrix} 0 & 3 & 4 \\ 3 & -3 & 4 \\ 3 & 0 & -4 \end{bmatrix}$$

and

$$S^{-1} = \frac{1}{36} \begin{bmatrix} -4 & 8 & 4 \\ 8 & -4 & 4 \\ 3 & 3 & -3 \end{bmatrix}.$$

The hexagonal lattice must give rise to values of Σ of 36 times that for the same rotation applied to the cubic lattice *or* an integral factor of this. Thus for the cubic $\Sigma = 5$ the hexagonal lattice must give Σ as one of 5 10 15 20 30 45 69 90 or 180. Different values will arise as cubic axes of the same form will be parallel to hexagonal axes of different forms.

Having found a solution for a given Σ it will represent, in general one of 12×12 symmetry related rotation matrices (the hexagonal lattice possesses 12 symmetry rotations, and rotations of both crystals must be taken into account). These matrices are related by suitable combinations of changes of signs of rows or columns or suitable interchanges and additions of the first two rows or columns. Any given solution is therefore characterised by the element r_{33}(or w_3). In addition for an axial ratio $\sqrt{m/n}$, where m and n are integers, equations (1) and (2) show that elements r_{31} and r_{32} will be divisible by n and that $u_3^2 + v_3^2 - u_3\, v_3$ will be divisible by m. In practice this latter condition means that both u_3 and v_3 are divisible by m.

The matrices presented in table I are those for the hexagonal disorientation, that is the crystal axes in crystals (1) and (2) and the designation of crystals (1) and (2) are such that the rotation axis lies within

TABLE I

Hexagonal lattice, $c/a = \sqrt{8/3}$ crystal coordinates

Σ	Disorientation Rotation matrix $R(x\Sigma)$			— Axis	— Angle	Basis vectors DSC($x\Sigma$)			Alternative		
7	8	—3	0	001	21.79	3	—1	0			
	3	5	0			1	3	0			
	0	0	7			0	0	7			
10	10	0	0	210	78.46	10	0	0			
	4	2	—16			0	2	—2			
	—3	6	2			0	1	4			
11	11	0	0	210	62.96	11	0	0			
	3	5	—16			0	1	5			
	—3	6	5			0	—1	6			
13	15	—7	0	001	27.80	4	—1	0			
	7	8	0			1	3	0			
	0	0	13			0	0	13			
14	14	0	0	210	44.42	14	0	0			
	2	10	—16			0	4	—2			
	—3	6	10			0	1	3			
17	17	—8	—16	100	86.63	9	1	6	1	0	0
	0	1	—32			1	2	—5	2	17	0
	0	9	1			—8	1	6	1	0	17
18	18	—6	—16	100	70.53	6	2	2	2	0	0
	0	6	—32			—6	4	4	4	18	0
	0	9	6			0	—3	6	—3	0	9
19	21	—5	0	001	13.17	3	2	0			
	5	16	0			—2	5	0			
	0	0	19			0	0	19			
22	22	—4	—16	100	50.48	10	2	—2	2	0	0
	0	14	—32			—2	4	—4	4	22	0
	0	9	14			5	1	10	1	0	11
25	25	0	0	210	23.07	25	0	0			
	1	23	—16			0	7	—1			
	—3	6	23			0	4	3			

C.S.L. disorientations for hexagonal lattice $c/a = \sqrt{8/3}$

Σ	$R(x\Sigma)$			Axis	Angle
26	28	—18	—16	801	87.796
	6	—2	—48		
	3	12	2		
27	27	—3	—16	100	38.942
	0	21	—32		
	0	9	21		
29	32	—17	—16	1603	66.637
	9	7	—48		
	3	12	13		
31	35	—11	0	001	17.897
	11	24	0		
	0	0	31		
31	32	—5	—16	510	56.744
	3	16	—48		
	—3	15	17		
34	38	—18	—16	401	53.968
	12	14	—48		
	3	12	22		

TABLE I (suite)

C.S.L. disorientations for hexagonal lattice $c/a = \sqrt{8/3}$

Σ	$R(x\Sigma)$			Axis	Angle
35	35	0	0	210	34.048
	3	29	—32		
	—6	12	39		
35	35	0	0	210	57.122
	8	19	—48		
	—9	18	19		
37	40	—7	0	001	9.430
	7	33	0		
	0	0	37		
37	39	—7	—16	720	72.705
	8	9	—64		
	—6	21	11		
38	38	—2	—16	100	26.525
	0	34	—32		
	0	9	34		
38	42	—14	16	1683	73.174
	26	4	—48		
	—6	21	14		
41	41	—9	—32	100	55.877
	0	23	—64		
	0	18	23		
43	48	—13	0	001	15.178
	13	35	0		
	0	0	43		
43	45	—16	—32	810	83.323
	5	3	—80		
	—3	24	5		
45	48	—9	—16	310	86.177
	15	0	—80		
	—9	27	3		
46	52	—22	—16	803	40.459
	18	26	—48		
	3	12	38		
46	50	—12	16	841	79.985
	30	2	—64		
	—9	27	10		
47	53	—21	16	32169	55.679
	29	16	—48		
	—6	21	31		
49	55	—16	0	001	16.426
	16	39	0		
	0	0	49		
49	49	0	0	210	88.831
	24	1	—80		
	—15	30	1		
50	54	—22	—34	801	60.000
	10	20	—80		
	3	21	26		
50	52	—6	—16	310	63.896
	10	20	—80		
	—9	27	22		

the stereographic triangle [100]-[210]-[001] and the rotation angle is a minimum positive value consistent with the operation of the symmetry rotations (Fig. 1) ([1]). This manner of presentation clearly

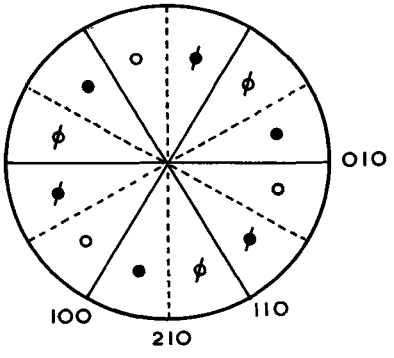


FIG. 1. — Stereographic projection showing symmetry related rotation axes of the form $< u\ v\ w >$. Symbols ● and ○ represent axes above and below the primitive and are related by the point group 32 ; symbols ◖ and ◇ show similarly the additional axes related by the point group 622. In addition an axis ● in the triangle 100-210-001 is related to an axis ○ in the triangle 100 001 210 by interchanging the labelling of crystals 1 and 2 and defining all rotations as positive and less than 180°. The disorientation rotations all lie within a parametral region with limits of 30° rotation along [001] and 90° rotation along [100] and [210].

indicates whether two Σ rotations are related by symmetry or not and also that no Σ values are omitted. These points are not clear when *CSL* rotations are derived about *chosen* axes by a generating function technique [11-12].

It is also seen that if the axial ratio is expressed as the ratio of integers of no common divisor then the parity of eq. (1) indicates that both odd *and* even values of Σ are possible provided a is odd.

3. **Determination of the DSC vectors for a given R.** — It has been shown that the volume of the *DSC* unit cell is given by V/Σ. While the volume of the *CSL* of the direct lattice is equal to $V\Sigma$, the volume of the *CSL* formed from the *reciprocal lattice* is Σ/V. This lattice, which may be designated coincident reciprocal site lattice or *CRSL*, is also present at any rotation giving rise to a *CSL*. In the case of the simple cubic lattice the *CSL* and the *CRSL* are coincident. A vector basis of the *DSC* lattice is therefore given by the matrix equation

$$(DSC)^{T}(CRSL) = I \qquad (3)$$

The meaning of this equation is that any chosen unit cell of the *CRSL*, designated by the three column vectors of a matrix (*CRSL*), is related to a unit cell of the *DSC* lattice, designated by the three column vectors of a matrix (*DSC*) or conversely the three row vectors of its transpose $(DSC)^{T}$. This statement has been formally proved by Grimmer [13] using the property of the *DSC* lattice that it is formed as the difference lattice of vectors of the two crystals. Equation (3) forms the simplest route to the determination of the *DSC* lattice for any crystal system. It is a highly convenient route when the coordinate systems of the crystal, and reciprocal lattices are used.

Let the coordinate system for the equation be an orthogonal (cartesian) system. Using crystal coordinates the (*DSC*) matrix is given by S (*DSC*) and hence the transpose by $(DSC)^{T}(S)^{T}$. Using reciprocal lattice coordinates the (*CRSL*) matrix is given by SG^{-1} (*CRSL*) or S^{T-1} (*CRSL*). Thus the equation still holds when the *DSC* lattice is expressed in crystal coordinates and the coincidence site lattice of the reciprocal lattice is expressed in reciprocal lattice coordinates. These latter coordinates are the natural choice for the *CRSL* which may be determined exactly as if it were the *CSL* of a fictional crystal (suitably oriented) having a lattice identical with that of the reciprocal crystal.

The route to the *DSC* lattice is to determine the *CRSL* either by number theory, or more conveniently by the O lattice technique [14], and then to apply the above equation. This technique is more direct than that previously used for cubic metal lattices [15] and demonstrates the advantages to be gained from a suitable choice of coordinate system. The transformation relationships between the various lattices and coordinate systems are summarized in figure 2.

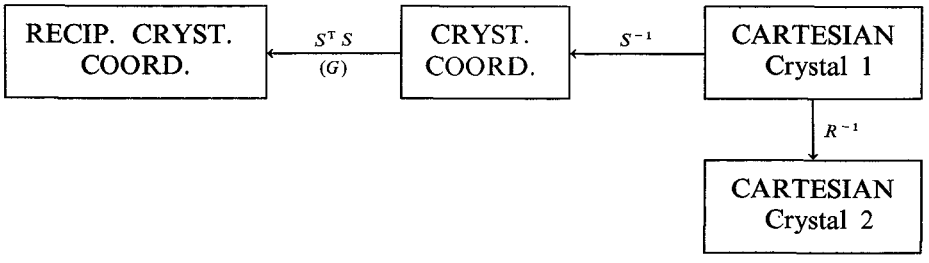
The bases for the various *DSC* lattices given in the tables are for the quoted disorientation matrices. They have been *reduced* only in the sense that they are the three vectors of minimum length in *the crystal coordinate system.* Occasionally an alternative description is given to indicate a symmetry with respect to the crystal axes ; this clearly demonstrates that, as expected, unit vectors along rotation axes are always allowed *DSC* vectors (Table I).

4. **Discussion.** — While linear features have been observed in grain boundaries of hexagonal metals [7], it is still too early to say whether minimum length *DSC* vectors will necessarily have the minimum energy within such boundaries and

([1]) Following the terminology used by Mackenzie (Mackenzie J. K. *Biometrika* **45** (1958) 229) for cubic crystals, and discussed in the calculations of the probabilities of given rotations occuring [18], the hexagonal disorientation is defined as the rotation with the least rotation angle that may be used to describe an arbitrary rotation. If Ui represents a hexagonal symmetry operation and H a rotation in hexagonal coordinates, the twelve rotations $H\ Ui$ represent the same physical situation but with a reindexed crystal 1. They include all the possible angles of rotation and all possible forms of rotation axes of the different possible descriptions. There are in general twelve descriptions of a given angle about axes of the same form given by $UjHUiUj^{-1}$. Putting $Ui = Uj$ we can see all possible combinations of rotation axes and rotation angles are also given by UjH (i. e. a set of descriptions obtained by reindexing crystal 2).

Coordinate transformations

with examples of natural coordinate system transformations



S^T	S^{-1}	I	Cartesian crystal 1
G	I	S	Crystal 1
$S^T RS$	$S^{-1} RS$	RS	Crystal 2
$G(CSL)$	(CSL)	$S(CSL)$	CSL
$G(CSL)^{T^{-1}}$	$(CSL)^{T^{-1}}$	$S(CSL)^{T^{-1}}$	Rec. CSL
I	G^{-1}	$S^{T^{-1}}$	Rec. crystal 1
$(CRSL)$	$G^{-1}(CRSL)$	$S^{T^{-1}}(CRSL)$	$CRSL$
$G(DSC)$	(DSC)	$S(DSC)$	DSC

FIG. 2. — Coordinate transformations between systems. Cartesian crystal 1 refers to a cartesian system of axes fixed with respect to crystal 1. The *CSL* systems are included (although not required by the procedures of this paper) to emphasize the distinction between the reciprocal *CSL* lattice and the coincidence site lattice of the reciprocal crystal (termed *CRSL*). The *DSC* and *CRSL* lattices are further related by equation (3).

indeed whether grain boundaries of given Σ value will have generally a comparable reduction in energy to that which occurs for cubic metals. True *CSL* data derived here are strictly valid only for ideal values of (c/a). However, the same order as for an ideal ratio may be maintained in a boundary of a metal of non ideal ratio by the introduction of misfit nets of the relevant *DSC* dislocations. These misfit nets would play the role of Van der Merwe dislocations and would increase the minimum energy of the boundary above the value for an ideal ratio or alternatively could lead to stepped or faceted boundary interface. Until now such interfaces have been interpreted only in terms of combinations of structural units [16].

The total numbers of different *CSL* solutions are compared in the accompanying table.

No. of Σ Solutions

$(c/a)^2$	Σ range			
	3 to 11	11 to 25	26 to 50	Total
1 (cubic)	5	12	30	47
5/2	4	11	31	46
8/3	3	7	23	33
7/2	2	10	18	30

The ideal values of $(c/a)^2$ correspond approximately to Ti, Mg, Zn respectively. It is seen that while in general low Σ values are fewer, higher Σ values occur with a frequency close to that of the cubic system.

The axes of the *CSL* disorientations lie mostly in mirror planes of symmetry of the holosymmetric class. Thus below $\Sigma = 50$ only $\Sigma = 49$ for $c/a = \sqrt{5/2}$ has an axis, [621], not in a symmetry plane, and thus this is the one *CSL* not having a twin description. In such a situation, a reversal of the roles of crystal 1 and 2, to maintain a positive rotation angle within the disorientation region, leads to a rotation matrix formed from different column vector solutions for equations (1) and (2). In order that the geometry of any particular interface can be described without confusion and with a minimum possibility of observer error it cannot be too strongly emphasised that the disorientation description is to be preferred, just as it is in the case of the cubic system. (A recent error in the hexagonal structure, fortunately not having serious consequences at this stage, is to be found in an incorrect solution to the *DSC* vectors in the $\Sigma = 13$ [001] case in reference [7]).

The values of Σ given are for the hexagonal *lattice*. Structures of lower symmetry (i. e. hexagonal close packed structure) will give rise to the same disorientations for the same Σ values provided that the relative displacement vector [2/3 1/3 1/2] is allowed in addition to a rotation. We believe this is the better approach rather than concentrating attention on atomic sites. An interface which would contain no dislocations in a case of ideal c/a ratio will contain, in the non ideal case, a network of *DSC* to restore coincidence between crystal sites and naturally lead to a facetted boundary. The approach of Bruggeman, Bishop and Hartt [16] in terms of structural units mixed from different *CSL* structures is nearly equivalent to the presence of *DSC* vectors in a *CSL* interface. Where it is

incomplete is in that the planes to either side of a tilt boundary contain additional distortions not allowed for in the simple structural unit model.

What proportion of boundaries of random rotation might be expected to fall within energy cusps corresponding to the formation of boundary structures of given *CSL* ? To answer this question, we need to specify the deviation from a true *CSL* to be allowed and the number of equivalent rotations to the disorientation that may be generated by operation of the full symmetry of both cyrstals. In order to make a comparison with the cubic case [17], a simple deviation of 1/4 radian will be allowed for $\Sigma = 1$ and that for other values of Σ be allowed to vary as $\Sigma^{-1/2}$. (It is noted that this is a simplification and will depend upon criteria which may be uncertain, but it is likely to give an upper limit to the proportions allowed.) The *coverage* of a given Σ, i. e. the probability that a random rotation will lie within an allowed deviation from an exact *CSL* rotation, is given by the product of the number of equivalent *CSL* rotations and the probability that a random rotation lies within a given deviation from one *CSL* rotation. Using the same method as described by Warrington [17], table II gives the data for coverage of the *CSL* regions for $\Sigma \leqslant 25$ and $c/a = \sqrt{8/3}$ and $\sqrt{5/2}$. Table III shows as an example, the derivation of equivalent rotations (axes and angles) to the disorientation values for $\Sigma = 13$, $c/a = \sqrt{5/2}$. An important difference from the cubic case is that the numbers of equivalent rotations do not increase so rapidly with Σ value. Thus for $c/a = \sqrt{8/3}$ only one tenth the number of random rotations satisfy a comparable criterion to

TABLE II

$c/a = \sqrt{8/3}$		$\Sigma^{-1/2}$ criterion	$c/a = \sqrt{5/2}$		$\Sigma^{-1/2}$ criterion
Σ	No. equivalent rotations	probability ($\times 10^{-2}$)	Σ	No. equivalent rotations	probability ($\times 10^{-2}$)
7	24	.108	7a	24	.108
10	72	.191	b	72	.324
11	72	.157	11a	72	.157
13	24	.042	b	72	.157
14	72	.112	13a	72	.126
17	72	.085	b	72	.126
18	72	.078	17a	72	.085
19	24	.024	17b	132	.156
22	72	.054	19a	72	.072
25	72	.048	19b	150	.150
			23a	72	.054
			b	72	.054
			23c	132	.099
Totals for hexagonal lattices $\Sigma = 7 - 25 =$		0.9×10^{-2}			1.67×10^{-2}
Total for cubic structure $\Sigma = 3 - 25 = 9.0 \times 10^{-2}$ [17]					

TABLE III

Equivalent rotations $\Sigma = 13$ $c/a = \sqrt{5/2}$

Angle	13a Axis	Number	Angle	13b Axis	Number
57.42	< 100 >	6	76.65	< 210 >	6
81.15	< 211 >	12	94.41	< 502 >	12
122.57	< 100 >	6	103.34	< 210 >	6
127.97	< 101 >	12	115.02	< 401 >	12
130.83	< 20.10.3 >	12	133.81	< 10.56 >	12
152.20	< 10.03 >	12	143.87	< 843 >	12
180	< 211 >	12	180	< 201 >	12
180	< 10.53* >	12	180	< 504 >	12

the cubic case and hence on a *random* basis it is much less likely that *CSL* boundaries will be observed for a hexagonal than for a cubic case. No attempt will be made here to assess the probability of two dimensional or one dimensional (plane matching) *CSL* boundaries as has been done for cubic materials [18].

The above argument is probably an oversimplification of a practical situation as no account is taken of the effect of boundary plane as distinct from boundary rotation. Balluffi and coworkers [19] have indicated that for given boundary planes, a structure, corresponding to the maintenance of a *CSL* interface, may be observed well beyond the deviation limit chosen for the above calculations. Nevertheless observations on randomly oriented boundary planes in cubic materials appear to support the approach used here [18].

5. **Conclusions.** — A numerical method for the determination of all rotations leading to any given Σ value for hexagonal crystals of a rational $(c/a)^2$. Determination of the corresponding *CSL* for the reciprocal crystal lattice (achieved easily via the O lattice technique) leads to the determination of the *DSC* vectors (vectors of grain boundary dislocations maintaining the structure of a *CSL* interface). The use of the disorientation description of a rotation leads to a simple, unambigous correlation between boundary structure and *DSC* dislocation burgers vectors.

Although the number of possible values of Σ for a hexagonal lattice is similar to that for a cubic lattice, the lower symmetry of hexagonal lattice leads to a lower number of equivalent descriptions of a given rotation. It is predicted, on a simple criterion, that the number of random boundaries possessing structure corresponding to a slight deviation from *CSL* structure is smaller by an order of magnitude than it is for a cubic lattice.

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DISCUSSION

R. BONNET : Pour trouver une base du réseau *DSC*, le Dr Warrington utilise la relation de réciprocité démontrée dans le cas général par Grimmer. Il faut pour cela connaître une base du réseau de coïncidence pour les réseaux réciproques. En fait, la simple considération de la matrice rotation *R* permet de connaître directement une base du réseau *DSC*. En choisissant correctement un vecteur colonne de *R*, la simple résolution de deux équations linéaires rationnelles fournit la base cherchée, comme nous le montrons dans un travail proposé pour publication.

D. H. WARRINGTON : The information required on the *DSC* lattice, and on the various coincidence site lattices, is of course contained in the rotation matrix *R*. The technique of M. Bonnet is similar to that presented in the Acta. Crystall. paper of Grimmer, Bollmann and Warrington and naturally I congratulate M. Bonnet in his similar approach. I

wished to emphasize the method in my present paper simply because it emphasises the physical relationship between the *DSC* lattice and the reciprocal lattice. In this way we may demonstrate more clearly that the *DSC* vectors are (generally) related to *plane normal vectors,* and the undue preoccupation of the importance of coinciding lattice site atoms in grain boundaries can be avoited. Thus the 0 lattice approach can be divorced from the structural unit approach and as M. Sainfrot has shown in this colloquium may predict studies very close to that computed from energy considerations. In addition it demonstrates that we way surely expect to find ordered boundaries in crystals of lower symmetry or when axial ratios are not rational.

K. LUCKE : Since you are concerned with boundaries in hexagonal metals I like to drag your attention to some boundaries showing very high mobility. They have been found in bicrystal experiments [1] of Zn and Cd and also by the analysis of recrystallisation textures [2] of Ti, Zn and Hf.

They are given in zero approximation by a 30° rotation around the hexagonal axis and by a 90° rotation around a two-fold axis. A closer inspection, however, shows that the rotation axis leave a distance of about 10° from these low index directions. Since the boundaries are similarly important for the recrystallisation of hexagonal metals as the $40° < 111 >$ boundary for the recrystallisation of aluminium, it might be interesting to look into the nature of these boundaries.

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D. H. WARRINGTON : Thank you for draining my attention to these two interesting papers.