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Fundamentals for the Description of Hexagonal Lattices in General and in Coincidence Orientation

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(*Received* 11 *April* 1986; *accepted* 24 *September* 1986)

Abstract

The connection between the rotation matrix in hexagonal lattice coordinates and an angle-axis quadruple is given. The multiplication law of quadruples is derived. It corresponds to multiplying two matrices and gives the effect of two successive rotations. The relation is given between two quadruples that describe the same relative orientation of two lattices owing to their hexagonal symmetry; a unique standard description of the relative orientation is proposed. The restrictions satisfied by rotations generating coincidence site lattices (CSL's) are derived for any value of the axial ratio $\rho = c/a$. It is shown that the law for cubic lattices, where the multiplicity Σ of the CSL is equal to the lowest common denominator of the elements of the rotation matrix, does not always hold for hexagonal lattices. A generalization of this law to lattices of arbitrary symmetry is given and another, quicker, method of determining Σ for hexagonal lattices is derived. Finally, convenient algorithms are described for determining bases of the CSL and the DSC lattice.

1. Introduction

Consider a boundary between two grains of the same homogeneous phase. The boundary energy per unit area depends on the relative orientation of the two grains. It has often been observed that this energy has a relative minimum if a significant fraction $1/\Sigma$ of symmetry translations of one grain are simultaneously symmetry translations of the other. The lattice formed by the common translations is called the coincidence site lattice (CSL), Σ its multiplicity. The relative orientation of the two grains can be described by a rotation mapping one set of symmetry translations onto the other.

Motivated by investigations into the frequency with which different relative orientations of grains occur in hexagonal materials, considerable attention has been given to coincidence rotations, *i.e.* rotations generating CSL's in hexagonal lattices (Warrington, 1975; Fortes & Smith, 1976; Bonnet, Cousineau & Warrington, 1981; Hagège, Nouet & Delavignette, 1980; Bleris, Nouet, Hagège & Delavignette, 1982). This last paper, which will be referred to as BNHD, uses an axis-angle description in lattice coordinates for the rotations, which turns out to be convenient for deriving the coincidence rotations.

BNHD and a recent paper by Hagège & Nouet (1985) have stimulated the present investigation because we have found that the two different rules proposed for determining the multiplicity Σ do not always give the correct result. The main purpose of the present investigation is to derive universally valid methods for determining Σ. At the same time, some gaps are filled in the derivation of the BNHD method to find the coincidence rotations and some arguments are simplified.

Some of the results on coincidence rotations including the first method of determining Σ have already been presented without complete proofs in two pre-

0108-7673/87/020232-12$01.50

liminary publications (Grimmer & Warrington, 1983, 1985). Colleagues have convinced us that a detailed derivation of those results would be welcome. We have tried to keep overlaps to a minimum without forcing the reader to switch back and forth between several papers. Examples that were published earlier have been omitted; in particular, we refer to earlier publications for lists of all equivalence classes of coincidence rotations with a given value of the axial ratio and a value of Σ less than a given limit.

Before considering the properties of coincidence rotations in §§ 5-8 results are derived which are valid for arbitrary rotations, as indicated in the *Abstract.*

2. The general rotation matrix in cubic and in hexagonal lattice coordinates, hexagonal quadruples and quaternions

It will be shown in this section how the rotation matrix expressed in lattice coordinates depends on the axial ratio $\rho = c/a$ of the hexagonal lattice, on the angle θ and on the axis of the rotation.

Any vector of three-dimensional space can be written in the form $\mathbf{e}_1x_1+\mathbf{e}_2x_2+\mathbf{e}_3x_3=\mathbf{e}x$, where $\mathbf{e}$ denotes a row of basis vectors, x a column of components. Two bases will be considered; a cubic basis $\boldsymbol{\varepsilon}$ consisting of three mutually orthogonal vectors $\boldsymbol{\varepsilon}_1$, $\boldsymbol{\varepsilon}_2$, $\boldsymbol{\varepsilon}_3$, each of length a, and a hexagonal basis $\mathbf{e}$ related to $\boldsymbol{\varepsilon}$ by $\mathbf{e}=\boldsymbol{\varepsilon}S$, where

$$S=\begin{pmatrix}1 & -1/2 & 0\\ 0 & \sqrt{3}/2 & 0\\ 0 & 0 & \rho\end{pmatrix}. \qquad (1)$$

$\mathbf{e}_1$ and $\mathbf{e}_2$ have length a, the angle between them is 120°; $\mathbf{e}_3$ has length $c=\rho a$ and is orthogonal to $\mathbf{e}_1$ and $\mathbf{e}_2$.

Consider a right-handed rotation by an angle $\theta = 2\varphi$ around an axis with cubic components ν satisfying $\nu_1^2+\nu_2^2+\nu_3^2=1$. With parameters

$$[\alpha, \beta, \gamma, \delta] = \pm[\cos\varphi, \nu_1\sin\varphi, \nu_2\sin\varphi, \nu_3\sin\varphi], \qquad (2)$$

the rotation is described in cubic coordinates by a matrix R_0 of the form [see *e.g.* Synge (1960) or Grimmer (1974*a*)]:

$$R_0=\begin{pmatrix}\alpha^2+\beta^2-\gamma^2-\delta^2 & 2(\beta\gamma-\alpha\delta) & 2(\beta\delta+\alpha\gamma)\\ 2(\beta\gamma+\alpha\delta) & \alpha^2-\beta^2+\gamma^2-\delta^2 & 2(\gamma\delta-\alpha\beta)\\ 2(\beta\delta-\alpha\gamma) & 2(\gamma\delta+\alpha\beta) & \alpha^2-\beta^2-\gamma^2+\delta^2\end{pmatrix}; \qquad (3)$$

it transforms the vector $\boldsymbol{\varepsilon}\xi$ into $\boldsymbol{\varepsilon}\xi'=\boldsymbol{\varepsilon}R_0\xi$.

The hexagonal components n of the rotation axis are given by $\mathbf{e}n=\boldsymbol{\varepsilon}Sn=\boldsymbol{\varepsilon}\nu$, *i.e.* $\nu=Sn$:

$$\nu_1=n_1-n_2/2, \quad \nu_2=\sqrt{3}n_2/2, \quad \nu_3=\rho n_3 \qquad (4)$$

and

$$1=\nu_1^2+\nu_2^2+\nu_3^2=n_1^2-n_1n_2+n_2^2+\rho^2n_3^2. \qquad (5)$$

Introducing parameters

$$(A, B, C, D)=\pm(\cos\varphi, n_1\sqrt{3}\rho\sin\varphi, n_2\sqrt{3}\rho\sin\varphi, n_3\sqrt{3}\rho\sin\varphi), \qquad (6)$$

one obtains from (2) and (4)

$$[\alpha, \beta, \gamma, \delta]=[A, (B-C/2)/\sqrt{3}\rho, C/2\rho, D/\sqrt{3}], \qquad (7)$$

so that R_0 becomes

$$R_0=\frac{1}{3}\begin{pmatrix}3A^2-D^2+\tau(B^2-BC-C^2/2) & \sqrt{3}[\tau C(B-C/2)-2AD] & \sqrt{\tau}[D(2B-C)+3AC]\\ \sqrt{3}[\tau C(B-C/2)+2AD] & 3A^2-D^2-\tau(B^2-BC-C^2/2) & \sqrt{3\tau}[CD-A(2B-C)]\\ \sqrt{\tau}[D(2B-C)-3AC] & \sqrt{3\tau}[CD+A(2B-C)] & 3A^2+D^2-\tau(B^2-BC+C^2)\end{pmatrix} \qquad (8)$$

where

$$\tau=1/\rho^2. \qquad (9)$$

Using (6) and (5) one finds that the parameters (A, B, C, D) satisfy the normalization condition

$$3A^2+D^2+\tau(B^2-BC+C^2)$$
$$=3[\cos^2\varphi+\sin^2\varphi(\rho^2n_3^2+n_1^2-n_1n_2+n_2^2)]=3. \qquad (10)$$

Expressing the original and rotated vectors in the basis $\mathbf{e}$, one obtains $\boldsymbol{\varepsilon}\xi=\mathbf{e}S^{-1}\xi=\mathbf{e}x$ and $\boldsymbol{\varepsilon}\xi'=\boldsymbol{\varepsilon}R_0\xi=\mathbf{e}S^{-1}R_0Sx=\mathbf{e}Rx$, where $x=S^{-1}\xi$ and $R=S^{-1}R_0S$, *i.e.*

$$R=\frac{1}{3}\begin{pmatrix}3A^2+2AD-D^2+\tau(B^2-C^2) & \tau B(2C-B)-4AD & 2[BD+A(2C-B)]\\ \tau C(2B-C)+4AD & 3A^2-2AD-D^2-\tau(B^2-C^2) & 2[CD-A(2B-C)]\\ \tau[D(2B-C)-3AC] & \tau[D(2C-B)+3AB] & 3A^2+D^2-\tau(B^2-BC+C^2)\end{pmatrix}. \qquad (11)$$

We summarize: a rotation by an angle $\theta=2\varphi$ around an axis with hexagonal coordinates $[B, C, D]$ satisfying the normalization condition

$$B^2-BC+C^2+\rho^2D^2=3\rho^2\sin^2\varphi \qquad (12)$$

is given by the matrix R (11), where $A=\cos\varphi$. The parameters (A, B, C, D), which (together with $\tau=a^2/c^2$) determine R, will be called a (hexagonal) quadruple. They satisfy the normalization condition

(10). The analogous cubic quadruple $[\alpha, \beta, \gamma, \delta]$ is usually called a unit quaternion.

3. The multiplication law for hexagonal quadruples

The rotations form a group. Its neutral element is the rotation by an angle $\theta = 0$, described by the quadruples $\pm(1, 0, 0, 0)$. If $\pm(A, B, C, D)$ describe the rotation n, $\theta = 2\varphi$ according to (6), the inverse rotation $-n$, θ is described by $(A, -B, -C, -D)$ or $(-A, B, C, D)$. The multiplication law of quadruples, which describes the effect of two successive rotations, will be derived for the general case where the two rotations may be described in crystal coordinate systems with different values of c/a. A practical application where this is used is the following: the relative orientation of a pair of neighbouring grains was found to be $(a, b, c, d)_r$, where r is the measured value of the axial ratio. This is approximated by a coincidence orientation $(A, B, C, D)_R$ of a lattice with R close to r. How big is the difference $(a, b, c, d)_r$ $(-A, B, C, D)_R$?

$$\begin{aligned}(a\ b\ c\ d)_r&(A\ B\ C\ D)_R\\ =\Bigg(&aA-\frac{dD}{3}-\frac{bB-(bC+cB)/2+cC}{3rR},\\ &\rho\left[\frac{aB}{R}+\frac{bA}{r}+\frac{(2c-b)D}{3r}-\frac{d(2C-B)}{3R}\right],\\ &\rho\left[\frac{aC}{R}+\frac{cA}{r}-\frac{(2b-c)D}{3r}+\frac{d(2B-C)}{3R}\right],\\ &aD+dA+\frac{bC-cB}{2rR}\Bigg)_\rho. \qquad (13a)\end{aligned}$$

This formula was obtained by replacing the quadruples on the left-hand side by quaternions according to (7), applying the law of quaternion multiplication [*e.g.* equation (3) in Grimmer (1974*a*)] and changing back to hexagonal quadruples. Equation (13*a*) simplifies in the special case $r = R = \rho$ to

$$\begin{aligned}(a\ b\ c\ d)&(A\ B\ C\ D)\\ =\tfrac{1}{3}(&3aA-dD-\tau[bB-(bC+cB)/2+cC],\\ &3aB+3bA+(2c-b)D-d(2C-B),\\ &3aC+3cA-(2b-c)D+d(2B-C),\\ &3[aD+dA+\tau(bC-cB)/2]). \qquad (13b)\end{aligned}$$

4. Equivalent rotations; choice of a representative in each equivalence class

Consider a pair of neighbouring grains of the same hexagonal phase. The relative orientation of their lattices can be described by different rotations: if R is a rotation that turns lattice 1 parallel to lattice 2 then any of the 12 symmetry rotations S_i followed by R, *i.e.* $R' = RS_i$, $i = 1, \ldots, 12$, has the same effect as R. The rotation may be expressed also in a symmetry-equivalent basis, $R' = S_j^{-1}RS_j$, and either lattice may be taken as lattice 1. Up to $2\times12^2 = 288$ different rotations $R' = S_j^{-1}RS_k$ and $R' = S_j^{-1}R^{-1}S_k$ are obtained in this way. They were called (hexagonally) equivalent by Grimmer (1980), who showed that the number N of different rotations in any (hexagonal) equivalence class is a divisor of 288 and a multiple of 12, *i.e.* $w = N/12$ is always an integer dividing 24. An example with $w = 1$ is the equivalence class consisting of the 12 hexagonal symmetry rotations (*i.e.* the elements of the group 622).* Consider one of the 24 stereographic triangles (ST) into which the sphere is divided by mirror planes of the group $6/mmm$ and consider the equivalent rotations with angle $\leq 180°$ and axis in the interior or on the surface of this triangle. Each ST contains the same numbers of equivalent rotations with the same rotation angles. If an equivalence class contains 288 rotations, each rotation will have an angle $< 180°$ and an axis in the interior of a ST. The maximum number of equivalent rotations with axis in or on the surface of a given ST is 12: the maximum number of different rotation angles in an equivalence class is also 12.

Grimmer (1980) gave also the relations between the quaternions corresponding to the rotations in an equivalence class. These relations between equivalent quaternions can be translated into relations between equivalent hexagonal quadruples by means of (7). Table 1 gives 12 quadruples representing the different rotation angles that occur in an equivalence class.† The $2\times288 = 576$ equivalent hexagonal quadruples are obtained from those in the table by arbitrary combinations of the following four operations: (*a*) sign change of the first component; (*b*) sign change of the fourth component; (*c*) interchanging the second and third components; (*d*) replacing the second and third components B, C by $B-C$, B. Applying this repeatedly one obtains $(B, C) \to (B-C, B) \to (-C, B-C) \to (-B, -C) \to (C-B, -B) \to (C, C-B) \to (B, C)$.

Quadruples connected by these operations correspond to rotations with the same angle and with axes related by symmetry operations of the hexagonal lattice: (*a*) inversion, (*b*/*c*) reflections in planes perpendicular/parallel to the sixfold axis, (*d*) 60° rotation.

Using the connection between equivalent quadruples one finds that one and only one quadruple in

* This definition of equivalence is appropriate for our purpose of dealing with coincidence site and DSC (dislocation shift complete) lattices. It may not be appropriate to classify the possible atomic arrangements in a bicrystal if the symmetry of the crystal structure differs from the lattice symmetry.

† A similar table was given by Hagège & Nouet (1985).

Table 1. 12 *equivalent quadruples representing the different rotation angles that occur in an equivalence class, obtained by letting operators I, J, K, L act on the quadruple* $q=(A, B, C, D)$

q	(	A	B	C	D	)
Iq	(	$[A+D]/2$	B	C	$[3A-D]/2$	)
Jq	(	$[D-A]/2$	B	C	$[3A+D]/2$	)
Kq	$(1/\sqrt{3})($	D	$B-2C$	$2B-C$	$3A$	)
IKq	$(1/\sqrt{3})($	$[3A+D]/2$	$B-2C$	$2B-C$	$3[D-A]/2$	)
JKq	$(1/\sqrt{3})($	$[3A-D]/2$	$B-2C$	$2B-C$	$3[A+D]/2$	)
Lq	$\rho($	$[B-C]\tau/2$	$A+D$	$2A$	$[B+C]\tau/2$	)
ILq	$\rho($	$B\tau/2$	$A+D$	$2A$	$[B-2C]\tau/2$	)
JLq	$\rho($	$C\tau/2$	$A+D$	$2A$	$[2B-C]\tau/2$	)
KLq	$(\rho/\sqrt{3})($	$[B+C]\tau/2$	$D-3A$	$2D$	$3[B-C]\tau/2$	)
$IKLq$	$(\rho/\sqrt{3})($	$[2B-C]\tau/2$	$D-3A$	$2D$	$3C\tau/2$	)
$JKLq$	$(\rho/\sqrt{3})($	$[B-2C]\tau/2$	$D-3A$	$2D$	$3B\tau/2$	)

each equivalence class satisfies the conditions*

$$B \geq 2C \geq 0, \qquad D \geq 0 \tag{14}$$

$$A \geq \sigma B/2, \qquad A \geq \sigma(2B-C)/\sqrt{12},$$

$$A \geq (2/\sqrt{3}+1)D \tag{15}$$

$$D \leq \sigma(B-2C)/2 \quad \text{if } A=\sigma B/2 \tag{16a}$$

$$D \leq \sqrt{3}\sigma C/2 \quad \text{if } A=\sigma(2B-C)/\sqrt{12} \tag{16b}$$

$$B \geq (2+\sqrt{3})C \quad \text{if } A=(2/\sqrt{3}+1)D. \tag{16c}$$

Equation (14) chooses among equivalent rotations one with axis in the standard stereographic triangle, (15) one with minimum rotation angle. If there are several such rotations, (16*a*)-(16*c*) will make a unique choice.

A quadruple satisfying (14)-(16) will be called the representative quadruple $\{A, B, C, D\}$ of its equivalence class, the corresponding rotation the representative rotation. A rotation that corresponds to a quadruple satisfying (14) and (15) is usually called a disorientation.

Table 2 gives for each equivalence class a number of properties that are determined by the form of its representative quadruple. This quadruple is given there with a first component equal to 1. To obtain the normalization condition (10), each of the four components $\{1, b, c, d\}$ has to be divided by $[1+(b^2-bc+c^2+\rho^2 d^2)/3\rho^2]^{1/2}$.

In Appendix *A*, Table 2 is expressed in the language of orthogonal coordinates and quaternions, which shows how the first three columns of the table follow from Figs. 2 and 3 in Grimmer (1980).

5. Coincidence rotations

We restrict our attention from now on to rotations that generate a three-dimensional lattice of coincidence sites. A rotation is of this type if and only if its matrix R expressed in lattice coordinates is rational, *i.e.* has only rational matrix elements (Warrington, 1975; Grimmer, 1976). From the algorithm for matrix inversion it follows that R^{-1} is rational if and only if R is rational. R^{-1} is obtained by replacing A by $-A$ in (11). We shall denote the elements of R by R^+_{ij}, the elements of R^{-1} by R^-_{ij}. It follows from (11) and (10) that

$$4A^2 = 1+R^+_{11}+R^+_{22}+R^+_{33} \tag{17a}$$

$$4AB = R^+_{13}-R^-_{13}-2R^+_{23}+2R^-_{23} \tag{17b}$$

$$4AC = 2R^+_{13}-2R^-_{13}-R^+_{23}+R^-_{23} \tag{17c}$$

$$4AD = 3(R^+_{11}-R^-_{11}) \tag{17d}$$

$$4BD = 3(R^+_{13}+R^-_{13}) \tag{17e}$$

$$4CD = 3(R^+_{23}+R^-_{23}) \tag{17f}$$

$$4D^2 = 3(1-R^+_{11}-R^+_{22}+R^+_{33}) \tag{17g}$$

$$\tau B^2 = 1+R^+_{11}-R^+_{22}-R^+_{33}+R^+_{12} \tag{17h}$$

$$2\tau BA = R^+_{32}-R^-_{32} \tag{17i}$$

$$2\tau BD = 2R^+_{31}+2R^-_{31}+R^+_{32}+R^-_{32} \tag{17j}$$

$$2\tau BC = 1-R^+_{33}+2R^+_{12}+2R^+_{21} \tag{17k}$$

$$2\tau AC = R^-_{31}-R^+_{31} \tag{17l}$$

$$2\tau DC = R^+_{31}+R^-_{31}+2R^+_{32}+2R^-_{32} \tag{17m}$$

$$\tau C^2 = 1-R^+_{11}+R^+_{22}-R^+_{33}+R^+_{21}. \tag{17n}$$

Since the right-hand sides of (17) are rational, it follows for irrational τ from (17*b*, *i*) that $AB=0$, from (17*c*, *l*) that $AC=0$, from (17*e*, *j*) that $BD=0$, from (17*f*, *m*) that $CD=0$, *i.e.* either $A=D=0$ or $B=C=0$. If $A\neq 0$, one obtains from (17*a*)-(17*d*) that there exists a number $k\neq 0$ and four coprime integers m, U, V, W such that

$$A^2=km, \quad AB=kU, \quad AC=kV, \quad AD=kW. \tag{18}$$

'Coprime' means that the greatest common divisor of the integers equals 1, *i.e.*

$$\text{g.c.d.}(m, U, V, W)=1. \tag{19}$$

From (18) and (10) one obtains

$$km = A^2 = A^2[3A^2+D^2+\tau(B^2-BC+C^2)]/3$$
$$= k^2[3m^2+W^2+\tau(U^2-UV+V^2)]/3 = k^2 s, \tag{20}$$

where

$$s=[3m^2+W^2+\tau(U^2-UV+V^2)]/3. \tag{21}$$

It follows that $k=m/s$, whence $A^2=m^2/s$ and

$$A=m/\sqrt{s}, \quad B=U/\sqrt{s}, \quad C=V/\sqrt{s}, \quad D=W/\sqrt{s}. \tag{22}$$

Equation (22) with m, U, V, W satisfying (19) remains true also if $A=0$. This follows from (17*h*)-(17*k*) if $B\neq 0$, from (17*k*)-(17*n*) if $C\neq 0$, from (17*d*)-(17*g*) if $D\neq 0$. $A=B=C=D=0$ is not

* Grimmer (1980) derived restrictions on quaternions equivalent to (14)-(16); restrictions on quaternions equivalent to (14), (15) were derived independently also by Bonnet (1980).

Table 2. *Some properties of an equivalence class that are determined by the form of its representative quadruple*

$n = 12w$ is the number of different rotations, n_{180} the number of 180° rotations in the class. The column * indicates (for $w < 24$) the conditions (16*a*)-(16*c*) that are satisfied.

w	Representative quadruple	*	n_{180}	Axes of 180° rotations in the SST
1	$\{1, 0, 0, 0\}$		7	$1, 0, 0; 2, 1, 0; 0, 0, 1$
1	$\{1, 0, 0, 2\sqrt{3}-3\}$	c	6	$1, 2-\sqrt{3}, 0$
2	$\{1, 0, 0, d\}$, $0<d<2\sqrt{3}-3$		12	$3+d, 2d, 0; 2, 1-d, 0$
3	$\{1, 2\rho, \rho, 0\}$	a	6	$\rho, 0, 1$
3	$\{1, \sqrt{3}\rho, 0, 0\}$	b	6	$2\rho, \rho, \sqrt{3}$
6	$\{1, 2c, c, 0\}$, $0<c<\rho$		12	$c, 0, 1; \rho^2, 0, c$
6	$\{1, b, 0, 0\}$, $0<b<\sqrt{3}\rho$		12	$2b, b, 3; 2\rho^2, \rho^2, b$
6	$\{1, 2\rho, 2(2-\sqrt{3})\rho, 2\sqrt{3}-3\}$	abc	0	
12	$\{1, b, c, 0\}$, $0<2c<b\begin{cases}\le 2\rho \\ \le \sqrt{3}\rho + c/2\end{cases}$	$=\to a$ $=\to b$	12	$2b-c, b-2c, 3$
12	$\{1, b, 0, d\}$, $0<b<\sqrt{3}\rho$, $0<d\le 2\sqrt{3}-3$	$=\to c$	12	$2\rho^2, \rho^2(1-d), b$
12	$\{1, 2c, c, d\}$, $0<c<\rho$, $0<d<2\sqrt{3}-3$		12	$\rho^2(3+d), 2\rho^2 d, 3c$
12	$\{1, 2\rho, \rho(1-d), d\}$, $0<d<2\sqrt{3}-3$	a	0	
12	$\{1, \rho(\sqrt{3}+x), 2\rho x, \sqrt{3}x\}$, $0<x<2-\sqrt{3}$	b	0	
12	$\{1, b, (2-\sqrt{3})b, 2\sqrt{3}-3\}$, $0<b<2\rho$	c	0	
24	All other representative quadruples	-	0	

possible because of (10). Substitution of (22) into (11) gives

$$R = \frac{1}{3s}\begin{pmatrix} 3m^2+2mW-W^2+\tau(U^2-V^2) & \tau U(2V-U)-4mW & 2[UW+m(2V-U)] \\ \tau V(2U-V)+4mW & 3m^2-2mW-W^2-\tau(U^2-V^2) & 2[VW-m(2U-V)] \\ \tau[W(2U-V)-3mV] & \tau[W(2V-U)+3mU] & 3m^2+W^2-\tau(U^2-UV+V^2) \end{pmatrix}, \quad (23)$$

where

$$m = W = 0 \text{ or } U = V = 0 \text{ if } \tau \text{ is irrational.} \quad (24)$$

Equations (23) and (21) show that the conditions (19) and (24) are also sufficient to guarantee that R is rational, *i.e.* that R describes a coincidence rotation. Coincidence rotations can therefore be denoted by quadruples (m, U, V, W) consisting of four coprime integers. To obtain this result we have replaced the normalization condition (10) by (19). The expressions $[B, C, D]$ for the axis and $\cos\varphi = A$ for the half-angle of the rotation become now $[U, V, W]$ and $\cos\varphi = m/\sqrt{s}$, *i.e.*

$$\cos\varphi = \left[\frac{3m^2}{3m^2+W^2+\tau(U^2-UV+V^2)}\right]^{1/2}. \quad (25)$$

It follows that

$$\tan\varphi = \left[\frac{\tau(U^2-UV+V^2)+W^2}{3m^2}\right]^{1/2} = \left[\frac{\tau(u^2-uv+v^2)+w^2}{3}\right]^{1/2}\frac{n}{m}, \quad (26)$$

where

$$n = \text{g.c.d.}(U, V, W), \qquad u = U/n, \quad v = V/n, \quad w = W/n. \quad (27)$$

From (27) it follows that

$$\text{g.c.d.}(u, v, w) = 1 \quad (28)$$

and [because of (19)] that

$$\text{g.c.d.}(m, n) = 1. \quad (29)$$

We conclude that a coincidence rotation is a rotation about a lattice vector $[u, v, w]$ by a half-angle φ, the tangent of which is the product of an arbitrary rational number n/m times the quantity $\{[\tau(u^2-uv+v^2)+w^2]/3\}^{1/2}$, which is proportional to the length of the vector $[u, v, w]$.* An additional restriction is imposed on coincidence rotations by (24) if τ is not rational. Then a coincidence rotation is either ($m = W = 0$) a 180° rotation around a lattice vector perpendicular to the sixfold axis or ($U = V = 0$) a rotation around the sixfold axis with a rational value for $\sqrt{3}\tan\varphi$. Equations (23) and (21) show that R does not depend on τ if $U = V = 0$ or $m = W = 0$. The coincidence rotations for irrational τ are therefore the same for each value of τ and they coincide with those coincidence rotations for any rational values of τ that satisfy $U = V = 0$ or $m = W = 0$.

If τ is rational, then there exist positive integers μ, ν satisfying

$$\nu/\mu = \tau \quad (30)$$

$$\text{g.c.d.}(\mu, \nu) = 1. \quad (31)$$

If we set

$$F = 3\mu s = \mu(3m^2+W^2)+\nu(U^2-UV+V^2), \quad (32)$$

* Fortes (1977) gave a similar characterization for coincidence rotations in arbitrary lattices.

(23) becomes

$$R=\frac{1}{F}\begin{pmatrix} \mu(3m^2+2mW-W^2)+\nu(U^2-V^2) & \nu U(2V-U)-4\mu mW & 2\mu[UW+m(2V-U)] \\ \nu V(2U-V)+4\mu mW & \mu(3m^2-2mW-W^2)-\nu(U^2-V^2) & 2\mu[VW-m(2U-V)] \\ \nu[W(2U-V)-3mV] & \nu[W(2V-U)+3mU] & \mu(3m^2+W^2)-\nu(U^2-UV+V^2) \end{pmatrix}. \quad (33)$$

The elements of the matrices $r^+=F.R$ and $r^-=F.R^{-1}$ are integers because μ, ν, U, V, W and $\pm m$ are integers. From (27) one can see that (33) is equivalent to equation (25) in BNHD and to equation (5) in Delavignette (1982). The additional parameter α in their equations stresses the fact that the elements of the matrix r may have a factor in common.

If one multiplies both sides of (17) by $F=3\mu s$ and defines $r^{\mp}_{ij}=FR^{\mp}_{ij}$ one obtains with (22) and (30):

$$12\mu m^2=F+r^+_{11}+r^+_{22}+r^+_{33} \quad (34a)$$
$$12\mu mU=r^+_{13}-r^-_{13}-2r^+_{23}+2r^-_{23} \quad (34b)$$
$$12\mu mV=2r^+_{13}-2r^-_{13}-r^+_{23}+r^-_{23} \quad (34c)$$
$$4\mu mW=r^+_{11}-r^-_{11} \quad (34d)$$
$$4\mu UW=r^+_{13}+r^-_{13} \quad (34e)$$
$$4\mu VW=r^+_{23}+r^-_{23} \quad (34f)$$
$$4\mu W^2=F-r^+_{11}-r^+_{22}+r^+_{33} \quad (34g)$$
$$3\nu U^2=F+r^+_{11}-r^+_{22}-r^+_{33}+r^+_{12} \quad (34h)$$
$$6\nu Um=r^+_{32}-r^-_{32} \quad (34i)$$
$$6\nu UW=2r^+_{31}+2r^-_{31}+r^+_{32}+r^-_{32} \quad (34j)$$
$$6\nu UV=F-r^+_{33}+2r^+_{12}+2r^+_{21} \quad (34k)$$
$$6\nu mV=r^-_{31}-r^+_{31} \quad (34l)$$
$$6\nu WV=r^+_{31}+r^-_{31}+2r^+_{32}+2r^-_{32} \quad (34m)$$
$$3\nu V^2=F-r^+_{11}+r^+_{22}-r^+_{33}+r^+_{21}. \quad (34n)$$

6. The multiplicity Σ of the CSL generated by R

Because the computation of Σ is the central theme of this paper, we shall digress for a moment in order to place it in a more general context. Consider a boundary between two arbitrary phases. If $\mathbf{b}^1$ and $\mathbf{b}^2$ are bases of the corresponding lattices and v_1 and v_2 the volumes of primitive cells, one can write

$$\mathbf{b}^2=\mathbf{b}^1T \quad \text{and} \quad v_2=\|T\|v_1,$$

where $\|T\|$ denotes the absolute value of the determinant of the matrix T. Grimmer (1976) showed that the two lattices have a CSL in common if and only if T is rational. The volume v of a primitive cell of the CSL can be written as

$$v=\Sigma_1v_1=\Sigma_2v_2,$$

where Σ_2 is the lowest positive integer such that $\Sigma_2\|T\|$ is an integer and that Σ_2T and $\Sigma_2\|T\|T^{-1}$ are integral matrices, $\Sigma_1=\|T\|\Sigma_2$ [Fortes (1983); see also Yang (1982)]. If T is the matrix R of a rotation (more generally if $\|T\|=1$) it follows that $\Sigma_1=\Sigma_2=\Sigma$ is the least positive integer such that ΣR and ΣR^{-1} are integral matrices (Grimmer, 1976). Σ is then the lowest common multiple of Σ' and Σ'',

$$\Sigma=\text{l.c.m.}(\Sigma',\Sigma''), \quad (35)$$

where Σ' and Σ'' denote the lowest common denominators of the matrix elements of R and R^{-1} respectively. In the case of orthonormal axes, R^{-1} is the transpose of R, *i.e.* $\Sigma=\Sigma'=\Sigma''$ for the primitive cubic lattice.* $\Sigma'=\Sigma''$ is not necessarily true for rotations expressed in terms of hexagonal axes. The implicit proposal (Warrington, 1975; BNHD) that $\Sigma=\Sigma'$ for hexagonal lattices is not always correct; examples to the contrary have been given by Grimmer & Warrington (1985).

Because $r^+=FR$ and $r^-=FR^{-1}$ have integral matrix elements, it follows that Σ', Σ'' and Σ are factors of F, *i.e.* there exist integers α', α'' and α such that

$$F=\alpha'\Sigma'=\alpha''\Sigma''=\alpha\Sigma. \quad (36)$$

Equations (34*a*, *h*, *n*, *g*) show that α' is a factor of $12\mu m^2, 3\nu U^2, 3\nu V^2, 4\mu W^2$. It follows because of (19) that α' is a factor of $12\mu\nu$, *i.e.* Σ' is a multiple of $F/12\mu\nu$.

Consider the case μ and ν odd, α' even (*i.e.* all the r^+_{ij} are even). The expression for r^+_{12} in (33) shows that U is even, the one for r^+_{21} that V is even. The expression for r^+_{33} shows then that $3m^2+W^2$ is even, *i.e.* m and W are both odd or both even. The latter is not compatible with (19). Equation (33) shows then that all the r^+_{ij} are multiples of 4. We conclude that α' has the form

$$\alpha'=\beta\gamma, \quad (37)$$

where $\beta=1,3,4$ or 12 and γ is a factor of $\mu\nu$. This remains true even if μ and ν are not both odd because (37) is then equivalent to the statement that α' is a factor of $12\mu\nu$. Equation (37) corresponds to equation (26) in BNHD. The proof presented above is more direct than the one given in the Appendix of BNHD.

The properties proved for α' can be proved similarly for α'' because (34*a*, *h*, *n*, *g*) remain true on replacing r^+_{ij} by r^-_{ij}. It follows that (37) remains true for α'' and α and also that Σ'' and Σ are multiples

* A given rotation leads to the same value Σ for f.c.c. and b.c.c. lattices as for the primitive cubic lattice.

of $F/12\mu\nu$. Because α is a divisor of F [see (36)] and of the $r_{ij}^{\pm}$, it follows from (34*a*)-(34*d*) and (19) that*

$$\alpha|12\mu m \qquad (38a)$$

and similarly that

$$\alpha|4\mu W \qquad (38b)$$

$$\alpha|6\nu U \qquad (38c)$$

$$\alpha|6\nu V, \qquad (38d)$$

which give because of (19) an alternative proof that

$$\alpha|12\mu\nu. \qquad (39)$$

7. A simplified procedure to compute Σ

Many calculations involving coincidence rotations can most easily be performed by using the quadruple description of the rotations. To determine Σ according to the method given in § 6, however, one has to return to the matrix description by determining first the two matrices R and R^{-1} and then computing Σ as the lowest positive integer such that ΣR and ΣR^{-1} are integral matrices.

Hagège & Nouet (1985) proposed a set of rules for computing $\alpha = F/\Sigma$ as a function of μ, ν, m, n, u, v and w without passing through R and R^{-1}. They tested their rules on many examples but did not give a proof of their general validity. The aim of the present section is to show that there are certain cases where their rules do not give the correct result and to propose as a theorem a modified procedure, which is even somewhat simpler.

If we write $\Sigma = F/\alpha$, where F is given by (32) as

$$F = \mu(3m^2 + W^2) + \nu(U^2 - UV + V^2),$$

α can be computed as follows.

α-hex theorem

$$\alpha = \alpha_1\alpha_2\alpha_3\alpha_4, \qquad (40)$$

where

$$\alpha_1 = \text{g.c.d.}(12, 3m^2 + W^2, U^2 - UV + V^2), \quad (41)$$

α_2 is the greatest common divisor of μ, $3U$ and $3V$ satisfying

$$\alpha_2^2|3(U^2 - UV + V^2)/\alpha_1, \qquad (42)$$

$$\alpha_3 = \text{g.c.d.}[4, \nu, (3m^2 + W^2)/\alpha_1], \qquad (43)$$

and α_4 is the greatest common divisor of ν/α_3, W and m satisfying

$$\alpha_4^2|(3m^2 + W^2)/\alpha_1\alpha_3. \qquad (44)$$

* $g|h$ where g and h are integers and $g \neq 0$ means that h is an integral multiple of g; $g \nmid h$ means that h is not an integral multiple of g.

The following examples illustrate the application of the theorem:

(1) $(m, U, V, W) = (1, 4, 2, 3)$
$\rightarrow \alpha_1 = 12$, $\alpha_2 = \alpha_3 = \alpha_4 = 1$
$\rightarrow \alpha = 12$ for any values of μ and ν.

(2) $(m, U, V, W) = (5, 2, 1, 5)$
$\rightarrow \alpha_1 = 1$, $\alpha_2 = \text{g.c.d.}(3, \mu)$, $\alpha_3 = \text{g.c.d.}(4, \nu)$, $\alpha_4 = \text{g.c.d.}(5, \nu)$
$\rightarrow \alpha = \text{g.c.d.}(3, \mu) \times \text{g.c.d.}(20, \nu)$.

(3) $(m, U, V, W) = (2, 3, 1, 2)$
$\rightarrow \alpha_1 = \alpha_2 = 1$, $\alpha_3 = \text{g.c.d.}(4, \nu)$, $\alpha_4 = \text{g.c.d.}(8, \nu)/\alpha_3$
$\rightarrow \alpha = \text{g.c.d.}(8, \nu)$.

Notice that α as given by the theorem satisfies (39) because $\alpha_1|12$, $\alpha_2|\mu$ and $\alpha_3\alpha_4|\nu$. Being an integer, α can be written in exactly one way in the form

$$\alpha = k_1 2^{k_2} 3^{k_3}, \qquad (45)$$

where the k_i are integers and

$$\text{g.c.d.}(6, k_1) = 1. \qquad (46)$$

The proof that the theorem gives k_1 correctly is rather simple but the proofs that it also gives k_2 and k_3 correctly are more involved. The latter proofs will be given in outline here and in detail in Appendix *B*. Each of these three proofs consists of two parts: (*a*) The numbers k_i given by the theorem are not too large, *i.e.* k_1, 2^{k_2} or 3^{k_3} divide all the $r_{ij}^{\pm}$. (*b*) The numbers k_i are not too small, *i.e.* if the l_i are integers such that l_1, 2^{l_2} or 3^{l_3} divides all the $r_{ij}^{\pm}$ then $l_1|k_1$, $l_2 \leq k_2$ or $l_3 \leq k_3$.

(1*a*) k_1 *is not too large.* Define

$$\beta = \text{g.c.d.}(\mu, U, V) \qquad (47)$$

and

$$\gamma = \text{g.c.d.}(\nu, m, W). \qquad (48)$$

Equation (33) shows that each term in each of the 18 numbers $r_{ij}^{\pm}$ contains at least one of the factors μ, U, V and at least one of the factors ν, m, W. It follows that $\beta\gamma|\text{all } r_{ij}^{\pm}$ (*i.e.* that $\beta\gamma$ divides all the $r_{ij}^{\pm}$). The theorem shows that k_1 has the form

$$k_1 = \beta_1\gamma_1, \qquad (49)$$

where β_1 is the largest divisor of β satisfying g.c.d. $(\beta_1, 6) = 1$ and where γ_1 is the largest divisor of γ satisfying g.c.d. $(\gamma_1, 6) = 1$. Because $k_1|\beta\gamma$ it follows that $k_1|\text{all } r_{ij}^{\pm}$.

(1*b*) k_1 *is not too small.* Let l_1 be an integer with

$$\text{g.c.d.}(l_1, 6) = 1 \qquad (50)$$

that divides all the $r_{ij}^{\pm}$. Because of (39) and (31) one can write

$$l_1 = bc, \qquad (51)$$

where

$$b = \text{g.c.d.}\ (l_1, \mu) \tag{52}$$

and

$$c = \text{g.c.d.}\ (l_1, \nu). \tag{53}$$

Because of (31) one has g.c.d. $(b, \nu) =$ g.c.d. $(c, \mu) = 1$. From (38) it follows then that $b|U$, $b|V$, $c|m$, $c|W$. These together with (52) and (53) show that $b|\beta_1$ and $c|\gamma_1$. It follows from (51) and (49) that $l_1|k_1$.

$(2a)$ k_2 *is not too large.* Let k be the number of factors 2 in $\beta\gamma$ defined by (47), (48). The theorem gives for k_2: $k_2 = k$ except for the cases (a)-(d), where $k_2 = k+2$ if (a) or (b) is satisfied, $k_2 = k+1$ otherwise:

(a) $2^k|\mu$, $2^{k+1}|U$, $2^{k+1}|V$, m and W odd
(b) $2^{k+2}|\nu$, $2^k|m$, $2^k|W$, $2^{k+1}|m+W$
(c) $2^k|\mu$, $2^k|U$, $2^k|V$, m and W odd, $k>0$
(d) $2^{k+1}|\nu$, $2^k|m$, $2^k|W$, $2|m+W$.

That $2^k|$all $r_{ij}^{\pm}$ has been shown in $(1a)$, that $2^{k+2}|$all $r_{ij}^{\pm}$ if (a) or (b) is satisfied and that $2^{k+1}|$all $r_{ij}^{\pm}$ if (c) or (d) is satisfied follows from (33).

$(2b)$ k_2 *is not too small.* Making use of (19), (38) and $(34h, n)$ one finds: $2^{k+3}|$not all $r_{ij}^{\pm}$, $2^{k+2}|$all $r_{ij}^{\pm}$ only if (a) or (b) is satisfied, $2^{k+1}|$all $r_{ij}^{\pm}$ only in the cases (a)-(d).

$(3a)$ k_3 *is not too large.* Redefine k to be the number of factors 3 in $\beta\gamma$ defined by (47), (48). The theorem gives for k_3: $k_3 = k$ except in the following three cases, where $k_3 = k+1$:

(a) $3^k|\nu$, $3^k|m$, $3^{k+1}|W$, $3|U+V$
(b) $3^k|\mu$, $3^k|U$, $3^k|V$, $3|W$, $k>0$
(c) $3^{k+1}|\mu$, $3^k|U$, $3^k|V$, $3^{k+1}|U+V$.

That $3^k|$all $r_{ij}^{\pm}$ has been shown in $(1a)$, that $3^{k+1}|$all $r_{ij}^{\pm}$ if one of the conditions (a)-(c) is satisfied follows from (33).

$(3b)$ k_3 *is not too small.* Making use of (19) and (38) one finds: $3^{k+2}|$not all $r_{ij}^{\pm}$, $3^{k+1}|$all $r_{ij}^{\pm}$ only if one of the conditions (a)-(c) is satisfied.

It is easy to see that the theorem can be written in the following simpler form if g.c.d. $(\mu, 6) = 1$ and g.c.d. $(\nu, 6) = 1$.

Corollary 1

If g.c.d. $(\mu\nu, 6) = 1$ then

$$\alpha = \alpha_1\beta\gamma, \tag{54}$$

where

$$\alpha_1 = \text{g.c.d.}\ (12, 3m^2 + W^2, U^2 - UV + V^2), \tag{41}$$

$$\beta = \text{g.c.d.}\ (\mu, U, V), \tag{47}$$

$$\gamma = \text{g.c.d.}\ (\nu, m, W). \tag{48}$$

An example is $(m, U, V, W) = (4, 1, 0, 1)$, $\mu = 1$, $\nu = 7$, where $\alpha_1 = \beta = \gamma = 1$, *i.e.* $\Sigma = F = 56$. The rules of Hagège & Nouet (1985) give in this case $\alpha = \alpha_3'' = 7$, *i.e.* $\Sigma = 8$, which is not correct.

Let us consider two other special cases of the theorem: $U = V = 0$ and $m = W = 0$. If $U = V = 0$ then $\alpha_1 =$ g.c.d. $(12, 3m^2 + W^2)$, $\alpha_2 = \mu$. $\alpha_4 = 1$ because (19) gives g.c.d. $(m, W) = 1$, from which it follows also that g.c.d. $(3m^2 + W^2, 8) = 1$ or 4. $(3m^2 + W^2)/\alpha_1$ is odd in both cases, *i.e.* $\alpha_3 = 1$. It follows that $\alpha = \mu \times$ g.c.d. $(12, 3m^2 + W^2)$. $\Sigma = F/\alpha = (3m^2 + W^2)/$ g.c.d. $(12, 3m^2 + W^2)$. We conclude that:

Corollary 2

If $U = V = 0$ then

$$\Sigma = \frac{3m^2 + W^2}{\text{g.c.d.}\ (3, W) \times [\text{g.c.d.}\ (2, m+W)]^2}.$$

If $m = W = 0$ then g.c.d. $(U, V) = 1$ because of (19). It follows that $U^2 - UV + V^2$ is odd. From g.c.d. $(U, V) = 1$ it follows also that $9 \nmid U^2 - UV + V^2$ and that $3|U^2 - UV + V^2$ if and only if $3|U+V$. It follows that $\alpha_1 =$ g.c.d. $(3, U+V)$, $\alpha_2 = 1$, $\alpha_3 =$ g.c.d. $(4, \nu)$, $\alpha_4 = \nu/\alpha_3$, *i.e.* $\alpha_3\alpha_4 = \nu$ and $\alpha = \nu \times$ g.c.d. $(3, U+V)$. $\Sigma = F/\alpha = (U^2 - UV + V^2)/$g.c.d. $(3, U+V)$. We conclude that:

Corollary 3

If $m = W = 0$ then

$$\Sigma = \frac{U^2 - UV + V^2}{\text{g.c.d.}\ (3, U+V)}.$$

Corollaries 2 and 3 show that Σ does not depend on μ and ν and hence on τ if $U = V = 0$ or $m = W = 0$. They remain true even if τ is irrational.

8. Determination of bases for the CSL and DSC lattices generated by *R*

If the relative orientation between two grains with a common boundary deviates by only a few degrees from a coincidence orientation with a low value of Σ, then it has often been observed that the deviation from exact coincidence is compensated by arrays of dislocations in the boundary. Bollmann showed that the Burgers vectors of such grain boundary dislocations are vectors of a lattice, which he called the 'dislocation shift complete lattice', abbreviated as DSC lattice or DSCL [see *e.g.* Bollmann (1970, 1982)].* To analyse experimentally observed boundaries and their dislocation arrays, it is therefore important to have a convenient algorithm for determining CSL's and the corresponding DSCL's. The

* The Burgers vectors are vectors of small length of the DSCL because the energy of a dislocation is proportional to b^2.

connection between these two lattices and a convenient algorithm to determine bases for both will be given in this section.

The hexagonal lattice formed by the translation vectors with integral components in the basis $\mathbf{e}=(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ will be called lattice 1, the rotated lattice with integral components in the basis $\mathbf{e}R=\mathbf{e}'=(\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3)$ will be called lattice 2. The CSL is the lattice formed by the vectors that belong simultaneously to both lattices, *i.e.* by the vectors with integral components in both bases. The DSCL is the lattice formed by the vectors that are a sum of a vector of lattice 1 and a vector of lattice 2.

If V, V_C and V_D denote the volumes of primitive cells of lattice 1, the CSL and the DSCL respectively, then one has $V_C=V\Sigma$ and $V_D=V/\Sigma$. The latter result was proved by Bonnet & Durand (1975) and by Iwasaki (1976). Grimmer (1974*b*) established a reciprocity relation between CSL and DSCL. Bonnet (1976) presented a convenient method to determine bases for the CSL and the DSCL. His method can also be used to determine Σ. If Σ is known from the α-hex theorem, his method can be further simplified.

(1) Determine $N_1>0$, the lowest integral factor of Σ such that $N_1R^+_{i1}$, $i=1,2,3$, are integers.

(2) Determine n_{12} and N_2, where $N_2>0$ is the lowest integral factor of Σ/N_1 such that $n_{12}R^+_{i1}+N_2R^+_{i2}$, $i=1,2,3$, are integers for a suitable choice of the integer n_{12} in the range $0\le n_{12}<N_1$.

(3) Compute $N_3=\Sigma/N_1N_2$.

A basis for the CSL is obtained as follows: determine the integers n_{13} and n_{23} satisfying $0\le n_{13}<N_1$ and $0\le n_{23}<N_2$, for which $n_{13}R^+_{i1}+n_{23}R^+_{i2}+N_3R^+_{i3}$, $i=1,2,3$, are integers. A basis for the CSL is then given by $\mathbf{e}^c_1=N_1\mathbf{e}'_1$, $\mathbf{e}^c_2=n_{12}\mathbf{e}'_1+N_2\mathbf{e}'_2$, $\mathbf{e}^c_3=n_{13}\mathbf{e}'_1+n_{23}\mathbf{e}'_2+N_3\mathbf{e}'_3$.

A basis for the DSCL is obtained as follows: compute the internal coordinates* of the vectors $n_1\mathbf{e}'_1+n_2\mathbf{e}'_2+n_3\mathbf{e}'_3$, where the n_i are integers satisfying $0\le n_i<N_i$ for $i=1,2,3$. Determine among these Σ triplets of internal coordinates

(*a*) the one of form $(k_{11},0,0)$ with the least $k_{11}>0$ (if there is no such triplet then $\mathbf{e}^D_1=\mathbf{e}_1$ and $k_{11}=1$, otherwise $\mathbf{e}^D_1=k_{11}\mathbf{e}_1$);

(*b*) the one of form $(k_{12}, k_{22}, 0)$ with the least $k_{22}>0$ and $0\le k_{12}<k_{11}$ (if there is no such triplet then $\mathbf{e}^D_2=\mathbf{e}_2$ and $k_{22}=1$, otherwise $\mathbf{e}^D_2=k_{12}\mathbf{e}_1+k_{22}\mathbf{e}_2$);

(*c*) the one of form (k_{13}, k_{23}, k_{33}) with the least $k_{33}>0$, $0\le k_{13}<k_{11}$ and $0\le k_{23}<k_{22}$ (if there is no such triplet then $\mathbf{e}^D_3=\mathbf{e}_3$, otherwise $\mathbf{e}^D_3=k_{13}\mathbf{e}_1+k_{23}\mathbf{e}_2+k_{33}\mathbf{e}_3$).

Another method of determining a basis for the DSCL has been proposed recently by Bleris, Doni, Karakostas, Antonopoulos & Delavignette (1985). Let us consider the same example ($\mu=8$, $\nu=3$, $m=7$, $U=V=0$, $W=3$) as they do to illustrate our method and to compare it with theirs. Corollary 2 gives $\Sigma=13$, (33) gives

$$R=\frac{1}{13}\begin{pmatrix}15 & -7 & 0\\ 7 & 8 & 0\\ 0 & 0 & 13\end{pmatrix}.$$

$N_1=13$, whence $N_2=N_3=1$. $n_{12}=10$. Determination of the CSL: $n_{13}=n_{23}=0$. Using the fact that $\mathbf{e}'$ is given by the columns of R, we obtain

$$\mathbf{e}^C=\begin{pmatrix}15 & 11 & 0\\ 7 & 6 & 0\\ 0 & 0 & 1\end{pmatrix}.$$

Determination of the DSCL: the internal coordinates of $n_1\mathbf{e}'_1$, $0\le n_1<13$ are

$$\frac{1}{13}\begin{pmatrix}0 & 2 & 4 & 6 & 8 & 10 & 12 & 1 & 3 & 5 & 7 & 9 & 11\\ 0 & 7 & 1 & 8 & 2 & 9 & 3 & 10 & 4 & 11 & 5 & 12 & 6\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}.$$

It follows that

$$\mathbf{e}^D=\frac{1}{13}\begin{pmatrix}13 & 4 & 0\\ 0 & 1 & 0\\ 0 & 0 & 13\end{pmatrix}.$$

This procedure is more efficient than the one proposed by Bleris, Doni, Karakostas, Antonopoulos & Delavignette (1985).

HG is grateful for stimulating discussions with Dr S. Hagège on methods of computing Σ. DHW is grateful for support by NATO grant 1650.

APPENDIX *A*
Table 2 expressed in orthogonal coordinates

Grimmer (1980) gave the number N of rotations in a hexagonal equivalence class in Figs. 2 and 3, where he used a normalized orthogonal coordinate system with z axis parallel to the sixfold symmetry axis and x axis parallel to a twofold symmetry axis. The information on $N=12w$ contained in those figures is completed in Table 3. Since 180° rotations are often used to describe twins, the number n_{180} of 180° rotations has been included as well as the axes of those that lie in the standard stereographic triangle (SST) defined by $x\ge\sqrt{3}y\ge0$, $z\ge0$.

A comparison of Tables 3 and 2 shows that the results look somewhat simpler in Table 3, which is no surprise because hexagonal equivalence does not depend on the value of $\rho=c/a$, *i.e.* ρ appears in Table 2 only because the results are expressed there in

* The triplet of non-negative numbers less than 1 obtained by adding appropriate integers to the components v of a vector expressed in the basis $\mathbf{e}$ is called the internal coordinates of the vector.

Table 3. *Table 2 expressed in orthonormal coordinates*

w	Representative quaternion	*	n_{180}	Axes of 180° rotations in the SST
1	$\{1, 0, 0, 0\}$		7	$1, 0, 0; \sqrt{3}, 1, 0; 0, 0, 1$
1	$\{1, 0, 0, 2-\sqrt{3}\}$	c	6	$1, 2-\sqrt{3}, 0$
2	$\{1, 0, 0, d\}, 0<d<2-\sqrt{3}$		12	$1, d, 0; \sqrt{3}+d, 1-\sqrt{3}d, 0$
3	$\{1, \sqrt{3}/2, 1/2, 0\}$	a	6	$1, 0, 1$
3	$\{1, 1, 0, 0\}$	b	6	$\sqrt{3}, 1, 2$
6	$\{1, \sqrt{3}c, c, 0\}, 0<c<1/2$		12	$2c, 0, 1; 1, 0, 2c$
6	$\{1, b, 0, 0\}, 0<b<1$		12	$\sqrt{3}b, b, 2; \sqrt{3}, 1, 2b$
6	$\{1, 1, 2-\sqrt{3}, 2-\sqrt{3}\}$	abc	0	
12	$\{1, b, c, 0\}, 0<\sqrt{3}c<b \begin{cases}\le (2-c)/\sqrt{3} \\ \le 1\end{cases}$	$= \to a$ $= \to b$	12	$\sqrt{3}b+c, b-\sqrt{3}c, 2$
12	$\{1, b, 0, d\}, 0<b<1, 0<d\le 2-\sqrt{3}$	$= \to c$	12	$\sqrt{3}+d, 1-\sqrt{3}d, 2b$
12	$\{1, \sqrt{3}c, c, d\}, 0<c<1/2, 0<d<2-\sqrt{3}$		12	$1, d, 2c$
12	$\{1, (\sqrt{3}+d)/2, (1-\sqrt{3}d)/2, d\}, 0<d<2-\sqrt{3}$	a	0	
12	$\{1, 1, d, d\}, 0<d<2-\sqrt{3}$	b	0	
12	$\{1, b, (2-\sqrt{3})b, 2-\sqrt{3}\}, 0<b<1$	c	0	
24	All other representative quaternions	-	0	

hexagonal lattice coordinates, which depend on ρ. These latter coordinates have been used in the bulk of the paper because they are much better suited to deal with coincidence rotations.

APPENDIX *B*
Details of the proof of the α-hex theorem

*B*1. *Introduction*

α can be written in the form

$$\alpha = k_1 2^{k_2} 3^{k_3}, \tag{45}$$

where k_1 contains the factors different from 2 and 3. It was shown in § 7 that k_1 is given correctly by the α-hex theorem and an outline was given of the proofs that k_2 and k_3 are determined correctly by the α-hex theorem. These proofs will be given here in detail. Each of them consists of three steps: (1) k_n ($n=2$ or 3) as given by the theorem is expressed in terms of k, the number of factors n in $\beta\gamma$, where

$$\beta = \text{g.c.d.}\ (\mu, U, V) \tag{47}$$

and

$$\gamma = \text{g.c.d.}\ (\nu, m, W). \tag{48}$$

(2) k_n is not too large, *i.e.* $n^{k_n}|\text{all } r_{ij}^{\pm}$. (3) k_n is not too small, *i.e.* if $n^{l_n}|\text{all } r_{ij}^{\pm}$ then $l_n \le k_n$.

*B*2. *The number of factors* 2 *in* α

If U and V are not both even then U^2-UV+V^2 is odd. From this follows:

Lemma 1. Let p be the largest integer such that $2^p|U$ and $2^p|V$, q the largest integer such that $2^q|U^2-UV+V^2$. Then $q=2p$.

If m and W are not both even then $4|3m^2+W^2$ and $8\nmid 3m^2+W^2$ if m and W are odd, $2\nmid 3m^2+W^2$ otherwise. From this follows:

Lemma 2. Let p be the largest integer such that $2^p|m$ and $2^p|W$, q the largest integer such that $2^q|3m^2+W^2$. Then $q=2p+2$ if $2^{p+1}|m+W$, $q=2p$ otherwise.

The reasoning that led to these lemmas shows also that α_1 defined by (41) is either odd or a multiple of 4. In fact, if α_1 is even then (a) U^2-UV+V^2 is even, whence U and V are even, *i.e.* $4|U^2-UV+V^2$; (b) $3m^2+W^2$ is even, whence m and W are odd [they cannot both be even because of (19)], *i.e.* $4|3m^2+W^2$. It follows that $4|\alpha_1$.

*B*2.1. k_2 *according to the theorem*

It will be shown here that the theorem gives four cases (a)-(d) with $k_2>k$, where k is the number of factors 2 in $\beta\gamma$. Equation (31) shows that either $2\nmid\mu$ or $2\nmid\nu$, *i.e.* at most one of the two numbers β and γ contains factors 2.

(1) $4|\alpha_1$. Then $2|(U, V)$, $2\nmid(m, W)$.*

(1.1) $k=0$. Then $2\nmid(\alpha_2, \alpha_4)$. $\alpha_3=1$ because lemma 2 shows that $(3m^2+W^2)/\alpha_1$ is odd. Then $k_2=k+2$ (a_1). This covers also the case $2\nmid\mu$ for arbitrary k because then $2^k|\text{g.c.d.}\ (\nu, m, W)$, whence $k=0$ because $2\nmid(m, W)$.

(1.2) $k>0$, $2\nmid\nu$, *i.e.* $2^k|\text{g.c.d.}\ (\mu, U, V)$. Then $2\nmid(\alpha_3, \alpha_4)$. (42) then gives $k_2=k+2$ if $2^{2k}|(U^2-UV+V^2)/4$. Lemma 1 shows that this is the case if and only if $2^{k+1}|(U, V)$ (a_2). Otherwise $k_2=k+1$ because $2^{2(k-1)}|(U^2-UV+V^2)/4$ is always satisfied (c).

(2) $4\nmid\alpha_1$.

(2.1) $2\nmid\mu$, *i.e.* $2^k|\text{g.c.d.}\ (\nu, m, W)$. Then $2\nmid\alpha_2$.

(2.1.1) $\alpha_3=1$. Equation (44) gives $k_2=k$.

(2.1.2) $\alpha_3>1$, *i.e.* $2|\nu$ and $2|m+W$. Then $k_2=k$ if $2^{k+1}\nmid\nu$, $k_2=k+2$ if $2^{k+2}|\nu$ and $2^{k+1}|m+W$ (because in this case $\alpha_3=4$ and $\alpha_4=2^k$ by lemma 2) (b), $k_2=k+1$ otherwise (d).

(2.2) $2\nmid\nu$, *i.e.* $2^k|\text{g.c.d.}\ (\mu, U, V)$. Then $2\nmid(\alpha_3, \alpha_4)$. Equation (42) gives $k_2=k$.

* $n|(p, q)$ means n divides p and q, *i.e.* $n|p$ and $n|q$; $n\nmid(p, q)$ means n divides neither p nor q, *i.e.* $n\nmid p$ and $n\nmid q$.

In summary, the theorem gives $k_2 = k$ except in the cases (a)-(d), where $k_2 = k+2$ if (a) or (b) is satisfied, $k_2 = k+1$ otherwise:

(a) $2^k|\mu$, $2^{k+1}|(U, V)$, m and W odd
(b) $2^{k+2}|\nu$, $2^k|(m, W)$, $2^{k+1}|m+W$
(c) $2^k|(\mu, U, V)$, m and W odd, $k>0$
(d) $2^{k+1}|\nu$, $2^k|(m, W)$, $2|m+W$.

B2.2. k_2 is not too large

It has to be shown that $2^{k_2}|$all $r_{ij}^{\pm}$. This follows from (33): for $k_2 = k$ it has been shown in $(1a)$ of § 7; for (b), (c) and (d) it is easily verified; to verify it for (a), the following hints may be useful: To see that 2^{k+2} divides $r_{11}^{\pm}$ and $r_{22}^{\pm}$ use the fact that $W \pm m$ are even, $3m^2 \pm 2mW - W^2 = 3m^2 + W^2 - 2W(W \mp m)$; to see that 2^{k+2} divides $r_{31}^{\pm}$ and $r_{32}^{\pm}$ use the fact that $W \pm 3m$ are even.

B2.3. k_2 is not too small

It has to be shown that (1) $2^{k+3}|$not all $r_{ij}^{\pm}$, (2) $2^{k+2}|$all $r_{ij}^{\pm}$ only if (a) or (b) is satisfied, (3) $2^{k+1}|$all $r_{ij}^{\pm}$ only in the cases (a)-(d).

(1) Assume $2^{k+3}|$all $r_{ij}^{\pm}$.

(1.1) $2\nmid\mu$. Equation (38) shows $2^{k+1}|(m, W, \nu U, \nu V)$. Equation (19) gives $2^{k+1}|\nu$, *i.e.* $2^{k+1}|\gamma$ contrary to the definition of k.

(1.2) $2\nmid\nu$. Equation (38) shows $2^{k+1}|(\mu m, \mu W, U, V)$. Equation (19) gives $2^{k+1}|\mu$, *i.e.* $2^{k+1}|\beta$ contrary to the definition of k.

(2) Assume $2^{k+2}|$all $r_{ij}^{\pm}$.

(2.1) $2\nmid\mu$. Equation (38) shows $2^k|(m, W)$, $2^{k+1}|(\nu U, \nu V)$.

(2.1.1) $k=0$ and U, V even. $4|r_{33}^{+}$ shows that $4|3m^2+W^2$. This is possible only if m and W are odd because they cannot both be even according to (19). It follows that (a) is satisfied.

(2.1.2) $k=0$ and U, V not both even or $k>0$. Equation (19) shows that U and V are not both even also if $k>0$. It follows then from $(34h)$ and $(34n)$ that $2^{k+2}|\nu$. $2^{k+2}|r_{33}^{+}$ shows that $2^{k+2}|3m^2+W^2$. Lemma 2 shows that $2^{k+1}|m+W$, *i.e.* (b) is satisfied.

(2.2) $2\nmid\nu$. Equations $(38c)$ and $(38d)$ show $2^{k+1}|(U, V)$. The definition of k gives $2^k|\mu$ and $2^{k+1}\nmid\mu$. $2^{k+2}|r_{33}^{+}$ shows that $4|3m^2+W^2$. This is possible only if m and W are odd because they cannot both be even according to (19). It follows that (a) is satisfied.

(3) Assume $2^{k+1}|$all $r_{ij}^{\pm}$.

(3.1) $2|\nu$. Then $2\nmid\mu$ because of (31). The definition of k gives $2^k|(\nu, m, W)$.

(3.1.1) $k>0$. Equations $(34h)$ and $(34n)$ show that $2^{k+1}|(\nu U^2, \nu V^2)$. Since U and V are not both even according to (19), it follows that $2^{k+1}|\nu$. Then (d) is satisfied.

(3.1.2) $k=0$. From $2|r_{33}^{+}$ follows $2|3m^2+W^2$, whence m and W are both even or both odd, *i.e.* (d) is satisfied.

(3.2) $2\nmid\nu$. The definition of k gives $2^k|(\mu, U, V)$. Equations $(34h)$ and $(34n)$ show that $2|(U, V)$ also if $k=0$. Equation (19) gives therefore for all values of k that m and W are not both even. 2^{k+1} divides r_{33}^{+}, r_{32}^{-} and r_{31}^{+} and therefore $\mu(3m^2+W^2)$, $U(3m+W)$ and $V(3m+W)$. If m or W is even then it follows that $2^{k+1}|$g.c.d. (μ, U, V) contrary to the definition of k, *i.e.* m and W are odd. It follows that (c) is satisfied if $k>0$ and (a) if $k=0$.

B3. The number of factors 3 in α

Use will be made of the following results:

Lemma 3. Let p be the largest integer such that $3^p|U$ and $3^p|V$, q the largest integer such that $3^q|U^2-UV+V^2$. Then $q=2p+1$ if $3^{p+1}|U+V$, $q=2p$ otherwise.

Proof: $q \geq 2p$ is obvious. $U^2-UV+V^2=(U+V)^2-3UV$. If $3^{p+1}\nmid U+V$ then $q=2p$ because $3^{2p+1}|3UV$, $3^{2p+1}\nmid(U+V)^2$. If $3^{p+1}|U+V$ then $q \geq 2p+1$ and $3^{2p+2}|(U+V)^2$. $q>2p+1$ is not possible because it would follow that $3^{p+2}|3UV$, *i.e.* $3^{p+1}|U$ or $3^{p+1}|V$. But then $3^{p+1}|U$ and $3^{p+1}|V$ because $3^{p+1}|U+V$, contradicting the definition of p.

If m and W are not both multiples of 3 then $3|3m^2+W^2$ and $9\nmid 3m^2+W^2$ if $3|W$, $3\nmid 3m^2+W^2$ otherwise. From this follows:

Lemma 4. Let p be the largest integer such that $3^p|m$ and $3^p|W$, q the largest integer such that $3^q|3m^2+W^2$. Then $q=2p+1$ if $3^{p+1}|W$, $q=2p$ otherwise.

B3.1. k_3 according to the theorem

It will be shown here that the theorem gives three cases (a)-(c) with $k_3>k$, where k has been redefined to be the number of factors 3 in $\beta\gamma$. Equation (31) shows that either $3\nmid\mu$ or $3\nmid\nu$, *i.e.* at most one of the numbers β and γ contains factors 3; (43) shows that $3\nmid\alpha_3$.

(1) $3|\alpha_1$. Then $3|(W, U+V)$.

(1.1) $k=0$. Then $3\nmid\alpha_4$. If $3|\alpha_2$ then $3|\mu$ and $9|U^2-UV+V^2$. Lemma 3 gives $3|U$ and $3|V$, *i.e.* $3|\beta$, contradicting $k=0$. It follows that $k_3=k+1$ (a_1).

(1.2.1) $k>0$, $3\nmid\mu$, *i.e.* $3^k|$g.c.d. (ν, m, W). $3\nmid\alpha_2$. Equation (44) gives because of lemma 4 $k_3=k+1$ if $3^{k+1}|W(a_2)$, $k_3=k$ otherwise.

(1.2.2) $k>0$, $3\nmid\nu$, *i.e.* $3^k|$g.c.d. (μ, U, V). $3\nmid\alpha_4$, $3^k|\alpha_2$. Lemma 3 shows similarly as in (1.1) that $3^{k+1}\nmid\alpha_2$. It follows that $k_3=k+1$ (b).

(2) $3\nmid\alpha_1$.

(2.1) $3\nmid\mu$, *i.e.* $3^k|$g.c.d. (ν, m, W). $3\nmid\alpha_2$. Equation (44) gives $k_3=k$.

(2.2) $3\nmid\nu$, *i.e.* $3^k|$g.c.d. (μ, U, V). $3\nmid\alpha_4$. Equation (42) gives because of lemma 3 $k_3=k+1$ if $3^{k+1}|(\mu, U+V)$ (c), $k_3=k$ otherwise.

In summary, the theorem gives $k_3=k$ except in the cases (a)-(c), where $k_3=k+1$:

(a) $3^k|(\nu, m)$, $3^{k+1}|W$, $3|U+V$
(b) $3^k|(\mu, U, V)$, $3\nmid W$, $k>0$
(c) $3^{k+1}|(\mu, U+V)$, $3^k|(U, V)$.

*B*3.2. k_3 *is not too large*

It has to be shown that $3^{k_3}|$all $r_{ij}^{\pm}$. This follows from (33): for $k_2=k$ it has been shown in $(1a)$ of § 7; for (b) it is easily verified because $k>0$; to verify it for (a) and (c) one makes use of $U^2-V^2=(U+V)(U-V)$, $U^2-UV+V^2=(U+V)^2-3UV$, $2U-V=3U-(U+V)$, $2V-U=3V-(U+V)$.

*B*3.3. k_3 *is not too small*

The proof that $3^{k+2}|$not all $r_{ij}^{\pm}$ is similar to the proof that $2^{k+3}|$not all $r_{ij}^{\pm}$, given in *B*2.3. It remains to show that $3^{k+1}|$all $r_{ij}^{\pm}$ only in the cases (a)-(c).

Assume $3^{k+1}|$all $r_{ij}^{\pm}$.

(1) $3\nmid\mu$. Equation (38) shows $3^{k+1}|W$, $3^k|(m, \nu U, \nu V)$. It follows that $3^k|\nu$ because of (19) if $k>0$ and trivially if $k=0$. Because $3\nmid\mu$, it follows from $3^{k+1}|r_{13}^{+}$ that $3^{k+1}|m(2V-U)$ and from $3^{k+1}|r_{33}^{+}$ that $3^{k+1}|\nu(U^2-UV+V^2)$. If $3|U+V$ then 3 divides both $2V-U$ and U^2-UV+V^2, otherwise none. If it divides none then $3^{k+1}|(m, \nu)$, *i.e.* $3^{k+1}|\gamma$ contrary to the definition of k. It follows that (a) is satisfied.

(2) $3|\mu$. Then $3\nmid\nu$ because of (31). Equation (38) shows $3^{k+1}|\mu W$, $3^k|(\mu m, U, V)$.

(2.1) $k>0$.

(2.1.1) $3|W$. Equation (19) shows that $3^k|\mu$, *i.e.* (b) is satisfied.

(2.1.2) $3\nmid W$. Then $3^{k+1}|\mu$. From $3^{k+1}|r_{31}^{+}$ follows $3^{k+1}|2U-V$, whence $3^{k+1}|U+V$, *i.e.* (c) is satisfied.

(2.2) $k=0$. It follows from $3|r_{33}^{+}$ that $3|U^2-UV+V^2$, *i.e.* $3|U+V$. It follows that (c) is satisfied.

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