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Coincidence orientations of grains in hexagonal materials

Koinzidenzorientierungen von Körnern in hexagonalen Materialien

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CONTENTS

Kurzfassung

Es werden Grenzen zwischen Körnern der gleichen homogenen Phase betrachtet. Die Energie/cm^2 der Grenzfläche hängt von der gegenseitigen Orientierung der beiden Körner ab. Experimentelle Untersuchungen zeigen häufig, dass diese Energie ein relatives Minimum aufweist, wenn ein grosser Bruchteil der Translationsvektoren des einen Gitters gleichzeitig Translationsvektoren des andern Gitters sind. Das von den gemeinsamen Vektoren erzeugte Gitter heisst Koinzidenzgitter, Σ seine Multiplizität.

Für hexagonale Materialien werden vorerst Resultate gegeben, die für beliebige gegenseitige Orientierungen der Körner gelten: Die Form der Drehmatrix in hexagonalen Gitterkoordinaten wird hergeleitet und mit einem Quadrupel aus Drehwinkel und Drehachse parametrisiert. Das Multiplikationsgesetz der Quadrupel wird hergeleitet. Es ersetzt die Multiplikation der Drehmatrizen und gibt die Wirkung von zwei aufeinanderfolgenden Drehungen. Eine gegebene gegenseitige Orientierung von zwei Gittern kann wegen ihrer hexagonalen Symmetrie durch verschiedene Quadrupeln beschrieben werden. Die Beziehung zwischen diesen wird dargestellt und es wird eine eindeutige standardisierte Beschreibung der gegenseitigen Orientierung vorgeschlagen.

Anschliessend werden für beliebige Werte des Achsenverhältnisses $\rho = c/a$ die Bedingungen hergeleitet, welche Drehungen erfüllen müssen, um Koinzidenzgitter zu erzeugen. Es wird gezeigt, dass die für kubische Gitter gültige Beziehung, wo Σ durch den kleinsten gemeinsamen Nenner der Elemente der Drehmatrix gegeben ist, für hexagonale Gitter nicht immer zutrifft. Für Gitter beliebiger Symmetrie ist Σ gegeben durch den kleinsten gemeinsamen Nenner der 18 Elemente der in Gitterkoordinaten ausgedrückten Drehmatrix und ihrer Inversen. Kernstück der vorliegenden Arbeit ist die Begründung eines vereinfachten Verfahrens zur Bestimmung von Σ für hexagonale Gitter. Zum Schluss werden einfache Algorithmen dargestellt, zur Bestimmung von Basen für das Koinzidenzgitter und für das zugehörige DSC Gitter, welches die geometrisch möglichen Burgers Vektoren von Versetzungen in der Korngrenze gibt.

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 due to their hexagonal symmetry; a unique standard description of the relative orientation is proposed. The restrictions satisfied by rotations generating coincidence site lattices (CSLs) 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 was equal to the least common denominator of the elements of the rotation matrix, does not always hold for hexagonal lattices. A generalisation of this law to lattices of arbitrary symmetry is given and another, quicker method to determine 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 CSLs 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 to determine Σ have been presented without complete proofs already in two preliminary publications (Grimmer & Warrington, 1983 and 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 Sections 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 3-dimensional space can be written in the form $\underline{e}_1x_1+\underline{e}_2x_2+\underline{e}_3x_3= \underline{e}x$, where $\underline{e}$ denotes a row of basis vectors, x a column of components. Two bases will be considered: a cubic basis $\underline{\varepsilon}$ consisting of 3 mutually orthogonal vectors $\underline{\varepsilon}_1$, $\underline{\varepsilon}_2$, $\underline{\varepsilon}_3$, each of length a and a hexagonal basis $\underline{e}$ related to $\underline{\varepsilon}$ by $\underline{e} = \underline{\varepsilon}\, S$, where

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

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

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

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

the rotation is described in cubic coordinates by a matrix R_o of the form (see e.g. Synge (1960) or Grimmer (1974a)).

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

it transforms the vector $\underline{\varepsilon}\xi$ into $\underline{\varepsilon}\xi' = \underline{\varepsilon}R_o\xi$.

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

$$\nu_1=n_1-n_2/2,\ \nu_2=\sqrt{3}n_2/2,\ \nu_3=\rho n_3 \tag{4}$$

and

$$1=\nu_1^2+\nu_2^2+\nu_3^2 = n_1^2-n_1n_2+n_2^2+\rho^2n_3^2. \tag{5}$$

Introducing parameters

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

one obtains from (2) and (4)

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

so that R_o becomes

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

where

$$\tau = 1/\rho^2. \tag{9}$$

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

$$3A^2+D^2+\tau(B^2-BC+C^2) = 3(\cos^2\phi+\sin^2\phi(\rho^2n_3^2+n_1^2-n_1n_2+n_2^2)) = 3. \tag{10}$$

Expressing the original and rotated vectors in the basis $\underline{e}$ one obtains $\underline{\varepsilon}\xi = \underline{e}S^{-1}\xi = \underline{\varepsilon}x$ and $\underline{\varepsilon}\xi' = \underline{\varepsilon}R_o\xi = \underline{e}S^{-1}R_oSx = \underline{e}Rx$, where $x = S^{-1}\xi$ and $R = S^{-1}R_oS$, i.e.

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

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

$$B^2 - BC + C^2 + \rho^2D^2 = 3\rho^2\ \sin^2\phi \tag{12}$$

is given by the matrix R (Eq. (11)), where $A = \cos\phi$. 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 ν, $\theta = 2\phi$ according to (6), the inverse rotation $-\nu$, 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 $(a,b,c,d)_r\ (-A,B,C,D)_R$?

$$(a\ b\ c\ d)_r\ (A\ B\ C\ D)_R = \Big(aA - \frac{dD}{3} - \frac{bB-(bC+cB)/2+cC}{3rR},$$

$$\rho\left(\frac{aB}{R} + \frac{bA}{r} + \frac{(2c-b)D}{3r} - \frac{d(2C-B)}{3R}\right),\quad \rho\left(\frac{aC}{R} + \frac{cA}{r} - \frac{(2b-c)D}{3r} + \frac{d(2B-C)}{3R}\right),$$

$$aD+dA+\frac{bC-cB}{2rR}\Big)_\rho . \tag{13a}$$

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. Eq. (3) in Grimmer (1974a)) and changing back to hexagonal quadruples. (13a) simplifies in the special case $r = R = \rho$ to

$$(a\ b\ c\ d)\ (A\ B\ C\ D) = 1/3\ \Big(3aA-dD-\tau(bB-(bC+cB)/2+cC),$$

$$3aB+3bA+(2c-b)D-d(2C-B),\ 3aC+3cA-(2b-c)D+d(2B-C),\ 3(aD+dA+\tau(bC-cB)/2)\Big). \tag{13b}$$

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 P is a rotation that turns lattice 1 parallel to lattice 2 then any of the 12 symmetry rotations of lattice 1 followed by R and by any of the 12 symmetry rotations of lattice 2 has the same effect as R. Because either lattice may be taken as lattice 1, up to $2 \cdot 12^2 = 288$ different rotations 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. $w = m/12$ 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 the mirror planes of the group 6/mmm and consider the equivalent rotations with angle $\leq 180^{\circ}$ 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 $<180^{\circ}$ 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.

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* This definition of equivalence is appropriate for our purpose of dealing with coincidence site and DSC 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.

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 Eq. (7).

Table 1*: 12 equivalent quadruples representing the different rotation angles that occur in an equivalence class. They are 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	ρ	((B−C)τ/2	A+D	2A	(B+C)τ/2)
ILq	ρ	(Bτ/2	A+D	2A	(B−2C)τ/2)
JLq	ρ	(Cτ/2	A+D	2A	(2B−C)τ/2)
KLq	$\rho/\sqrt{3}$	((B+C)τ/2	D−3A	2D	3(B−C)τ/2)
IKLq	$\rho/\sqrt{3}$	((2B−C)τ/2	D−3A	2D	3Cτ/2)
JKLq	$\rho/\sqrt{3}$	((B−2C)τ/2	D−3A	2D	3Bτ/2)

Table 1 gives 12 quadruples representing the different rotation angles that occur in an equivalence class. The 2 · 288 = 576 equivalent hexagonal quadruples are obtained from those in the table by arbitrary combinations of the following 4 operations

a) sign change of the 1st component
b) sign change of the 4th component
c) interchanging the 2nd and 3rd component
d) replacing the 2nd and 3rd components B,C by B−C,B. Applying this repeatedly one obtains (B,C)→(B−C,B)→(−C,B−C)→(−B,−C)→(C−B,−B)→(C,C−B)→(B,C).

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

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 6-fold axis, d) 60° rotation.

Using the connection between equivalent quadruples one finds that one and only one quadruple in each equivalence class satisfies the conditions*

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

$$A \geq \sigma B/2, \qquad A \geq \sigma(2B-C)/\sqrt{12}, \qquad A \geq (2/\sqrt{3}+1)D \tag{15}$$

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

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

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

(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, (16a-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 (14,15) 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 $\sqrt{(1+(b^2-bc+c^2+\rho^2d^2)/3\rho^2)}$.

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* 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 (16a-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
	$\{1,0,0,2\sqrt{3}-3\}$	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	ρ 0 1
	$\{1,\sqrt{3}\rho,0,0\}$	b	6	2ρ ρ $\sqrt{3}$
6	$\{1,2c,c,0\}$, $0<c<\rho$		12	c 0 1, ρ^2 0 c
	$\{1,b,0,0\}$, $0<b<\sqrt{3}\rho$		12	2b b 3, $2\rho^2$ ρ^2 b
	$\{1,2\rho,2(2-\sqrt{3})\rho, 2\sqrt{3}-3\}$	abc	0	
12	$\{1,b,c,0\}$, $0<2c<b \begin{cases}\leq 2\rho \\ \leq\sqrt{3}\rho+c/2\end{cases}$	$\overset{=}{\to}$a $\overset{=}{\to}$b	12	2b-c b-2c 3
	$\{1,b,0,d\}$, $0<b<\sqrt{3}\rho$, $0<d\leq 2\sqrt{3}-3$	$\overset{=}{\to}$c	12	$2\rho^2$ $\rho^2(1-d)$ b
	$\{1,2c,c,d\}$, $0<c<\rho$, $0<d<2\sqrt{3}-3$		12	$\rho^2(3+d)$ $2\rho^2 d$ 3c
	$\{1,2\rho,\rho(1-d),d\}$, $0<d<2\sqrt{3}-3$	a	0	
	$\{1,\rho(\sqrt{3}+x),2\rho x,\sqrt{3}x\}$, $0<x<2-\sqrt{3}$	b	0	
	$\{1,b,(2-\sqrt{3})t,2\sqrt{3}-3\}$, $0<b<2\rho$	c	0	
24	all other representative quadruples	-	0	

In Appendix A, Table 2 is expressed in the language of orthogonal coordinates and quaternions, which shows how the first 3 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 3-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

$4A^2 = 1+R_{11}^{+}+R_{22}^{+}+R_{33}^{+}$	(17a)	$\tau B^2 = 1+R_{11}^{+}-R_{22}^{+}-R_{33}^{+}+R_{12}^{+}$	(17h)
$4AB = R_{13}^{+}-R_{13}^{-}-2R_{23}^{+}+2R_{23}^{-}$	(17b)	$2\tau BA = R_{32}^{+}-R_{32}^{-}$	(17i)
$4AC = 2R_{13}^{+}-2R_{13}^{-}-R_{23}^{+}+R_{23}^{-}$	(17c)	$2\tau BD = 2R_{31}^{+}+2R_{31}^{-}+R_{32}^{+}+R_{32}^{-}$	(17j)
$4AD = 3(R_{11}^{+}-R_{11}^{-})$	(17d)	$2\tau BC = 1-R_{33}^{+}+2R_{12}^{+}+2R_{21}^{+}$	(17k)
$4BD = 3(R_{13}^{+}+R_{13}^{-})$	(17e)	$2\tau AC = R_{31}^{-}-R_{31}^{+}$	(17l)
$4CD = 3(R_{23}^{+}+R_{23}^{-})$	(17f)	$2\tau DC = R_{31}^{+}+R_{31}^{-}+2R_{32}^{+}+2R_{32}^{-}$	(17m)
$4D^2 = 3(1-R_{11}^{+}-R_{22}^{+}+R_{33}^{+})$	(17g)	$\tau C^2 = 1-R_{11}^{+}+R_{22}^{+}-R_{33}^{+}+R_{21}^{+}$	(17n)

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

$$A^2=km,\ AB=kU,\ AC=kV,\ AD=kW. \qquad (18)$$

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

$$\gcd\ (m,U,V,W)=1. \qquad (19)$$

Using (18) and (10) one obtains

$$km=A^2=A^2\left(3A^2+D^2+\tau(B^2-BC+C^2)\right)/3=k^2\left(3m^2+W^2+\tau(U^2-UV+V^2)\right)/3=k^2s, \qquad (20)$$

where

$$s=(3m^2+W^2+\tau(U^2-UV+V^2))/3. \qquad (21)$$

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

$$A=m/\sqrt{s},\ B=U/\sqrt{s},\ C=V/\sqrt{s},\ D=W/\sqrt{s}. \qquad (22)$$

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

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

(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. Doing this we have replaced the normalization condition (10) by (19). The expressions [B,C,D] for the axis and $\cos\phi=A$ for the half-angle of the rotation become now [U,V,W] and $\cos\phi=m/\sqrt{s}$, i.e.

$$\cos\phi=\sqrt{\frac{3m^2}{3m^2+W^2+\tau(U^2-UV+V^2)}}\;. \quad (25)$$

It follows that

$$\tan\phi=\sqrt{\frac{\tau(U^2-UV+V^2)+W^2}{3m^2}}=\sqrt{\frac{\tau(u^2-uv+v^2)+w^2}{3}}\cdot\frac{n}{m} \quad (26)$$

where

$$n=\gcd(U,V,W),\; u=U/n,\; v=V/n,\; w=W/n. \quad (27)$$

From (27) it follows that

$$\gcd(u,v,w)=1 \quad (28)$$

and (because of (19)) that

$$\gcd(m,n)=1 \quad (29)$$

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 $\sqrt{(\tau(u^2-uv+v^2)+w^2)/3}$, which is proportional to the length of the vector [u,v,w].* An additional

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

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 6-fold axis or ($U=V=0$) a rotation around the 6-fold axis with a rational value for $\sqrt{3}\tan\phi$. (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 value of τ that satisfy $U=V=0$ or $m=W=0$.

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

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

and

$$\gcd(\mu,\nu) = 1\ . \qquad (31)$$

Putting

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

(23) becomes

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

The elements of the matrices $r^{+} = F\cdot R$ and $r^{-} = F\cdot R^{-1}$ are integers because μ,ν,U,V,W and $\pm$ m are integers. Using (27) one can see that (33) is equivalent to Eq. (25) in BNHD and to Eq. (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.

Multiplying both sides of (17) with $F=3\mu s$, one obtains defining $r_{ij}^{\pm} = FR_{ij}^{\pm}$ and using (20) and (30)

$$12\mu m^2=F+r_{11}^{+}+r_{22}^{+}+r_{33}^{+} \qquad (34a)$$

$$12\mu mU=r_{13}^{+}-r_{13}^{-}-2r_{23}^{+}+2r_{23}^{-} \qquad (34b)$$

$$12\mu mV=2r_{13}^{+}-2r_{13}^{-}-r_{23}^{+}+r_{23}^{-} \qquad (34c)$$

$$4\mu mW=r_{11}^{+}-r_{11}^{-} \qquad (34d)$$

$$4\mu UW=r_{13}^{+}+r_{13}^{-} \qquad (34e)$$

$$4\mu VW=r_{23}^{+}+r_{23}^{-} \qquad (34f)$$

$$4\mu W^2=F-r_{11}^{+}-r_{22}^{+}+r_{33}^{+} \qquad (34g)$$

$$3\nu U^2=F+r_{11}^{+}-r_{22}^{+}-r_{33}^{+}+r_{12}^{+} \qquad (34h)$$

$$6\nu Um=r_{32}^{+}-r_{32}^{-} \qquad (34i)$$

$$6\nu UW=2r_{31}^{+}+2r_{31}^{-}+r_{32}^{+}+r_{32}^{-} \qquad (34j)$$

$$6\nu UV=F-r_{33}^{+}+2r_{12}^{+}+2r_{21}^{+} \qquad (34k)$$

$$6\nu mV=r_{31}^{-}-r_{31}^{+} \qquad (34l)$$

$$6\nu WV=r_{31}^{+}+r_{31}^{-}+2r_{32}^{+}+2r_{32}^{-} \qquad (34m)$$

$$3\nu V^2=F-r_{11}^{+}+r_{22}^{+}-r_{33}^{+}+r_{21}^{+} \qquad (34n)$$

6. THE MULTIPLICITY Σ of the CSL generated by R

The computation of Σ being 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 $\underline{b}^1$ and $\underline{b}^2$ are bases of the corresponding lattices and v_1 and v_2 the volumes of primitive cells, one can write

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

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

$$v=\Sigma_1 v_1=\Sigma_2 v_2,$$

where Σ_2 is the least positive integer such that $\Sigma_2\|T\|$ is an integer and that $\Sigma_2 T$ 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 least common multiple of Σ' and Σ'',

$$\Sigma = \mathrm{lcm}(\Sigma',\Sigma''), \qquad (35)$$

where Σ' and Σ'' denote the least 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 and 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

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* A given rotation leeds to the same value Σ for fcc and bcc lattices as for the primitive cubic lattice.

$$F=\alpha'\Sigma'=\alpha''\Sigma''=\alpha\Sigma. \tag{36}$$

(34a,h,n and g) show that α' is a factor of 12 μm^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). (33) shows then that all the r_{ij}^+ are multiples of 4. We conclude that α' has the form

$$\alpha'=\beta \cdot \gamma, \tag{37}$$

where β= 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: α' is a factor of $12\mu\nu$. (37) corresponds to Eq. (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 (34a,h,n and g) remain true on replacing r_{ij}^+ by r_{ij}^-. It follows that (37) remains true for α'' and α and that also Σ'' and Σ are multiples of $F/12\mu\nu$. α being a divisor of F (see (36)) and of the $r_{ij}^{\pm}$, it follows from (34a-d) and (19) that *

$$\alpha | 12\mu m \tag{38a}$$

and similarly that

$$\alpha | \ 4\mu W \tag{38b}$$

$$\alpha | \ 6\nu U \tag{38c}$$

$$\alpha | \ 6\nu V , \tag{38d}$$

which give because of (19) an alternative proof that

$$\alpha | 12\mu\nu. \tag{39}$$

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* $g|h$ 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.

7. A SIMPLIFIED PROCEDURE TO COMPUTE Σ

Many calculations involving coincidence rotations can most easily be done by using the quadruple description of the rotations. To determine Σ according to the method given in Section 6, however, one has to return to the matrix description by determining first the two matrices R and R^{-1} and computing then Σ as the least 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.

Writing $\Sigma=F/\alpha$, 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

$$\alpha=\alpha_1\alpha_2\alpha_3\alpha_4, \tag{40}$$

where

$$\alpha_1=\gcd(12,3m^2+W^2,U^2-UV+V^2), \tag{41}$$

α_2 is the largest common divisor of μ, 3U and 3V satisfying $\alpha_2^2\,|\,3(U^2-UV+V^2)/\alpha_1$, (42)

$$\alpha_3=\gcd(4,\nu,(3m^2+W^2)/\alpha_1), \tag{43}$$

α_4 is the largest common divisor of ν/α_3, W and m satisfying $\alpha_4^2\,|\,(3m^2+W^2)/\alpha_1\alpha_3$. (44)

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) $(m,U,V,W)=(5,2,1,5) \rightarrow \alpha_1=1,\ \alpha_2=\gcd(3,\mu),\ \alpha_3=\gcd(4,\nu),\ \alpha_4=\gcd(5,\nu) \rightarrow \alpha=\gcd(3,\mu)\cdot\gcd(20,\nu)$.
3) $(m,U,V,W)=(2,3,1,2) \rightarrow \alpha_1=\alpha_2=1,\ \alpha_3=\gcd(4,\nu),\ \alpha_4=\gcd(8,\nu)/\alpha_3 \rightarrow \alpha=\gcd(8,\nu)$.

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

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

where the k_i are integers and

$$\gcd(6,k_1)=1. \tag{46}$$

The proof that the Theorem gives k_1 correctly is rather simple but the proofs that it gives also 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 $l_3\leq k_3$.

1A) <u>k_1 is not too large</u>

Define

$$\beta=\gcd(\mu,U,V) \tag{47}$$

and

$$\gamma=\gcd(\nu,m,W). \tag{48}$$

Eq. (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 $\beta\cdot\gamma|$all $r_{ij}^{\pm}$ (i.e. that $\beta\cdot\gamma$ divides all the $r_{ij}^{\pm}$). The Theorem shows that k_1 has the form

$$k_1=\beta_1\gamma_1, \tag{49}$$

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

1B) k_1 is not too small

Let l_1 be an integer with

$$\gcd(l_1,6)=1 \quad (50)$$

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

$$l_1=b\cdot c, \quad (51)$$

where

$$b=\gcd(l_1,\mu) \quad (52)$$

and

$$c=\gcd(l_1,\nu). \quad (53)$$

Because of (31) one has $\gcd(b,\nu) = \gcd(c,\mu) = 1$. From (38) it follows then that $b|U$, $b|V$, $c|m$, $c|W$. These together with (52,53) 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 $\beta\cdot\gamma$ 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 (34 h,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 $\beta\cdot\gamma$ 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 $\gcd(\mu,6)=1$ and $\gcd(\nu,6)=1$.

Corollary 1

If $\gcd(\mu\nu,6)=1$ then

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

where

$$\alpha_1=\gcd(12,3m^2+W^2,U^2-UV+V^2), \tag{41}$$

$$\beta=\gcd(\mu,U,V), \tag{47}$$

$$\gamma=\gcd(\nu,m,W). \tag{48}$$

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 $\alpha_1=\gcd(12,3m^2+W^2)$, $\alpha_2=\mu$. $\alpha_4=1$ because (19) gives

$\gcd(m,W)=1$, from which it follows also that $\gcd(3m^2+W^2,8)=1$ or 4. $(3m^2+W^2)/\alpha_1$ is odd in both cases, i.e. $\alpha_3=1$. It follows that $\alpha=\mu\cdot \gcd(12,3m^2+W^2)$. $\Sigma=F/\alpha=(3m^2+W^2)/\gcd(12,3m^2+W^2)$. We conclude

Corollary 2

If $U=V=0$ then

$$\Sigma = \frac{3m^2+W^2}{\gcd(3,W)\cdot(\gcd(2,m+W))^2} \ .$$

If $m=W=0$ then $\gcd(U,V)=1$ because of (19). It follows that U^2-UV+V^2 is odd. From $\gcd(U,V)=1$ 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 $\alpha_1=\gcd(3,U+V)$, $\alpha_2=1$, $\alpha_3=\gcd(4,\nu)$, $\alpha_4=\nu/\alpha_3$, i.e. $\alpha_3\alpha_4=\nu$ and $\alpha=\nu\cdot\gcd(3,U+V)$. $\Sigma=F/\alpha=(U^2-UV+V^2)/\gcd(3,U+V)$. We conclude

Corollary 3

If $m=W=0$ then

$$\Sigma = \frac{U^2-UV+V^2}{\gcd(3,U+V)}.$$

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 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 or 1982).* To analyze experimentally observed boundaries and their dislocation arrays, it is therefore important to have a convenient algorithm for determining CSLs and the corresponding DSCLs. The 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 $\underline{e}=(\underline{e}_1,\underline{e}_2,\underline{e}_3)$ will be called lattice 1, the rotated lattice with integral components in the basis $\underline{e}R=\underline{e}'=(\underline{e}_1',\underline{e}_2',\underline{e}_3')$ 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 of 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 $V_C = V\cdot\Sigma$ and $V_D = V/\Sigma$. The latter result was proved by Bonnet & Durand (1975) and by Iwasaki (1976). Grimmer (1974b) 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 be used also to determine Σ. Knowing Σ from the α-hex Theorem, his method can be further simplified.

1) Determine $N_1>0$, the least 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 least 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 $\underline{e}_1^C=N_1\underline{e}_1'$, $\underline{e}_2^C=n_{12}\underline{e}_1'+N_2\underline{e}_2'$, $\underline{e}_3^C=n_{13}\underline{e}_1'+n_{23}\underline{e}_2'+N_3\underline{e}_3'$.

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

A basis for the DSCL is obtained as follows: Compute the internal coordinates * of the vectors $n_1\underline{e}_1'+n_2\underline{e}_2'+n_3\underline{e}_3'$, where the n_i are integers satisfying $0\leq n_i<N_i$ 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 $\underline{e}_1^D=\underline{e}_1$ and $k_{11}=1$, else $\underline{e}_1^D=k_{11}\underline{e}_1$.

b) the one of form $(k_{12}, k_{22}, 0)$ with the least $k_{22}>0$ and $0\leq k_{12}<k_{11}$. If there is no such triplet then $\underline{e}_2^D=\underline{e}_2$ and $k_{22}=1$, else $\underline{e}_2^D=k_{12}\underline{e}_1+k_{22}\underline{e}_2$.

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

Another method to determine 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 to 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 that $\underline{e}'$ is given by the columns of R, we obtain

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

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

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

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* 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 $\underline{e}$ is called the internal coordinates of the vector.

It follows that

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

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

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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. 180^{o} rotations being often used to describe twins, also the number n_{180} of 180^{o} rotations has been included as well as the axes of those that lie in the standard stereographic triangle (SST) defined by $x \geq \sqrt{3}y \geq 0$, $z \geq 0$.

Table 3: Table 2 expressed in orthonormal coordinates

w	representative quaternion	*	n_{180}	axes of 180^{o} rotations in the SST
1	$\{1,0,0,0\}$		7	1 0 0, $\sqrt{3}$ 1 0, 0 0 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
	$\{1,1,0,0\}$	b	6	$\sqrt{3}$ 1 2
6	$\{1,\sqrt{3}c,c,0\}$, $0<c<1/2$		12	2c 0 1, 1 0 2c
	$\{1,b,0,0\}$, $0<b<1$		12	$\sqrt{3}b$ b 2, $\sqrt{3}$ 1 2b
	$\{1,1,2-\sqrt{3}, 2-\sqrt{3}\}$	abc	0	
12	$\{1,b,c,0\}, 0<\sqrt{3}c<b$ $\begin{cases} \leq (2-c)/\sqrt{3} \\ \leq 1 \end{cases}$	↔a ↔b	12	$\sqrt{3}b+c$ $b-\sqrt{3}c$ 2
	$\{1,b,0,d\}$, $0<b<1$, $0<d\leq 2-\sqrt{3}$	↔c	12	$\sqrt{3}+d$ $1-\sqrt{3}d$ 2b
	$\{1,\sqrt{3}c,c,d\}$, $0<c<1/2$, $0<d<2-\sqrt{3}$		12	1 d 2c
	$\{1,(\sqrt{3}+d)/2,(1-\sqrt{3}d)/2,d\}, 0<d<2-\sqrt{3}$	a	0	
	$\{1,1,d,d\}$, $0<d<2-\sqrt{3}$	b	0	
	$\{1,b,(2-\sqrt{3})b,2-\sqrt{3}\}$, $0<b<1$	c	0	
24	all other representative quaternions	-	0	

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 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 TO THE PROOF OF THE α-HEX THEOREM

B1) 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 Section 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 $\beta \cdot \gamma$, where

$$\beta = \gcd(\mu, U, V) \tag{47}$$

and

$$\gamma = \gcd(\nu, m, W). \tag{48}$$

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

B2) 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

<u>Lemma 2</u> 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 can not both be even because of (19)), i.e. $4|3m^2+W^2$. It follows that $4|\alpha_1$.

B2.1) <u>k_2 according to the Theorem</u>

It will be shown here that the Theorem gives 4 cases a)-d) with $k_2>k$, where k is the number of factors 2 in $\beta\cdot\gamma$. (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 $2^k|\gcd(\nu,m,W)$, whence k=0 because $2\nmid(m,W)$.

1.2) k>0, $2\nmid\nu$, i.e. $2^k|\gcd(\mu,U,V)$. Then $2\nmid(\alpha_3,\alpha_4)$. (42) gives then $k_2=k+2$ 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. $2^k|\gcd(\nu,m,W)$. Then $2\nmid\alpha_2$.

2.1.1) $\alpha_3=1$. (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).

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* $n|(p,q)$ 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 $n\nmid q$.

2.2) $2 \nmid \nu$, i.e. $2^k | \gcd(\mu,U,V)$. Then $2 \nmid (\alpha_3,\alpha_4)$. (42) gives $k_2=k$.
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 Section 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 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 that $W \pm 3m$ are even.

B2.3) k_2 is not too small

It has to be shown 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) $2 \nmid \mu$. (38) shows $2^{k+1}|(m,W,\nu U,\nu V)$. (19) gives $2^{k+1}|\nu$, i.e. $2^{k+1}|\gamma$ contrary to the definition of k.
1.2) $2 \nmid \nu$. (38) shows $2^{k+1}|(\mu m,\mu W,U,V)$. (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) $2 \nmid \mu$. (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 can not both be even according to (19). It follows that a) is satisfied.

2.1.2) $k=0$ and U,V not both even or $k>0$. (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) $2\nmid\nu$. (38c,d) 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 can not 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) $k>0$. (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 $2^{k}|(\mu,U,V)$. (34h) and (34n) show that $2|(U,V)$ also if $k=0$. (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 $2^{k+1}|\gcd(\mu,U,V)$ 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) <u>The number of factors 3 in α</u>

Use will be made of the following results

<u>Lemma 3</u> Let 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

<u>Lemma 4</u> 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) <u>k_3 according to the Theorem</u>

It will be shown here that the Theorem gives 3 cases a)-c) with $k_3>k$, where k has been redefined to be the number of factors 3 in $\beta\cdot\gamma$. (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. $3^k|\gcd(\nu,m,W)$. $3\nmid\alpha_2$. (44) gives because of Lemma 4 that $k_3=k+1$ if $3^{k+1}|W$ a$_2$), $k_3=k$ otherwise.

1.2.2) $k>0$, $3\nmid\nu$, i.e. $3^k|\gcd(\mu,U,V)$. $3\nmid\alpha_4$, $3^k|\alpha_2$. 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. $3^k|\gcd(\nu,m,W)$. $3\nmid\alpha_2$. (44) gives $k_3=k$.

2.2) $3\nmid\nu$, i.e. $3^k|\gcd(\mu,U,V)$. $3\nmid\alpha_4$. (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) $3^k|(\mu,U,V)$, $3|W$, $k>0$

c) $3^{k+1}|(\mu,U+V)$, $3^k|(U,V)$

B3.2) 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 Section 7); for b) it is easily verified because $k>0$; to verify it for a) and c) one makes use of

$U^2-V^2=(U+V)(U-V)$, $U^2-UV+V^2=(U+V)^2-3UV$, $2U-V=3U-(U+V)$, $2V-U=3V-(U+V)$.

B3.3) 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 B2.3). 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) $3\nmid\mu$. (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). (38) shows $3^{k+1}|\mu W$, $3^k|(\mu m,U,V)$.

2.1) $k>0$.

2.1.1) $3|W$. (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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