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The Generating Function for Coincidence Site Lattices in the Cubic System

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Abstract

The derivation of the generating function given by Bleris & Delavignette [*Acta Cryst.* (1981), A**37**, 779–786] is simplified and made rigorous. It is shown that their main result can also be deduced directly from Grimmer [*Acta Cryst.* (1974), A**30**, 685–688]. The following applications of the generating function are described: determining all rotations that generate coincidence site lattices (CSLs) by giving their axis and angle or their matrix, determining the equivalence classes of rotations with respect to cubic symmetry and the 180° and minimum-angle rotations that they contain, determining the number of rotations in each equivalence class and the total number of rotations that generate a CSL with given unit-cell volume Σ. We also discuss how a basis for the CSL can be computed and how a bicrystal with a plane grain boundary can be characterized.

1. Introduction

Ranganathan (1966) showed that a rotation about an axis $[u, v, w]$ of a cubic lattice by an angle θ such that

$$\tan\frac{\theta}{2}=\frac{n}{m}(u^2+v^2+w^2)^{1/2}, \tag{1}$$

while m and n are integers, generates a coincidence site lattice (CSL) with multiplicity Σ equal to an odd factor of

$$S=m^2+(u^2+v^2+w^2)n^2. \tag{2}$$

(The multiplicity Σ tells us that the volume of a unit cell is Σ times larger for the CSL than for the cubic lattice.) To give this result its strongest form, Ranganathan (1966) chooses the integers u, v, w and the integers m, n coprime, *i.e.* with greatest common divisor (g.c.d.) equal to 1,

$$\text{g.c.d.}\,(u, v, w)=1 \quad \text{and} \quad \text{g.c.d.}\,(m, n)=1. \tag{3}$$

and suggests without proof that Σ becomes then the largest odd factor of S.

Warrington & Bufalini (1971) showed that a rotation that generates a CSL is described in a cubic crystal coordinate system by a matrix R with rational matrix elements. They stated also the stronger result that Σ is equal to the least-common denominator D of the matrix elements of R, a fact which was proved rigorously by Grimmer, Bollmann & Warrington (1974) and which was used by Bleris & Delavignette (1981) to show that Σ is in fact the largest odd factor of S. The latter paper will be referred to as BD.

Putting

$$S=\alpha\Sigma, \tag{4}$$

it follows that α must be either 1, 2 or 4 because it follows from (3) that S cannot be a multiple of 8.

It will be shown in § 2 that this connection between S and the multiplicity Σ follows immediately from lemma 1 in Grimmer (1974*b*) and that his quaternions are equivalent to Ranganathan's generating function. Also that paper quoted the result $\Sigma=D$ and gave the connection between the generating function (expressed as a quaternion) and the form of the rotation matrix.

The important feature of BD is the emphasis put on the fact that a generating function can be derived by examining the form of the rotation matrices with a given value of D. In fact, Bleris, Nouet, Hagège & Delavignette (1982) have shown that CSLs in hexagonal lattices can be investigated analogously. Unfortunately, the proof presented by BD contains a few errors and gaps. Instead of just correcting them, a new, simpler and more lucid proof is presented in § 3. § 4 describes applications of the generating function.

2. The connection between Grimmer (1974*b*) and Bleris & Delavignette (1981)

Equations from Grimmer (1974*b*) will be put between brackets [ ], equations from BD between braces { }.

Lemma 1 in Grimmer (1974*b*) can be stated as

(1) Each quadruple of coprime integers m, U, V, W,

$$\text{g.c.d.}\,(m, U, V, W)=1, \tag{5}$$

defines (by [10] and [4]) a rotation matrix

$$R=\frac{1}{S}\begin{bmatrix} m^2+U^2-V^2-W^2 & 2(UV-mW) & 2(UW+mV) \\ 2(UV+mW) & m^2-U^2+V^2-W^2 & 2(VW-mU) \\ 2(UW-mV) & 2(VW+mU) & m^2-U^2-V^2+W^2 \end{bmatrix}, \tag{6}$$

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where $S = m^2 + U^2 + V^2 + W^2$. D, the least-common denominator of the matrix elements of R, is equal to the largest odd factor of S:

$$\Sigma = D = (m^2 + U^2 + V^2 + W^2)/\alpha, \quad \Sigma \text{ odd}, \quad \alpha = 1, 2 \text{ or } 4. \tag{7}$$

(2) Two different quadruples define the same rotation matrix if and only if $m' = -m$, $U' = -U$, $V' = -V$, $W' = -W$.

(3) Each rotation matrix with rational matrix elements can be obtained in this way.

[Grimmer (1974*b*) refers to these quadruples as quaternions to indicate that the product of two rotation matrices corresponds to multiplying the corresponding quadruples according to the (non-commutative) law of quaternion multiplication. The connection between different ways of expressing rotations was given by Synge (1960).]

Putting g.c.d. $(U, V, W) = n$, $u = U/n$, $v = V/n$, $w = W/n$, we obtain (3) from (5) and (4) from (7), which shows that our quaternions are equivalent to Ranganathan's generating function.

The main equations {31} and {32} of BD are obtained as follows: introducing $d = u^2 + v^2 + w^2$ we find that (6) is equivalent to {31} and that (7) is equivalent to {32}.

3. Derivation of a generating function for the rotations generating CSLs with multiplicity Σ

From the general form of a rotation matrix, a new derivation of the generating function for the rotations generating CSLs will be given in this section, *i.e.* no use will be made of the results stated in § 2.

Expressed in a cubic crystal coordinate system, a rotation by an angle θ around an axis with direction cosines p_1, p_2, p_3 is given by the matrix

$$R = \begin{bmatrix} p_1^2(1-\cos\theta)+\cos\theta & p_1p_2(1-\cos\theta)-p_3\sin\theta & p_1p_3(1-\cos\theta)+p_2\sin\theta \\ p_1p_2(1-\cos\theta)+p_3\sin\theta & p_2^2(1-\cos\theta)+\cos\theta & p_2p_3(1-\cos\theta)-p_1\sin\theta \\ p_1p_3(1-\cos\theta)-p_2\sin\theta & p_2p_3(1-\cos\theta)+p_1\sin\theta & p_3^2(1-\cos\theta)+\cos\theta \end{bmatrix}, \tag{8}$$

where

$$p_1^2 + p_2^2 + p_3^2 = 1. \tag{9}$$

Putting, $t = \tan(\theta/2)$ if $\theta \neq 180°$, we obtain $\sin\theta = 2t/(1+t^2)$, $\cos\theta = (1-t^2)/(1+t^2)$, $1-\cos\theta = 2t^2/(1+t^2)$, so that (8) becomes

$$R = \frac{1}{1+t^2}\begin{bmatrix} 2t^2p_1^2+1-t^2 & 2t^2p_1p_2-2tp_3 & 2t^2p_1p_3+2tp_2 \\ 2t^2p_1p_2+2tp_3 & 2t^2p_2^2+1-t^2 & 2t^2p_2p_3-2tp_1 \\ 2t^2p_1p_3-2tp_2 & 2t^2p_2p_3+2tp_1 & 2t^2p_3^2+1-t^2 \end{bmatrix}. \tag{10}$$

As stated in the *Introduction*, R generates a CSL if and only if its matrix elements R_{ij} are rational numbers. It follows from (10) that

$$(R_{32}-R_{23}):(R_{13}-R_{31}):(R_{21}-R_{12}) = p_1:p_2:p_3. \tag{11}$$

$R_{32}-R_{23}$, $R_{13}-R_{31}$ and $R_{21}-R_{12}$ being rational numbers, there exist three coprime integers u, v, w,

$$\text{g.c.d.}\,(u, v, w) = 1, \tag{12}$$

such that

$$p_1:p_2:p_3 = u:v:w, \tag{13}$$

i.e. a rational matrix describes a rotation around a lattice direction $[u, v, w]$, which was proved first by Fortes (1972*a*). It follows from (9) that

$$p_1 = u/\sqrt{d},\ p_2 = v/\sqrt{d},\ p_3 = w/\sqrt{d}, \quad \text{where} \quad d = u^2+v^2+w^2, \tag{14}$$

$$\frac{R_{21}+R_{12}}{R_{21}-R_{12}} = \frac{tp_1p_2}{p_3} = \frac{tuv}{\sqrt{d}\,w} \tag{15}$$

being a rational number, it follows that $t/\sqrt{d}$ is rational, too, so that we can write

$$t/\sqrt{d} = n/m, \tag{16}$$

where n and m are coprime integers,

$$\text{g.c.d.}\,(m, n) = 1. \tag{17}$$

Introducing (14) and (16) into (10) we obtain

$$R = \frac{1}{m^2+dn^2} \times \begin{bmatrix} 2u^2n^2+m^2-dn^2 & 2uvn^2-2wmn & 2uwn^2+2vmn \\ 2uvn^2+2wmn & 2v^2n^2+m^2-dn^2 & 2vwn^2-2umn \\ 2uwn^2-2vmn & 2vwn^2+2umn & 2w^2n^2+m^2-dn^2 \end{bmatrix}. \tag{18}$$

Consider now the case $\theta = 180°$, which we excluded after (9). Equation (8) gives then $\frac{1}{2}(R_{11}+1) = p_1^2$, $\frac{1}{2}R_{12} = p_1p_2$, $\frac{1}{2}R_{13} = p_1p_3$. These numbers being rational, one concludes similarly, as above, that the p_i can be written in the form (14), (12). Specializing (8) to $\theta = 180°$ and using (14), we find that R is of the form (18) with $m = 0$ and $n = 1$, *i.e.* (17) also remains true.

Putting

$$U = un, \quad V = vn, \quad W = wn$$

and

$$S = m^2 + dn^2 = m^2 + U^2 + V^2 + W^2, \tag{19}$$

we obtain from (12) and (17)

$$\text{g.c.d.}\,(m, U, V, W) = 1 \tag{20}$$

and (18) becomes

$$R = \frac{1}{S}\begin{bmatrix} m^2+U^2-V^2-W^2 & 2(UV-mW) & 2(UW+mV) \\ 2(UV+mW) & m^2-U^2+V^2-W^2 & 2(VW-mU) \\ 2(UW-mV) & 2(VW+mU) & m^2-U^2-V^2+W^2 \end{bmatrix} = \frac{[r_{ij}]}{S}. \tag{21}$$

If α denotes the greatest common divisor of the nine integers r_{ij}, we can write, according to Warrington & Bufalini (1971),

$$\begin{aligned}\Sigma = D = S/\alpha &= (m^2 + dn^2)/\alpha \\ &= (m^2 + U^2 + V^2 + W^2)/\alpha. \end{aligned} \tag{22}$$

It remains to determine α:

$$\begin{aligned} r_{11}^2 + r_{21}^2 + r_{31}^2 &= S^2 \\ -r_{11} - r_{22} - r_{33} &= S - 4m^2 \\ -r_{11} + r_{22} + r_{33} &= S - 4U^2 \\ r_{11} - r_{22} + r_{33} &= S - 4V^2 \\ r_{11} + r_{22} - r_{33} &= S - 4W^2. \end{aligned} \tag{23}$$

Let $k|l$ express that k and l are integers and that k divides l. Equation (23) shows that $\alpha^2|S^2$, *i.e.* $\alpha|S$. Equation (24) shows then that $\alpha|4m^2$, $\alpha|4U^2$, $\alpha|4V^2$, $\alpha|4W^2$, *i.e.* $\alpha|4$ because of (20). Let N denote the number of odd integers among m, U, V, W. Equation (20) excludes $N=0$, whence $N = 1$, 2, 3 or 4. The square of an odd number being of the form $8k+1$ (k an integer) and the square of an even number being of the form $4k$, it follows that S has the form $4k+N$. From $\alpha|4$ and $\alpha|S$ follows then (1) $\alpha = 1$ if $N = 1$ or 3; (2) $\alpha = N$ if $N = 2$ or 4 because (21) shows that each r_{ij} is a multiple of N.

The results can be summarized as follows. A rotation R of a cubic lattice generates a CSL if its axis $[U, V, W]$ is a lattice direction, *i.e.* if U, V and W are integers, and if its angle θ satisfies (16), *i.e.*

$$\tan\frac{\theta}{2} = \frac{(U^2 + V^2 + W^2)^{1/2}}{m}, \tag{24}$$

where m is an integer. We can choose g.c.d. $(m, U, V, W) = 1$ without restricting generality. The matrix describing R is given by (21), where $S = m^2 + U^2 + V^2 + W^2$. The least common denominator of its matrix elements (equal to the multiplicity Σ of the CSL) is given by $\Sigma = S/\alpha$, where

$$\alpha = 1 \text{ if } N = 1 \text{ or } 3, \quad \alpha = 2 \text{ if } N = 2, \quad \alpha = 4 \text{ if } N = 4, \tag{25}$$

N being the number of odd integers among m, U, V, W. Σ is an odd integer.

The term 'generating function' introduced by Ranganathan (1966) is appropriate for $\Sigma = (m^2 + U^2 + V^2 + W^2)/\alpha$ because of the one-to-one correspondence between rotation matrices generating CSLs with multiplicity Σ and the pairs $\pm[m, U, V, W]$ of quadruples of coprime integers satisfying $m^2 + U^2 + V^2 + W^2 = \alpha\Sigma$, $\alpha = 1$, 2 or 4, Σ odd. Because $\pm[m, U, V, W]$ determine the same matrix, we may choose the first non-vanishing component of the quadruple to be positive. With this restriction, we obtain a one-to-one correspondence between quadruples and matrices. The three integers U, V, W, which need not be coprime, determine the rotation axis $[U, V, W]$, the rotation angle θ is given by (24), the rotation matrix by (21).

Table 1. *The possible forms of the characteristic* $\{m_0, U_0, V_0, W_0\}$ *of an equivalence class, the number* $N = 24M$ *of rotations in it and the symmetry of the CSL it generates*

$\{m_0, U_0, V_0, W_0\}$	M	Symmetry of the CSL	
$m_0 > U_0 > V_0 > W_0 > 0$	48	Triclinic or monoclinic	(28*a*)
$m_0 > U_0 > V_0 > W_0 = 0$ $W_0 > 0$, two numbers equal	24	Monoclinic or orthorhombic	(28*b*)
$V_0 > W_0 = 0$, two numbers equal	12	Orthorhombic	(28*c*)
$W_0 > 0$, three numbers equal	8	Hexagonal if $3\|\Sigma$, rhombohedral otherwise	(28*d*)
$m_0 > U_0 > V_0 = W_0 = 0$	6	Tetragonal	(28*e*)
{1 1 1 0}	4	Hexagonal	(28*f*)
{1 0 0 0}	1	Cubic	(28*g*)

4. Some applications of the generating function

The relative orientation between two neighbouring grains of the same phase with point group 432 or $m3m$ can be described in different ways: carry out one of the 24 symmetry rotations of one grain, then a rotation that orients it parallel to the other grain, then a symmetry rotation in its new orientation. Because also the roles of the two grains can be interchanged, up to $2 \times 24^2 = 1152$ different rotations are obtained in this way. They were called (cubically) equivalent by Grimmer (1973, 1974*b*) because they all describe the same relative orientation of the two grains and of two cubic lattices.

Exactly one representative of each equivalence class is obtained by considering only the quadruples of coprime integers $[m_0, U_0, V_0, W_0]$ satisfying

$$\begin{aligned} m_0^2 + U_0^2 + V_0^2 + W_0^2 &= \Sigma, \\ m_0 \geq U_0 \geq V_0 \geq W_0 &\geq 0. \end{aligned} \tag{26}$$

Each equivalence class is therefore determined by its characteristic $\{m_0, U_0, V_0, W_0\}$. The quadruples equivalent to $[m_0, U_0, V_0, W_0]$ are obtained by arbitrary permutations and sign changes in the six quadruples

$$\begin{aligned} &[m_0, U_0, V_0, W_0] \\ &[m_0 + U_0, m_0 - U_0, V_0 + W_0, V_0 - W_0] \\ &[m_0 + V_0, m_0 - V_0, U_0 + W_0, U_0 - W_0] \\ &[m_0 + W_0, m_0 - W_0, U_0 + V_0, U_0 - V_0] \\ &[m_0 + U_0 + V_0 + W_0, m_0 + U_0 - V_0 - W_0, \\ &\quad m_0 - U_0 + V_0 - W_0, m_0 - U_0 - V_0 + W_0] \\ &[m_0 + U_0 + V_0 - W_0, m_0 + U_0 - V_0 + W_0, \\ &\quad m_0 - U_0 + V_0 + W_0, m_0 - U_0 - V_0 - W_0], \end{aligned} \tag{27}$$

i.e. there is a maximum number of $4! \times 2^4 \times 6 = 2304$ equivalent quadruples or 1152 equivalent rotations. Generally, the number N of different equivalent rotations is a multiple of 24, $N = 24M$, and a divisor of $1152 = 24 \times 48$.

Table 1 shows the possible forms of the characteristic $\{m_0, U_0, V_0, W_0\}$ of an equivalence class, the num-

Table 2. *For each equivalence class with $\Sigma < 40$ are listed its number of rotations, its minimum angle rotation with axis $[U, V, W]$ in the reference triangle $U \geq V \geq W \geq 0$ and its 180° rotations with axis $[u, v, w]$ in the reference triangle ($u^2+v^2+w^2=\Sigma$ in the left column, $u^2+v^2+w^2=2\Sigma$ in the right column)*

The equivalence classes are marked by their characteristic and by a short symbol consisting of Σ and a label arranging classes with equal Σ in order of increasing θ_{min}.

Equivalence class			Representative		Axes of 180° rotations with $u \geq v \geq w \geq 0$	
Symbol	$\{m_0, U_0, V_0, W_0\}$	M	$[m, U, V, W]$	θ_{min} (°)		
1	1 0 0 0	1	1 0 0 0	0	1 0 0	1 1 0
3	1 1 1 0	4	3 1 1 1	60	1 1 1	2 1 1
5	2 1 0 0	6	3 1 0 0	36·87	2 1 0	3 1 0
7	2 1 1 1	8	5 1 1 1	38·21		3 2 1
9	2 2 1 0	12	4 1 1 0	38·94	2 2 1	4 1 1
11	3 1 1 0	12	3 1 1 0	50·48	3 1 1	3 3 2
13*a*	3 2 0 0	6	5 1 0 0	22.62	3 2 0	5 1 0
13*b*	2 2 2 1	8	7 1 1 1	27·80		4 3 1
15	3 2 1 1	24	5 2 1 0	48·19		5 2 1
17*a*	4 1 0 0	6	4 1 0 0	28·07	4 1 0	5 3 0
17*b*	3 2 2 0	12	5 2 2 1	61·93	3 2 2	4 3 3
19*a*	3 3 1 0	12	6 1 1 0	26·53	3 3 1	6 1 1
19*b*	4 1 1 1	8	4 1 1 1	46·83		5 3 2
21*a*	3 2 2 2	8	9 1 1 1	21·79		5 4 1
21*b*	4 2 1 0	24	6 2 1 1	44·42	4 2 1	
23	3 3 2 1	24	9 3 1 1	40·46		6 3 1
25*a*	4 3 0 0	6	7 1 0 0	16·26	4 3 0	7 1 0
25*b*	4 2 2 1	24	9 3 3 1	51·68		5 4 3
27*a*	5 1 1 0	12	5 1 1 0	31·59	5 1 1	5 5 2
27*b*	4 3 1 1	24	7 2 1 0	35·43		7 2 1
29*a*	5 2 0 0	6	5 2 0 0	43·60	5 2 0	7 3 0
29*b*	4 3 2 0	24	7 2 2 1	46·40	4 3 2	
31*a*	3 3 3 2	8	11 1 1 1	17·90		6 5 1
31*b*	5 2 1 1	24	5 2 1 1	52·20		7 3 2
33*a*	4 4 1 0	12	8 1 1 0	20·05	4 4 1	8 1 1
33*b*	4 3 2 2	24	11 3 1 1	33·56		7 4 1
33*c*	5 2 2 0	12	5 2 2 0	58·99	5 2 2	5 5 4
35*a*	5 3 1 0	24	8 2 1 1	34·05	5 3 1	
35*b*	4 3 3 1	24	11 3 3 1	43·23		6 5 3
37*a*	6 1 0 0	6	6 1 0 0	18·92	6 1 0	7 5 0
37*b*	4 4 2 1	24	8 3 1 0	43·14		8 3 1
37*c*	5 2 2 2	8	11 3 3 3	50·57		7 4 3
39*a*	6 1 1 1	8	6 1 1 1	32·20		7 5 2
39*b*	5 3 2 1	48	8 3 2 1	50·13		

ber $N = 24M$ of rotations in it and the symmetry of the CSL it generates. Notice that no other cases than those listed in Table 1 are possible because either one or three of the numbers m_0, U_0, V_0, W_0 are odd. The results on the symmetry of the CSL hold at least for $\Sigma < 200$ (Grimmer, 1976). The crystal system of the CSL does not depend on whether the original lattice was primitive, body or face centered (Fortes, 1972*b*). All the rotations of an equivalence class obviously create congruent CSLs. The reverse is not true: congruent CSLs are created, for example, by the classes {4 4 1 0} and {5 2 2 0}.

Grimmer (1976) lists the numbers of equivalence classes of rotations with $\Sigma < 100$ and $\Sigma < 200$ that give rise to a CSL belonging to a given crystal system. The total number of 147 equivalence classes with $\Sigma < 100$ is 1 larger than the number given by BD because the trivial case $\Sigma = 1$ is included.

The total number of rotations generating CSLs with multiplicity Σ was determined by Grimmer (1976) to be $N(\Sigma) = 24M(\Sigma)$, where

$$M(\Sigma) = (p_1+1)(p_2+1)\ldots(p_s+1)p_1^{m_1}p_2^{m_2}\ldots p_r^{m_r}, \quad (28)$$

if the decomposition of the odd number Σ into a product of primes contains s different primes, r of which appear more than once:

$$\Sigma = p_1 p_2 \ldots p_s p_1^{m_1} p_2^{m_2} \ldots p_r^{m_r}, \quad (29)$$

e.g. $45 = 3\times5\times3^1$, $M(45) = 4\times6\times3^1 = 72$.

It follows from (27) that each equivalence class contains quadruples $[m, U, V, W]$ satisfying $m \geq (\sqrt{2}-1)U$ and $m \geq U+V+W$. The corresponding rotations have the least value θ_{min} of the rotation angle. Among these rotations there is at least one with $U \geq V \geq W \geq 0$, *i.e.* with axis in the reference (stereographic) triangle. If the equivalence class generates a CSL, there is only one such rotation (Grimmer, 1974*b*), which will be chosen as its representative. It is usually called the disorientation.

180° rotations are of special interest, too, being convenient to describe twins (*cf. e.g.* Fortes, 1972*b*). Equivalence classes of type (28*a*) contain no 180° rotations, those of types (28*b*–28*e*) contain 24, the class {1 1 1 0} contains 16 and {1 0 0 0} contains nine 180° rotations. One of the 180° rotations has an axis $[u, v, w]$ with $u \geq v \geq w \geq 0$ and $u^2+v^2+w^2=\Sigma$ if $W_0=0$, one has an axis with $u \geq v \geq w \geq 0$ and $u^2+v^2+w^2=2\Sigma$ if at least two of the four components m_0, U_0, V_0, W_0 are equal.

Table 2 lists for each equivalence class with $\Sigma < 40$ its number of rotations, its minimum angle rotation with axis $[U, V, W]$ in the reference triangle $U \geq V \geq W \geq 0$ and its 180° rotations with axis $[u, v, w]$ in the reference triangle.

Table 2 shows that Fig. 2 in BD needs a correction: [5 1 0] belongs to 13*a*, [5 4 1] to 21*a*.

Table 1 in Mykura (1980) extends our Table 2 to $\Sigma \leq 101$. Although his definition of equivalence differs from ours, only the asterisks in his table remind us of his different definition.

Expressed in crystal coordinates of one of the two lattices, which we call lattice 1, a bicrystal in CSL orientation with a plane grain boundary may be characterized by the disorientation that maps lattice 1 onto lattice 2 and by a vector perpendicular to the grain boundary and pointing towards lattice 2. As an example, we consider a bicrystal in 39*b* orientation with a boundary plane that is for one of the two lattices of type {1 0 0}. There are 12 physically distinct such bicrystals forming six enantiomorphous pairs. They can be characterized by the disorientation

$$R = \frac{1}{39}\begin{bmatrix} 34 & -2 & 19 \\ 14 & 29 & -22 \\ -13 & 26 & 26 \end{bmatrix} \tag{30}$$

and one of the 12 vectors

$$\pm\begin{pmatrix}1\\0\\0\end{pmatrix}, \quad \pm\begin{pmatrix}0\\1\\0\end{pmatrix}, \quad \pm\begin{pmatrix}0\\0\\1\end{pmatrix}, \tag{31a}$$

$$\pm\begin{pmatrix}34\\14\\-13\end{pmatrix}, \quad \pm\begin{pmatrix}-2\\29\\26\end{pmatrix}, \quad \pm\begin{pmatrix}19\\-22\\26\end{pmatrix}. \tag{31b}$$

An alternative characterization is given by one of the two matrices R, R^{-1} and one of the six vectors (31*a*).

If $M < 48$ then R^{-1} [or (31*b*)] is not needed to list all physically distinct bicrystals with a boundary plane of type {1 0 0} for one of the two lattices.

Given a rotation matrix, different methods, often not described in detail, have been used by different authors to determine a basis for the CSL. A systematic and easily programmed method for primitive cubic lattices was described by Grimmer (1974*a*). Other systematic methods and the transition from primitive to centered cubic lattices were described by Grimmer, Bollmann & Warrington (1973). A generalization of the first-mentioned method to arbitrary lattices was given by Bonnet (1976).

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