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A New Formulation for the Generation of Coincidence Site Lattices (CSL's) in the Cubic System*

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Abstract

The generation of tables of CSL's in the cubic system is presented with three parameters giving easy and rapid access to all the significant data characterizing a CSL: it is given by the rotation matrix from which the rotation axis and the rotation angle are easily determined. A method for the experimental determination of a CSL is presented, based on this new formulation.

1. Introduction

Two identical crystal lattices related by a special rotation operation (defined by an axis $[uvw]$ and an angle θ) may have certain common sites located on a single lattice of larger cell dimension (Ranganathan, 1966). This larger lattice is called the coincidence site lattice (CSL). The volume ratio of the primitive cells of the CSL and the crystal lattice is called the multiplicity Σ (Warrington & Bufalini, 1971). CSL's are of importance in connection with the study of grain boundaries. It is an extension of the concept of twinning. This paper will more specifically be devoted to the determination of these special rotation operations describing a CSL and their symmetrically equivalent descriptions. This information is included in the rotation matrix. The properties of that matrix (Grimmer, Bollmann & Warrington, 1974) will be extensively used for the establishment of a new simple formulation of that well-known matrix. This is a useful tool for the rapid establishment of extended tables of CSL's. It will be applied to other systems in future work.

Ranganathan (1966) proposed the following relationships between the variables uvw in the cubic system:

$$\tan(\theta/2) = \frac{y}{x}(u^2 + v^2 + w^2)^{1/2} \qquad (1)$$

and

$$\Sigma = x^2 + (u^2 + v^2 + w^2)y^2, \qquad (2)$$

where x, y are integers.

As a consequence, Grimmer (1973) showed that all the CSL's in the cubic system can be deduced from all different decompositions of the multiplicity Σ into a sum of the squares of four integers:

$$\Sigma = a^2 + b^2 + c^2 + d^2. \qquad (3)$$

Grimmer (1974) also discussed the possibility of different or equivalent descriptions of a CSL and showed that there are $24^2 \times 2$ possible 'cubically equivalent' descriptions of a particular CSL.

Warrington & Bufalini (1971) proposed another method for the generation of a CSL. According to them, the rotation matrix describing a CSL has the form

$$\mathsf{R} = \frac{1}{\Sigma}[r_{ij}], \qquad (4)$$

where Σ is the multiplicity and r_{ij} are integers without a common divisor. The column vector $(r_{i1}/\Sigma,\ r_{i2}/\Sigma,\ r_{i3}/\Sigma)$ forms a unitary orthonormal basis.

The general procedure for the generation of the CSL's is therefore the following:

(*a*) determine for every Σ all the lattice vectors of length Σ;

(*b*) from these, choose all the possible orthonormal bases;

(*c*) finally, eliminate the bases for which the numbers r_{ij} have a common divisor.

With the same basic arguments, the last method was extended to the hexagonal system by Warrington (1975) and CSL rotation axes–rotation angles have been given for $c/a = \sqrt{8/3}$. It was similarly used by Grimmer, Bollmann & Warrington (1974) for the determination of the CSL and the DSC lattice.

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Ranganathan's formula gives a simple and fast criterion for the determination of the existence of a CSL for a given axis or a given Σ. Grimmer's method has the advantage of being a more systematic method for the generation and description of all CSL's for the cubic system. Moreover, as far as we know, there is no extension of the two theories to another system.

It is the purpose of this paper to give the principles of a method for the generation of all possible CSL's for the cubic system, based on properties of integer numbers. The expression of the rotation matrix will be given, from which the other data may be deduced. The main advantage of this formulation is that the correlation of Ranganathan's formulas and Warrington's approach will be given with firstly a better insight into the properties of formulas (2) and (4) and secondly the obvious possibility of the extension to other systems.

2. The rotation matrix describing a CSL

Any rigid body displacement leaving one point fixed is described by a rotation of an angle θ around an axis with direction cosines p_1, p_2, p_3 (Euler's theorem). The rotation matrix is of the form

$$\mathrm{R}=\begin{bmatrix} p_1^2(1-\cos\theta)+\cos\theta & p_1p_2(1-\cos\theta)-p_3\sin\theta & p_1p_3(1-\cos\theta)+p_2\sin\theta \\ p_2p_1(1-\cos\theta)+p_3\sin\theta & p_2^2(1-\cos\theta)+\cos\theta & p_2p_3(1-\cos\theta)-p_1\sin\theta \\ p_3p_1(1-\cos\theta)-p_2\sin\theta & p_3p_2(1-\cos\theta)+p_1\sin\theta & p_3^2(1-\cos\theta)+\cos\theta \end{bmatrix}, \quad (5)$$

where $p_1^2+p_2^2+p_3^2=1$.

Expressing the rotation axis with its Miller indices u, v, w, one has

$$p_1=\frac{u}{\sqrt{d}} \quad p_2=\frac{v}{\sqrt{d}} \quad p_3=\frac{w}{\sqrt{d}} \quad d=u^2+v^2+w^2, \quad (6)$$

with

$$(u,v,w) \doteqdot 1^* \quad (7)$$

and introducing the multiplicity Σ in agreement with relation (4), for a rotation describing a CSL, the rotation matrix (5) becomes:

$$\mathrm{R}=[R_{ij}]=\frac{1}{\Sigma}[r_{ij}]$$

$$=\frac{1}{\Sigma}\begin{bmatrix} u^2\frac{\Sigma}{d}(1-\cos\theta)+\Sigma\cos\theta & uv\frac{\Sigma}{d}(1-\cos\theta)-w\frac{\Sigma}{\sqrt{d}}\sin\theta & uw\frac{\Sigma}{d}(1-\cos\theta)+v\frac{\Sigma}{\sqrt{d}}\sin\theta \\ uv\frac{\Sigma}{d}(1-\cos\theta)+w\frac{\Sigma}{\sqrt{d}}\sin\theta & v^2\frac{\Sigma}{d}(1-\cos\theta)+\Sigma\cos\theta & vw\frac{\Sigma}{d}(1-\cos\theta)-u\frac{\Sigma}{\sqrt{d}}\sin\theta \\ uw\frac{\Sigma}{d}(1-\cos\theta)-v\frac{\Sigma}{\sqrt{d}}\sin\theta & vw\frac{\Sigma}{d}(1-\cos\theta)+u\frac{\Sigma}{\sqrt{d}}\sin\theta & w^2\frac{\Sigma}{d}(1-\cos\theta)+\Sigma\cos\theta \end{bmatrix}. \quad (8)$$

The matrix (8) describes a CSL of multiplicity Σ (an integer) if and only if the elements r_{ij} are integers (Warrington, 1975).

It is known that the Miller indices of the rotation axis are given according to the following relations:

$$u=\frac{\sqrt{d}(r_{32}-r_{23})}{2\Sigma\sin\theta}, \quad v=\frac{\sqrt{d}(r_{13}-r_{31})}{2\Sigma\sin\theta},$$

$$w=\frac{\sqrt{d}(r_{21}-r_{12})}{2\Sigma\sin\theta} \quad (9)$$

and the rotation angle is deduced from the trace of the matrix:

$$\mathrm{tr}=\frac{S}{\Sigma}=1+2\cos\theta \quad \text{or} \quad \cos\theta=\frac{S-\Sigma}{2\Sigma}, \quad (10)$$

where S is the sum of the diagonal elements of $[r_{ij}]$:

$$S=r_{11}+r_{22}+r_{33}. \quad (11)$$

3. A direct correlation of Ranganathan's formula and Warrington's approach

With the following transformations,

$$\cos\theta=\frac{x^2-dy^2}{\Sigma}, \quad \sin\theta=\frac{2xy\sqrt{d}}{\Sigma}, \quad (12)$$

* $(q_1, q_2, q_2\dots)\doteqdot p$ means that the greatest common divisor of q_i $(i=1, 2,\dots)$ is the integer p.

easily deduced from Ranganathan's relations (1) and (2), the matrix (5) becomes

$$\mathsf{R} = \frac{1}{\Sigma}\begin{bmatrix} 2u^2y^2 + x^2 - dy^2 & 2uvy^2 - 2wxy & 2uwy^2 + 2vxy \\ 2uvy^2 + 2wxy & 2v^2y^2 + x^2 - dy^2 & 2vwy^2 - 2uxy \\ 2uwy^2 - 2vxy & 2vwy^2 + 2uxy & 2w^2y^2 + x^2 - dy^2 \end{bmatrix}, \quad (13)$$

where obviously the matrix elements obey the conditions for the matrix (4). We can see from (13) that for three given integers x, y and d satisfying the relation $\Sigma = x^2 + y^2 d$, the matrix R is rapidly established. Therefore, a superficial analysis indicates that this is a simple procedure for the determination of all the rotation relationships for a given Σ. It should however be noted that some uncertainties remain, as already mentioned by Ranganathan (1966): that, for example, erroneous determinations of multiple Σ values arise. Relation (13) would therefore more strictly be written in the form

$$\mathsf{R} = \frac{1}{\Sigma}\left[\frac{r_{ij}}{\alpha}\right] \quad \text{and} \quad \Sigma = \frac{x^2 + dy^2}{\alpha}, \quad (14)$$

where α is a possible common factor of the r_{ij} elements.

Up till now a particular form of the rotation matrix has been deduced from Ranganathan's formula. A different procedure will be presented later based exclusively on the form of the rotation matrix and on arithmetical properties of its elements when the rotation describes a CSL. This will lead to the demonstration of expressions similar to (13) and (14).

4. Effect of the symmetries on the elements of the rotation matrix

If G_i are the symmetry-element rotation matrices of the cubic point group (see, for example, Karakostas, Bleris & Antonopoulos, 1979), then other descriptions R_i of the same CSL are produced with the expression:

$$\mathsf{R}_i = \mathsf{R}G_i \quad i = 1, 2, \ldots, 24, \quad (15)$$

where R and R_i are matrices of type (8). On the other hand, for every description R_n of type (15), a description of another symmetrically equivalent CSL is given by the expression:

$$\mathsf{R}_{nj} = G_j \mathsf{R}_n G_j^{-1} \quad j = 1, 2, \ldots, 24. \quad (16)$$

This shows that 24^2 symmetrically equivalent descriptions exist for a particular CSL. Since the role of lattices 1 and 2 can be exchanged, there are actually 2×24^2 symmetrically equivalent descriptions of a CSL (Grimmer, 1974).

Taking into account the form of the matrices R_{ij}, it is easily established, as a consequence of the form of G_i, that the absolute values of the nine terms of all the matrices of symmetrically equivalent descriptions of CSL's in the cubic systems are all equal two by two.

5. Rotation matrix describing a CSL for which $\theta = 180°$

Firstly, the simplified problem of the form of a rotation matrix with the description for which $\theta = 180°$ will be examined. The rotation matrix (8) for $\theta = 180°$ becomes

$$\mathsf{R}_{180} = \frac{1}{\Sigma}\begin{bmatrix} 2u^2\frac{\Sigma}{d} - \Sigma & 2uv\frac{\Sigma}{d} & 2uw\frac{\Sigma}{d} \\ 2uv\frac{\Sigma}{d} & 2v^2\frac{\Sigma}{d} - \Sigma & 2vw\frac{\Sigma}{d} \\ 2uw\frac{\Sigma}{d} & 2vw\frac{\Sigma}{d} & 2w^2\frac{\Sigma}{d} - \Sigma \end{bmatrix}. \quad (17)$$

The matrix (17) describes a CSL if the r_{ij} are all integers, *i.e.* the numbers

$$2vw\frac{\Sigma}{d}, \quad 2uw\frac{\Sigma}{d}, \quad 2uv\frac{\Sigma}{d} \quad (18)$$

must be integers. Since $(u,v,w) \doteqdot 1$, one has $(uv,uw,uw) \doteqdot 1$, therefore 2Σ must be a multiple of d:

$$2\Sigma = fd \quad (19)$$

and the rotation matrix (17) becomes

$$\mathsf{R}_{180} = \frac{1}{\Sigma}\begin{bmatrix} f(u^2 - d/2) & fuv & fuw \\ fuv & f(v^2 - d/2) & fvw \\ fuw & fvw & f(w^2 - d/2) \end{bmatrix}. \quad (20)$$

Since the elements of matrix (20) have no common divisor and taking into account the form of the elements r_{ij}, $i \neq j$, it is clear that f may take only the following values:

$$f = 1 \quad \text{if } d \equiv 0 (\text{mod } 2)$$

or (21)

$$f = 2 \quad \text{if } d \equiv 1 (\text{mod } 2).$$

This proves the well-known relation (Ranganathan, 1966; Grimmer, 1973; Karakostas *et al.*, 1979):

$$d = u^2 + v^2 + w^2 = \Sigma \text{ or } 2\Sigma. \quad (22)$$

Moreover, since the only forbidden values for Σ are $\Sigma \equiv 0 (\text{mod } 2)$ (which is treated in Appendix II), and since it is known that forbidden values for d are of the form (*International Tables for X-ray Crystallography*, 1959)

$$d \equiv 0 \pmod 4, \qquad d \equiv 7 \pmod 8 \tag{23}$$

[d is a sum of squares of three integers (Mordell, 1969)]. From the first of these expressions it is concluded that there is no other condition relating Σ and d.

On the other hand, since (9) are undetermined for a 180° rotation, they are replaced by the following expressions [(20), (21)]:

$$u = [f(r_{11} + \Sigma)]^{1/2}, \quad v = [f(r_{22} + \Sigma)]^{1/2}, \quad w = [f(r_{33} + \Sigma)]^{1/2}, \tag{24}$$

where the signs of u, v and w are deduced from

$$\begin{aligned} \text{sign}(uv) &= \text{sign}(r_{21}) = \text{sign}(r_{12}) \\ \text{sign}(uw) &= \text{sign}(r_{13}) = \text{sign}(r_{31}) \\ \text{sign}(vw) &= \text{sign}(r_{32}) = \text{sign}(r_{23}). \end{aligned} \tag{25}$$

The matrix (20) with the conditions (21) is the general form for the description of 180° leading to a CSL. It allows a direct determination of all the elements of the CSL. In particular, it allows, with (22), a simple and fast determination of all possible CSL's of a particular multiplicity Σ which have a 180° rotation description.

Finally, it is possible, from the form of matrix (20), to propose a criterion for the recognition of a CSL which can be described by a rotation of 180°. This criterion is a direct consequence of the symmetry properties discussed in § 4.

Criterion. If a matrix R describes a CSL relationship, this CSL has a 180° rotation description, if R has at least three pairs of terms equal in absolute value.

6. The general form of a rotation matrix describing a CSL

With the following transformation, according to (10):

$$\cos\theta = \frac{S-\Sigma}{2\Sigma}, \quad 1-\cos\theta = \frac{3\Sigma - S}{2\Sigma},$$

$$\sin\theta = \frac{1}{2\Sigma}(3\Sigma - S)^{1/2}(S+\Sigma)^{1/2},$$

the rotation matrix (8) takes the general form

$$\mathrm{R} = \frac{1}{\Sigma}\begin{bmatrix} u^2\frac{3\Sigma-S}{2d} + \frac{S-\Sigma}{2} & uv\frac{3\Sigma-S}{2d} - w\frac{[(3\Sigma-S)(S+\Sigma)]^{1/2}}{2\sqrt{d}} & uw\frac{3\Sigma-S}{2d} + v\frac{[(3\Sigma-S)(S+\Sigma)]^{1/2}}{2\sqrt{d}} \\ uv\frac{3\Sigma-S}{2d} + w\frac{[(3\Sigma-S)(S+\Sigma)]^{1/2}}{2\sqrt{d}} & v^2\frac{3\Sigma-S}{2d} + \frac{S-\Sigma}{2} & vw\frac{3\Sigma-S}{2d} - u\frac{[(3\Sigma-S)(S+\Sigma)]^{1/2}}{2\sqrt{d}} \\ uw\frac{3\Sigma-S}{2d} - v\frac{[(3\Sigma-S)(S+\Sigma)]^{1/2}}{2\sqrt{d}} & vw\frac{3\Sigma-S}{2d} + u\frac{[(3\Sigma-S)(S+\Sigma)]^{1/2}}{2\sqrt{d}} & w^2\frac{3\Sigma-S}{2d} + \frac{S-\Sigma}{2} \end{bmatrix}. \tag{26}$$

This expression makes use exclusively of integer variables (Σ, u, v w, S and d), so that all the terms r_{ij} must be integers in order to express a rotation describing a CSL. In this event, a new formulation of (26) is proposed with new parameters m, n and f obtained by expressing the following obvious properties.

1. Since $2r_{ij}$ for $i=j$ are integers, and since their second terms are integers, $S-\Sigma$, their first terms must also be integers; taking into account (7), one concludes that $(3\Sigma - S)/d$ is an integer.

2. The differences $r_{ij} - r_{ji}$ for $i \neq j$ are also integers, this implies that the product $(3\Sigma - S)(S+\Sigma)$ is a perfect square multiple of the integer d.

Therefore, if m and n are any integers, and f is unity or a square-free integer (*i.e.* an integer without a square factor), then the expressions $3\Sigma - S$ and $S + \Sigma$ are necessarily of one of the forms:

$$\begin{cases} 3\Sigma - S = fd \\ S+\Sigma = fm^2 \end{cases} \text{ or } \begin{cases} 3\Sigma - S = dn^2 \\ S+\Sigma = m^2 \end{cases} \text{ or } \begin{cases} 3\Sigma - S = fdn^2 \\ S+\Sigma = fm^2 \end{cases}, \tag{27}$$

the last being the most general. Moreover, we have

$$f(m^2 + dn^2) \equiv 0 \pmod 4, \qquad f(3m^2 - dn^2) \equiv 0 \pmod 4, \tag{28}$$

since the determinant of the transformation (27) is equal to 4.

With (27), (26) becomes

$$R = \frac{1}{\Sigma}\begin{bmatrix} \frac{f}{4}(2u^2n^2 + m^2 - dn^2) & \frac{f}{4}(2uvn^2 - 2wmn) & \frac{f}{4}(2uwn^2 + 2vmn) \\ \frac{f}{4}(2uvn^2 + 2wmn) & \frac{f}{4}(2v^2n^2 + m^2 - dn^2) & \frac{f}{4}(2vwn^2 - 2umn) \\ \frac{f}{4}(2uwn^2 - 2vmn) & \frac{f}{4}(2vwn^2 + 2umn) & \frac{f}{4}(2w^2n^2 + m^2 - dn^2) \end{bmatrix} \quad (29)$$

and

$$\Sigma = \frac{f}{4}(m^2 + dn^2). \quad (30)$$

The factor 1/4 in (29) and (30) may be eliminated if compatibility conditions are introduced between the parameters m,n and the variables Σ,d. This will be done later on. The factor f may then be considered as a superfluous common factor, therefore $f = 1$. Finally, the elements of the matrix (29) may have a common factor, which will be eliminated by introducing a new parameter α, which has to be determined. The relations (29), (30) then have the following form:

$$R = \frac{1}{\Sigma}\begin{bmatrix} (2u^2n^2 + m^2 - dn^2)/\alpha & (2uvn^2 - 2wmn)/\alpha & (2uwn^2 + 2vmn)/\alpha \\ (2uvn^2 + 2wmn)/\alpha & (2v^2n^2 + m^2 - dn^2)/\alpha & (2vwn^2 - 2umn)/\alpha \\ (2uwn^2 - 2vmn)/\alpha & (2vwn^2 + 2umn)/\alpha & (2w^2n^2 + m^2 - dn^2)/\alpha \end{bmatrix} \quad (31a)$$

or

$$R = \frac{1}{\Sigma}[r^*_{ij}/\alpha] \quad \text{with} \quad r^*_{ij}/\alpha = r_{ij}, \quad (31b)$$

where r^*_{ij} all express integer values; α is the common factor of the terms r^*_{ij} and

$$\Sigma = (m^2 + dn^2)/\alpha = \Sigma^*/\alpha. \quad (32)$$

Allowed values of α will be determined, and the selection rules for the m and n values for given α and d values will also be established. Thereafter any CSL of a given Σ value is simply deduced from the relation (32) giving all compatible values for the four parameters m, n, α and d.

The relation (32) is more general than Ranganathan's generating function. It is a direct consequence of Warrington's approach applied to the matrix (26).

7. Definitive form of the rotation matrix

Expression (31) for the rotation matrix was obtained starting from the general form of a rotation matrix and based on some evident conditions that its elements are expressed with integer numbers. It makes exclusive use of the following integers:

Σ, defining the multiplicity of the CSL;

u, v and w, the Miller indices of the rotation axis, taking (7) into account;

d, the square of the length of the vector $[uvw]$;

m, n and α, three parameters; the conditions limiting their possible values will be established; this will allow the generation of all possible expressions of a CSL.

Expression (31) satisfies two conditions presented by Warrington: all the elements r_{ij} are integers (for compatible α values), and the three column vectors form an orthonormal base. It must still be noted that all the r_{ij} elements have no common divisor. This condition will be fulfilled if the α value is the greatest common divisor of the elements r^*_{ij}. Therefore all possible α values will be determined.

In order to avoid obvious α values, we will express a limiting condition on the parameters m and n:

$$(m,n) \doteq 1 \quad (33)$$

since the elements r^*_{ij} are homogeneous in m and n.

A detailed analysis of the possible α values is given in Appendix I. The reasoning is essentially centered on the consideration of the non-diagonal elements. It is concluded that the only possible values for α are $\alpha = 1$, 2 or 4.

A last analysis is still necessary in order to determine under which conditions these α values will be attributed. This will be given in terms of selection rules limiting possible α, m and n values for given d values. Their determination is given in Appendix II and summarized in Table 1.

The determination of these selection rules, based on the condition that (32) expresses an integral Σ value, has shown that they are compatible with the condition that the elements r_{ij} of (31) are all integers. Moreover, it has also been proved that only the odd values of Σ are allowed.

Therefore, it has been proved that (31), including the conditions limiting the values of m, n and α [(33) and

Table 1. *Selection rules – α values*

	$d = 1 \pmod 4$	$d = 2 \pmod 4$	$d = 3 \pmod 4$
$m = 1 \pmod 2$, $n = 1 \pmod 2$	2	1	4
$m = 0 \pmod 2$, $n = 1 \pmod 2$	1	2	1
$m = 1 \pmod 2$, $n = 0 \pmod 2$	1	1	1

Table 1], always describes a CSL and that any CSL may be expressed in that form.

8. Determination of CSL's in the cubic system

Any values given to the parameters m, n and α for a given multiplicity Σ allow a simple and fast determination of the rotation elements: the corresponding d value is given by (32) and any possible decomposition of d according to (6) gives the Miller indices of possible rotation axes. The corresponding rotation angle is given by the trace of the matrix (31):

$$\cos\theta = \frac{m^2 - dn^2}{m^2 + dn^2} \quad \text{or} \quad \tan\frac{\theta}{2} = \frac{n}{m}\sqrt{d}; \qquad (34)$$

the rotation matrix (31) is also rapidly determined.

Reciprocally a given rotation operation, $[uvw]$, θ, is rapidly converted into d,m,n parameters according to (34), taking into account (33); then α is determined according to (32) and the rotation matrix is determined according to (31).

It is clear in particular that u, v and w may take any value compatible with Miller indices, and that m and n are always positive integers, since $0 < \theta \leq 180°$.

An appreciable interest of this approach is direct access to all the symmetrically equivalent descriptions according to (16), since u,v,w are introduced as parameters. Therefore, all the significant different descriptions of a particular CSL may be generated in a reference triangle without useless duplication (as occurs in Warrington's approach) stating, for example,

$$u \geq v \geq w \geq 0, \qquad (35)$$

then all compatible m,n,α,d values will give all possible descriptions allowing a systematic generation of tables of CSL's.

The identity is described by $n = 0$ $(m = 1)$; this trivial case will not be considered. For $m = 0$ and $n = 1$, the rotation angle is $\theta = 180°$ and the matrix (31) takes the form of the matrix (20).

9. A systematic generation of CSL's

In practice, for a particular mutliplicity Σ, the generation of all possible different descriptions of existing CSL's is obtained without duplication (*i.e.* there is no double description with the same rotation angle and a symmetrically equivalent rotation axis) by varying m and n from 0 to a maximum allowed value determined by (32) in agreement with (33). The corresponding d value is determined and then all its possible decompositions according to (6), (7) and (35).

The role played by the parameters m, n and α is illustrated in Fig. 1 for Σ values up to $\Sigma = 35$, which shows that the characteristic elements of rotation operations describing a CSL fall on lines of equal m/n ratios.

An application of the method has allowed us to establish the list of all CSL's up to $\Sigma < 100$, where 146 CSL's appear, from which 17 have no 180° description. This list is in agreement with the list obtained by application of (3), but all equivalent descriptions are given since all significant data are rapidly determined with the fundamental equations (31), (32) and (34) and Table 1.

10. Characterization of a bicrystal in terms of a CSL

Limiting ourselves to multiplicities up to $\Sigma = 35$, the establishment of a table of CSL's suggests a method of characterization of a bicrystal since all of these CSL's have a 180° description. Relations (15) and (16) allow one to refer a bicrystal to its greatest-rotation-angle description through a rotation axis situated in the reference triangle. A graphical determination is therefore possible. Fig. 2 represents all rotation axes corresponding to a 180° rotation for CSL's with $\Sigma \leq 35$. The experimental rotation axis is shown on this stereographic projection and the deviation from an ideal CSL description is given by two components: the difference in rotation angle and the difference in

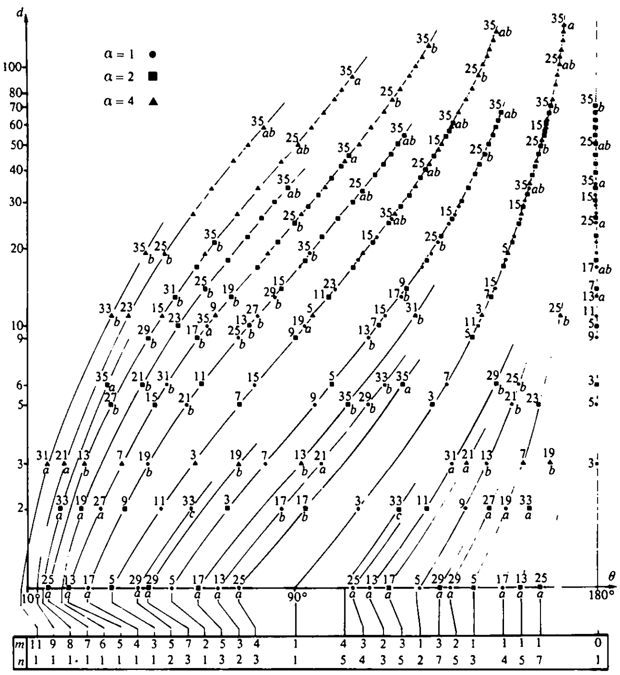

Fig. 1. A graph of the d values ($d = u^2 + v^2 + w^2$, $[uvw]$ is the rotation axis) as a function of the rotation angle, θ, showing that all CSL's are described with two main parameters m and n, taking into account three values for the third parameter, α. ● $\alpha = 1$; ■ $\alpha = 2$; ▲ $\alpha = 4$.

rotation axis. A rigorous method has been proposed by Bleris, Antonopoulos, Karakostas & Delavignette (1981) for the calculation of this deviation. A general procedure for the characterization of a bicrystal in terms of CSL's has also been given by Bleris, Hagège, Nouet, Antonopoulos, Karakostas & Delavignette (1980).

11. Conclusion

A bridge is laid between the theories of Ranganathan and Warrington leading to the generalization of Ranganathan's generating function and allowing a simple and fast establishment of tables of CSL's in the cubic system. Rotation matrices describing CSL's are established with the parameters m,n,α. The arguments are general and will be applied in a future paper to the hexagonal system.

APPENDIX I
Determination of the possible α values

The rotation matrix (31) describes a CSL of multiplicity Σ if the r_{ij} elements are relatively prime, *i.e.* if α is the common divisor of the elements r^*_{ij}. A generation of CSL's with (31) is therefore possible if the values α are determined.

If $\alpha | n$,* then according to (32) it is concluded that $\alpha | m$, which is impossible according to (33); therefore it will be supposed that

$$(\alpha,n) \div 1. \qquad (AI.1)$$

* $\alpha | n$ has the meaning 'α divides n'.

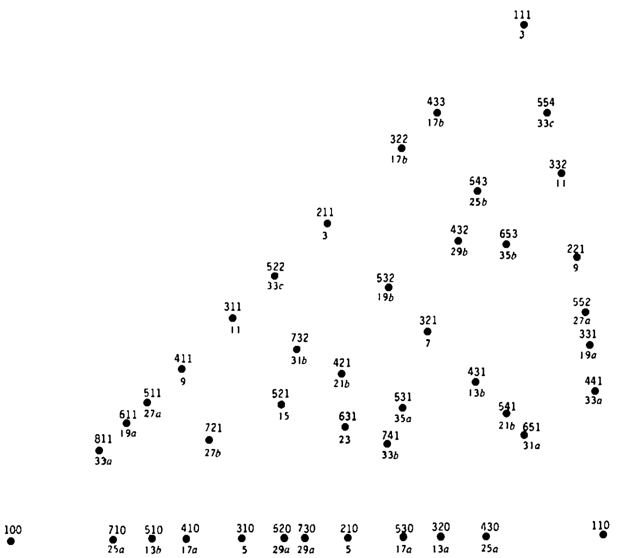

Fig. 2. Stereographic projection of the 180° rotation axes for all CSL's up to $\Sigma = 35$ in the reference triangle (cubic system).

The determination of possible α values will be based on the consideration of the non-diagonal elements r^*_{ij} for $i \neq j$. The common divisors of both terms of the algebraic sums of $r^*_{ij}/2n$ $(i \neq j)$ will be considered:

$$(uvn,wm) \div p_1; \quad (uwn,vm) \div p_2 \quad \text{and}$$
$$(vwn,um) \div p_3. \qquad (AI.2)$$

Supposing first that at least one of these three pairs is relatively prime, it is known that its sum and its difference, which are $r^*_{ij}/2n$ and $r^*_{ji}/2n$, may have only one common factor: the number 2. Therefore, according to (AI.1), the only common divisors for r^*_{ij} and r^*_{ji}, which are the only possible α values, are $\alpha = 1$, 2 or 4.

The values of α must then be determined in the event that p_1, p_2 and p_3 are all different from unity. Without restricting the generality, it will be supposed that p_1 is the smallest of the three.

A possible α value (different from 2 or 4) must obviously divide p_1:

$$\alpha | p_1 \quad \text{or} \quad 2p_1 \quad \text{or} \quad 4p_1.$$

Considering the corresponding relation (AI.2), we will show that this implies the possible occurrence of five different events separately or in different simultaneous combinations. The occurrence of all combinations of these events leads to an internal contradiction proving that the only possible α values are still in this case 1, 2 or 4:

$$E_1{:}\,\alpha|(n,w); \quad E_2{:}\,\alpha|(u,w); \quad E_3{:}\,\alpha|(v,w);$$
$$E_4{:}\,\alpha|(u,m); \quad E_5{:}\,\alpha|(v,m). \qquad (AI.3)$$

[A sixth event is clearly self contradictory – $E_6{:}\,\alpha|(m,n)$ – according to (33).]

All the possible combinations of the five events are given in Table 2 by a Boolean representation where '1' indicates that the corresponding relation (AI.3) is realized and '0' in the opposite case.

The rejection of different combinations is based on four different arguments *a* to *d*. They are indicated in Table 2:

Table 2. *Boolean analysis with binary description for five events*

	E_1	E_2	E_3	E_4	E_5	Exclusions		E_1	E_2	E_3	E_4	E_5	Exclusions
1	1	1	1	1	1	*a b c*	17	0	0	0	1	1	*c*
2	0	1	1	1	1	*a c*	18	0	0	1	0	1	*c*
3	1	0	1	1	1	*b c*	19	0	0	1	1	0	*c d*
4	1	1	0	1	1	*b c*	20	0	1	0	0	1	*c d*
5	1	1	1	0	1	*a b c*	21	0	1	0	1	0	*c*
6	1	1	1	1	0	*a b c*	22	0	1	1	0	0	*a*
7	0	0	1	1	1	*c*	23	1	0	0	0	1	*b c d*
8	0	1	0	1	1	*c*	24	1	0	0	1	0	*b c d*
9	0	1	1	0	1	*a c*	25	1	0	1	0	0	*b d*
10	0	1	1	1	0	*a c*	26	1	1	0	0	0	*b d*
11	1	0	0	1	1	*b c*	27	0	0	0	0	1	*d*
12	1	0	1	0	1	*b c*	28	0	0	0	1	0	*d*
13	1	0	1	1	0	*b c d*	29	0	0	1	0	0	*d*
14	1	1	0	0	1	*b c d*	30	0	1	0	0	0	*d*
15	1	1	0	1	0	*b c*	31	1	0	0	0	0	*b*
16	1	1	1	0	0	*a b*	32	0	0	0	0	0	

a: If E_2 and E_3 occur simultaneously, then $\alpha\,|\,(u,v,w)$ is improper because of (7).

b: If E_1 occurs, $\alpha\,|\,(m,n)$ or $\alpha\,|\,(u,v,w)$ is improper because of (7) or (33).

c: If α divides two Miller indices, as well as m, then, according to (32), since it divides Σ, it should divide d (and therefore divide the third Miller index) or divide n, both improper. This excludes the following simultaneous occurrences: E_1E_4, E_1E_5, E_2E_4, E_2E_5, E_3E_4, E_3E_5 and E_4E_5.

d: The occurrence of one event (E_2 to E_5) implies the occurrence of another event according to relation (*A*I.2), improper when labeled 0, or contradicts relation (33). E_2 implies E_3 or E_4; E_3 implies E_2 or E_5; E_4 implies E_2 or E_5 or contradicts (33); E_5 implies E_3 or E_4 or contradicts (33).

Only combinations 32 in Table 2 remains, proving that the only possible values for α are 1, 2 or 4.

APPENDIX II
Selection rules

Compatibility conditions between m, n, α and d will be expressed in terms of selection rules. Forbidden α values will be determined first considering the parity of the parameters m and n [m and n even is excluded according to (33)], then for each case three forms of d are considered since $d \equiv 0 (\mathrm{mod}\ 4)$ is excluded according to (23). Use is made of the well known property:

$$\text{if } p \text{ is any integer } (2p+1)^2 \equiv 1 (\mathrm{mod}\ 8). \quad (A\mathrm{II}.1)$$

Also, we will use:

$$\text{if } d \equiv 3 (\mathrm{mod}\ 4) \text{ then } u, v \text{ and } w \text{ are all odd and } d = 3 (\mathrm{mod}\ 8). \quad (A\mathrm{II}.2)$$

(I) m and n are odd.

(i) $d \equiv 1 (\mathrm{mod}\ 4)$.

From (32) it is concluded that $\Sigma^* \equiv 2 (\mathrm{mod}\ 4) \rightarrow \alpha = 2$, Σ is odd. This α value is compatible with r^*_{ij} (in particular this becomes obvious for the r_{ii} elements after the substitution $m^2 = 2\Sigma - dn^2$).

(ii) $d \equiv 2 (\mathrm{mod}\ 4)$.

From (32) it is concluded that $\Sigma^* \equiv 3 (\mathrm{mod}\ 4) \rightarrow \alpha = 1$, Σ is odd.

(iii) $d \equiv 3 (\mathrm{mod}\ 4)$, according to (*A*II.2) $d \equiv 3 (\mathrm{mod}\ 8)$.

From (32) it is concluded that $\Sigma^* = 4 (\mathrm{mod}\ 8) \rightarrow \alpha = 4$, Σ is odd. This α value is obviously compatible with r^*_{ij}, taking into account (*A*II.2).

(II) m is even, n is odd.

(i) $d \equiv 1 (\mathrm{mod}\ 4)$.

From (32) it is concluded that $\Sigma^* = 1 (\mathrm{mod}\ 4) \rightarrow \alpha = 1$, Σ is odd.

(ii) $d \equiv 2 (\mathrm{mod}\ 4)$.

From (32) it is concluded that $\Sigma^* = 2 (\mathrm{mod}\ 4) \rightarrow \alpha = 2$, Σ is odd. This α value is obviously compatible with r^*_{ij}.

(iii) $d \equiv 3 (\mathrm{mod}\ 4) \rightarrow d \equiv 3 (\mathrm{mod}\ 8)$.

From (32) it is concluded that $\Sigma^* = 3 (\mathrm{mod}\ 4) \rightarrow \alpha = 1$, Σ is odd.

(III) m is odd, n is even.

For any character of the d value, the second term of (32) is 0(mod 4), since n is even, and the first term is 1(mod 8), therefore $\alpha = 1$, Σ is odd.

Conclusion

Selection rules have been established. They also allow one to prove that Σ is always odd.

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