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Group-Theoretical Consideration of the CSL Symmetry

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Abstract

A theoretical analysis for the computation of the coincidence site lattice (CSL) symmetry is presented. It is shown that three types of symmetry elements can exist and each one can be found by properly using the CSL's rotation matrix of the smallest-angle description. Thus, from the existence of the subgroup H_1, the order of which is directly connected with the number of the different orientations that the sublattice Λ_1^1 can have, a low-symmetry H_1 group implies more possibilities for the formation of the corresponding CSL. From the existence of the symmetry elements of the second type, the smallest-angle rotation matrix can be a symmetry element but only of the fourth or sixth order. From the third type of elements a connection between CSLs of different Σ values can exist. Since the analytical form of this smallest-angle rotation matrix can be deduced for every crystallographic system, the procedure described here is of general use. Thus a new classification of the different CSLs is possible according to their symmetry group. This allows the study of the CSL model from the symmetry point of view.

1. Introduction

In this paper we present results of a study of the CSL model, which is based on the theory established by Bleris & Delavignette (1981). According to this theory a rotation matrix, which produces the CSL describing a bicrystal, can be expressed as a function of the integral numbers m, n, α and the rotation axis $[uvw]$. The algorithms for the calculation of these values have been recently given (Bleris, Karakostas & Delavignette, 1983) for any CSL of the cubic and hexagonal systems. With a complete classification of all CSLs according to the rotation matrix of their smallest-angle description, the question to be answered was 'how can we use this rotation matrix in order to define the crystallographic elements of a given CSL, *i.e.* the crystal system of the CSL and its base?'.

In this paper we shall give the group-theoretical information for the computation of the symmetry of a given CSL. The use of group theory for the study of the CSL was first introduced by Pond & Bollmann (1979), where the stability of a CSL boundary was examined by means of some selection rules based on the black and white symmetries. Later, Gratias & Portier (1982) presented an extension of Pond's idea. Neither of these works deals with the CSL symmetry. Thus, the only existing information for comparison with our results is the Bravais classes of the cubic CSLs, which have been determined by a method described by Mighell, Santoro & Donnay in *International Tables for X-ray Crystallography* (1969), and have been given for the CSLs up to $\Sigma = 49$ by Grimmer, Bollmann & Warrington (1974).

In the following paper (Bleris, Doni, Karakostas, Antonopoulos & Delavignette, 1985) we shall present the necessary analytical expressions for the CSL's base computation, using some of the results of the present work.

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2. Basic definitions

Two lattices Λ_1 and Λ_2, related by the equation

$$\Lambda_2 = R\Lambda_1, \quad (1)$$

where R is a rotation matrix, form a CSL Λ_{12} if

$$\Lambda_{12} = \Lambda_1 \cap R\Lambda_1 \quad (2)$$

is not the empty set.

In the following the CSL, which is the common sublattice of the two lattices, will be considered as part of one of the two lattices only, which will be called 'the parent lattice'. Let us now suppose that g is a symmetry operator of this sublattice. If we apply this operator to the parent lattice, the following possibilities only can exist:

(i) the sublattice and the parent lattice remain invariant;

(ii) the sublattice remains invariant but not the parent lattice;

(iii) a sublattice with a smaller Σ value, which contains all the points of the first (higher Σ value) sublattice, remains invariant, but not the parent lattice.

The above cases lead to the following obvious properties. Firstly, if we take into account the fact that every symmetry element may be a pure rotation or a combination of a rotation and the inversion operator I, we can say that, in the case of simple lattices, it is sufficient to deal with pure rotations only. Secondly, the axis of the g operator should be a vector of the sublattice and its angle can only have one of the allowable values $2\pi/2$, $2\pi/3$, $2\pi/4$ or $2\pi/6$. Furthermore, in case (i), g is a symmetry element of the parent lattice as well. In case (ii), the new orientation of the parent lattice and the old one have a common sublattice and also g is a CSL rotation, having a rotation angle equal to one of the previously mentioned values. In case (iii), g should be a CSL rotation of the higher Σ value sublattice and also a symmetry element of that with the smaller Σ value. Moreover, in this case the unit volume of the former sublattice is a multiple of the unit volume of the latter sublattice. Since the smaller Σ value sublattice has a unit volume that is a multiple of the unit volume of the parent lattice, we can conclude that the one with the higher Σ value has a unit volume that is a composite multiple of the unit volume of the parent lattice.

Let us now examine (2). This relation implies that the existence of a CSL is equivalent to the existence of two sublattices Λ_1^1 and Λ_1^2 of Λ_1 such that

$$R\Lambda_1^1 = \Lambda_1^2. \quad (3)$$

The previous argument becomes clear in a typical example taken from the cubic system. The CSL $\Sigma = 5$, which is produced by a 36·87° rotation around the [001] axis, is shown in Fig. 1. The meaning of the rotation matrix R becomes clear from this figure. This matrix, expressing a rotation of $\theta°$ around the $[uvw]$ axis, when it is applied to the parent lattice Λ_1, brings the sublattice Λ_1^1 into coincidence with the sublattice Λ_1^2, forming a CSL according to (3).

The sublattices Λ_1^1, Λ_1^2 have exactly the same geometry and also the same symmetry. Let $G_{\Lambda_1^1}$ be the symmetry group of Λ_1^1 and $G_{\Lambda_1^2}$ the symmetry group of Λ_1^2. These two groups are connected by the similarity transformation:

$$G_{\Lambda_1^2} = RG_{\Lambda_1^1}R^{-1}. \quad (4)$$

Relation (4) expresses the one-to-one correspondence between the elements of these two groups; therefore, it suffices for our purpose to find the group $G_{\Lambda_1^1}$ only. Then the symmetry group $G_{\Lambda_1^2}$, *i.e.* the CSL's symmetry, is immediately obtained by the similarity transformation (4).

In the following sections we shall determine the symmetry elements of the three types classified above. Moreover, since we are dealing with matrices and their numerical properties, we choose a constant base, that of Λ_1^1, for their representation.

3. The elements of the first type (the subgroup H_1)

Let G be the symmetry group of the parent lattice Λ_1 and H_1 the set of the elements of G defined by the relation:

$$H_1 = \{g_i = R^{-1}g_jR\colon g_j\Lambda_1^2 = \Lambda_1^2, g_i, g_j \in G\}. \quad (5)$$

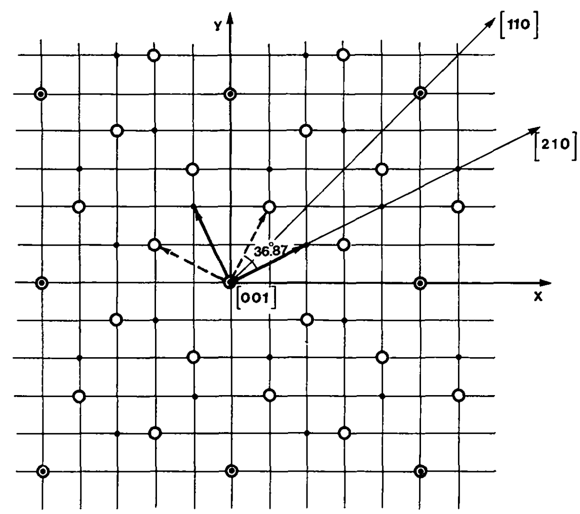

Fig. 1. [001] section of a cubic lattice. Dots: sublattice Λ_1^1. Open circles: sublattice Λ_1^2. Coincidence rotation around [001] by 36·87°. Rotation of 90° around [001] leaves Λ_1^1, Λ_1^2 invariant, rotation of 180° around [110] brings dots Λ_1^1 to open circles Λ_1^2, rotation of 180° around [210] leaves Λ_1^1 invariant, but not the parent lattice. Miller indices are referred to the indices of the lattice Λ_1.

In fact, H_1 is a subgroup of $G_{\Lambda_1^1}$ because

$$\forall\, g_i \in H_1 \to g_i\Lambda_1^1 = R^{-1}g_jR\Lambda_1^1 = R^{-1}\Lambda_1^2 = \Lambda_1^1 \quad (6)$$

and also H_1 is a subgroup of G.

It is well known that every group can be analysed as a coset sum of one of its subgroups (see for instance Bradley & Cracknell, 1972; Van Tendeloo & Amelinckx, 1974). By using this property, G can be written as a coset sum of H_1:

$$G = g_1H_1 + g_2H_1 + \cdots + g_vH_1, \quad (7)$$

where g_i ($i = 1, 2, 3, \ldots, v$) does not belong to H_1 and $g_1 = E$ is the identity operator. The integer v, named the index of H_1 in G, is the ratio of the orders $[G]$ and $[H_1]$ of the groups G and H_1, respectively.

All of the cosets in (7) correspond to a variant, *i.e.* to a different orientation of the sublattice Λ_1^1 within lattice Λ_1, produced by the application on Λ_1 of one of the g_i elements that do not belong to H_1. There are v possible variants of Λ_1^1, the integer v being dependent on the order of H_1. The smaller the order of H_1 the larger the number of variants. As an example of the relation between the symmetry elements of the parent lattice Λ_1 and the variants of Λ_1^1 let us again consider the previously examined case of $\Sigma = 5$, in Fig. 1. If we consider a 90° rotation around the [001] axis, which is a symmetry element of Λ_1, it can be easily seen that this is also a symmetry element of Λ_1^1, that is this rotation is a symmetry element of H_1. On the contrary, if we consider a 180° rotation around the [110] axis, which is also a symmetry element of Λ_1, when this rotation is applied on Λ_1^1 it produces Λ_1^2, so that this rotation is one of the $g_i \notin H_1$ elements.

Similarly, $G_{\Lambda_1^1}$ can be analysed as

$$\begin{gathered} G_{\Lambda_1^1} = h_1H_1 + h_2H_1 + \ldots + h_tH_1, \\ h_j \notin H_1\ (j = 1, 2, \ldots, t), \end{gathered} \quad (8)$$

where the $h_j \notin H_1$ elements are not symmetry elements of G. Since h_j are symmetry elements of $G_{\Lambda_1^1}$, they are of the second or third kind, according to our classification in § 2. An example of the second kind of operations is a 180° rotation around the [210] axis in the previously examined case of $\Sigma = 5$ (Fig. 1), which leaves Λ_1^1 invariant while it changes the orientation of Λ_1.

4. The elements of the second type ($h_i \notin H_1$)

As was pointed out before, the elements of the second type are CSL rotations. This means that h_i corresponds to one of the symmetrically equivalent descriptions of the same CSL discussed by Karakostas, Bleris & Antonopoulos (1979). By its definition every symmetrically equivalent description is a rotation connecting a variant of Λ_1^1 with Λ_1^2. Thus the general expression of the rotation matrix describing a CSL and operating on Λ_1^1 is

$$R_i = g_i^{-1}R. \quad (9)$$

Let us consider the set of the elements h_i for which it holds that

$$h_i = g_i^{-1}R \in G_{\Lambda_1^1} \quad (10)$$

and $g_i^{-1} \neq E$, the identity operator. Since h_i is an element of $G_{\Lambda_1^1}$ and a CSL rotation as well, for a convenient t, it follows that

$$G_{\Lambda_1^1} \ni h_i^{-1} = g_t^{-1}R. \quad (11)$$

Let us now consider an element $h \in G_{\Lambda_1^1}$ to be constant. Then, for every other $h_i \in G_{\Lambda_1^1}$, we have either

$$h_i^{-1}h = R^{-1}g_ig^{-1}R = g_k^{-1}R \in G_{\Lambda_1^1}, \quad (12a)$$

for a convenient k, or

$$h_i^{-1}h = R^{-1}g_ig^{-1}R = g_t^{-1} \in G_{\Lambda_1^1}, \quad (12b)$$

for a convenient t. Relation (12*a*) leads to $R \in G$, which is impossible. On the other hand, from (12*b*) one can see that

$$h_i^{-1}h \in H_1. \quad (13)$$

Moreover, from (12*b*) it is obvious that

$$\forall\, h_i \in G_{\Lambda_1^1} \to \exists g_t \in H_1 : hg_t = h_i \quad (14)$$

and this means that all the symmetry elements h_i of (14) belong to the left coset hH_1. Since (12*b*) is unique for the existence of h_i, we can conclude that

$$H_1 + hH_1 \subset G_{\Lambda_1^1} \quad (15)$$

and if there are no elements of the third type in $G_{\Lambda_1^1}$ we have

$$H_1 + hH_1 = G_{\Lambda_1^1}. \quad (16)$$

From (16) it is obvious that $[G_{\Lambda_1^1}]/[H_1] = 2$, which means that H_1 is an invariant subgroup of $G_{\Lambda_1^1}$ (see Bradley & Cracknell, 1972). The previous statement immediately implies that $hH_1 = H_1h$ and therefore

$$(hH_1)(hH_1) = h(H_1h)H_1 = h^2H_1 = H_1, \quad (17)$$

which means that $h^2 = E$ and so h is a 180° rotation.

Let us examine the order p that h may have in (15). Supposing that $p > 2$, we have

$$E = \underbrace{h\,.\,h\,.\,h \ldots h}_{p} = g^{-1}Rg^{-1}R \ldots g^{-1}R, \quad (18)$$

where E is the identity operator. From (11) we have

$$Rg^{-1}R = g_t. \quad (19)$$

By substituting (19) into (18) $p - 1$ times, we have

$$E = g^{-1}Rg^{-1}g_t \ldots g^{-1}g_t. \quad (20)$$

This relation cannot be true, since $R \notin G$. Thus, if R is the smallest-angle rotation matrix of a given CSL, then

$$G_{\Lambda_1^1} \ni h = g^{-1}R, \text{ if and only if } h^2 = E.$$

Finally, there remains the case

$$h_i = g_i^{-1}R \quad \text{and} \quad g_i^{-1} = E. \tag{21}$$

In this case (11) is still valid and therefore

$$h_i^{-1} = R^{-1} = g_t^{-1}R \tag{22}$$

for an appropriate $g_t \in G$. From this relation we have

$$R^2 = g_t \tag{23}$$

and, since $R \in G_{\Lambda_1^1}$, the element R^2 belongs to $G_{\Lambda_1^1}$ and $g_t \in H_1$. Thus, the smallest-angle rotation matrix R can be a symmetry element if its square is an element of H_1.

In the case where R is an element of $G_{\Lambda_1^1}$, we also form the product

$$h_i^{-1}R = R^{-1}g_iR, \quad \forall\, h_i \in G_{\Lambda_1^1}$$

and (24)

$$h_i \neq R,\ h_i \neq R^{-1}.$$

From (24), following the procedure used for (12), it can be easily proved that

$$h_i^{-1}R = R^{-1}g_iR = g_m^{-1} \in H_1. \tag{25}$$

Relation (25) can be rewritten as

$$h_i^{-1}R = h_iR = g_m^{-1} = g_i^{-1}RR = g_i^{-1}R^2 = g_i^{-1}g_t. \tag{26}$$

But $g_t \in H_1$, so it is obvious that $g_i^{-1} \in H_1$. Moreover, (25) implies that

$$\forall\, h_i \in G_{\Lambda_1^1} \rightarrow \exists\, g_m \in H_1\colon h_i = Rg_m \in RH_1,$$

which means that all the symmetry elements h_i belong to the left coset RH_1 of H_1 in $G_{\Lambda_1^1}$. From (25) it is also obvious that

$$\forall\, h_i \in G_{\Lambda_1^1} \rightarrow \exists\, g_k \in H_1\colon R = h_ig_k \in h_iH_1, \tag{27}$$

which means that R is among the elements of h_iH_1. The same is true for R^{-1}. This can be possible only if H_1 contains a number of elements equal to the number of 180° rotations that it has plus two. So, when $R \in G_{\Lambda_1^1}$, H_1 contains two more elements, besides the g_t element, which are given by (23).

As we have mentioned before, R, being a symmetry element, can be a rotation of the third, fourth or sixth order. If R is of the third order, then necessarily $R^3 = E$ and because of (23) we have $R = g_t^{-1}$. This is impossible and we may conclude that R can only be of the fourth or sixth order.

5. The elements of the third type

As has been pointed out above (§ 2), this case can only exist if Σ is a composite integer. Let us now suppose that $\Sigma = pq$, where p, q are prime integers. Then, a symmetry element of the third type for the CSL with volume Σ can be found from the symmetry elements of the CSLs with volume either $\Sigma = p$ or $\Sigma = q$.

For the symmetry element R_p (or R_q) to be a symmetry element of the CSL with volume Σ, in both cases the following conditions are necessary:

(i) R_p is not a symmetry element of G. Then R_p is either a 180° rotation or one of the exceptional cases of 90 or 60° rotations.

(ii) The axis r of R_p is a vector of the CSL. This condition can be easily checked by taking the transformation $R_\Sigma^{-1}r$, where R_Σ is the smallest-angle rotation matrix of the CSL with volume Σ.

(iii) The product $R_\Sigma^{-1}R_pR_\Sigma$ gives a rotation matrix that describes a CSL with volume p.

If such an element exists, then the symmetry group $G_{\Lambda_1^1}$ of this composite CSL can be obtained by joining this element to the group of the elements that have been found by the steps of §§ 3 and 4.

6. Practical procedure for the construction of $G_{\Lambda_1^1}$

In this section we shall develop the practical procedure for the construction of $G_{\Lambda_1^1}$, taking into account the previously established properties of the symmetry group $G_{\Lambda_1^1}$.

Let G be the symmetry group of the parent lattice. Since we are dealing with simple lattices, G has the form

$$G = G_0 + IG_0, \tag{28}$$

where I is the inversion operator and G_0 is a subgroup of G containing only pure rotations. As we have mentioned before, we shall use the subgroup G_0. For the cubic system G_0 is the O (432) group containing 24 elements (Karakostas *et al.*, 1979), and for the hexagonal system G_0 is the D_6 (622) group containing 12 elements (Hagège, Nouet & Delavignette, 1980).

Let R be the rotation matrix that gives a CSL with multiplicity Σ when it operates on Λ_1. We compute the products

$$\left.\begin{array}{ll}(a) & R^{-1}gR \\ (b) & g^{-1}R\end{array}\right\} \forall\, g \in G_0. \tag{29}$$

Relation (29*a*) gives the subgroup H_1 while (29*b*) gives the set of the different descriptions of the same CSL.

We can easily see that the order of H_1, *i.e.* the number of the symmetry elements $R^{-1}gR$, can never be equal to the order of G_0. (Otherwise all the elements of G_0 would be symmetry elements of Λ_1^1 and there would be no variants of Λ_1^1, so that all the $g^{-1}R$ rotations would describe one and the same geometrical operation.) On the other hand, the number of 180° rotations from the set of the $g^{-1}R$ elements should be smaller or equal to one half of the order of G_0. This happens because, as we have seen before,

Table 1. *Possible CSL symmetry according to the number of* 180° *rotations*

Number of 180° rotations	Σ prime	Σ composite
None	Triclinic	Triclinic or higher
1	Monoclinic	Monoclinic or higher
2	Orthorhombic	Orthorhombic or higher
3	Rhombohedral	Rhombohedral or higher
4	Tetragonal	Tetragonal
5	Impossible, because there are no subgroups of order 5	
6	Hexagonal	Hexagonal or cubic

if there exists a set of 180° rotations, then the number of the elements of this set is equal to the number of the elements of hH_1. This number is equal to the number of the elements of hH_1 minus 2 in the special cases where R is an element of $G_{\Lambda_1^1}$. Taking into account that in all cases the symmetry elements of $G_{\Lambda_1^1}$ that do not belong to G are included in the products hH_1, we can write

$$[H_1+hH_1]\leq[G_0] \tag{30}$$

and

$$[H_1+hH_1]=2[H_1]\leq[G_0]\rightarrow[H_1]\leq[G_0]/2. \tag{31}$$

The possibilities existing for the symmetry of the sublattice Λ_1^1 are shown in the following diagram, holding for both cubic and hexagonal systems.

Cubic $O(432)$			Hexagonal $D_6(622)$
Rhombohedral	$D_3(32)$	:	$[D_3]=6$
Tetragonal	$D_4(422)$	:	$[D_4]=8$
Orthorhombic	$D_2(222)$	:	$[D_2]=4$ (32)
Monoclinic	$C_2(2)$	:	$[C_2]=2$
Triclinic	$C_1(1)$	:	$[C_1]=1.$

Taking this diagram into account, we have classified all the possibilities as a function of the existing 180° rotations in Table 1.

In all the above cases one must also take into account the possibility of R being a symmetry element of the CSL. In this case the symmetry of the CSL does not follow the rules of Table 1, but it is characterized by the order of R.

In what follows, we shall treat two typical examples of constructing $G_{\Lambda_1^1}$, one of a composite Σ-value CSL and the case $\Sigma=2$ CSL of the hexagonal system. Moreover, tables have been constructed for CSLs up to $\Sigma=49$ for both cubic and hexagonal ($\mu=\nu=1$; $\mu=5$, $\nu=2$; $\mu=8$, $\nu=3$) systems. These tables present the step by step procedure for the computation of $G_{\Lambda_1^1}$ of every CSL.*

* Supplementary material giving the results of the application of the theory has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42161 (15pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Cubic system: $\Sigma=15$, $[uvw]=[210]$, $\theta=48{\cdot}18°$.

In this CSL the application of (29) gives the subgroup H_1, which contains only the identity operator and one element of the 180° type. This element corresponds to a 180° rotation around the $[1\bar{2}\bar{5}]$ axis and it is in a matrix form:

$$h=\frac{1}{15}\begin{bmatrix}\overline{14} & \bar{2} & \bar{5}\\ \bar{2} & \overline{11} & 10\\ \bar{5} & 10 & 10\end{bmatrix}.$$

So the subgroup H_1+hH_1 is

$$H_1+hH_1=\{E\}+h\{E\}=\{E,h\}.$$

Since the volume of this CSL is a composite number, we have to look for symmetry elements of the third type before the final classification. But the CSL rotation around the [210] axis of $\Sigma=15$ corresponds to a symmetry element of 180°, because a symmetrical equivalent of this axis is among the equivalent descriptions of $\Sigma=5$, corresponding to a 180° symmetry element. So, the 180° rotation around the [210] axis of $\Sigma=5$ is a symmetry element of the third type of $\Sigma=15$ and $G_{\Lambda_1^1}$ is constructed by joining this element, given in a matrix representation with the form

$$R_5=\frac{1}{5}\begin{bmatrix}3 & 4 & 0\\ 4 & \bar{3} & 0\\ 0 & 0 & \bar{5}\end{bmatrix},$$

to the subgroup H_1+hH_1 according to the following relation:

$$G_{\Lambda_1^1}=\{E,h\}+R_5\{E,h\}.$$

The element R_5h is in a matrix form:

$$R_5h=hR_5=\frac{1}{3}\begin{bmatrix}\bar{2} & \bar{2} & 1\\ \bar{2} & 1 & \bar{2}\\ 1 & \bar{2} & \bar{2}\end{bmatrix}=R_3$$

and corresponds to a 180° rotation around the $[1\bar{2}1]$ axis of $\Sigma=3$, which is also a symmetry element of the third type of $\Sigma=15$. It can be easily checked that the $[1\bar{2}1]$ axis is an axis of the CSL $\Sigma=15$.

So, $G_{\Lambda_1^1}$ containing the identity operator E and three other elements corresponding to 180° rotations is isomorphic to the D_2 orthorhombic symmetry group.

Hexagonal system: $\Sigma=2$, $[uvw]=[210]$, $\theta=90°$ ($\mu=\nu=1$).

By using (29) we obtain

$$H_1=\{E,C_2,C'_{22},C''_{22}\}$$

and two rotations of 180°. Taking into account that R is of the fourth order, we have a typical example of the case discussed in § 4. The different powers of

R have the following matrix form:

$$R=\frac{1}{2}\begin{bmatrix} 2 & 0 & 0 \\ 1 & 0 & \bar{2} \\ \bar{1} & 2 & 0 \end{bmatrix}, \quad R^2=\begin{bmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix},$$

$$R^3=\frac{1}{2}\begin{bmatrix} 2 & 0 & 0 \\ 1 & 0 & 2 \\ 1 & \bar{2} & 0 \end{bmatrix}, \quad R^4=E.$$

R^2 is the $C'_{22} \in H_1$ element and we may construct $G_{A_1^1}$ by making use of the $C_2 \in H_1$ element. Therefore,

$$\begin{aligned} G_{A_1^1} &= \{R, R^2, R^3, R^4\} + C_2\{R, R^2, R^3, R^4\} \\ &= \{E, C'_{22}, C''_{22}, C_2, R, R^{-1}, C_2R, C_2R^3\} \end{aligned}$$

and $G_{A_1^1}$ is isomorphic to the D_4 tetragonal symmetry group.

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Use of the CSL Symmetrically Equivalent Descriptions Tables in the DSC Lattice Base Computation

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Abstract

A combination of analytical expressions and a knowledge of symmetry is employed for the displacement shift complete lattice (DSCL) base computation. The method is of general use and its application to cubic and hexagonal systems is given. Tables containing all the symmetrically equivalent descriptions of one and the same coincidence site lattice (CSL) as a function of one description are given for both cubic and hexagonal systems.

1. Introduction

Since the grain boundary (GB) cannot be described only on the basis of absolutely exact coincidence site lattice (CSL) orientations, the study of equilibrium grain boundaries in the vicinity of a CSL condition is a real necessity and a completion to a full CSL study. It has been experimentally shown that the deviation of a few degrees from the exact CSL condition is usually accommodated by a dislocation array. The Burgers vectors of such a dislocation array are related with the approximate CSL if they are members of the corresponding displacement shift complete lattice (DSCL) (Bollmann, 1970).

According to the reciprocity theorem, which has been established by H. Grimmer, there is a one-to-one correspondence between the CSL and the DSCL, and the DSCL base can be found if the CSL base is known (Grimmer, 1974). An application of this elegant statement, which is of general character, was given for the DSCL of the cubic system for CSLs up to $\Sigma = 49$ by Grimmer, Bollmann & Warrington (1974). Unfortu-

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