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Symmetry Properties of Grain Boundary Junctions*

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Abstract

The symmetry group of the coincidence site lattice (CSL) is used for the study of the properties of triple junctions formed by plane boundaries. The experimental evidence that there are junctions with an obviously symmetrical relationship among the adjacent planes is analysed systematically. The analysis concerns the triple junctions in which the grain boundaries (GBs) are described by 180° CSL rotations. For these triple junctions the common intersection is a CSL rotation axis of the three GBs. Two cases need to be distinguished. In the first case the common intersection is a symmetry axis of the three CSLs, while in the second case the common intersection is a general direction. Thus in the first case the corresponding symmetry element is a common symmetry element of the three CSLs participating in the junction.

1. Introduction

In the framework of grain boundary (GB) structural studies many different observations have been reported dealing with the study of the intersections of GBs, *i.e.* interfaces which meet each other at multiple junctions or faceted interfaces (Komninou, Karakostas, Bleris & Economou, 1982; Vaudin, Cunningham & Ast, 1982; Sukhomlin & Andreeva, 1983; Komninou & Karakostas, 1984; Fionova, 1985; Iijima, 1987). A detailed account of rules concerning GB configurations during grain growth from the thermodynamical and topological points of view is given in a very recent review (Atkinson, 1988). In this paper, the mutual symmetry relations among the various grains of the junction and their connection with the CSL model are not taken into consideration. Moreover, an important question is whether there exist simple geometric criteria for low interfacial energy for any GB structure. This question has been extensively analysed by Sutton & Balluffi (1987) who concluded that there is no simple answer. They suggest a more fundamental physical study for the relation of the structural and energetic properties of grain boundaries. In this particular study some faceted GBs have also been examined from the energetic point of view. Almost all of these faceted GBs might be considered as a joint pattern of double and triple junctions. Consideration of the atomic structure and the details of the bonding at the interface show that the symmetry properties of interfacial configurations can be a useful tool because symmetry is an abstraction which serves as a guide for many developments. From our study of polycrystalline materials and from the observations reported in the literature we have seen that in junctions with thermodynamically favorable CSL boundaries some systematic symmetry properties exist. Numerical identifications of these systems are obtained by the use of CSL rotational operations such as those proposed by Warrington (1979) for CSL triple junctions. Such identifications can be used for the prediction of all possible CSL junctions and are based on relationships between coordinate systems, but cannot give the symmetry properties of the interfaces.

We argue below that all triple junctions can be classified into two categories in a unique way. The first category contains junctions formed by special GBs, *i.e.* GBs described by 180° CSL rotations. The second category contains junctions where some or all GBs are not 180° CSL boundaries. These two categories have the critical distinction that some systematic symmetry properties are present in the first which are absent in the second. Our interest is focused on the first category only, since the special GBs retain the coherence of the structure as much as possible, as was first suggested by Friedel (1926). Moreover, in the first category we have seen that there are cases where the common intersection is a symmetry axis. The corresponding symmetry element is a member of the symmetry group of each of the three CSLs participating in the junction. For this type of junction the intersection retains continuity in the three GBs. For the special GBs the breaking of the initial symmetry (the symmetry of the single crystal) implies the elimination of at least one symmetry element of the initial symmetry group. This dissymmetrization process has been analysed extensively by Pond (1989).

Application of our analysis is made on two typical examples, one of which has already been experimentally confirmed (Komninou & Karakostas, 1984). The general physical property which can be established by our results is that there are junctions in

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which the common intersection has the property of keeping a common symmetry element in the composite lattice.

2. Description of a triple junction

If we consider the junction of three grains whose lattices are Λ_i, $i=1, 2, 3$, there are three rotation matrices R_i, $i=1, 2, 3$, giving the relation between the three lattices one by one. By expressing the three matrices in the same coordinate system the mutual relation of the grains is described by

$$R_3 = R_1 R_2^{-1}. \tag{1}$$

Warrington (1979) was the first to point out that if two of the above matrices describe a CSL rotation relationship then the third matrix also represents a CSL rotation matrix. This property immediately implies a relation between the multiplicities Σ of the three CSLs, and it can be shown that there also exists an equation of the form

$$\Sigma_3 = \Sigma_1 \Sigma_2. \tag{2}$$

Many applications of the above description of a triple junction have already been made in different polycrystalline materials (Perevezentsev, Shcherban, Soldatov & Belov, 1982; Komninou *et al.*, 1982; Sukhomlin & Andreeva, 1983; Komninou & Karakostas, 1984; Hasimoto, Fujii & Miura, 1987). Moreover, its simple form allows its use for the experimental characterization of a junction, if one also uses the convenient algorithms that exist (Bleris, Karakostas & Delavignette, 1983). Typical examples of this procedure have been reported elsewhere (Komninou *et al.*, 1982; Komninou & Karakostas, 1984). The first of them concerns a fully characterized triple junction by means of relation (1). It is the $\Sigma = 3, 13, 39$ CSLs case where the third GB, *i.e.* $\Sigma = 39$ CSLs, lacks a 180° description. The second concerns a fully symmetric triple junction with $\Sigma = 3, 3, 9$ CSLs where the GBs are special. In this case one can characterize the junction very quickly. Since the rotation axes are perpendicular to the GBs the dihedral angles are directly estimated by the corresponding angles of the axes. Nevertheless (1) cannot be used for theoretical predictions without some assumption being added. For example, we cannot get information about the common intersection axis and the symmetry of the participating CSLs *a priori*. In what follows we shall consider only triple junctions with special GBs.

Following our previous assumption we shall consider two of the operators, *i.e.* R_1 and R_2, to describe CSL rotations of 180°. It is rather obvious that these operators can describe the special CSL boundaries and rotate across a crystallographic plane, according to the natural rule which produces the grain boundaries of a given material. Since R_1 and R_2 are rotation operators of 180° the operator R_3 is exactly defined; it is a rotation around an axis perpendicular to the axes of R_1 and R_2 through an angle 2φ (where φ is the angle between the axes of R_1 and R_2). This axis is the common intersection axis of the three boundaries participating in the junction (Landau & Lifshitz, 1952).

Recalling that a given CSL rotation operation is of the form $g_j R$, where g_j is a symmetry element of the symmetry group G of the parent lattice (Doni, Bleris, Karakostas, Antonopoulos & Delavignette, 1985), we shall examine the case that the axis r of the rotation R_3 is also a CSL rotation axis of one of the other two. Then the following relations should simultanously hold:

$$\begin{aligned} R_3 r &= r \\ g_j R_1 r &= r, \end{aligned} \tag{3}$$

from which it is obvious that

$$R_1 r = g_j^{-1} r. \tag{4}$$

By making use of relation (1) and of the fact that R_1 and R_2 are 180° operators we get from (4)

$$R_2 R_3^{-1} r = R_2 r = g_j^{-1} r,$$

or

$$g_j R_2 r = r, \tag{5}$$

which means that r is also a CSL rotation axis of the third CSL. Thus, if the triple junction contains two special CSL boundaries and their intersection is a CSL axis for one of them, then it is a common CSL rotation axis for the three grains. This kind of junction forms one category of triple junctions. Another category is that in which the axis of the rotation R_3 is a CSL rotation axis for this rotation only. An example of this category of junctions is the triple junction of $\Sigma = 3, 13, 39$ CSLs studied by Komninou *et al.* (1982). In this case the intersection axis is the [283] axis, which is a CSL rotation axis only of $\Sigma = 39$ CSL. We adopt the terminology 'CSL triple junctions' for the first category of junctions.

3. Symmetry properties

In order to study CSL triple junctions we need to make use of some symmetry properties of the CSL. We recall the meaning of the sublattice Λ_1^1 of the parent lattice. The existence of this sublattice is the necessary condition in order for a CSL to be formed (Doni *et al.*, 1985). The symmetry of Λ_1^1 is given by the symmetry group

$$G_{\Lambda_1^1} = H + RH, \tag{6}$$

where H is a subgroup of G and R is the CSL 180° operator describing the GB. By taking into account the fact that H is a subgroup of G we can decompose

G into left cosets (Van Tendeloo & Amelinckx, 1974):

$$G = g_1H + g_2H + \ldots + g_pH, \tag{7}$$

where $g_1 = E$, $g_i \in G$, $i = 1, 2, \ldots, p$ and $g_i \notin H$. The integer p is the ratio of the orders ^oG of G and ^oH of H as is implied by the Langrange theorem (Bradley & Cracknell, 1972). Let $g(\neq E)$ be any element of G; then by using the decomposition (7) we can take $g = g_ih$ and

$$g\Lambda_1^1 = g_ih\Lambda_1^1 = g\Lambda_{1g}^1 \tag{8}$$

is a variant of Λ_1^1. Moreover every element g belonging to a coset in (7) produces one and only one variant; there are at most p variants. Any physical property concerning the sublattice Λ_1^1 can also be considered to exist on any other variant of Λ_1^1. This remark allows the investigation of the CSL descriptions of one and the same CSL taking into account that there are as many CSL descriptions as the elements of G (Bleris, Doni, Karakostas, Antonopoulos & Delavignette, 1985). In order to clarify this property let us consider a 180° rotation operator R_1. Since R_1 is a symmetry element of $G_{\Lambda_1^1}$ we have

$$R_1\Lambda_1^1 = \Lambda_1^1 \tag{9}$$

and there is a vector $r_0 \in \Lambda_1^1$ such that

$$R_1r_0 = r_0 \in \Lambda_1^1. \tag{10}$$

From (9) we get

$$g \in G: \quad gR_1\Lambda_1^1 = \begin{cases} \Lambda_1^1 & \text{if } g \in H \\ \Lambda_{1g}^1 & \text{if } g \notin H, \end{cases} \tag{11}$$

and it is obvious that there are ^oH different descriptions of the same CSL inside the variant Λ_1^1 and $(p-1)^oH$ descriptions of the same CSL in $p-1$ different variants. Thus a CSL description gR is referred to one and only one variant H if the symmetry element g belongs to the subgroup H.

Let us suppose now that r_0 is the intersection axis of the grain boundaries of a CSL triple junction. Then we can always find some symmetry elements of G such that

$$\begin{aligned} h_\mu R_1 r_0 &= r_0, \quad h_\mu \in G \\ h_\nu R_2 r_0 &= r_0, \quad h_\nu \in G \\ R_3 r_0 &= r_0, \end{aligned} \tag{12}$$

or

$$\begin{aligned} R_1 r_0 &= h_\mu^{-1} r_0, \quad h_\mu \in G \\ R_2 r_0 &= h_\nu^{-1} r_0, \quad h_\nu \in G \\ R_3 r_0 &= r_0, \end{aligned} \tag{13}$$

and by making use of (1) we get

$$R_2r_0 = R_1^{-1}r_0 = R_1r_0 = h_\mu^{-1}r_0. \tag{14}$$

By combining (14) with the second of equations (13) we obtain for the common axis r_0 [which belongs to Λ_1^1, equation (10)]

$$h_\mu h_\nu^{-1} r_0 = r_0. \tag{15}$$

Equation (15) creates a strong distinction. In fact since h_μ, h_ν^{-1} are elements of G their product is also an element of G. If $h_\mu h_\nu^{-1} = E$, the identity operator of G, then r_0 may be any CSL vector, but if $h_\mu h_\nu^{-1} \neq E$ then r_0 is a CSL symmetry axis. Since r_0 is a CSL axis of the three CSLs, this symmetry axis is a common symmetry axis of the three CSLs participating in the junction. Thus the symmetry groups of the three CSLs contain a common symmetry element. For this case we adopt the terminology 'special triple junctions'. Thus there are restricted possibilities for the existence of special triple junctions in each crystal system. For example, the only special triple junctions can exist around the ⟨100⟩, ⟨110⟩ and ⟨111⟩ type of axes for cubic CSLs.

4. Variant description of a triple junction

We can now summarize the above results as follows: if in a given triple junction the intersection axis is a CSL rotation axis of the three CSLs, then it may be a symmetry axis of the three CSLs. This particular case implies that a mutual symmetrical relation may exist between the three CSLs. This investigation can be based analytically on relation (1). Such an investigation is a very long process so we shall try to organize the symmetry properties on the basis of the properties implied by the decomposition of (7).

At first we recognize that, given two special CSL boundaries, whether they are related or not, they can have some common CSL characteristics which cannot be directly seen, since for every one of them there exist many different CSL rotation operations and one has to combine them one by one in order to arrive at the properties of the third grain boundary. However, we know that the symmetry group of a given CSL has the form of (6) and a property existing in the variant Λ_1^1 can also exist in any other variant. Coming back to (6) and taking into account that R is a second-order element we can define the factor group F,

$$F = G_{\Lambda_1^1}/H \tag{16}$$

of the order $^oF = 2$. Thus $G_{\Lambda_1^1}$ is homomorphic to F and every $h \in H$ corresponds to the unit element of F, while every element of the form $Rh \in G_{\Lambda_1^1}$ corresponds to the second-order element of F. Thus the symmetry of the CSL given in the variant Λ_1^1 is completely defined by the symmetry group $G_{\Lambda_1^1}$ and the symmetry of the bicrystal by the factor group F.

For every CSL operator R_k which describes the grain boundaries under consideration a factor group similar to that of (16) exists. A correspondence

between the different factor groups can be found by considering the conjugate groups of the different variants. In fact every variant has a conjugate group H_g of H given by the equation

$$H_g = g^{-1}Hg. \tag{17}$$

The meaning of (17) is that all the symmetry properties of Λ_1^1 are transformed by a similarity transformation into the same symmetry properties in the variant Λ_{1g}^1 and *vice versa*. By substituting (17) into (6) we get

$$G_{\Lambda_1^1} = gH_gg^{-1} + RgH_gg^{-1}$$

or

$$g^{-1}G_{\Lambda_1^1}g = H_g + g^{-1}RgH_g. \tag{18}$$

Thus a new factor group is now defined and the second-order element of it is $g^{-1}Rg$. It is rather obvious that the symmetry laws referring to different variants may or may not be the same, but if we want to make a mapping into one and the same variant the similarity transformation (18) is always needed.

We can now make a distinction between some special cases. If, for example, $gH = Hg$ holds, then (18) becomes

$$g^{-1}G_{\Lambda_1^1}g = H + g^{-1}RgH \tag{19}$$

and if R and $g^{-1}Rg$ are of the same CSL law then we have a crystallographically equivalent symmetric boundary in the same variant provided that $gR \neq Rg$. If $gH \neq Hg$ we have two special CSL boundaries in different variants and the third is defined by the equation

$$R_3 = (R)_1(g^{-1}Rg)_2, \tag{20}$$

according to (1). Relation (20) is the final relation for the characterization of a triple junction and its identification according to the CSL model. It is similar to the relation proposed by Pond (1989) for the characterization of degenerate defects, *i.e.* defects related by symmetry. Since the operators R_1 and R_2 in the right part of (20) are 180° CSL rotation operators the operator R_3 is a well established CSL rotation operator. By contrast, if R_1 and R_2 are not 180° CSL rotation operators, then the rotation operator R_3 cannot be *a priori* defined. Moreover, if the common intersection axis is a symmetry axis, then the corresponding symmetry element g is such that

$$g \in H \cap g^{-1}Hg \tag{21}$$

and is also a symmetry element of the third CSL. By using the expressions giving the rotation angles for the CSLs of the cubic system (Bleris *et al.*, 1985), we can easily see that if a CSL axis of the type ⟨100⟩, ⟨110⟩ or ⟨111⟩ exists, the CSL has at least one 180° description and the three CSLs forming the triple junction are all described by a 180° CSL rotation. (A similar property can also be found for the hexagonal system.)

5. Application

We shall present junctions based on the $\Sigma = 3$ cubic CSL twin boundary which is the most favorable cubic special CSL boundary from thermodynamic considerations. In fact a considerable number of these systems of grain boundaries has already been observed in polycrystalline Si (Komninou, 1987). Regardless of the reason for their origin this kind of CSL triple junction of Si may be considered as the best example since the symmetry of $\Sigma = 3$ is described by the greatest subgroup $H = D_3$ of O (the symmetry group of the cubic lattice).

The $\Sigma = 3$ forms two types of CSL twin boundaries, *i.e.* ⟨111⟩ and ⟨211⟩. We consider first the case which is described by a 180° rotation around the [111] axis, *i.e.* the first-order twin. The second-order symmetry element which acts as a twin generator is described by the operator

$$R = 1/3\begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix}. \tag{22}$$

The symmetry of the CSL is

$$G(\Sigma = 3) = H + RH \tag{23}$$

where

$$H = \{E,\ C_{31}^-,\ C_{31}^+,\ C_{2b},\ C_{2e},\ C_{2f}\}. \tag{24}$$

The elements of the coset RH in (23) are

$$R_1 = RC_{31}^- = \tfrac{1}{3}\begin{bmatrix} 2 & -1 & 2 \\ 2 & 2 & -1 \\ -1 & 2 & 2 \end{bmatrix}$$

rotation of 60° around the [111] axis

$$R_2 = RC_{31}^+ = \tfrac{1}{3}\begin{bmatrix} 2 & 2 & -1 \\ -1 & 2 & 2 \\ 2 & -1 & 2 \end{bmatrix} = R_1^{-1}$$

$$R_3 = RC_{2b} = \tfrac{1}{3}\begin{bmatrix} -2 & 1 & -2 \\ 1 & -2 & -2 \\ -2 & -2 & 1 \end{bmatrix}$$

rotation of 180° around the $[11\bar{2}]$ axis

$$R_4 = RC_{2e} = \tfrac{1}{3}\begin{bmatrix} -2 & -2 & 1 \\ -2 & 1 & -2 \\ 1 & -2 & -2 \end{bmatrix}$$

rotation of 180° around the $[1\bar{2}1]$ axis

$$R_5 = RC_{2f} = \tfrac{1}{3}\begin{bmatrix} 1 & -2 & -2 \\ -2 & -2 & 1 \\ -2 & 1 & -2 \end{bmatrix}$$

rotation of 180° around the $[\bar{2}11]$ axis.

Table 1. *Group multiplication table of the group* $G(\Sigma=3)$

E	C_{31}^{+}	C_{31}^{-}	C_{2b}	C_{2e}	C_{2f}	R	RC_{31}^{+}	RC_{31}^{-}	RC_{2b}	RC_{2e}	RC_{2f}
C_{31}^{-}	E	C_{31}^{+}	C_{2f}	C_{2b}	C_{2e}	RC_{31}^{-}	R	RC_{31}^{+}	RC_{2f}	RC_{2b}	RC_{2e}
C_{31}^{+}	C_{31}^{-}	E	C_{2e}	C_{2f}	C_{2b}	RC_{31}^{+}	RC_{31}^{-}	R	RC_{2e}	RC_{2f}	RC_{2b}
C_{2b}	C_{2f}	C_{2e}	E	C_{31}^{-}	C_{31}^{+}	RC_{2b}	RC_{2f}	RC_{2e}	R	RC_{31}^{-}	RC_{31}^{+}
C_{2e}	C_{2b}	C_{2f}	C_{31}^{+}	E	C_{31}^{-}	RC_{2e}	RC_{2b}	RC_{2f}	RC_{31}^{+}	R	RC_{31}^{-}
C_{2f}	C_{2e}	C_{2b}	C_{31}^{-}	C_{31}^{+}	E	RC_{2f}	RC_{2e}	RC_{2b}	RC_{31}^{-}	C_{31}^{+}	R
R	RC_{31}^{+}	RC_{31}^{-}	RC_{2b}	RC_{2e}	RC_{2f}	E	C_{31}^{+}	C_{31}^{-}	C_{2b}	C_{2e}	C_{2f}
RC_{31}^{-}	R	RC_{31}^{+}	RC_{2f}	RC_{2b}	RC_{2e}	C_{31}^{-}	E	C_{31}^{+}	C_{2f}	C_{2b}	C_{2e}
RC_{31}^{+}	RC_{31}^{-}	R	RC_{2e}	RC_{2f}	RC_{2b}	C_{31}^{+}	C_{31}^{-}	E	C_{2e}	C_{2f}	C_{2b}
RC_{2b}	RC_{2f}	RC_{2e}	R	RC_{31}^{-}	RC_{31}^{+}	C_{2b}	C_{2f}	C_{2e}	E	C_{31}^{-}	C_{31}^{+}
RC_{2e}	RC_{2b}	RC_{2f}	RC_{31}^{+}	R	RC_{31}^{-}	C_{2e}	C_{2b}	C_{2f}	C_{31}^{+}	E	C_{31}^{-}
RC_{2f}	RC_{2e}	RC_{2b}	RC_{31}^{-}	RC_{31}^{+}	R	C_{2f}	C_{2e}	C_{2b}	C_{31}^{-}	C_{31}^{+}	E

We construct the multiplication table (Table 1), where all group properties are included. From this table it is easily seen that

$$g^{-1}Rg=R$$

for all $g\in G(\Sigma=3)$, and we cannot find any crystallographically equivalent boundaries of the same type. Thus a possible coexistence of $\Sigma=3$ $\langle 111\rangle$ CSL twin boundaries can be found in two different variants. We have to analyse the group O of the parent lattice according to (7). The easiest way for that is to look for a subgroup of O of order 4, *i.e.* the index of H in G. We may easily see that two groups

$$\begin{aligned} D_2&=\{E,\ C_{2x},\ C_{2y},\ C_{2z}\}\\ C_4&=\{E,\ C_{2x},\ C_{4x}^{+},\ C_{4x}^{-}\}\end{aligned}\tag{25}$$

can be used for the decomposition of (7). The above two groups lead to the same type of conjugate subgroups, which are

$$\begin{aligned} H_{C_{2x}}&=C_{2x}HC_{2x}=\{E,\ C_{33}^{-},\ C_{33}^{+},\ C_{2a},\ C_{2c},\ C_{2f}\}\\ H_{C_{2y}}&=C_{2y}HC_{2y}=\{E,\ C_{34}^{-},\ C_{34}^{+},\ C_{2a},\ C_{2d},\ C_{2e}\}\\ H_{C_{2z}}&=C_{2z}HC_{2z}=\{E,\ C_{32}^{-},\ C_{32}^{+},\ C_{2b},\ C_{2c},\ C_{2d}\}.\end{aligned}\tag{26}$$

The second-order elements of the corresponding factor groups (18) for the coset representatives are

$$C_{2x}RC_{2x}=R_{C_{2x}}=\tfrac{1}{3}\begin{bmatrix}-1&-2&-2\\-2&-1&2\\-2&2&-1\end{bmatrix}$$

rotation of 180° around the $[\bar{1}11]$ axis or the $[1\bar{1}\bar{1}]$ axis

$$C_{2y}RC_{2y}=R_{C_{2y}}=\tfrac{1}{3}\begin{bmatrix}-1&-2&2\\-2&-1&-2\\2&-2&-1\end{bmatrix}\tag{27}$$

rotation of 180° around the $[\bar{1}1\bar{1}]$ axis or the $[1\bar{1}1]$ axis

$$C_{2z}RC_{2z}=R_{C_{2z}}=\tfrac{1}{3}\begin{bmatrix}-1&2&-2\\2&-1&-2\\-2&-2&-1\end{bmatrix}$$

rotation of 180° around the $[11\bar{1}]$ axis or the $[\bar{1}\bar{1}1]$ axis.

The following cases are the only possible ones that exist:

$$\begin{aligned}&\text{(i)}\quad H\cap H_{C_{2x}}=\{E,\ C_{2f}\}\\&\text{(ii)}\quad H\cap H_{C_{2y}}=\{E,\ C_{2e}\}\\&\text{(iii)}\quad H\cap H_{C_{2z}}=\{E,\ C_{2b}\}.\end{aligned}\tag{28}$$

The possible third boundary may have as symmetry element of the first type a second-order element. The rotation axis is of the $\langle 110\rangle$ type and this is the only direction for the coexistence of two $\Sigma=3$ twins of the (111) boundary type. We shall examine only the first case from the three equivalent ones of (28).

Consider the coexistence of twins having (111) and $(\bar{1}11)$ boundary planes. The angle between the two 180° axes is 70·53° and the corresponding product (20) will give a rotation of 141·06°, the common axis is the $[0\bar{1}1]$ which is exactly the axis of the C_{2f} element and the third special CSL boundary is a $\Sigma=9$. Using the angles of the rotation axes we can represent the possible coexistence geometrically as in Fig. 1.

As a second example let us take the second-order twin which is described by a 180° rotation around the [211] axis. In this case the corresponding second-order element which acts as a twin generator is given by the operator

$$R_1=\tfrac{1}{3}\begin{bmatrix}1&2&2\\2&-2&1\\2&1&-2\end{bmatrix}.\tag{29}$$

Its symmetry group is conjugate to the group given by (23) and it contains the elements

$$H=\{E,\ C_{33}^{-},\ C_{33}^{+},\ C_{2a},\ C_{2c},\ C_{2f}\}.\tag{30}$$

We can also use the groups (25) for the decomposition (7) and we make use of the group C_4. The same results are obtained if we use the group D_2.

In this case the second-order elements of the factor group (18) are

$$C_{2x}R_1C_{2x}=R_{C_{2x}}=\tfrac{1}{3}\begin{bmatrix}1&-2&-2\\-2&-2&1\\-2&1&-2\end{bmatrix}$$

rotation of 180° around the $[2\bar{1}\bar{1}]$ axis or the $[\bar{2}11]$ axis

$$C_{4x}^{-}R_1C_{4x}^{+} = R_{C_{4x}^{+}} = \tfrac{1}{3}\begin{bmatrix} 1 & 2 & -2 \\ 2 & -2 & -1 \\ -2 & -1 & -2 \end{bmatrix}$$

rotation of 180° around the $[21\bar{1}]$ axis or the $[\bar{2}\bar{1}1]$ axis

$$C_{4x}^{+}R_1C_{4x}^{-} = R_{C_{4x}^{-}} = \tfrac{1}{3}\begin{bmatrix} 1 & -2 & 2 \\ -2 & -2 & -1 \\ 2 & -1 & -2 \end{bmatrix}$$

rotation of 180° around the $[2\bar{1}1]$ axis or the $[\bar{2}1\bar{1}]$ axis.

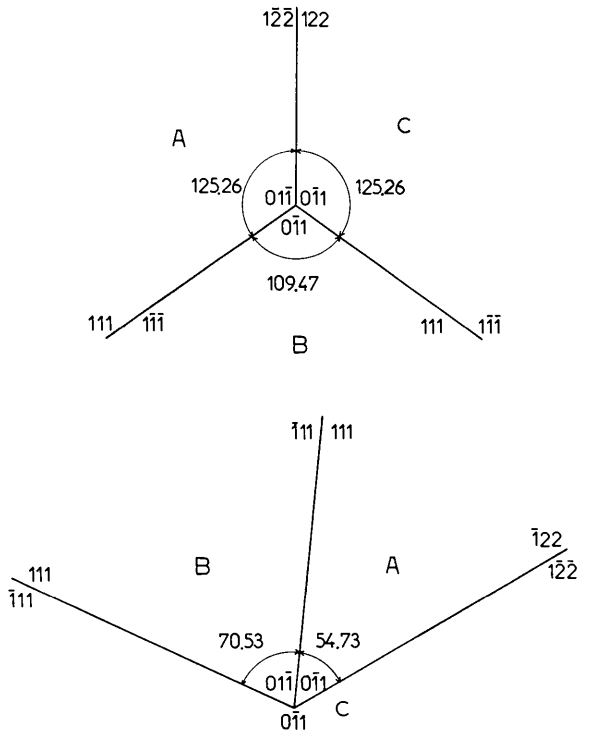

Fig. 1. The special triple junction of first-order twins {111} with $\Sigma = 3, 3, 9$.

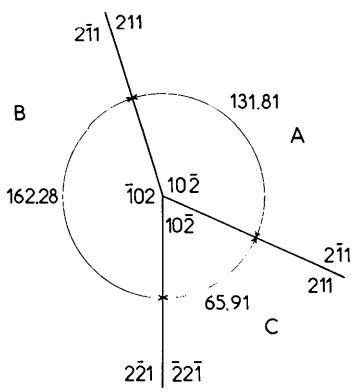

Fig. 2. The CSL triple junction of second-order twins {211} with $\Sigma = 3, 3, 9$.

We shall examine the coexistence of twins having (211) and $(2\bar{1}1)$ boundary planes. The angle between the two 180° axes is 48·19° and the corresponding product (20) gives a rotation angle of 96·38° and the common rotation axis which is the $[10\bar{2}]$ axis. The third CSL boundary is a $\Sigma = 9$. This is a typical case in which the common intersection axis in a CSL triple junction is not a symmetry axis. The geometrical representation of this triple junction is given in Fig. 2.

6. Discussion

We have presented an analytical procedure showing that the possible coexistence of special CSL boundaries is uniquely defined by using the CSL symmetry. It is rather obvious that our conclusions are independent of those of relation (1). This does not mean that (1) is not useful. It is very efficient for the experimental characterization and recognition of the junctions (Doni & Bleris, 1989).

However, this work has concluded that a CSL triple junction implies the conservation of the parent lattice symmetry as well as the symmetry of a common sublattice. This property may be directly connected to the idea that some structural building element at the microscopic level, *i.e.* an atomic cluster having the conserved symmetry, should exist. The junction may be built from this unit and the symmetry elements which have been eliminated by the symmetry breaking. However, we have seen an example in which two special GBs intersect on a CSL axis but not on a symmetry axis. In this case the absence in the symmetry continuation may lead to a linear defect by taking into account the translational symmetry.

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Linear Algebraic Analyses of Structures with One Predominant Type of Anomalous Scatterer

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Abstract

Further studies have been made of the information content of the exact linear equations for analyzing anomalous dispersion data in one-wavelength experiments. The case of interest concerns structures containing atoms that essentially do not scatter anomalously and one type of anomalously scattering atoms. For this case, there are three alternative ways of writing the equations. The alternative sets of equations and the transformations for transforming one set into the other are given explicitly. Comparison calculations were made with different sets of equations. Isomorphous replacement information is readily introduced into the calculations and the advantage of doing so is clearly illustrated by the results. Another aspect of the potential of the exact linear algebraic theory is its application to multiple-wavelength experiments. Successful applications of the latter have been made by several collaborative groups of investigators.

Introduction

By means of an algebraic analysis in which the contributions to a structure factor from the real and imaginary anomalous corrections to normal atomic scattering factors are treated separately from that from the normal part, it was possible to develop an exact linear system of simultaneous equations for extracting phase and intensity information from multiwavelength anomalous-dispersion experiments (Karle, 1980). The system of equations applies to any number and types of anomalous scatterers.

It was further indicated that essentially unique values for the phase differences that occur in the equations can be obtained in a one-wavelength experiment for the case of structures composed of non-anomalous scatterers and one predominant type of anomalous scatterer (Karle, 1985) even though the equations in this case contain a twofold ambiguity. This is achieved by using a least-squares technique for solving the equations in which the process is initiated with statistically reasonable starting values for the unknown quantities. In the one-wavelength calculation, the number of unknown quantities exceeds the number of equations by one. Therefore, one of the starting values obtained from the statistical estimates is held fixed throughout the calculation.

This investigation is concerned with the case of structures composed of non-anomalous scatterers and one predominant type of anomalous scatterer (Karle, 1985). An alternative algebraic description of this case was derived by Hendrickson (1987) in which somewhat different unknown quantities occur. The relationship between the two forms of the equations is described here. In addition, a third form for the equations is presented. The alternatives combined with the original formulation give rise to a new system of equations whose characteristics were investigated.

The purpose of these studies is to examine further the information content of the linear algebraic equations. One-wavelength data are considered here. For one-wavelength data, errors in the unknown phase differences depend on the accuracy of the quantities estimated to make the equations definitive as well as the accuracy of the data and the starting values for the unknown quantities in a least-squares process. The latter values determine whether the more accurate of two possible answers in an ambiguous calculation will be obtained.

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