

The authors would like to thank M. More for communicating his new results on CBr_4I prior to publication. They are also grateful to K. Mika and K. Wingerath for their support in computational problems.

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Crystallographic Description of Coincidence-Site Lattice Interfaces in Homogeneous Crystals

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(Received 16 June 1978; accepted 3 May 1979)

Abstract

Coincidence-site lattice interfaces (CSLI) are frequently observed in crystals where a rigid framework remains invariant on both sides of the interface. They also seem to minimize the interface energy, for example, in metals where, empirically, the greater the density of the coincidence-site lattice the more stable the grain boundary becomes. Group-theory considerations allow the determination of all the possible interface operations which leave a given sublattice invariant. A classification of these CSLI with respect to the number of equivalent sublattices they leave invariant is a guide for the prediction of the most stable type of interfaces with respect to the sublattice

considered. Examples from different types of crystals illustrate the method, which also applies for translation boundaries, twins and grain boundaries.

Introduction

It has often been verified that, in homogeneous crystals which present coherent boundaries, a fraction of the structure – which may be an atomic lattice or a partial set of atoms distributed on a lattice – remains undisturbed when crossing the boundary. This idea was first proposed by Mallard and Friedel (see, for instance, Friedel, 1926) for explaining the merohedral (or penetration) twins and the twins formed by reticular

merohedry. The undisturbed lattice was thereafter called the coincidence-site lattice (CSL) and the interfaces, which leave it invariant, the Coincidence-Site Lattice Interfaces (CSLI).

A geometrical approach to the CSLI was given by Bollmann (1970) starting from the knowledge of the interface operation. It has been more or less successfully applied, in particular, to the study of grain boundaries in metals.

In the present paper, on the contrary, our starting point is the knowledge of the CSL; we shall derive a systematic method for characterizing and numbering all possible interface operations which leave the given coincidence-site lattice invariant. This method is able to include all the cases of CSLI as well as pure translation boundaries, twins by merohedry or by reticular merohedry, for any type of structure.

The actual shape of the boundaries between the adjacent crystals, depending on energy and kinetic factors, is of no concern here, where only the geometrical relationships between the crystals are considered: we may define a geometrical space operator $(\alpha|\tau)$ which relates the homologous points \mathbf{r}^I and \mathbf{r}^{II} between the two crystals (I) and (II) by:

$$\mathbf{r}^{II} = (\alpha|\tau) \mathbf{r}^I = \alpha \mathbf{r}^I + \tau, \quad (1)$$

where α is a point operation (inversion, rotation, rotation-inversion, reflection) and τ the associated translation part (Seitz, 1936). However, every point \mathbf{r}^I deduced from \mathbf{r}^I by any $(g|t)$ space operation of the space operation

$$(\alpha|\tau)(g|t) = (\alpha g|\alpha t + \tau) \quad (2)$$

is equivalent to $(\alpha|\tau)$ and defines the same boundary: the set of the equivalent operators $(\alpha|\tau)(g|t)$ associated with the same boundary is called the *coset* of the boundary (see, for instance, Aizu, 1970; Van Tendeloo & Amelinckx, 1974; Guymont, Gratiias, Portier & Fayard, 1976; Guymont, 1978). In the following we shall denote this coset as $\{(\alpha|\tau)\}$.

I. General considerations

The structure of the crystal is assumed to be known.

I. 1. Partial and total sublattices

Any structure may be described by the superposition of atomic lattices, the nodes of which are occupied by equivalent atoms. It is always possible to build up a 'sublattice'* by selecting a subset from among the Wyckoff positions involved and which shows a translation group. Rigorously, any sublattice

* For simplicity, the term 'sublattice' will always be used even if its translation group is not a subgroup of the translation group of the structure.

has to be built up from *one* Wyckoff set so that the nodes are strictly equivalent. However, it is frequently useful to consider a 'pseudo-sublattice' built up from atoms of the same chemical species but belonging to different Wyckoff sets. We shall include these pseudo-sublattices in our description and call these *atomic* sublattices as opposed to *site* sublattices when built up from only *one* Wyckoff set.

We may define two types of atomic – or site – sublattices:

- (i) a sublattice whose nodes are defined by *all* the positions of one (or more for the case of atomic sublattices) Wyckoff set is called a *total* sublattice;
- (ii) if at least one Wyckoff set is *partially* included in the sublattice, it will be called a *partial* sublattice.

We shall illustrate these definitions by some well known examples in holohedral and hemihedral crystals. The notations used are those in *International Tables for X-ray Crystallography* (1969).

I.2. Examples (Wyckoff, 1963)

(a) Diamond

Holohedral space group $Fd\bar{3}m$.

Carbon in $8(a)$: $\left. \begin{array}{l} 0,0,0 \\ \frac{1}{4},\frac{1}{4},\frac{1}{4} \end{array} \right\} + \text{f.c.c.}$

The C atoms form two *partial* atomic sublattices translated from each other by $\frac{1}{4},\frac{1}{4},\frac{1}{4}$. It is easily shown that atoms located at $0,0,0$ and $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ cannot belong to the same atomic sublattice for there is no atom at $\frac{1}{2},\frac{1}{2},\frac{1}{2}$: The $8(a)$ Wyckoff set is only partially described by any one of these two partial atomic sublattices.

(b) Rutile, TiO_2

Holohedral, space group $P4_2/mnm$.

Titanium in $2(a)$: $0,0,0; \frac{1}{2},\frac{1}{2},\frac{1}{2}$.

Oxygen in $4(f)$: $x,x,0; \bar{x},\bar{x},0;$

$$\frac{1}{2} + x, \frac{1}{2} - x, \frac{1}{2}; \frac{1}{2} - x, \frac{1}{2} + x, \frac{1}{2},$$

with $x = 0.305$.

The Ti atoms form a *total* atomic sublattice (body-centred tetragonal) because *all* the positions of the $2(a)$ Wyckoff set are included. On the other hand, the oxygen atoms define four equivalent partial atomic sublattices (primitive tetragonal).

(c) Pyrite, FeS_2

Hemihedral, space group $Pa\bar{3}$.

Iron in $4(a)$: $0,0,0; \frac{1}{2},\frac{1}{2},0; \frac{1}{2},0,\frac{1}{2}; 0, \frac{1}{2},\frac{1}{2}$.

Sulfur in $8(c)$: $\pm(x,x,x; x + \frac{1}{2}, \frac{1}{2} - x, \bar{x}; \bar{x}, x + \frac{1}{2}, \frac{1}{2} - x; \frac{1}{2} - x, \bar{x}, x + \frac{1}{2}),$

with $x = 0.386$.

The iron atoms form a *total* f.c.c. sublattice, while the sulfur atoms form eight partial primitive cubic sublattices.

(d) *F.c.c. metals*

Holohedral, space group $Fm\bar{3}m$.

Metal in 4(a): 0, 0, 0 + f.c.c.

This is a trivial total f.c.c. lattice.

(e) *Building up of partial sublattices out of a sublattice*

In all the previous examples, we may build up an infinite number of *partial* sublattices starting from a total or partial sublattice. For instance, in case (d) any subset of the 4(a) Wyckoff set showing a translation group is a partial sublattice; for example, the subset generated by the vectors $a/2[1\bar{1}0]$, $a/2[01\bar{1}]$ and $a[111]$ defines a partial hexagonal sublattice. This sublattice is the CSL for the usual $[111]$ mirror twin.

II. Fundamental symmetry properties

Any sublattice, considered alone, shows the point symmetry of a holohedral class consistent with the crystal metrics. It can then be described by a symmorphic space group (taking into account its own translation group).

The difference between *partial* and *total* sublattices can be characterized as follows: all the elements of the space group G_o of the structure leave any total sublattice invariant because G_o is the invariance group for the Wyckoff sets involved. On the contrary, a partial sublattice is transformed into an equivalent sublattice by some operators of G_o . Let G_R be the space group associated with a given sublattice R (total or partial); the symmetry operators which leave both R and the structure *simultaneously* invariant define a group G_I which is the intersection of G_o and G_R :

$$G_I = G_o \cap G_R. \quad (3)$$

This is obviously a common space subgroup of G_o and G_R for which the R sublattice is total because G_I leaves R invariant. If R is total with respect to G_o , G_I is identical to G_o which is then a subgroup of G_R (Fig. 1).

Considering the previous examples, we find:

(a) *Diamond*

$G_R = Fm\bar{3}m$ with $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ unit cell centred on a carbon atom $(0,0,0$ or $\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$,

$G_o = Fd\bar{3}m$ with the same basis, then

$$G_I = Fm\bar{3}m \cap Fd\bar{3}m = F\bar{4}3m.$$

(b) *Rutile*

The Ti atoms form a total sublattice with space group

$G_R = I4/mmm$ with $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ unit cell centred on 0,0,0,

$G_o = P4_2/mnm$ taken with the same basis is in fact a subgroup of G_R so that:

$$G_I = P4_2/mnm \cap I4/mmm = P4_2/mnm = G_o.$$

The oxygen atoms form four partial sublattices, each one of group $P4/mmm$ centred on the atoms considered. Only the symmetry operators passing through these atoms (which are centres of symmetry in $P4/mmm$) have to be retained for building the intersection group with $P4_2/mnm$ centred on 0,0,0. For instance, the $(x,x,0)$ atomic sublattice shows a centre of symmetry at $(x,x,0)$ which is obviously not the case for $P4_2/mnm$. Hence, there will be no centre of symmetry in the intersection group G_I ; the only symmetry elements which are kept are the site symmetry elements: two perpendicular mirrors $m_{[11\bar{1}0]}$ and $m_{[001]}$ and the diad axis $2_{[110]}$ which is their intersection. Thus, one obtains the space group $Amm2$ with $(\mathbf{c}, \mathbf{b} - \mathbf{a}, \mathbf{a} + \mathbf{b})$ as unit cell:

$$G_I = Amm2(\mathbf{c}, \mathbf{b} - \mathbf{a}, \mathbf{a} + \mathbf{b}).$$

In this group, the oxygen position $x,x,0$ now constitutes the complete 2(a) Wyckoff set: 0,0,Z; it is a *total* sublattice with respect to $Amm2$.

(c) *Pyrite*

The Fe atoms form a *total* atomic sublattice of group $Fm\bar{3}m$, and then

$$G_I = G_o = Pa\bar{3}.$$

The S atoms form eight *partial* atomic sublattices of group $Pm\bar{3}m$, each one centred on the S atoms

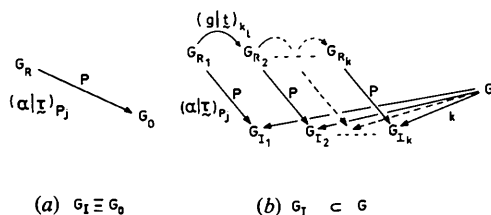


Fig. 1. Group-subgroup relation (a) for total sublattices and (b) for partial sublattices of space group G_R . p and k are the indices of G_I in G_R and G_o respectively. For the partial sublattices the different G_R space groups associated with the different equivalent R_j sublattices are conjugated by operators of G_o : $G_{R_j} = (g|t)_j G_{R_1} (g|t)_j^{-1}$.

considered. Here again, centres of symmetry disappear and only a triad axis is kept: for the (x,x,x) sublattice, for example, we obtain:

$$G_I = Pa3 \cap Pm3m = R3.$$

For this group $R3$, the (x,x,x) positions now form the complete 1(a) Wyckoff set.

(d) *F.c.c. metal*

We consider the partial atomic sublattice previously chosen (§ I.2e): $0,0,0$; $\frac{1}{2}, -\frac{1}{2}, 0$; $0, \frac{1}{2}, -\frac{1}{2}$; $1, 1, 1$. This sublattice has space group $P6/mmm$. The intersection group with $Fm3m$ is:

$$G_I = Fm3m(\mathbf{a}, \mathbf{b}, \mathbf{c})$$

$$\cap P6/mmm \{(\mathbf{a} - \mathbf{b})/2, (\mathbf{b} - \mathbf{c})/2, \mathbf{a} + \mathbf{b} + \mathbf{c}\} \\ = P\bar{3}m1 \{(\mathbf{a} - \mathbf{b})/2, (\mathbf{b} - \mathbf{c})/2, \mathbf{a} + \mathbf{b} + \mathbf{c}\}$$

with atoms now in 1(a) Wyckoff positions.

III. Numbering and characterization of interface operations

III.1. Numbering

A twinned material exhibits several types of domains; the domains which are related by a symmetry operation of the space group of any one of them define a unique variant (*i.e.* if adjacent, these domains would reduce to a single crystal). The number of different possible interfaces bordering a given domain depends on the following:

(i) to be crystallographically different, (with respect to G_I) two interface operations have to belong to two different cosets of the decomposition of G_R with respect to G_I : the index p of G_R in G_I gives the number of different interfaces which leave R invariant without being symmetry operations of the structure;

(ii) R may also be transformed into any one of its equivalents. The number k of the equivalent sublattices (which is different from unity for partial sublattices) is equal to the index of G_o in G_I (these two decompositions will be explicitly performed in § III.3).

Thus, starting from one given domain, it is possible to build up

$$n = k(p - 1) \quad (4)$$

adjacent domains which leave any one of the sublattices equivalent to R , or R itself, invariant.

However, n is *not* the actual number of the different types of possible interfaces because any interface leaving at least l sublattices simultaneously invariant ($l \leq k$) has here been taken into account l times (once per invariant sublattice).

We then have to subtract from n , $(l - 1)$ times the number of interfaces which simultaneously leave at least l equivalent sublattices invariant, l running from 2 to k . Let there be R_1, R_2, \dots, R_l sublattices; to leave these invariant the interface operations have to belong simultaneously to $G_{R_1}, G_{R_2}, \dots, G_{R_l}$, *i.e.* to the intersection group

$$G_{123\dots l} = G_{R_1} \cap G_{R_2} \cap \dots \cap G_{R_l}. \quad (5)$$

Since these interface operations must not belong to G_o one obtains all these possible interface operations by decomposing $G_{123\dots l}$ in cosets of $G_o \cap G_{123\dots l}$. Their number is the index $p_{123\dots l}$ of $G_{123\dots l}$ in $G_o \cap G_{123\dots l}$:

$$n_{123\dots l} = p_{123\dots l} - 1. \quad (6)$$

By now considering all the possible combinations of the l invariant sublattices in the k equivalent ones we obtain the total number N_l of different interfaces which leaves at least l sublattices invariant:

$$N_l = \sum_{j_1 > j_2} \dots \sum_{j_l} n_{j_1 j_2 \dots j_l}. \quad (7)$$

The total number of different possible interfaces is therefore

$$N = k(p - 1) - \sum_{j_2 > j_1} \sum_{j_3 > j_2 > j_1} n_{j_1 j_2} - 2 \sum_{j_3 > j_2 > j_1} \sum_{j_4} n_{j_1 j_2 j_3} \\ - (l - 1) \sum_{j_1 > j_2 > j_3} \dots \sum_{j_l} n_{j_1 j_2 \dots j_l} - \dots \\ - (k - 1) n_{123\dots k}, \quad (8)$$

where the summations run over the k partial equivalent sublattices.

For the case of total sublattices, a group-subgroup relationship between G_R and G_o holds ($k = 1$) which reduces relation (8) to

$$N = p - 1. \quad (9)$$

This is the usual number of different possible domains adjacent to a given domain when generated after a phase transition between two structures which are group-subgroup related (Guymont, Gratias, Portier & Fayard, 1976).

It seems reasonable to assume that, if an interface with CSL exists in a crystal, the fault energy will be minimized (independently of the shape of the boundary) for those interfaces which leave a maximum of equivalent sublattices simultaneously invariant. These interfaces are found by building up the different intersection groups (5). A necessary condition for an interface to leave l equivalent sublattices invariant is that at least one of the intersection groups is not a subgroup of the space group G_o of the structure. Obviously, if one has an intersection of order l which is a subgroup of G_o , all further intersections are also subgroups of G_o and do

not have to be considered. Practically, it is convenient to consider first the intersection defining a maximum number, say L , of invariant partial sublattices (*i.e.* all further intersections $G_{12\dots L,L+1}$ are subgroups of G_o). There are C_l^k possible different combinations of l sublattices among k sublattices. However, one given combination, say $\{j\}$, belongs to $v_{\{j\}}^l$ equivalent combinations with respect to the structure and then the initial C_l^k combinations are distributed among only J_l different families with respect to the structure with

$$\sum_{j=1}^{J_l} v_{\{j\}}^l = C_l^k. \quad (10)$$

Let us denote by $H_{\{j\}}^l$ the subgroup of G_o which leaves the combination $\{j\}$ of l sublattices globally invariant (Fig. 2). The index of G_o in $H_{\{j\}}^l$ is the searched $v_{\{j\}}^l$ of relation (10):

$$v_{\{j\}}^l = \text{index of } G_o \text{ in } H_{\{j\}}^l. \quad (11)$$

Thus the number of interface operations leaving the combination $\{j\}$ or its equivalents invariant is:

$$N_{\{j\}}^l = v_{\{j\}}^l (p_{\{j\}}^l - 1), \quad (12)$$

where $p_{\{j\}}^l$ has the same meaning as in (6). By performing the same calculation over the J_L families we finally obtain the total number of interface operations leaving L sublattices invariant:

$$N_L = \sum_{j=1}^{J_L} v_{\{j\}}^L (p_{\{j\}}^L - 1). \quad (13)$$

The number N_l of interface operations leaving exactly l sublattices invariant is then

$$N_l = \sum_{j=1}^{J_l} v_{\{j\}}^l (p_{\{j\}}^l - 1) - (l+1)N_{l+1} - \dots - LN_L. \quad (14)$$

This procedure considerably reduces the number of intersection groups to be determined in relation (8): we need only one intersection group per family. We shall illustrate the method in detail for pyrite and rutile.

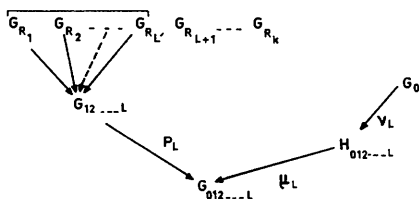


Fig. 2. Group-subgroup relations for CSLI leaving L equivalent sublattices simultaneously invariant. The number of the equivalent combinations of L sublattices is given by the index v_L of $H_{012\dots L}$ in G_o .

III.2. Examples

(a) Diamond

$$\begin{aligned} G &= Fd3m(\mathbf{a}, \mathbf{b}, \mathbf{c}; 0, 0, 0); \\ G_{R_1} &= Fm3m(\mathbf{a}, \mathbf{b}, \mathbf{c}; 0, 0, 0); \\ G_{R_2} &= Fm3m(\mathbf{a}, \mathbf{b}, \mathbf{c}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}). \end{aligned}$$

We first perform the intersection $G_{12} = G_{R_1} \cap G_{R_2}$.

Because of the $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ translation between the two groups the common symmetry elements reduce to the triad axis $3_{[111]}$ and the mirrors $m_{[1\bar{1}0]}$, $m_{[01\bar{1}]}$ and $m_{[10\bar{1}]}$, thus:

$$G_{12} = R3m\{(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} + \mathbf{c})/2, (\mathbf{b} + \mathbf{c})/2; 0, 0, 0\}.$$

But G_{12} is a subgroup of $Fd3m$: there are no possible interfaces which leave R_1 and R_2 simultaneously invariant (this is a trivial result because the structure here consists only of the superposition of these two sublattices).

The total number of different possible interfaces is simply

$$N = k(p - 1)$$

with

$$k = \text{index of } F\bar{4}3m \text{ in } Fd3m = 2$$

and

$$p = \text{index of } F\bar{4}3m \text{ in } Fm3m = 2,$$

then

$$N = 2.$$

(b) Rutile

The case of the Ti sublattice is trivial because it is a total sublattice:

$$N = p - 1$$

with

$$p = \text{index of } P4_2/mnm \text{ in } I4/mmm = 2.$$

There is only one possible interface leaving the Ti sublattice invariant.

We designate by 1, 2, 3, 4, respectively, the oxygen sublattices built up from $x, x, 0; \bar{x}, \bar{x}, 0; \frac{1}{2} + x, \frac{1}{2} - x, \frac{1}{2}$ and $\frac{1}{2} - x, \frac{1}{2} + x, \frac{1}{2}$. These four sublattices obviously constitute a complete Wyckoff set of $P4_2/mnm$ and may therefore be used as a basis of representation of this group. This representation is isomorphic with a permutation group of four objects as shown in Table 1. One set $\{j\}$ of i sublattices being given, we obtain the numbers $v_{\{j\}}^i$ by counting the number of the different combinations which appear in the i considered columns of the permutation group. For instance, the representation of $P4_2/mnm$ at the $4(f)$ Wyckoff position is isomorphic with a permutation group of order eight. Let us consider the sublattice 1 alone. Any other sub-

lattices appear twice in the first column (this is obvious because the four sublattices are equivalent and the permutation group is of order eight), so that 1, 2, 3, 4 belong to the same family and then

$$v_1^1 = 4.$$

Moreover, $C_4^1 = 4$ so that there is only one family of one sublattice (trivial result!). We have then only to determine G_1 and G_{01} ; also, H_1^1 is trivial and reduces to G_{01} .

Let us now consider the couple (1, 2): it exchanges with (3, 4) only, and then

$$v_{12}^2 = 2.$$

Taking now (1, 3) we obtain (1, 4) (2, 3) and (2, 4), so that:

$$v_{13}^2 = 4.$$

Remembering that $\sum v = C_4^2$ we see that we have to consider two families only for finding the possible interfaces which leave two sublattices invariant. We shall then build up (G_{12}, G_{012}) and (G_{13}, G_{013}) .

The different intersection groups are given in Table 2. Finally we obtain:

$$N_4 = 0$$

$$N_3 = 0$$

$$N_2 = v_{12}^2(p_{12} - 1) + v_{13}^2(p_{13} - 1) = 2(1 - 1) + 4(2 - 1) = 4$$

$$N_1 = v_1^1(p_1 - 1) - 2N_2 = 4(4 - 1) - 2 \times 4 = 4.$$

There are then four possible interfaces with two simultaneously invariant sublattices, and four possible interfaces with only one invariant sublattice.

Table 1. Representation of $P4_2/mnm$ in the $4(f)$ Wyckoff position

$G_o = P4_2/mnm$	Permutations of the $4(f)$ position*
(1 000)	1 2 3 4
$(m_{1001} 000)$	1 2 3 4
$(m_{11\bar{1}0} 000)$	1 2 4 3
$(2_{110} 000)$	1 2 4 3
$(2_{1\bar{1}0} 000)$	2 1 4 3
$(1 000)$	2 1 4 3
$(m_{110} 000)$	2 1 3 4
$(2_{1\bar{1}0} 000)$	2 1 3 4
$(m_{1010} \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	3 4 1 2
$(2_{1100} \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	3 4 1 2
$(4_{21001} \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	3 4 2 1
$(4_{2\bar{1}001} \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	3 4 2 1
$(m_{1100} \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	4 3 2 1
$(2_{1010} \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	4 3 2 1
$(4_{21001} \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	4 3 1 2
$(4_{1001} \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	4 3 1 2

* $4(f)$: (1) $x, x, 0$, (2) $\bar{x}, \bar{x}, 0$, (3) $\frac{1}{2} + x, \frac{1}{2} - x, \frac{1}{2}$, (4) $\frac{1}{2} - x, \frac{1}{2} + x, \frac{1}{2}$.

Table 2. Intersection groups for partial oxygen sublattices in TiO_2 .

The unit-cell vectors are expressed in the reference frame of the structure. X and Y denote respectively the [110] and $\bar{1}\bar{1}0$ directions. The origins different from 000 are indicated.

Number i of sublattices considered	1	2	3	4
C_i^1	4	6	6	6
Number J of different sets $\{j\}$	1	2	2	2
$v_{(j)}$	4	4	4	4
$H_{0(j)}$	$H_{01} = C2_x m_y m$ (a + b, b - a, c)	$H_{013} = P2_1 nm$ (a, b, c)	$H_{012} = Cm_x m_y m$ (a + b, b - a, c)	$H_{014} = Cm_x m_y m$ (a + b, b - a, c)
$G_{0(j)}$	$G_{01} = H_{01}$	$G_{013} = Pm_2$ (a, b, c)	$G_{012} = C2_x m_y m$ (a + b, b - a, c)	$G_{014} = C2_x m_y m$ (a + b, b - a, c)
$G_{(j)}$	$G_1 = P4/mmm$ (a, b, c; x, x, 0)	$G_{13} = Pm2m$ (a, b, c; x, 0, 0)	$G_{12} = G_{012}$	$G_{14} = G_{014}$
$p_{(j)}$	4	2	2	1*

* No possible interlaces.

This example illustrates fairly well the fact that the notion of CSL has to be generalized because the actual geometrical locus of zero displacement obtained for the interfaces with two invariant sublattices does not reduce to a single lattice; this treatment is presented elsewhere (Gratias, Portier & Fayard 1979).

(c) Pyrite

The Fe sublattice being total, we directly obtain:

$$N = p - 1 \text{ with } p = \text{index of } Fm\bar{3}m \text{ in } Pa\bar{3} = 8.$$

Then

$$N = 7.$$

For the S sublattices, we proceed in the same way as for rutile. However, the workings are rather tedious so that we shall give here only the principal results. A careful examination of the intersection groups obtained for more than four sublattices shows that they all are subgroups of G_o . Then $N_8 = N_7 = N_6 = N_5 = 0$.

For four sublattices, we obtain six different families characterized by the combinations:

$$(1, 4, 5, 8); v_{1458}^4 = 6$$

$$(1, 2, 3, 4); v_{1234}^4 = 6$$

$$(1, 3, 5, 7); v_{1357}^4 = 2$$

$$(1, 3, 5, 8); v_{1358}^4 = 8$$

$$(1, 2, 3, 5); v_{1235}^4 = 24$$

$$(1, 2, 3, 6); v_{1236}^4 = 24,$$

where the sublattices are labelled as follows:

$$(1) x, x, x \quad (5) x, \frac{1}{2} + x, \frac{1}{2} - x$$

$$(2) \bar{x}, \bar{x}, \bar{x} \quad (6) \bar{x}, \frac{1}{2} - x, \frac{1}{2} + x$$

$$(3) \frac{1}{2} + x, \frac{1}{2} - x, \bar{x} \quad (7) \frac{1}{2} - x, x, \frac{1}{2} + x$$

$$(4) \frac{1}{2} - x, \frac{1}{2} + x, x \quad (8) \frac{1}{2} + x, \bar{x}, \frac{1}{2} - x.$$

We can verify that $\sum v = C_8^4 = 70$.

We have then to consider only six intersection groups. We find therefore:

$$N_4 = 6(2-1) + 6(1-1) + 2(1-1) + 8(1-1) \\ + 24(1-1) + 24(1-1) = 6.$$

For three sublattices we have only three families:

$$(1,4,5); v_{145}^3 = 24$$

$$(1,2,3); v_{123}^3 = 24$$

$$(1,3,5); v_{135}^3 = 8.$$

Also, $\sum v = C_8^3 = 56$; by considering the three corresponding intersection groups we obtain

$$N_3 = 24(2-1) + 24(1-1) + 8(1-1) - 4 \times 6 = 0.$$

There are no possible interfaces leaving three sublattices only invariant. For two sublattices we find three families:

$$(1,4); v_{14}^2 = 12$$

$$(1,2); v_{12}^2 = 4$$

$$(1,3); v_{13}^2 = 12; \sum v = C_8^2 = 28$$

and

$$N_2 = 12(4-1) + 12(2-1) + 4(2-1) \\ - 3 \times 0 - 4 \times 6 = 28.$$

Finally, there is one family only ($v = k = 8$) for one sublattice, then

$$N_1 = 8(16-1) - 2 \times 28 - 3 \times 0 - 4 \times 6 = 40.$$

(d) *F.c.c. metals*

The number of equivalent hexagonal sublattices, k , is given by the index of $G_o = Fm\bar{3}m(\mathbf{a}, \mathbf{b}, \mathbf{c})$:
in

$$G_I = P\bar{3}m1[(\mathbf{a} - \mathbf{b})/2, (\mathbf{b} - \mathbf{c})/2, \mathbf{a} + \mathbf{b} + \mathbf{c}] \\ k = 12;$$

p is the index of $P6/mmm$ in $P\bar{3}m1$ (same unit cell):

$$p = 2.$$

Moreover, it can be verified that all the intersection groups are subgroups of G_o : the interfaces all leave only one partial sublattice invariant; their number is then:

$$N = k(p-1) = 12.$$

III.3. Characterization of the boundary operations

As we have said in the *Introduction* any interface is crystallographically characterized by a coset of operations denoted by $(\alpha|\tau)$. Let us perform the two coset decompositions of G_R and G_o with respect to G_I :

$$G_R = G_I + (\alpha|\tau)_2 G_I + \dots + (\alpha|\tau)_p G_I \quad (15)$$

$$G_o = G_I + (g|t)_2 G_I + \dots + (g|t)_k G_I. \quad (16)$$

$(\alpha|\tau)_j G_I$ represents the j th coset of equivalent operators which leave the R sublattice invariant but change the structure (in orientation and/or translation). Since any right multiplication of this coset by an operator of G_o leaves the structure invariant, the complete j th coset with respect to the structure becomes:

$$(\alpha|\tau)_j G_I G_o = (\alpha|\tau)_j G_o. \quad (17)$$

Looking for the other equivalent sublattices of R , we see from the second coset decomposition that they are deduced from R by:

$$R_i = (g|\tau)_i G_I R. \quad (18)$$

To obtain their corresponding interface operations we have to conjugate (17) by the operations (18) which relate the equivalent sublattices; the expression for a CSLI operation is then:

$$(g|t)_i G_I (\alpha|\tau)_j G_I^{-1} (g|t)_i^{-1} = \{(g|t)_i\}' \{(\alpha|\tau)_j\}. \quad (19)$$

The associated interface leaves the l th sublattice invariant by the j th symmetry operation of this sublattice which does not belong to the space group of the structure. The symbol $\{\dots\}'$ denotes a coset with respect to G_I only, because we have arbitrarily differentiated the k equivalent sublattices by choosing one of the equivalent reference frames for describing the structure. The general expression for a CSLI may be written as:

$$\{G_o\} (\alpha|\tau) \{G_o^{-1}\}, \quad (20)$$

where $\{G_o\}$ (of course $\{G_o^{-1}\} = \{G_o\}$) denotes any operator belonging to G_o .

If we are only interested in the interfaces which leave several, say i , sublattices invariant the second coset decomposition (16) has to be performed with respect to $H_{o(i)}$ only, because the further decomposition of $H_{o(i)}$ with respect to $G_{o(i)}$ gives no new interface operations.

We are now able to calculate the total number of variants which may be generated in the bulk material. Let us consider a succession of domains belonging to the variants $V_0, V_1, \dots, V_{l-1}, V_l, \dots$. All the boundaries between any two succeeding domains are assumed to be CSLI. For instance, the interface (V_{l-1}, V_l) corresponds to a coset (10) where the operators are expressed in the reference frame of V_{l-1} or V_l , say V_{l-1} . This coset now expressed in the reference frame of V_0 has to be conjugated by the (V_0, V_{l-1}) interface operation:

$$(V_{l-1}, V_l)_0 = (V_0, V_{l-1}) G_o (\alpha|\tau)_i G_o^{-1} (V_0, V_{l-1})^{-1}, \quad (21)$$

so that the operation between V_0 and V_l expressed in V_0 is

$$(V_0, V_l)_0 = (V_0, V_{l-1}) G_o (\alpha|\tau)_i G_o^{-1} (V_0, V_{l-1})^{-1} \\ \times (V_0, V_{l-1}). \quad (22)$$

By iterating this recurrent relation $l - 1$ times we finally obtain

$$(V_0, V_l) = G_o(\alpha|\tau)_1 G_o(\alpha|\tau)_2 G_o \dots (\alpha|\tau)_l G_o^{-1}. \quad (23)$$

Thus, the boundary operations between domains are obtained by sequential products of operators belonging to G_o and to G_R . Generally, such products generate an infinite number of operators so that we obtain an infinite number of variants.

The condition for the number of variants to be finite is that G_R and G_o be subgroups of a least-common space supergroup J . In fact, all the products of (18) remain in J and the total number of possible variants N_V is then the index of the space supergroup J in G_o (as in the case of variants generated from a group-subgroup phase transition):

$$N_V = \text{index of } J \text{ in } G_o. \quad (24)$$

Furthermore, it is important to emphasize that the boundaries defined in (20) are not always CSLI if the sublattice considered is partial. For total sublattices, J is identical to G_R : the number of variants N_V is always finite and is the index of G_R in G_o : all the boundaries are CSLI because the invariant sublattice is the same in all variants. Let us illustrate these results with the previous examples.

III.4. Examples

(a) Diamond

$$G_o = Fd3m(\mathbf{a}, \mathbf{b}, \mathbf{c}); G_R = Fd3m(\mathbf{a}, \mathbf{b}, \mathbf{c}); \\ G_l = F\bar{4}3m(\mathbf{a}, \mathbf{b}, \mathbf{c}).$$

We have previously shown that $p = 2$, $k = 2$ and then $N = 2$ with one invariant carbon sublattice. These two boundaries bordering a given variant are characterized by the cosets of (15) and (16):

$$Fm3m = \{(1|000) + (m_{1001}|000)\} F\bar{4}3m, \\ Fd3m = \{(1|000) + (m_{1001}|\frac{1}{4}, \frac{1}{4}, \frac{1}{4})\} F\bar{4}3m,$$

so that the boundary operations are

$$(m_{1001}|000)Fd3m \text{ and } (m_{1001}|\frac{1}{4}, \frac{1}{4}, \frac{1}{4})(m_{1001}|000)Fd3m.$$

These may obviously be written as pure translation operations:

$$(m_{1001}|000)Fd3m = (m_{1001}|000)(m_{1001}|\frac{1}{4}, \frac{1}{4}, \frac{1}{4})Fd3m \\ = (1|\frac{1}{4}, \frac{1}{4}, \frac{1}{4})Fd3m$$

and

$$(m_{1001}|\frac{1}{4}, \frac{1}{4}, \frac{1}{4})(m_{1001}|000)Fd3m = (1|\frac{1}{4}, \frac{1}{4}, \frac{1}{4})Fd3m.$$

We obtain two pure translations with fault vectors:

$$\mathbf{R}_1 = [\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}] \text{ and } \mathbf{R}_2 = [\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$$

(or any of their equivalent pure translation operators belonging to their cosets with respect to G_o).

Moreover, $Fm3m$ and $Fd3m$ are common subgroups of the space group

$$J = Im3m(\mathbf{a}/2, \mathbf{b}/2, \mathbf{c}/2),$$

and the total number of variants is the index of

$$Im3m(\mathbf{a}/2, \mathbf{b}/2, \mathbf{c}/2) \text{ in } Fd3m(\mathbf{a}, \mathbf{b}, \mathbf{c}).$$

Because there are two types of CSLI and four types of variants here we may obtain boundaries [see boundaries (V_0, V_3) or (V_1, V_2) in Fig. 3] which are not CSLI; for instance:

$$(1|\frac{1}{4}, \frac{1}{4}, \frac{1}{4})(1|\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) = (1|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) = (1|0, 0, \frac{1}{2})$$

does not leave any carbon sublattice invariant.

Though we are not able to describe the geometrical shape of the boundaries with this approach we may assume that the $(1|0, 0, \frac{1}{2})$ type of boundary shows a higher fault energy than the $(1|\frac{1}{4}, \frac{1}{4}, \pm\frac{1}{4})$ ones. A way of decreasing the $(1|0, 0, \frac{1}{2})$ boundary surfaces is for the intersections between CSLI to present an even number of adjacent boundaries. Unfortunately no observations have been made on possible translation faults in diamond.

(b) Rutile

The Ti sublattice needs only the decomposition of G_R with respect to G_o :

$$I4/mmm = \{(1|000) + (1|\frac{1}{2}, \frac{1}{2}, \frac{1}{2})\} P4_2/mnm.$$

We obtain a unique possible CSLI which is a pure translation, with a fault vector

$$\mathbf{R} = [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}].$$

For the oxygen sublattices, we shall consider only the most probable CSLI, *i.e.* those which simultaneously leave two partial sublattices invariant. We

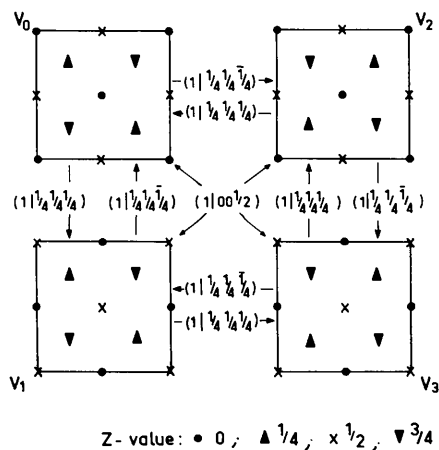


Fig. 3. The four possible variants for diamond with CSLI ($V_0 - V_1$, $V_0 - V_2$): here they are pure translation boundaries.

then perform the two coset decompositions of G_{13} with respect to G_{013} and G_o with respect to H_{013} :

$$P4_2/mnm(\mathbf{a},\mathbf{b},\mathbf{c}; 000) = [(1|000) + (m_{[110]}|000)] \\ \times [(1|000) + (m_{[100]}|\frac{1}{2},\frac{1}{2},\frac{1}{2})] \\ \times P2_{1x}n_y m_z(\mathbf{a},\mathbf{b},\mathbf{c}; 000), \\ Pm_x2_y m_z(\mathbf{a},\mathbf{b},\mathbf{c}; x,0,0) = \{(1|000) + (m_{[100]}|2x,0,0)\} \\ \times Pm_z(\mathbf{a},\mathbf{b},\mathbf{c}; 000).$$

The translation $2x,0,0$ associated with the mirror $m_{[100]}$ appears because of the change $(x,0,0)$ of the origin of Pm with respect to $Pm2m$: by a translation \mathbf{p} of the origin, any space operator $(g|t)$ transforms into $(g|t + g\mathbf{p} - \mathbf{p})$.

If we now perform the different products (19), we obtain in all cosets at least one pure translation operation; for example:

$$(m_{[100]}|\frac{1}{2},\frac{1}{2},\frac{1}{2})(m_{[100]}|-2x,0,0) = (1|\frac{1}{2} + 2x, \frac{1}{2}, \frac{1}{2}),$$

with $x \simeq 0.305$. The fault vector is:

$$\mathbf{R} \simeq \frac{1}{10}[1.5.5].$$

This result is in agreement with the careful experimental determination of Van Landuyt, de Ridder, Gevers & Amelinckx (1970). Moreover, there is no common supergroup between G and G_R because the value of x is not a submultiple of the unit-cell parameter a .

This generates an infinite number of variants. The products of any two CSLI operations not being a CSLI operation, we see that the minimization of the total fault energy in the crystal is obtained for parallel interfaces, i.e. if the CSLI do not intersect. In fact, the faults observed in rutile correspond to a shear structure where the CSLI are parallel walls.

(c) Pyrite

Fe sublattice: since this sublattice is total only the decomposition of G_R with respect to G_o is required:

$$Fm3m = \{(1|000) + (1|\frac{1}{2},\frac{1}{2},0) + (1|\frac{1}{2},0,\frac{1}{2}) \\ + (1|0,\frac{1}{2},\frac{1}{2})(1|000) + (m_{[110]}|000)\}Pa3.$$

We obtain three pure translation boundaries with fault vectors $[\frac{1}{2},\frac{1}{2},0]$ and four merohedral twins: $(m_{[110]}|000)$; $(m_{[110]}|\frac{1}{2},\frac{1}{2},0)$; $(m_{[110]}|\frac{1}{2},0,\frac{1}{2})$ and $(m_{[110]}|0,\frac{1}{2},\frac{1}{2})$.

The number of variants is the index of $Fm3m$ in $Pa3$: $N_V = 8$.

Finally, as for all cases of total sublattices, the intersections of any CSLI always generate another CSLI. These merohedral twins and translation boundaries in pyrite have recently been observed (Donnay, Donnay & Iijima, 1977).

S sublattice: as for the case of rutile, we restrict our example to the case interfaces leaving four sublattices

invariant. The groups involved are

$$G_{1458} = Pm_y(\mathbf{a},\mathbf{b},\mathbf{c}; 0,x,0)$$

$$G_{01458} = P1(\mathbf{a},\mathbf{b},\mathbf{c}; 0,0,0)$$

and

$$H_{01458} = Pa_x2_{1y}c_z(\mathbf{a},\mathbf{b},\mathbf{c}; 0,0,0).$$

We obtain the following coset decompositions:

$$Pa3(\mathbf{a},\mathbf{b},\mathbf{c}; 000) = \{(1|000) + (\bar{1}|000)\}(1|000) \\ + (3_{[111]}|000) \\ + (3_{[111]}^2|000)\}Pa_x2_{1y}c_z(\mathbf{a},\mathbf{b},\mathbf{c}; 000) \\ Pm_y(\mathbf{a},\mathbf{b},\mathbf{c}; 0,x,0) = \{(1|000) + (m_{[010]}|0,2x,0) \\ \times P1(\mathbf{a},\mathbf{b},\mathbf{c}; 000)\}.$$

As for the case of rutile all cosets of the different products (19) contain one pure translation operator:

$$(m_{[010]}|0,\frac{1}{2},\frac{1}{2})(m_{[010]}|0,2x,0) = (1|0, \frac{1}{2} - 2x, \frac{1}{2}).$$

The fault vector is then ($x = 0.386$)

$$\mathbf{R} \simeq [0, -0.27, \frac{1}{2}]$$

and its equivalents with respect to $Pa3$.

This result is to be compared with the experimental determination of Fagot, Levade, Couderc & Bras (1978) who did not find the $\frac{1}{2}$ component along z . However, the extinction condition $l = 2n$ of $Pa3$ for the $h0l$ planes, which still applies in two-dimensional electron dynamical diffraction (Gjønnes & Moodie, 1965), leads to a possible half-integer value along z of the \mathbf{R} vector that the authors have not considered.

(d) F.c.c. metals

We have to decompose $Fm3m$ and $P6/mmm$ with respect to $P\bar{3}m1$. By expressing the operators in the cubic reference frame we obtain:

$$P6/mmm = \{(1|000) + (2_{[111]}|000)\}P\bar{3}m1 \\ Fm3m = \{(1|000) + 1|\frac{1}{2},\frac{1}{2},0) + (1|\frac{1}{2},0,\frac{1}{2}) + (1|0,\frac{1}{2},\frac{1}{2})\} \\ \times \{(1|000) + (m_{[100]}|000) \\ + (m_{[110]}|000)\}P\bar{3}m1,$$

so that the 12 CSLI are defined by binary axes along $\langle 111 \rangle$ but located at different positions in the unit cell.

Since G_o and G_R have no common crystallographic space supergroup the number of variants is infinite.

IV. The particular case of total sublattices

The general method proposed here is greatly simplified if the invariant sublattice is total because G_I is then identical to G_o , so that G_R is a supergroup of G_o . It follows that the number of variants is the index of G_o in G_R .

If the structure has a holohedral symmetry class, the CSLI operations all reduce to pure translations; their number is equal to the sum of the multiplicity of the Wyckoff set(s) which defines the sublattice divided by the Bravais cell multiplicity of the structure. The boundary operations have the form:

$$(1|\mathbf{T}_R),$$

where \mathbf{T}_R are the translations of the sublattice, reduced modulo the primitive cell of the structure.

If the structure is not holohedral the decomposition of G_R with respect to G_o may be performed in two steps:

(i) decomposition of G_R with respect to an intermediate *Translationengleich* subgroup G' .

(ii) decomposition of G' with respect to G_o (*Klassengleich*).

The first decomposition generates only pure orientation operations referred to as:

$$(h_R|000),$$

in the reference frame centred on any node of the R total sublattice. The second decomposition generates only pure translation operations so that the general form of CSLI may be written

$$(h_R|000)(1|\mathbf{T}_R) = (h_R|h_R \mathbf{T}_R).$$

The number of variants is equal to the sum of the multiplicities of the Wyckoff set(s) concerned, divided by the multiplicity of the Bravais cell of the structure and multiplied by the index of the point group associated with the structure in the holohedral symmetry class of the crystal system.

For instance, we find that for the Ti sublattice in rutile

$$N_V = 2 \times 1 = 2.$$

The Ti are in the 2(a) Wyckoff positions (multiplicity 2) and the Bravais lattice of the structure is primitive (multiplicity 1).

For the Fe sublattice, in pyrite, we find

$$N_V = 4 \times 2 \times 1 = 8.$$

The Fe atoms are in the 4(a) Wyckoff positions (multiplicity 4); the index of $m3m$ in $m3$ is 2 and the Bravais lattice of the structure ($Pa3$) is primitive (multiplicity 1).

V. Conclusions

The method presented here only requires knowledge of the invariant sublattice (as far as this sublattice is defined as a subset of the Wyckoff positions of one type of atom involved in the structure).

There is no formal difference between pure translation boundaries and twins because the translation subgroups of the space groups of the structure and of the sublattice do not play a particular role in the determination of the CSLI with respect to the other symmetry operators.

Furthermore, it should be noted that all the boundary operations which leave a site sublattice (built up from only one Wyckoff set) invariant are always translation reducible (their cosets contain pure rotations or pure reflections) since they leave at least one site, of the same type, invariant for the two crystals. This is the case in our examples; only site sublattices have been considered. The translation boundaries we have obtained may all be replaced by pure point-symmetry operators.

This property disappears for the case of atomic sublattices built up from *several* different Wyckoff sets, because here some CSLI exchange different Wyckoff positions between the adjacent crystals. Hence, it is possible to obtain mixed boundaries (Wondratschek & Jeitschko, 1976; Guymont, Gratias, Portier & Fayard, 1976).

A major advantage of the present group approach is that one obtains all the possible boundary operations classified with respect to the number of equivalent sublattices they leave invariant. This includes the case where an interface leaves not only one sublattice but a fraction of the structure invariant (see, for example, the case of rutile), *i.e.* certain substructures which are not reducible to one atom per unit cell. A detailed study of the interfaces leaving a substructure (built up from different types of atoms) invariant is discussed in a following paper (Gratias, Portier & Fayard, 1979).

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