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GENERAL GEOMETRICAL MODELS OF GRAIN BOUNDARIES

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Résumé - A la suite des travaux de Bollmann, de nombreux modèles géométriques ont été proposés pour décrire les joints de grains. Ces modèles ne s'appliquent qu'aux structures symorphiques ne contenant qu'un atome par maille. Les restrictions peuvent être facilement évitées en introduisant quelques concepts élémentaires de cristallographie qui conduisent à une description unifiée des interfaces homophases. La notion d'extrema imposés par la symétrie est discutée pour la relaxation de la translation rigide en relation avec les travaux originaux de G. Kalonji et J.W. Cahn.

Abstract - Geometric models of grain boundaries have been extensively studied following Bollmann's original ideas. These models apply only for symorphic structures with one atom per primitive unit cell. These restrictions may be easily avoided by introducing some elementary concepts of crystallography which lead to an unified description of homophase interfaces. The notion of symmetry dictated extrema is discussed for the relaxation of the rigid body translation in connection with Kalonji and Cahn's original works.

Introduction - Translation boundaries, twins or grain boundaries between identical or enantiohromorphic crystals define a general class of extended defects called homophase interfaces. These defects have been extensively studied in different research fields according to their nature: the translation defects, which are not detectable by diffraction, have essentially been observed in Electron Microscopy by metallurgists whereas twins have been mostly studied by mineralogists. The resulting approaches in the 60's were therefore apparently quite different, the ones using basically the translational symmetry, the other mostly the orientation symmetry. In fact, it is obviously clear that stacking faults or grain boundaries are fundamentally the same kind of interfaces, as far as the geometry is concerned, the only difference being the low crystallographic coherency of the latter with respect to the former.

The major property of all these homophase interfaces resides in the fact that each of the adjacent crystals has an internal symmetry which results in a pseudo periodicity for the interface structure.

Most of the geometric models of grain boundaries derive from the basic notions introduced by W. Bollmann like coincidence site lattice (CSL), O-lattice, Displacement Shift Complete Lattice (DSC) and have been successfully applied in numerous cases for simple structures. A careful analysis of Bollmann's original and subsequent studies shows, however, a serious lack of generality of these kind of models: they apply only for the description of lattices and not of general crystals. Moreover the terminology to day in common use in grain boundary scientific community is often very unfortunate and confuse, for example, lattice nodes and crystal sites.

Two equivalent alternative unified methods have been proposed, these last years, one to G. Kalonji (see for instance [2]), and the other one due to the present authors (see [8]). Some advantages of these approaches are:
i - unification in the geometric description of any homophase interface;
ii - terminology consistent with both crystallography and group theory requirements;
iii - use of all the symmetry properties;
iv - simplification in the understanding of the usual concepts.

In the first part of the present paper, we will briefly recall the basic ingredients of the unified methods and give the definitions of the usual concepts in the scope of group theory. In the second part, we will treat one application - among many others - of the symmetry induced extrema for the relaxation of the rigid body translation.

I - Geometric parameters in homophase interfaces - The first step for describing a grain boundary consists in characterizing which spatial operations relate the two crystals independently of the shape and the location of the boundary.

Formally, this step requires 7 parameters: 3 Euler angles, the chirality factors (if the two crystals are inverse from each other) and the 3 coordinates of the rigid body translation [2].

They define an isometry \((R|\gamma)\) where \(R\) designates the point operation that the initial crystal has to undergo in order to superimpose its lattice to the lattice of the second crystal and \(\gamma\) designates the additional rigid body translation needed for superimposing the homologous sites.

I - Coset of the interface - Any generic point \(x^I\) in crystal I is related to its homologous point \(x^{II}\) in crystal II by:

\[
x^{II} = (R|\gamma)x^I = R x^I + \gamma
\]

If \(G^I\) is the space group of crystal I then the space group \(G^{II}\) of crystal II is isomorphic to \(G^I\):

\[
G^{II} = (R|\gamma) G^I (R|\gamma)^{-1}
\]

The existence of a space group tells us essentially that any generic point \(x\) has a set of equivalent points called the \(G -\) orbit of \(x\). For example the class of equivalence defined in Bollmann's theory is a subset of the \(G -\) orbit: it is the set of all points deduced from \(x\) by the translation subgroup \(T\) of \(G\). In fact, except for certain high symmetry special positions in symmorphic space groups, the class of equivalence does not include the complete \(G -\) orbit and therefore does not reflect the whole symmetry of the crystal. The consequence of the crystal symmetry is that the two crystals are related by an infinite set of equivalent operations: any \((R'|\gamma')\) isometry which relates any point of a \(G^I -\) orbit to any point of the homologous \(G^{II} -\) orbit obviously describes the same misorientation between the two crystals:

\[
(R'|\gamma') \equiv (R|\gamma) \Leftrightarrow \exists g^{II} \in G^{II} ; (R'|\gamma') x^I = g^{II} x^{II}
\]

Using (1) and (2) we easily obtain the set of the equivalent \((R'|\gamma')\) isometries:

\[
(R'|\gamma') = (R|\gamma) G^I
\]

Physically, relation (3) says that the original \((R|\gamma)\) operation may be preceded by any operation of \(G^I\) and followed by any operation of \(G^{II}\):

\[
(R'|\gamma') = G^{II} (R|\gamma) G^I = (R|\gamma) G^I (R|\gamma)^{-1} (R|\gamma) G^I = (R|\gamma) G^I
\]

The set (4) of all equivalent isometries is called the coset of the homophase interface. Let be \(a = (R|\gamma)\) in short notation; the general relations between the two crystals are:

\[
\begin{align*}
& G = a G^I = G^{II} a \\
& G = a G^I = G^{II} a
\end{align*}
\]
I - 2 - Coïncidence lattice $I$ ; Union lattice (or DSC) - Let $H$ be the intersection group :

$$H = \bigcap_{\alpha \in G} G^\alpha = G \bigcap_{\alpha \in G} G^\alpha$$

(7)

$H$ represents the set of all the common symmetry elements of both crystals.

For certain orientations, $H$ has a translational subgroup which defines a 1,2 or 3-dim lattice called the coïncidence lattice $I$ ($I$ for intersection) :

$$I = T \bigcap (R \mid T) \, T \, (R \mid T)^{-1} = T \bigcap R^T$$

(8)

where $T$ is the translation subgroup of $G$.

This coïncidence lattice does not depend on the rigid body translation and is not a coïncidence site lattice : it is an abstract translation subgroup of $T$. For example a pure translation boundary ($R = 1$) has the whole lattice $T$ as coincidence lattice but does not necessarily show any coincidence site lattice.

For the case where the coïncidence lattice $I$ is a 3-dim lattice, its index $\Sigma$ on to $T$ is a finite integer number :

$$\Sigma = \text{index} \,(I \mid T)$$

(9)

and gives the number of times $I$ is includes into $T$. This $\Sigma$ index is sometimes called the "generating function".

Again, $\Sigma$ being of finite order (3-dim coincidence lattice) then the union group (i.e. the group generated by the union) :

$$U = T^I \times T^{II}$$

(10)

is also a discrete 3-dim lattice. A partial order relation exists in the tree $U > (T^I,T^{II}) > I$ and all the groups are invariant into each other. Hence the order tree is a "lattice" (french : treillis). Even if the two initial lattices $T^I$ and $T^{II}$ correspond to different crystalline systems, as in the case for some heterophase interfaces the order tree remains the same : in both direct and reciprocal space representations there is a perfect symmetry between the indices $\Sigma$ and $\Sigma'$ ($\Sigma = \Sigma'$ in homophase interfaces).

Although the union group $U$ is isomorphic to the reciprocal $I^*$ of the intersection group it is still incorrect, for obvious crystallographic reasons, to claim that the $U$ lattice is the reciprocal lattice of the coïncidence lattice.

For practical purposes the determination of the $U$ lattice is quite easy ; its reciprocal $U^*$ is the coincidence lattice of the reciprocal lattices $T^{I\times}$ and $T^{II\times}$, i.e. the lattice defined by the common reflexions of the two crystals. This union lattice is called the DSC lattice. Here again this DSC lattice is an abstract translation group and is by no mean attached to any site.

I - 3 - Coïncidence sites and $G$-lattice - Contrary to the previous $I$ and $U$ lattices the coïncidence sites depend on the rigid body translation $I$. A generic site $x$ is a coïncidence site if it remains invariant through the interface operation. At such invariant sites, the two crystals fit perfectly together. Due to the crystal symmetry the term "invariant" means "invariant inside the $G$-orbit"; Hence a coïncidence site is such that at least one element of the coset $\alpha G$ leaves $x$ invariant. The complete $O^G$ coïncidence site pattern is then :

$$O^G = \{ x \ ; \ \exists \alpha \in G \, , \, \alpha x = x \}$$

(12)
Now it is well known that there are two categories of isometries: those which are translation reducible (inversion, mirrors rotations) and those which are irreducible (glide mirrors, screw rotations). The geometrical locus \( M^\alpha \) defined by:

\[ M^\alpha = \{ x ; \ \alpha x = x \} \]

is called the support of the isometry \( \alpha \). For example if \( \alpha \) is a mirror, \( M^\alpha \) is the mirror plane: if \( \alpha \) is a rotation, \( M^\alpha \) is the rotation axis, ...

A translation irreducible isometry is characterized by the fact that its support is an empty set:

\[ \alpha \text{ irreducible } \iff M^\alpha = \emptyset \]  

So the coincidence site pattern \( O^G \) simply is the set of all the supports of the elements of the coset of the boundary:

\[ O^G = \bigcup_{\alpha \in G} M^\alpha \]

The algebraic calculation of \( O^G \) consists in solving the set of equation:

\[ (R|_g) \ (g|t) = x \]  

where \((g|t)\) runs over all the symmetry operations of the space group (and not only over the translation subgroup as in Bollmann's derivation of the \( \theta \)-lattice formula).

Explicit form of (16) is:

\[ (1 - Rg) \ x = Rt + \tau \]

this equation generalizes the well known Bollmann' equation for the so-called \( \theta \)-lattice.

A point to be outlined here is that equation (17) is very well known in crystallography and is called the irreducibility criterion [3].

I - 4 - Terminology and concept - Usual geometric models of grain boundaries are based on the following concepts:

- CSL, \( \Sigma \) generating function, DSC, \( \Theta \)-lattice
- CSL: the CSL is not a site lattice but an abstract translation group which is the intersection of the translation groups of the two crystals. We propose then to call it the coincidence lattice;
- \( \Sigma \): this integer number reflects the index of the coincidence lattice into the translation lattice of the crystal. It does not take into account the complete symmetry properties since the point symmetry has been disregarded. We propose to replace this index by a more natural one: the index of \( H \) into \( G \), a crystallographic index:

\[ \Gamma = \text{index} \ (H/G) \]

\( \Gamma \) depends, through \( H \), on both orientation and translation between the two crystals. Reduced to the sole orientation symmetry \( \Gamma \) is the so called twin index \( \gamma \) and reduces to the translation symmetry it is the usual \( \Sigma \) index:

\[ \Gamma = \gamma . \Sigma \]

For example, for translation and inversion boundaries or more generally for the case of merohedral twins, the \( \Sigma \) index is equal to 1 whereas the \( \Gamma \) index may vary drastically according to the value of the rigid body translation \( \tau \).
- DSC: originally defined as the lattice generated by the difference (why not the sum ?) of the two lattices it is simply the union of the translation groups of the individual crystals. It may be best defined as the inverse reciprocal of the coincidence lattice of the reciprocal lattices. A point of interest that will be developed in § II-6 is that the DSC is isomorphic to the initial lattice: to any translation of the DSC there corresponds a physically equivalent translation of the crystal. Therefore the use of the DSC, as a support of Burgers vectors of grain boundary dislocations seems us a redundant procedure as far as the geometry is concerned.
O-lattice: the O-lattice is, sensu stricto, a coincidence site lattice. It is a non empty set only if the coset \( \alpha G \) has reducible elements. If it is the case, its lattice nodes are located on the support of these reducible elements. Generally the O-lattice is only a fraction of the coincidence site pattern. We prefer therefore replace the notion of the O-lattice by the more general one of coincidence site pattern.

II - The dichromatic pattern - symmetry dictated extrema -

II - 1 - The dichromatic pattern - Symmetry arguments tell us in which cases two physical situations are identical. So far, the previous concepts have been derived using the fact that any generic point is equivalent to any other point belonging to the same orbit. The next question will now turn around the symmetry dictated constraints on the possible relaxations of the interface parameters. The basic ingredient to be used for describing that kind of problem is the abstract construct called the dichromatic pattern. The dichromatic pattern (d.c.p) is the result of the extension of the two adjacent crystals beyond the boundary. Here too, a complete description of the symmetry properties of the d.c.p. requires the use of the crystal space groups and not only on the lattice. In particular the Pond & Bollmann's description [4] may be applied only for the special case of symmetric space groups with one atom per unit cell.

The symmetry group of the d.c.p. is very easy to derive by the unified methods. In fact two kinds of symmetry elements have to be considered:

i - those which leave both crystals invariant
ii - those which exchange the two crystals

the first have already been found: it is the intersection group \( H \); the second set is obtained by collecting all operations of the coset \( \alpha G \) (which transforms I into II) which also belong to the inverse coset \( G\alpha^{-1} \) (which transforms II into I). The symmetry group \( S \) of the d.c.p. is then:

\[
S = (G \cap \alpha G^{-1}) \cup (\alpha G \cap G^{-1})
\]

(20)

It is easily shown that the product of any two elements belonging to the exchange set \( G \cap \alpha G^{-1} \) is an element of \( H \). In coset representation, \( S \) may be written as:

\[
S = H \cup \varepsilon H
\]

(21)

where \( \varepsilon \) is any one of the element of the exchange set. By this way the practical determination of \( S \) requires the determination of only one element of the exchange set (if not empty).

The symmetry group of the d.c.p. has numerous interesting properties. It tells us essentially which are all the equivalent physical situations of two horophase adjacent crystals. Since there are two kinds of symmetry elements (\( H \) and \( \varepsilon H \)), the \( S \)-group may better be described by a two-color space group (see G. Kalonji [2]). It may as well be understood as the direct product of two groups: the space group \( H \) and the permutation group of 2 elements \( \Pi \):

\[
S = \Pi \times H \equiv H \times \Pi
\]

(22)

This last property may be useful for determining the ways \( S \) acts on different physical properties.

For example Kalonji & Cahn [5] used the \( S \)-action for deriving the possible morphologies of an embedded crystal: assuming planar boundaries with normal \( \eta \) and a given \( (u|v) \) operation they searched for all possible equivalent orientations of the boundary normal. In the group action terminology they derived the \( S \)-orbit of \( \eta \): the representation space is the normal space. Any element of \( H \) acts on this space through its sole point operation:

\[
(h|t) \ \eta \equiv h\eta
\]

(23)

Now the \( \Pi \) action on \( \eta \) either leaves \( \eta \) invariant (identity permutation) or transforms \( \eta \) into its inverse (the permutation of crystals I and II inverses the boundary normal):

\[
(h|t) \ \eta \equiv h\eta
\]
Therefore the S-action on the normal space is isomorphic to the point group W:

\[ W = h \cup (Ih) \]

where \( h \) designates the point group of the space group H.

The point group W has been recognized as the symmetry group of the Wulff plot of the interfacial energy by Kalonji & Cahn [5] from which they inferred the symmetry dictated extrema and the morphologies of the embedded crystal.

Another very parallel application of use of the symmetry group of the dichromatic pattern consists in searching for the symmetry dictated extremum with respect to relaxations of the rigid body translation.

II - 2 - Special point and symmetry dictated extrema - Most problem in physics can be solved through variational principles: once a certain energy functional, depending on a set of physical parameters, has been defined, a possible stationary state of the system is obtained by minimizing the energy functional with respect to the involved physical parameters. In many cases the minimization is such a difficult task that it is often more convenient to extract first among all the possible values of the physical parameters, those which certainly lead to an extremum of the energy functional. Assuming that the energy functional is a scalar function \( E(x) \) of \( \mathbb{R}^3 \), where \( x \) designates a vector the components of which are the independent physical parameters, it is well known that the gradient \( \nabla_x E(x) \) has the same little group as the considered point \( x_0 \):

\[
G(x_0) = \{ g \in \mathbb{O} \mid g x_0 = x_0 \} \tag{26}
\]

\[
G(\nabla_x E(x)) = \{ g \in \mathbb{O} \mid g \nabla_x E(x) = \nabla_x E(x) \} \equiv G(x_0) \tag{27}
\]

Now we can define the support of \( G(x_0) \), \( M^G(x_0) \), as the geometrical locus in the configurational vector space \( \{x\} \) of all the points \( x \) which are invariant by all the symmetry elements of \( G(x_0) \):

\[
M^G(x_0) = \{ x \mid \forall g \in G(x_0), gx = x \} \tag{28}
\]

If \( M^G(x_0) \) has dimension zero there are no finite non zero vectors that can exist at \( M^G(x_0) \). Therefore from (28), the gradient must vanish. The point \( x_0 \), the supports of the little groups of which have dim zero, are called the special points. In other terms, the energy functional has a maximum, a saddle point or a minimum at the special points.

II - 3 - Isotropic interfacial energy functional - Consider a bicrystal where one of the two crystals is totally embedded in the other and shows a perfect spherical shape. Once the radius of this homophase precipitate is sufficiently large, the interfacial energy per surface unit depends only on the orientation translation of the crystals; we call it the isotropic interfacial energy. For a given fixed orientation this energy depends on the three remaining variables \( \tau_x, \tau_y, \tau_z \) that we designate from now by \( x, y, z \). The problem we have to solve is to find the symmetry group \( \mathbb{O} \) for \( E(x,y,z) \) in this 3-dim configurational space.

First it is easily shown that, for a fixed matrix, say crystal I, the set of the equivalent boundary's cosets is \( G \alpha G \). If \( \gamma \) belongs to the symmetry group, the new coset generated by \( \alpha(\gamma) = (\alpha | \gamma) \) is such that, either:

\[
\alpha(\gamma) G \subset G \alpha G \quad (I \rightarrow II) \tag{29}
\]

or:

\[
G \alpha(\gamma)^{-1} \subset G \alpha G \quad (II \rightarrow I) \tag{30}
\]

In full notations, relation (29) leads to:

\[
(\alpha | \gamma) = (g | t) (\alpha | \gamma') (g' | t') \tag{31}
\]
and then $\gamma = (|h|t + h|t')$ (32)

where $h$ designates the elements of the intersection group of the point groups of the crystals. Relation (30) leads to:

$$ (\alpha^{-1} | -\alpha^{-1} \gamma' T) = (|g|t) (\alpha|T) (g'|t') $$

or:

$$ \gamma = (T_{\varepsilon} | -\Delta \varepsilon - \varepsilon x t') $$

(34)

where $\varepsilon$ designate the elements of intersection of the point exchange coset $(ag \cap gb^{-1})$. Relations (32) and (34) define the generators of the searched symmetry group.

In particular the translation group of $G$ is the DSC lattice:

Suppose that a $\gamma$ operation has been found from (32). We may replace in (31) the operators $(|g|t)$ and $(g'|t')$ by respectively $(|g|t + T)$ and $(g'|t' + T')$ where $T$ and $T'$ are any translations of crystal I. The new $\gamma'$ operation is:

$$ \gamma' = (|h|t + T + h|t' + hoT') $$

(35)

Since $h$ is an element of the intersection point group, $h|t' + hoT'$ is a translation of crystal II and therefore $\gamma'$ may be written as:

$$ \gamma' = (1|T + T') $$

(36)

A similar demonstration holds for the $\gamma$ elements issued from (34): the union translation group (DSC) belongs then to $G$.

II - 4 - The special points of the isotropic interfacial energy functional - Formally the special points are totally determined once the symmetry group $G$ has been found. However they may be found independently from in a straightforward way.

Consider a given $\tau$ point in the configurational space; we know that $\tau$ is a special point if:

$$ \dim H(G) = 0 \text{ with } G(\tau) = \{ \gamma \in G ; \gamma \tau = \tau \} $$

(37)

Using relations (32) and (34) it turns out, after a few algebraic manipulations, that the little group of $G(\tau)$, $(\tau)$, is isomorphic to the Wulff plot point group:

$$ G(\tau) \equiv H(\tau) \cup I_{\varepsilon}(\tau) h(\tau) $$

(38)

where $h(\tau)$ and $\varepsilon(\tau)$ $h(\tau)$ designate the point symmetries of the intersection space group $H(\tau)$ and exchange coset $\varepsilon(\tau) H(\tau)$. Obviously any change in the rigid body translation $\tau$ modifies $H(\tau)$ and $\varepsilon(\tau) H(\tau)$ and therefore the corresponding little group in the configurational space. The physical significance of $G(\tau)$ is clearly shown from (38). Suppose we add a new translation $\Delta \tau$ to a given chosen $\tau$. The dichromatic pattern having the symmetry $S(\tau)$ it is equivalent, instead of $\Delta \tau$, to add any transformed of $\Delta \tau$ by $H(\tau)$. Since $\Delta \tau$ is a free vector the $H(\tau)$ action on $\Delta \tau$ simply reduces to its point operation:

$$ H(\tau) \Delta \tau \equiv h(\tau) \Delta \tau $$

(39)

If we now apply any exchange element the new additional displacement transforms into $\varepsilon(\tau) H(\tau) \Delta \tau = \varepsilon(\tau) h(\tau) \Delta \tau$ but of the crystal I with respect to the crystal II. Therefore the equivalent translation of II with respect to I is $-\varepsilon(\tau) h(\tau) \Delta \tau$.

Hence, the complete orbit of equivalent additional $\Delta \tau$ translations starting from a given $\tau$ one is described by $W(\tau)$. In other terms, the little group $(\tau)$ gives us all the equivalent ways of relaxing a certain $\tau$ rigid body translation for a perfect isotropic homophase precipitate. If we now allow the precipitate to have non spherical shape, $W(\tau)$ tell us which kind of morphologies may appear : $W(\tau)$ is the minimal macroscopical symmetry of the precipitate (see J.W. Cahn [6]).

For the practical use an easy way for deciding if a $\tau$ translation is or not a special point consists in searching for the sole $h(\tau)$ point group. In fact it may be demonstrated that (§ II-6):

$$ \widehat{W}(\tau) \equiv H(h(\tau)) $$

(40)

so that $\tau$ is a special point if and only if $h(\tau)$ has a support of dimension zero.

Now since $h(\tau)$ is a subgroup of the little group of $\tau$, $h(\tau)$ is a subgroup of the symmetry class $W_0$ of $G$:
where \( h \) and \( \& h \) defined in (32) and (34) are independent of \( \tau \). Therefore \( h(x) \) may have a support of dimension zero only if the orientation of the two crystals leads to an intersection point group \( W \) the support of which has dimension zero. The practical procedure for determining the symmetry induced extrema of the rigid body translation is the following:

1. determine the intersection \( W_0 \) of the point groups of the crystals; there can be special points only if \( \text{dim} M_{W_0} = 0 \);
2. list all subgroups of \( W_0 \) which also have a support of dimension zero;
3. search for which translations \( \tau \) these subgroups may be little group of \( \tau \).

\[ \theta = 2 \tan^{-1} \frac{\sqrt{3} (n-p)}{n+p} \]

around the origin at \( 3\text{m} \) (\( \theta \) superimposes the lattice node \((n,p)\) to the lattice node \((p,n)\)). Find the symmetry dictated extrema for:

1. except for \( n = 2, p = 1 \) (\( \theta = \Pi/3 \)) \( W_0 = 3 \) of support zero in 2-dim space
2. only one subgroup \( W_0 = 3 \) with dimension zero
3. \( \tau \) is any translation which superimposes a 3 fold axis to another 3 fold axis.

Representatives of these special orbits are:

\( \tau = 0,0 \) and \( \tau = \frac{1}{3}, \frac{2}{3} \)

(expressed as well on \( T^{I}, T^{II}, \text{DSC or C.L. unit cells} \))

for \( \tau = 0,0 \) \( W(\tau) = 3 \text{m} \); \( \tau = \frac{1}{3}, \frac{2}{3} \) \( W(\tau) = 3 \)

Another simple example is the case of translation boundaries (\( T^{I} = T^{II} = \text{DSC} = \text{C.L.} \)) of centered crystals.

The inversion is always present into the exchange set \( eH(\tau) \) such that \( 1 \text{cH}(\tau) \) confuses with \( H(\tau) \) itself (see Kalonji [2]). Table 1 gives the little groups \( W(\tau) \) for any translation of the \( \text{P3m} \) crystal structure. It is interesting to notice here that the fault vector compatible with an inclusion of symmetry 43m is \( \frac{1}{3} \frac{1}{3} \frac{1}{3} \) and not \( \frac{1}{2} \frac{1}{2} \frac{1}{2} \) as it is usually assumed for stacking fault tetrahedra in F.C.C. metals [7].

<table>
<thead>
<tr>
<th>( \tau )</th>
<th>( W(\tau) )</th>
<th>( \text{dim} M_{W(\tau)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x,y,z )</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>( x,y,y )</td>
<td>m</td>
<td>2</td>
</tr>
<tr>
<td>( o,y,z )</td>
<td>m</td>
<td>2</td>
</tr>
<tr>
<td>( \frac{1}{2},y,y )</td>
<td>mm2</td>
<td>1</td>
</tr>
<tr>
<td>( o,y,y )</td>
<td>mm2</td>
<td>1</td>
</tr>
<tr>
<td>( x,x,x )</td>
<td>3m</td>
<td>1</td>
</tr>
<tr>
<td>( x,o,o )</td>
<td>4mm</td>
<td>1</td>
</tr>
<tr>
<td>( \frac{1}{2},x,0 )</td>
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<td>0</td>
</tr>
<tr>
<td>( \frac{1}{2},1,1 )</td>
<td>43m</td>
<td>0</td>
</tr>
<tr>
<td>( \frac{1}{2},0,0 )</td>
<td>m3m</td>
<td>0</td>
</tr>
<tr>
<td>( 0,0,0 )</td>
<td>m3m</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 1: little groups of the isotropic Interfacial Energy for translation boundary in F.C.C. \( \text{Pn3m} \) crystals. The symmetry dictated extrema occur at \( \frac{1}{3} \frac{1}{3} \) (morphology mm), \( \frac{1}{3} \frac{1}{3} \frac{1}{3} \) (morphology 43m) and \( \frac{1}{2} \frac{1}{2} \frac{1}{2} \) (morphology m3m). This table has been derived from G. Kalonji Ph. D. Thesis Table IV [2].
II - 6 - The particular case of symmorphic structures (*) - The procedure is very simple for symmorphic space groups where the sole translation parts are the lattice translations (\(t = T\)). From (32) and (34) the symmetry group of the isotropic interfacial energy is immediately obtained:

\[
\mathcal{G} = \mathcal{W}_0 \times \mathcal{U} = (\mathcal{W}_0 \cup \mathcal{I}_{\text{ch}_0}) \times \mathcal{U}
\]  

(41)

It is the symmorphic space group resulting in the direct product of the Union Lattice DSC with the point group of the orientation Wulff plot. We can choose the origin of the \(x, y, z\) configurational space (\(t = 0\)) on a point of the high symmetry orbit defined by little group \(\mathcal{W}_0\) (being symmorphic such points exist). All other points of this orbit are deduced from each others by a DSC translation. As we already pointed out all these translations lead to an identical pattern. But using the fact that the DSC is a supergroup of \(\mathcal{N}, \mathcal{N}^2\) and \(\mathcal{I}\), we obtain the result that the translation of the second crystal by a vector belonging to the DSC is perfectly equivalent to a translation of the second crystal itself or of the first crystal or of the coincidence lattice. In particular a secondary dislocation defined by a translation of either the first or the second crystals. From the sole geometric considerations, there are no need of the DSC lattice for defining secondary dislocations.

This complete equivalence between the DSC and the crystal lattice has further applications.

Let be \(\mathcal{I}_{\text{ch}_0}\) the intersection point group of the crystals point groups: \(\mathcal{I}_{\text{ch}_0}\) is a subgroup of \(\mathcal{W}_0\). Let be \(\mathcal{X}\) the space group

\[
\mathcal{X} = \mathcal{H}_0 \times \mathcal{U}
\]  

(42)

- all special points of \(\mathcal{G}\) are special points of \(\mathcal{X}\) (the inverse is obvious): any special point of \(\mathcal{G}\) has a little group \(\mathcal{W}\) which is a subgroup of \(\mathcal{H}_0 \cup \mathcal{I}_{\text{ch}_0}\) and which may be written as:

\[
\mathcal{W} = \mathcal{H} \cup \mathcal{I}_{\text{ch}_0}
\]  

(43)

where \(\mathcal{H}\) is a subgroup of \(\mathcal{H}_0\) (from (38)); the same point in \(\mathcal{X}\) has little group \(\mathcal{H}\). \(\mathcal{W}\) is therefore a supergroup of \(\mathcal{H}\) and then:

\[
\mathcal{M}^\mathcal{W} \subset \mathcal{M}^\mathcal{H}
\]  

(44)

but from (43)

\[
\mathcal{M}^\mathcal{W} = \mathcal{M}^\mathcal{H} \cap \mathcal{I}_{\text{ch}_0}
\]  

(45)

Now take a point \(x \in \mathcal{I}_{\text{ch}_0}\)

\[
\forall \epsilon \in \mathcal{I}_{\text{ch}_0}, \quad \mathcal{I}_{\text{ch}_0}x = x
\]  

(46)

or:

\[
chx = -x
\]  

(47)

a further application of any element of the coset leads to:

\[
\mathcal{I}_{\text{ch}}x' - (\mathcal{I}_{\text{ch}}x) = -x
\]  

(48)

then

\[
ch x' = x
\]  

(49)

but \(ch x'\) is an element of \(\mathcal{H}\) and any element of \(\mathcal{H}\) may be written as such product therefore \(x \in \mathcal{M}^\mathcal{H}\) and:

\[
\mathcal{M}^\mathcal{I}_{\text{ch}_0} = \mathcal{M}^\mathcal{H} \Rightarrow \mathcal{M}^\mathcal{W} = \mathcal{M}^\mathcal{H}
\]  

(50)

This achieves the demonstration of i.

\[\text{ii - Consider the space group :}\]

\[
\mathcal{X}' = \mathcal{H}_0 \times \mathcal{N}
\]  

(51)

\[\text{Although we have not been able to derive these properties for the general case it is plausible that they also partially hold.}\]
Since \( h \) is a subgroup of the symmetry class of \( G \), \( \chi' \) is a subgroup of \( G \). Also since \( O_1 \) is a subgroup of \( U \), \( \chi' \) is a subgroup of \( G \). Moreover there is an isomorphism between \( G \) and the special points of \( G \) which themselves are special points of \( G \).

We obtain finally the following amazingly simple result:

For symmorphic structures the symmetry dictated extremal of the isotropic interfacial energy with respect to the rigid body translation are obtained for translations which correspond to certain special points of the structure. This result is independent of the relative orientations of the two crystals as far as they lead to a coincidence lattice. The physical significance of this property is that a rigid body translation corresponding to a special point of coordinates \( x_0, y_0, z_0 \) expressed in the DSC unit cell is equivalent to a rigid body translation with the same coordinates expressed in either crystal I and II unit cells. It easily shown that this result also holds for the coincidence lattice unit cell.

For practical purposes we can see from (51) that the only requirement for determining the symmetry dictated extremal of the isotropic interfacial energy is the determination of \( h_0 \). Therefore, regardless of the relative orientation of the crystals, there will be only a few number of possible \( h_0 \) point groups. Also all point orientations leading to the same \( h_0 \) intersection will generate isosymbolic homologous symmetry groups (and identical special points).

These results hold partially for the case of non symmorphic space groups. Any space group \( G \) has a largest symmorphic subgroup \( G_0 \) (which sometimes reduces to \( P1 \)). The preceding demonstration holds for this \( G_0 \) subgroup, the special points of which are also special points of \( G \). The main difference here is that they may be other extrema which are not special points of \( G \) since the crystal symmetry has been arbitrarily reduced from \( G \) to \( G_0 \).

References: