

ON GROUPOIDS IN CRYSTALLOGRAPHY

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Introduction

The theory of groups has been the mathematical background of all the well-established parts of symmetry theory in crystallography. This is valid not only for the classical symmetry consideration in 3-dimensional space. It holds, however, for such well-known generalizations as symmetry in spaces of higher dimensions, black and white symmetry, colour symmetry.

The aim of this paper is to show that there are serious reasons to introduce other algebraic notions into crystallographic symmetry theory

The classical symmetry of a crystal structure is given by the coincidence operations of this structure. The set of motions which bring the crystal structure into coincidence with itself constitutes a group, the symmetry group of the crystal structure. In addition to the classical (total) symmetry operations, there may exist partial symmetry operations: motions which bring only a part of the crystal structure into coincidence with itself or with another part of the crystal structure.

In order to illustrate this, a very simple example will be given. For the fictitious molecule of Fig.1, the regularity of the distribution of atoms is only partly reflected by the symmetry group. Obviously, the molecule consists of two parts, and three kinds of coincidence operations may be considered:

1. Total symmetry operations transforming the whole molecule into itself, e.g. the inversion in the centre of gravity of the molecule.
2. Local symmetry operations transforming one of the two parts into itself, e.g. 3-fold rotations.
3. Partial coincidence operations transforming one of the parts into the other one, e.g. a rotation by an angle of 60 degrees.

The term "symmetry operations" of an object is used for the (total) coincidence operations. Accordingly, for a partial coincidence operation, the term partial symmetry operation is used. This notion refers to the coincidence operations of the second and third type, although

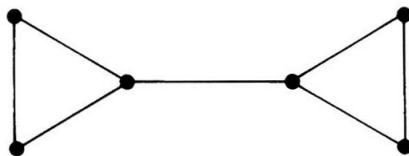


Fig. 1 A fictitious molecule consisting of two parts

it is sometimes avoided to use the word "symmetry" in connection with operations of the third type.

Partial symmetry operations have been considered in crystallography for different reasons. The main part of this paper is concerned with the OD theory of Dornberger-Schiff for polytypic structures. In this theory, the notion of a groupoid has been successfully used for more than 20 years. Moreover, some other examples are given, where partial symmetries play an important role, and the notion of a groupoid seems to be adequate. In an appendix, rigorous mathematical definitions are given.

Polytypic structures. The OD theory of Dornberger-Schiff

The OD theory of Dornberger-Schiff (see /4,6,7/) deals with polytypic structures, i.e. structures consisting of layers periodic in two dimensions. The layers may be stacked in different ways. Ordered as well as disordered structures may result from the different kinds of stacking. Often the OD theory has been mis-understood as a theory restricted to disordered structures. Nevertheless, for a substance having an OD structure there may exist many different arrangements periodic in three dimensions. In this way OD theory is closely related to traditional crystallography.

The OD theory explains the phenomenon of polytypism by the presence of partial symmetry operations and uses these partial symmetry operations as a powerful tool in solving such structures.

To illustrate an OD structure, let us regard the most typical polytypic structure, silicon carbide. In SiC any layer of the structure consists of the close packed layer of C-atoms with one Si-atom below each C-atom at a distance of 1.89 Å. (see Fig.2). If one layer, say I_0 is fixed, then the atoms of the next layer may occupy one of the two possible positions. Any layer is transformed into the next one by a translation either to the left or to the right. The symmetry relations of neighbouring layers may be seen in Fig.3. Any layer has the

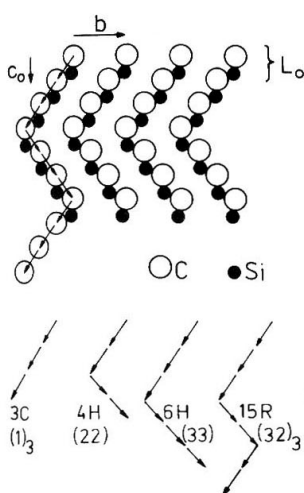


Fig. 2 Stacking possibilities in SiC

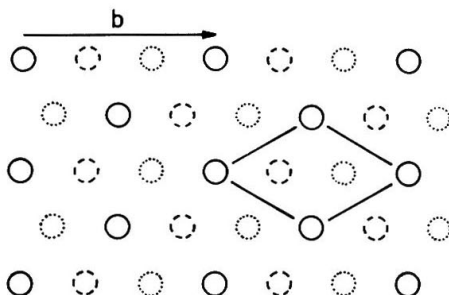


Fig. 3 Possible positions of neighboring layers in SiC. The thick circles represent the atoms of the layer L_0 . The atoms of the layer L_1 are either in the positions of the broken or of the dotted circles.

symmetry $P(6)mm$. The threefold axes and one of the two mirror planes are common to all layers. But the other mirror plane is valid only for one particular layer. It is a partial symmetry operation. This partial reflection transforms the two possible positions of L_1 into each other. Thus the existence of the partial reflection may be considered as the reason for the fact that the position of the next layer is not uniquely determined.

More than 100 different ordered SiC polytypes have been described so far (see /24/). Polycrystalline samples investigated in our institute contained mainly the polytypes 3C, 4H, 6H, and 15R (see Fig.2), but in addition to these ordered polytypes about 20 per cent thoroughly disordered SiC.

The description of the symmetry of any SiC polytype may be split into two parts. One part describes the stacking of the layers. Different notations to characterize the stacking have been developed. Hägg's notation describes the two stacking possibilities by + and - , so that for instance 6H is characterized by +++--- or shorter in the Zhdanov

symbol by (33), (see /23/). The second part describes the symmetry data common to all SiC polytypes. This second part is formed by the layer group, the net constants, and the possible translational vectors leading from one layer to the next one. An appropriate description of any polytypic substance will be discussed later.

SiC is the classic example of a polytypic substance. Other polytypic substances as for instance ZnS or CdI_2 may also be described as consisting of close packed layers. An increasing number of other polytypic substances with completely different symmetry relations has been studied. Examples may be found among layer silicates, framework silicates, oxalates as well as among organic substances as polymethins and biologically important substances (compare /8,16/).

Generally speaking, the phenomenon of polytypism is connected with two conditions:

1. Energetical condition

The influence of next but one layers on the position of a layer may be neglected.

2. Geometrical condition

There are two or more geometrically equivalent ways in which neighboring layers may be arranged with respect to one another.

Let us consider the geometrical condition in more detail. We suppose that a layer of the structure is fixed, say L_0 . Let L_1 and L_1' be two possible positions of the first layer. Then the geometrical condition means that there is a motion transforming the pair (L_0, L_1) into the pair of layers (L_0, L_1') . This transformation of layers may be performed by one of the following possibilities.

$$(1) \quad \begin{array}{l} L_0 \longrightarrow L_0 \\ L_1 \longrightarrow L_1' \end{array} \quad (11) \quad \begin{array}{l} L_1 \longleftrightarrow L_0 \\ L_0 \longrightarrow L_1' \end{array}$$

In either case, there exist partial symmetry operations. In the first case, there is a motion transforming L_0 into itself, but this motion is not a coincidence operation of the layer L_1 . In the second case L_1 is transformed into L_0 , but this motion transforms L_0 into a new position of the first layer.

Let us consider two different layers of the same kind, say L_i, L_j . For a polytypic structure, it is a reasonable condition that the relative position of the layer L_i to its adjacent layers is the same as the relative position of the layer L_j to its adjacent layers.

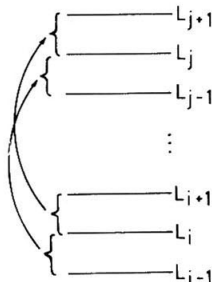


Fig. 4a

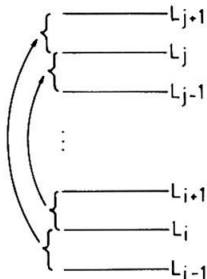


Fig. 4b

In detail: L_i is of the same kind as L_j means that there is a coincidence operation transforming L_i into L_j . Let us suppose (Fig. 4a) that the upper side of L_i is transformed into the upper side of L_j . Then there exists a motion that brings the pair (L_{i-1}, L_i) into coincidence with (L_{j-1}, L_j) . Moreover, there exists a motion that brings the pair (L_i, L_{i+1}) into the pair (L_j, L_{j+1}) . If on the other hand, a partial symmetry operation from L_i into L_j transforms the upper side of L_i into the lower side of L_j (Fig. 4b), then there exist motions which transform (L_{i-1}, L_i) into (L_j, L_{j+1}) and (L_i, L_{i+1}) into (L_{j-1}, L_j) , respectively. From these considerations we may draw the following conclusion.

- For a polytypic structure, always (strictly) partial symmetry operations exist.
- The phenomenon of polytypism may be understood on the basis of partial symmetry operations.

Polytypic structures as discussed so far are OD structures in the sense of Dornberger-Schiff. They are defined as follows.

An OD structure consists of an infinite number of layers stacked one onto another. All the layers are the same kind. Further we suppose that the layers are numbered according to the stacking. The following conditions are fulfilled:

- (i) The layers are periodic in two different directions. Any translation of a particular layer is a translation of the whole structure
- (ii) Let L_i, L_j be two layers of the structure. Then the pairs of adjacent layers (L_{i-1}, L_i) , (L_i, L_{i+1}) are of the same kind(s) as the pairs of adjacent layers (L_{j-1}, L_j) , (L_j, L_{j+1}) .

Remarks: (1) The notion OD structure may be generalized. The building units may be periodic only in one direction. That means, they are rods. Further the structure may be built of different kinds of building units. Layer silicates, for instance, are known as being built of two or three kinds of layers.

(2) The condition (i) can be weakened supposing that all layers have a common set of translational vectors into two direction. Any layer, however, may have additional translations.

The symmetry of an OD structure may be characterized by the set of all partial coincidence operations transforming the layers into one another. This set of partial coincidence operations does not form a group. A more general notion is necessary. In mathematics there are several appropriate notions:

Groupoid	(Brandt /2/, Ehresmann /10/)
Mischgruppe	(Loewy /17/)
Category with invertible morphisms	(Eilenberg, MacLane /11/, compare /22/)
Inverse semigroup	(Preston, Clifford /3/)
Inductive groupoid	(Ehresmann /10/)

From the mathematical point of view, these notions are equivalent or closely related. The definition used here is a mixture between the notions "groupoid" and "category". From the content it is the same as a groupoid, but the language used is taken mainly from category theory. It seems that this definition is the most appropriate one for the application to polytypic structures.

A groupoid \underline{G} consists of

- (i) $\text{ob } \underline{G}$, the set of objects of \underline{G}
(object: building unit of the crystal structure, e.g. layer)
- (ii) $[i, j]$, $i, j \in \text{ob } \underline{G}$, sets of morphisms leading from the object i to the object j .
(morphism: partial coincidence operation)
- (iii) a partial composition of morphisms. The morphisms $g_1 \in [i_1, j_1]$ and $g_2 \in [i_2, j_2]$ may be composed then and only then, if $j_1 = i_2$. The product $g_2 g_1$ belongs to $[i_1, j_2]$
(The composition is the usual composition of mappings)

For these data the following axioms have to be fulfilled

- (1) Existence of identical morphisms

For any $i \in \text{ob } \underline{G}$ there is an $1_i \in [i, i]$ with

$1_i \cdot f = f$, $g \cdot 1_i = g$,
whenever the left sides are defined.
(1_i : identical map of the object i)

(2) Existence of inverse morphisms

For any $g \in [i, j]$ there is a $g^{-1} \in [j, i]$, and

$$g g^{-1} = 1_j \quad g^{-1} g = 1_i$$

(As the partial symmetry operations are 1:1 mappings, the inverse mapping is again a partial symmetry operation).

(3) Associative law

$$g_3(g_2 g_1) = (g_3 g_2) g_1$$

if the products are defined

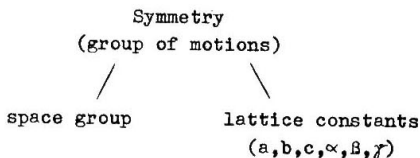
(For mappings, the associative law is always fulfilled)

Obviously, the set of all partial symmetry operations transforming the layers of an OD structure into each other forms a groupoid.

In the following we shall consider two problems: How to describe the symmetry of an OD structure? How to classify OD structures?

Description of the symmetry of an OD structure

We know that this symmetry may be described by a groupoid. But this groupoid is infinite and it is necessary to characterize it by a finite number of data. For comparison, let us consider the classical case of normal crystal structures. The symmetry of a crystal structure is fully described by the group of coincidence operations. This group is also infinite and has to be described by a finite data set. The data commonly used are the space group and the lattice constants.

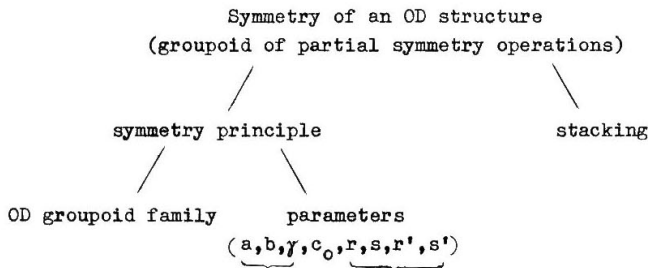


Now let us return to OD structures. For the example of SiC, we have seen that the stacking may be separated. The idea of stacking is, which of the possible positions of a layer is really occupied. The first notation for the stacking have been developed for SiC and may be used for quite a number of other polytypic substances. More general symbols have been

developed by Zvyagin /27/ for layer silicates. General rules for the construction of polytype symbols are the result of discussions between Dornberger-Schiff, Đurovič and Zvyagin and have been submitted to Acta Cryst.

With the stacking, a great part of infinity of the groupoid is separated. Here we will deal only with the remaining part. This part has been named symmetry principle, because it describes the features common to all structures of a polytypic substance, ordered as well as disordered structures. To this second part belongs the symmetry of a single layer. It may be described by the layer group and the net constants. Over this, to the second part belong all partial symmetry operations transforming adjacent layers one into another. Any partial symmetry operation may be split into a homogeneous part and into parameters describing the translational part.

The notion OD groupoid family covers the layer group and the homogeneous parts of the partial symmetry operations transforming different layers one into another. Thus, the symmetry principle consists of two parts, OD groupoid family and parameters as shown in the scheme:



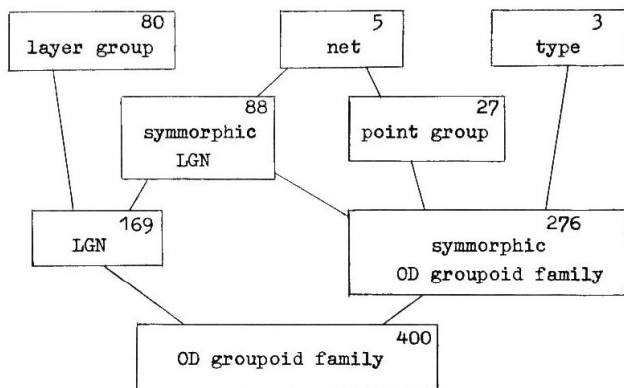
The notion OD groupoid family may be compared with the notion space group. As in the case of space groups, the number of OD groupoid families is also finite. Two problems arise immediately: how many essentially different OD groupoid families exist? How to characterize them by symbols? We will return to these problems after a more detailed discussion of the classification of OD groupoids.

Classification of OD groupoids

In order to have a reasonable classification, we have to arrange within a class all those groupoids which do not differ with respect to certain

features. The classifications of OD groupoids partly correspond to the classifications of normal crystallographic groups. In addition, there are classifications resulting from the fact that we have not the symmetry relations of a single object, but the symmetry relations of a set of objects.

The most simple classification considers the number of kinds of objects. In the language of category theory: how many connectivity components exist in the groupoid. In the following we refer only to OD structures of one kind of layers. Then we have the following hierarchy of notions:



Every OD groupoid is associated with one of the 80 layer groups. The net of an OD groupoid is determined not only by the layer group, but also by the restrictions following from the partial symmetry operations transforming different layers one into another.

For an OD structure consisting of one kind of layers, there are three cases how neighbouring layers may be transformed into each other. Accordingly, three types of OD groupoids exist (Fig.5). In the first case the layers are apolar. Hence, there are transformations bringing the upper side of L_0 into the upper side of L_1 as well as transformations bringing the upper side of L_0 into the lower side of L_1 . In the second and third cases the layers are polar. In the second case there is a transformation bringing the upper side of L_0 into the upper side of L_1 , but there is no coincidence operation bringing the upper side of L_0 into the lower side of L_1 . In the third case we have coincidence operations bringing the upper side of L_0 into the lower side of L_1 , but no coincidence operation brings the upper side of L_0 into the upper side of L_1 .

Remark: Instead of the notion type, in other papers (e.g. /6,9/), the notion category is used.

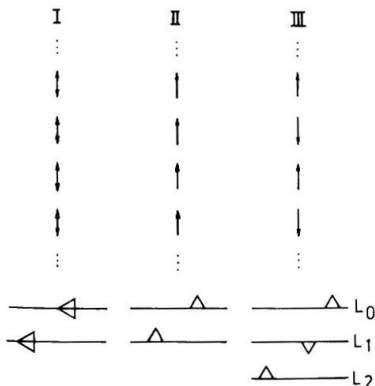


Fig. 5 The three types of OD structures

For any OD groupoid there is a point group. It is the group generated by the homogeneous parts of all partial symmetry operations of the groupoid. It is easy to see that there occur all non-cubic point groups.

The notion OD groupoid family has already been introduced. It is that part of an OD groupoid which remains if we abstract from the stacking and from the parameters. An exact mathematical definition of the notion OD groupoid family has been developed on the basis of category theory (see /13/).

The other notions in the scheme are of interest only in connection with the derivation of a complete list of OD groupoid families.

Dornberger-Schiff and Grell-Niemann /9/ reported on a first list of OD groupoid families in 1961. On the basis of mainly geometrical considerations they obtained 333 OD groupoid families. A second list /6/ published by Dornberger-Schiff in 1964 contained 339 OD groupoid families, but was still incomplete. In order to obtain a complete list and to avoid errors, I have generated a new list with an algebraically based method and by means of a computer (compare /12,14/). The method consists of three steps. In the first step the possible combinations of net and layer group have been derived. This combination of layer group and net

has been indicated by the three letters LGN. Then in a second step, for OD groupoid families the symmmorphic layer groups have been calculated. This is the most complicated step. In a last step the list was extended to all layer groups.

The new list contains 400 OD groupoid families. This number may be reduced, if those OD groupoid families are excluded, for which the position of a layer is uniquely determined with respect to the preceeding layer. Among the remaining OD groupoid families there are 14 enantio-morphic pairs, so that the number may be further reduced to 363.

Symbols for the OD groupoid families have been developed in the late fifties by Dornberger-Schiff (compare /6,7,15/). The symbols give in the first line the layer group and in the second line all possible transformations from a layer to an adjacent layer. For the example of Fig.6 the symbol is

$$P \quad m \quad m \quad (n)$$

$$\left\{ \begin{array}{cc} \frac{2_{1,25}}{n_{0,5,2}} & \frac{2_{1,5}}{n_{2,0,25}} \quad \left(\frac{2_2}{n_{1,25,1,5}} \right) \end{array} \right\}$$

In many cases these full symbols are rather complicated. Therefore, in /15/ short symbols have been proposed. In these short symbols only one of the possible transformations from layer to layer is given. In our example the layers are translationally equivalent. Therefore, the symbol may be given as

$$P \ m \ m \ (n) \mid 1, \ r=0.125, \ s=0.25$$

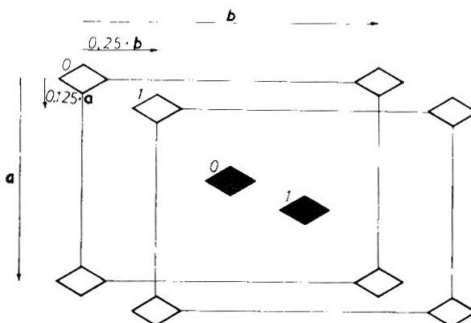


Fig. 6 Schematic example of an OD groupoid with translationally equivalent layers.

Diffraction enhancement of symmetry due to partial symmetry

Whereas the basic idea of OD theory is to express the features common to a whole set of polytypes, partial symmetries may be of importance, if we consider only one particular crystal structure. It is supposed to be periodic in three dimensions. Therefore, a space group for the characterization of symmetry exists. But in addition to the total symmetries partial symmetries are present, and they may influence the symmetry of physical properties of a structure. The notion "Diffraction enhancement of symmetry", introduced in /21/, has been used for the following phenomenon. The symmetry of the diffraction pattern of a crystal is higher than expected from the point group symmetry of the crystal and Friedel's law. A number of Japanese crystallographers has theoretically dealt with this problem (compare /20/). Although rather complicated theoretical examples may be constructed, the actually known examples are among polytypes of SiC, ZnS, mica etc. In these examples the diffraction enhancement of symmetry may be understood as a result of the existing partial symmetries. The OD theory provides a very good tool to understand the phenomenon.

As an example, let us take the polytype 10H of SiC (see /19/). This polytype is trigonal (space group $P\bar{3}m1$), but the diffraction symmetry is strictly hexagonal (point group $6/mmm$). This may be understood as a result of partial symmetries. The single layer has the symmetry $P(6)mm$. For any stacking, the 3-fold axes and the mirror plane perpendicular to the main axes are total. From Friedel's law it follows that the diffraction symmetry is at least $\bar{3}m1$. Enhancement of the symmetry of the dif-

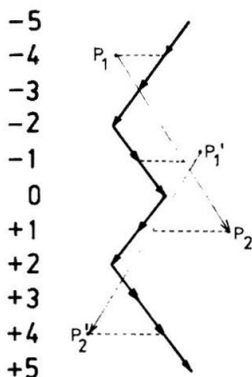


Fig. 7 Stacking sequence in the polytype 10H. The structure is strictly trigonal, but the symmetry of the diffraction pattern is $6/mmm$. The vector $\vec{P_1P_2}$ is transformed into $\vec{P_1'P_2'}$ by a twofold (screw) rotation.

$$P_1: (x_1, y_1, z_1)(n)$$

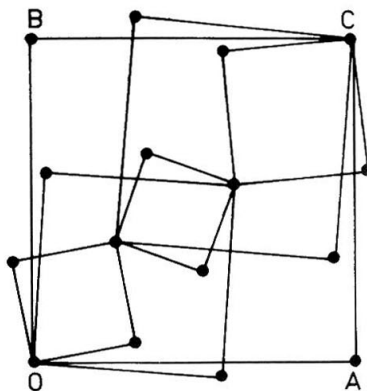
$$P_2: (x_2, y_2, z_2)(m)$$

$$P_1': (\bar{x}_1, \bar{y}_1, \bar{z}_1)(\bar{m})$$

$$P_2': (\bar{x}_2, \bar{y}_2, \bar{z}_2)(\bar{n})$$

fraction pattern to $6/mmm$ occurs for all polytypes, for which the stacking sequence is symmetric as for $10H$.

Fig. 8 Theoretical example for diffraction enhancement of symmetry (after /20/). OABC indicates a unit cell. The total symmetry is $p\ 1$; the diffraction symmetry is 4.



From the existence of two-fold symmetry axes for any layer and the symmetry of the stacking, it follows that there is a 1:1 correspondence between interatomic vectors in this structure (Fig.7). Every vector is transformed into its counterpart by a twofold rotation around an axis perpendicular to the layers. This correspondence of interatomic vectors is a sufficient condition for the symmetry of the diffraction pattern.

In /20/ the term "enhancement due to local symmetry" has been used in a far more general sense. Let us consider the theoretical example of the plane structure given in /20/ (see Fig.8). OACB indicates a unit cell. Obviously, the symmetry of the whole structure is $p\ 1$, but it can be proved that the diffraction symmetry is 4. The structure may be considered as consisting of several substructures, each formed by the orbits of the vertices of a square. All the substructures have the symmetry $p\ 4$. From this higher symmetry of the substructures originates the enhancement of symmetry of the diffraction pattern. This example is more general compared with the previous one with regard to three points.

1. Any two squares of different substructures are different in size and may be transformed one into the other only by an affine transformation.
2. Different substructures have common atoms.
3. The transformation of one substructure into another one is possible only by a rather complex transformation.

The notion of a groupoid may also be used for this example. The different substructures are the objects of the groupoid. The transformations of substructures are the morphisms. The axioms of a groupoid are fulfilled. It should be pointed out that the morphisms between different substructures are no longer partial symmetry operations (compare point 1 and 3).

Non-crystallographic symmetry in proteins

Other examples of non-traditional symmetries in crystallography are the so-called non-crystallographic symmetries. For many proteins, each crystal asymmetric unit contains several identical or closely related subunits. The operation which superimposes one of these subunits onto another one is only a partial symmetry operation. It is not in agreement with the crystal lattice and therefore it has been named a "non-crystallographic" symmetry. But these partial symmetries may facilitate the determination of such a structure. In some extent the effect of non-crystallographic symmetry is the same as the effect of normal crystallographic symmetry. It results in decreasing the size of the structural unit to be determined.

By Blow /1/ some important cases of non-crystallographic symmetry have been quoted:

1. Particle symmetry is not that of a crystallographic point group
 - (a) non-crystallographic point group
 - (b) helical symmetry
2. Particle has exact point group symmetry which is not incorporated into the lattice.
3. Several identical particles are in crystallographic unit, without systematic relationship.
4. Particle symmetry is approximate.

It is obvious that such partial symmetries may occur not only in case of proteins and viruses, but also in less complicated structures. Examples have been given by Watanabe /25/ and by Zorkii /26/.

Let us now consider the question how the symmetry of a structure of this kind may be described. The aim is to include the total symmetries as well as the partial symmetries. The structure may be divided into appropriately chosen building units. These units may be, for instance, molecules or parts of molecules. The building units are considered as the objects of a groupoid, and the coincidence operations of the objects are the morphisms of the groupoid. The groupoid includes the total and

the partial coincidence operations of the structure.

Let u_0 be one of the building units and M the set of all coincidence operations which start from u_0 . Then any total symmetry operation belongs to M , and we may consider M as the sum of the group G of total symmetry operations and a set H of strictly partial symmetry operations, $H = M \setminus G$. Only the total symmetry operations g fulfill the following condition: The composition of any h of M with g is again a motion h' of M . $M = G + H$ is a "Mischgruppe" as defined by Loewy /17/. G is the kernel or nucleus of this Mischgruppe and H its shell.

The great advantage of this characterization of total and partial symmetries is that the total symmetries obviously play a special role. The classical crystallographic groups are included into this characterization. For them, the shell is empty. As building unit, the asymmetric unit of the crystal structure may be chosen. The investigation and application of groupoids or Mischgruppen of this kind is in its starting phase. In the abstract /18/ of a lecture given in 1978 W. Nowacki informed that the derivation of all 3-dimensional crystallographic space groupoids is being performed.

The survey on the application of groupoids in crystallography is still incomplete. Modulated structures form an example for which partial symmetries play an important role. Up to now the groupoid theory has not been applied to modulated structures, although an application seems to be possible. The symmetry of all kinds of composite crystals as twins, for instance, may also be described by groupoids.

Summary

Finally, I would like to summarize the main ideas on groupoids in crystallography

- There are various branches of crystallography, in which partial symmetries are of relevance in addition to normal (total) symmetries
- Structure determinations are facilitated, if partial symmetries are taken into account.
- Groupoids as well as some other mathematical structures closely related to groupoids are adequate to describe partial symmetries.
- There is a profound mathematical background for the description of partial symmetries. In addition to papers on groupoids parts of category theory and the theory of semigroups are applicable. Nevertheless, this mathematical background has not been used extensively so far.

- If only one crystal structure with total and partial symmetries is considered, the notion of a Mischgruppe equivalent to that of a Brandt groupoid seems to express the symmetry of the structure in the most appropriate way.
- The OD theory of Dornberger-Schiff explains the phenomenon^{of}/polytypism by the existence of partial symmetries.
- In the OD theory groupoids are used
 - (i) to describe the symmetry of polytypes;
 - (ii) to split the symmetry of a polytype into a part characteristic for an individual polytype and a second part describing the common features of all polytypes of a polytypic substance;
 - (iii) to classify all the polytypes consisting of equivalent layers into a set of 400 families which essentially differ with respect to their symmetry.
- The phenomenon that the symmetry of the diffraction pattern of a crystal structure is higher than expected from the point group of the structure is often a result of the presence of partial symmetries.
- For many proteins the asymmetric unit becomes less complex, if in addition to normal crystallographic symmetries so-called non-crystallographic symmetries (i.e. partial symmetries) are considered.

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The aim of this appendix is to give precise mathematical definitions of the notion of an OD groupoid and of the equivalence classes for OD groupoids described in this paper. In more detail, these notions have been considered in /13/, /14/, and /28/. At first, some notations and some useful auxiliary definitions will be given (1-7).

1. A denotes the group of all affine transformations of the 3-dimensional Euclidean space, BCA is the subgroup of all motions, and TCB is the group of all translations. Z is the set of all integers.

2. \underline{A} denotes the groupoid of affine transformations:

$$\begin{aligned} \text{ob } \underline{A} &= Z \\ \text{mor } \underline{A} &= \{ (i, j, \alpha) \mid i, j \in Z, \alpha \in A \} \\ \text{composition: } (j, k, \alpha_2) \cdot (i, j, \alpha_1) &= (i, k, \alpha_2 \alpha_1) \end{aligned}$$

3. The groupoid of motions \underline{B} is a subgroupoid of \underline{A} with

$$\begin{aligned} \text{ob } \underline{B} &= \text{ob } \underline{A} \\ (i, j, \alpha) \in \text{mor } \underline{B} &\iff \alpha \in B \end{aligned}$$

4. $\nu: \text{mor } \underline{A} \rightarrow A$ is a mapping, which "forgets" the objects that are connected by the morphisms of \underline{A} : $(i, j, \alpha) \mapsto \alpha$.

5. The subgroupoids $\underline{V}_1, \underline{V}_2 \subseteq \underline{B}$ are geometrical equivalent in $\underline{G} \subseteq \underline{A}$ (notation: $\underline{V}_1 \stackrel{G}{\cong} \underline{V}_2$) then and only then, if there exists a mapping $\omega: \text{ob } \underline{V}_1 \rightarrow \text{mor } \underline{G}$ such that

(i) ω induces a bijective mapping (isomorphism of groupoids)

$F: \underline{V}_1 \rightarrow \underline{V}_2$, defined by

if $i \in \text{ob } \underline{V}_1$ and $\omega(i) \in [i, i']_{\underline{G}}$, then $F(i) := i' \in \text{ob } \underline{V}_2$;

if $g \in [i, j]_{\underline{V}_1}$, then $F(g) := \omega(j)g\omega(i)^{-1} \in [F(i), F(j)]_{\underline{V}_2}$.

(ii) $\nu(\omega(i)) = \nu(\omega(j))$ for all $i, j \in \text{ob } \underline{V}_1$.

The condition (ii) may be weakened. We say that the subgroupoids $\underline{V}_1, \underline{V}_2 \subseteq \underline{B}$ are geometrical equivalent up to translations, if there exists a mapping $\omega: \text{ob } \underline{V}_1 \rightarrow \text{mor } \underline{G}$ such that the conditions (i) and (ii)' are fulfilled.

(ii)' The homogeneous parts of $\nu(\omega(i))$ and $\nu(\omega(j))$ are equal, for all $i, j \in \text{ob } \underline{V}_1$.

6. $\underline{V}_{\underline{G}}(i, i+1, \dots, j)$ denotes the full subgroupoid of \underline{G} with $\{i, i+1, \dots, j\}$ as set of objects.

7. Let τ be a vector of the 3-dimensional space and τ_τ denote the corresponding translation. Then we define a function $\chi_\tau: B \longrightarrow \{0, 1, -1\}$ by

$$\chi_\tau(B) = \begin{cases} +1 & \text{if } B\tau_\tau B^{-1} = \tau_\tau \\ -1 & \text{if } B\tau_\tau B^{-1} = \tau_{-\tau} \\ 0 & \text{otherwise} \end{cases} \quad (B \in B)$$

As for any OD groupoid \underline{G} a vector $\tau = \alpha \times \epsilon$ exists, we may denote the corresponding function χ_τ by $\chi_{\underline{G}}$ or simply by χ , if confusion cannot arise.

8. A subgroupoid $\underline{G} \subset B$ is said to be an OD groupoid, if it satisfies the following conditions:

- (i) If $i \in Z$, then $T_i := \{ \tau \mid (i, i, \tau) \in \underline{G}, \tau \in T \}$ forms in T a subgroup, generated by two non-parallel translations. We suppose $T_i = T_0$ for all $i \in Z$ and denote the vectors of two generating translations by α, ϵ .
- (ii) If $(i, j, B) \in \underline{G}$, then

$$\chi(B) = +1 \implies \underline{V}_{\underline{G}}(i, i+1) \stackrel{G}{\cong} \underline{V}_{\underline{G}}(j, j+1) \wedge \underline{V}_{\underline{G}}(i, i-1) \stackrel{G}{\cong} \underline{V}_{\underline{G}}(j, j-1)$$

$$\chi(B) = -1 \implies \underline{V}_{\underline{G}}(i, i-1) \stackrel{G}{\cong} \underline{V}_{\underline{G}}(j, j+1) \wedge \underline{V}_{\underline{G}}(i, i+1) \stackrel{G}{\cong} \underline{V}_{\underline{G}}(j, j-1)$$
- (iii) $(i, j, B) \in \underline{G} \wedge (i+1, j+1, B) \in \underline{G} \implies \chi(B) = +1$;
 $(i, j, B) \in \underline{G} \wedge (i+1, j-1, B) \in \underline{G} \implies \chi(B) = -1$;
 $(i, j, B) \in \underline{G} \wedge i \neq j \wedge \chi(B) = +1 \implies$ The translational part of B is linearly independent of α, ϵ .
- (iv) \underline{G} is connected, i.e. $[i, j]_{\underline{G}}$ is nonempty for all pairs of objects $i, j \in Z$.

In a more general definition of the notion of an OD groupoid, the condition (i) may be weakened and (iv) omitted.

9. The OD groupoids \underline{G}_1 and \underline{G}_2 are of the same type then and only then, if there exists a mapping $\varphi: Z \longrightarrow Z$ with the following properties:

- (i) φ is an order-isomorphism or an order-anti-isomorphism (in reference to the usual order in Z).
- (ii) $(i, j, B) \in \underline{G}_1$ with $\chi(B) = +1$ exists if and only if there exists a $(\varphi(i), \varphi(j), \bar{B}) \in \underline{G}_2$ with $\chi(\bar{B}) = +1$; $(i, j, B) \in \underline{G}_1$ with $\chi(B) = -1$ exists if and only if there exists a $(\varphi(i), \varphi(j), \bar{B}) \in \underline{G}_2$ with $\chi(\bar{B}) = -1$.

10. In the following, a crystallographic group G is a group of motions, whose subgroup of translations T_G is generated by two linearly independent translations.

11. The crystallographic groups G_1, G_2 belong to the same layer group (more exactly affine layer group type), if there is an affine transformation $\alpha \in A$ such that $G_1 = \alpha G_2 \alpha^{-1}$.

12. Let T_1, T_2 be two translational groups, each of them generated by two linearly independent translations. They belong to the same Bravais net, if in each of the 80 layer groups (types), either both T_1 and T_2 or none of them occur as subgroups of all translations.

13. The crystallographic groups G_1, G_2 belong to the same LGN, if there exists an affine mapping α such that

$$(i) \quad G_2 = \alpha G_1 \alpha^{-1}$$

(ii) If G_3 is a crystallographic group with $T_{G_3} = T_{G_1}$ and G_4 is a crystallographic group with $T_{G_4} = T_{G_2}$, then $\alpha G_3 \alpha^{-1}$ and $\alpha G_4 \alpha^{-1}$ are crystallographic groups, too.

14. The crystallographic group G is called symmorphic, if it is the semidirect product of a subgroup $G_0 \subset G$ and T_G . Correspondingly, we speak of a symmorphic OD groupoid, if the crystallographic group belonging to a single object is symmorphic. A layer group is called symmorphic, if its members are symmorphic.

15. OD groupoid family

Let $\underline{G}_1, \underline{G}_2$ be two OD groupoids, P a positive integer, and $(O, P, B) \in \underline{G}_1$ satisfying $\chi(B) = +1$. $\underline{G}_1, \underline{G}_2$ belong to the same OD groupoid family, if and only if an OD groupoid \underline{G} and integers $i, j \in \mathbb{Z}$ exist such that

$$\underline{V}_{\underline{G}}(i, \dots, i+P) \text{ and } \underline{V}_{\underline{G}_1}(O, \dots, P)$$

$$\text{as well as } \underline{V}_{\underline{G}}(j, \dots, j+P) \text{ and } \underline{V}_{\underline{G}_2}(O, \dots, P)$$

are geometrical equivalent in \underline{A} up to translations.

This definition leads to 383 OD groupoid families. 17 of them split into pairs of enantiomorphic families, if we accept only geometrical equivalences which do not change the orientation of an appropriately chosen triple of vectors (e.g. α_1, ℓ_1 , and the translational part of B).