greater computational time, in applying this method to larger structures than illustrated here.

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The Derivation of Twin Laws for (Pseudo-)Merohedry by Coset Decomposition

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Abstract

The generation of possible twin laws for (pseudo-)merohedry by left coset decomposition of the point symmetry of the crystal lattice (metric symmetry) with respect to the crystal point group is presented. Two algorithms for the generation of the system of representatives have been devised. The first produces twin laws in the form of pure rotations of 180° wherever possible, and the second associates operations in pairs related by a centre of symmetry for crystals lacking an inversion centre. The metric symmetry should be determined by means of cell reduction from the measured cell dimensions and the crystal point group derived from the assumed space group. The automatic generation of twinning operations by this algorithm greatly facilitates the testing of twinning and orientation ambiguities by way of least-squares refinement of the twin fractions.

Introduction

Twinning by (pseudo-)merohedry results in the exact superposition of the reciprocal lattices of the twin components and hence leads to the modification of the intensities of Bragg reflections. The automatic treatment of (pseudo-)merohedry should hence be an essential component of any modern computer system undertaking structure solution and refinement. Even for the treatment of untwinned single crystals, a knowledge of the possible twin laws by (pseudo-)merohedry can be crucial, as these represent the alternative orientations of the crystal structure with respect to its own lattice.

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It is the object of this paper to present the theory and algorithms for the generation of possible twin laws by (pseudo-)merohedry. The method presented is applicable for arbitrary cell dimensions, for any orientation of the space-group symmetry with respect to the basis vectors and is very readily implemented on a computer. The classical analysis of merohedry [see, for example, Le Page, Donnay & Donnay (1984)] considers a lattice of arbitrary dimensions and leads to 44 oriented point groups. However, the twinning possibilities of a crystal, for example, in the monoclinic point group m but with a metric symmetry in the point group $m\bar{3}m$, cubic system, are not considered. In the analysis given below all group–subgroup relations between the metric symmetry and the crystal point group are taken into account. In this paper the term merohedry applies to the classical situation where the crystal point symmetry and the lattice symmetry are in the same system, and the term pseudo-merohedry to the more general case of metrical specialization. As a referee has pointed out, in pseudo-merohedry, the metrically higher symmetry of the lattice is never exact and exists only within the experimental error. In fact, it even changes with temperature, pressure, impurities *etc.* Moreover, the orientation of the tensor representation surfaces (especially the indicatrix ellipsoid) does not follow the pseudosymmetry but depends on the structure. It is, for example, possible to observe 'metrically merohedral' twins in the microscope by different optical extinction orientations.

One particular example of the use of possible twinning by merohedry is to be found in the very successful technique of determining absolute structure (chirality and polarity) during least-squares refinement by considering any non-centrosymmetric crystal as an inversion twin (Flack, 1983; Bernardinelli & Flack, 1985, 1987). This example clearly illustrates a possible twin law's power to define orientation (in this case chirality or polarity) even in the absence of twinning [*e.g.* in Bernardinelli & Flack (1985) the vast majority of the samples proved to be untwinned single crystals]. The capability of treating real twins is an additional asset.

Basic theory

Let H be the point-symmetry group of the crystal and G the point group of its lattice, *i.e.* its metric symmetry. H is a subgroup of G. As the relation of G to H is one of group to subgroup, it is natural to bring some of the tools of group theory to bear on the problem [for an excellent *exposé* of this subject with applications to crystallography see Klee & Wondratschek (1984)]. In particular, it is the technique of coset decomposition which is fruitful in this instance. Consider the coset decomposition of G with respect to H. In the following we take left cosets to conform to the convention of carrying out the right symmetry operation first in a product. Any system of representatives of the decomposition is a set of symmetry operations drawn from G which produces G from H by operating individually with each element of the set on all the operations in H. The operations in this set are precisely those which lead to the superposition of the lattice onto itself but which are not symmetry operations of H (apart from the identity operation). Hence any system of representatives of the coset decomposition of G with respect to H contains the possible (pesudo-)merohedral twin laws for a crystal of point symmetry H in a lattice of point symmetry G. The relationship between coset decomposition and merohedral twin laws seems not to have been treated in the literature to date. It should be noted that coset decomposition is a complete way of deriving the index of a subgroup (crystal point group) with respect to a supergroup (holohedry). The index gives the number of different orientation states of the twin domains and the number of classes of twin elements (including the identity).

The left coset decomposition is unique, but the system of representatives is not because it can be built by selecting an arbitrary element from each coset. The same arbitrariness is present in the definition of twin laws, and it is customary to use twin axes rather than twin planes if the crystal is centrosymmetric and to use 180° rotations about twin axes as much as possible. For example, in this prescription the decompositions of point group $2/m$ with respect to point groups 2 and m lead to $2/m = \{1; 2; \bar{I}; m\} = \{1; 2\} + \{\bar{I}; m\} = 1\{1; 2\} + \bar{I}\{1; 2\}$ and $2/m = \{1; 2; I; m\} = \{1; m\} + \{2; \bar{I}\} = 1\{1, m\} + 2\{1, m\}$. However, in the evaluation of structure factors and their derivatives much benefit is to be derived from choosing twin laws which embody relationships through a centre of symmetry; *i.e.* where possible the system of representatives should contain pairs of operators, one of which is a pure rotation and the second of which is related to the first by a centre of symmetry. For the cases cited above one obtains $2/m = \{1; \bar{I}; 2; m\} = \{1; 2\} + \{\bar{I}; m\} = 1\{1; 2\} + \bar{I}\{1; 2\}$ and $2/m = \{1; \bar{I}; 2; m\} = \{1; m\} + \{\bar{I}; 2\} = 1\{1; m\} + \bar{I}\{1; m\}$. This system is also to be preferred on physical grounds. Since the Laue symmetry is always a minimal supergroup of index 2 of a non-centrosymmetric point group within its Laue class, the inversion as first twin element would always produce the Laue symmetry, so important in diffraction and crystal physics. Furthermore, any merohedral twinning within one Laue class can always be considered as inversion twinning. Consequently two algorithms are presented: algorithm A produces a system of representatives according to the customary first prescription and algorithm B a system strongly bound to the centre of symmetry but nevertheless using twofold operations wherever possible.

The metric symmetry G is obtained by the process of cell reduction from the measured cell dimensions of the crystal. We have made use of the routine of Le Page (1982) to our entire satisfaction. Other excellent programs also exist (*e.g.* Zimmermann & Burzlaff, 1985). The cell-reduction routine produces a flag indicating the metric symmetry and a 3×3 matrix giving the orientation of this symmetry group in its conventional form with respect to the declared cell. The operations of the seven holosymmetric Laue groups ($\bar{1}$, $2/m$, mmm, $4/mmm$, $\bar{3}2/m$, $6/mmm$, $m\bar{3}m$) can be stored in the program and may readily be rotated into the orientation of the declared cell. The crystal point symmetry H may very simply be obtained from the declared space-group symmetry of the crystal.

Algorithm *A*

We wish here to select representatives which are symmetry operations of the first kind (determinant positive) and binary (applying an operation twice leads to the identity operation) as much as possible. This goal can be achieved by ranking the symmetry operations in G as follows: the identity operation appears first, then the binary operations of the first kind (twofold rotations), then the other first-kind operations (non-twofold rotations), then the same operations multipled by $\bar{1}$ giving respectively the inversion, the mirror reflections and finally the non-twofold second-kind operations. The first operation in H must be the identity, the remaining operations being in any order.

The coset decomposition of G with respect to H is then performed by 'crossing out' those operations in G which can be generated from pre-multiplication of a representative selected in G with any operation in H except identity, which would lead to crossing out the selected representative. The algorithm is as follows:

Flag each operation in G with a TRUE Boolean flag
Loop, in sequence, over the operations in G: $G[i]$
  If $G[i]$ is flagged TRUE, then
    Loop, starting at 2, over the operations in H: $H[j]$
      Loop, starting at $i+1$, over the operations in G: $G[k]$
        If $G[k]=G[i]H[j]$ then flag $G[k]$ as FALSE
      End of loop over $G[k]$
    End of loop over $H[j]$
  End of if $G[i]$ flagged TRUE
End of loop over $G[i]$.

The operations in G which are still flagged TRUE after applying the algorithm constitute a system of representatives for the coset decomposition of G with respect to H. They are the identity operation followed by possible operations (or twin laws) selected essentially in the traditional way.

Algorithm *B*

G is always centrosymmetric. Let G' be the subgroup of index 2 of G such that G' is composed only of pure rotations $G=G'+(\bar{1})G'$. G' will be one of the point-symmetry groups 1, 2, 222, 422, 32, 622 and 432 - the holoaxial hemihedral groups of Le Page, Donnay & Donnay (1984) - which should be ordered as for algorithm *A*. However, H may or may not be centrosymmetric:

(1) *H centrosymmetric.* Each coset of G contains pairs of elements related by a centre of symmetry. We will always choose pure rotation operations to include in the system of representatives. We may thus write $G=e_+H+f_+H+g_+H+\ldots$ for the coset decomposition of G with respect to H with e_+, f_+, g_+ *etc.* being pure rotation operations. Let H' be a subgroup of index 2 of H such that $H=H'+(\bar{1})H'$. H' may or may not contain only pure rotations. Clearly, then $G=e_+H'+f_+H'+g_+H'+\cdots+e_-H'+f_-H'+g_-H'+\ldots$, where $e_-=(\bar{1})e_+$, $f_-=(\bar{1})f_+$, *etc.* The required coset decomposition of G with respect to H may thus be obtained from the coset decomposition of G with respect to H' by taking only the pure rotations of the system of representatives of the latter. This is most readily carried out by generating pairs of centrosymmetrically related elements of G from stored values of G'.

(2) *H non-centrosymmetric.* Write $H'=H$. As G has pairs of operations related by a centre of symmetry, we have again $G=e_+H'+f_+H'+g_+H'+\cdots+e_-H'+f_-H'+g_-H'+\ldots$ as in (1). We may perform the coset decomposition as in (1) but keeping both elements of the centrosymmetrically related pairs.

Note that the definitions of H' given above correspond to the way in which space group is coded in many crystallographic least-squares programs as (*a*) a flag to indicate the type of lattice centring, (*b*) a flag to indicate whether there is a centre of symmetry and (*c*) the remaining symmetry operations in matrix form. With G stored as G', H' may be compared against pairs of elements generated from G', and only elements of G' kept in the system of representatives. For H centrosymmetric, this calculation gives the complete system of representatives whereas for H non-centrosymmetric only half the system is obtained, those outstanding being obtained from the former by multiplication by a centre of symmetry. The identity operators of G' and H' should be first in the sequence of elements. The algorithm is as follows:

Flag each operation of G' with a TRUE Boolean flag.
Loop, in sequence, over the operations in G', $G'[i]$

If $G'[i]$ is flagged TRUE, then
Loop, starting at 2, over the operations in H', $H'[j]$
Loop, starting at $i+1$, over the operations in G', $G'[k]$
If $G'[k]$ is flagged TRUE then
If $G'[k] = \pm G'[i]H'[j]$ then flag $G'[k]$ as FALSE
End of if $G'[k]$ is flagged TRUE
End of loop over $G'[k]$
End of loop over $H'[j]$
End of if $G'[i]$ is flagged TRUE
End of loop over the $G'[i]$.

At the end of this procedure, the elements of G' flagged TRUE will represent the possible twin laws of the (pseudo-)merohedry. Should the space group of the crystal be non-centrosymmetric, each element of G' flagged TRUE should be understood to represent two twinning operations - the element of G' itself and the element multiplied by $\bar{I}$.

It is possible to make use of group-subgroup relations to economize space in storing the symmetry operations of the holoaxial hemihedral point groups, ordered as for algorithm *A*. For 1, 2, 222, 422 and 432 one stores the operations of 432 in the following sequence of the operations given in *International Tables for Crystallography* (1983) for space group *P*432: 1, 3, 2, 4, 13, 14, 18, 19, 22, 24, 16, 15, 5, 6, 7, 8, 9, 10, 11, 12, 17, 20, 21, 23. In the order of the stored elements one finds the operations of: 432, 1 to 24; 422, 1 to 6 and 11 to 12; 222, 1 to 4; 2, 1 to 2; 1, 1. Likewise for 32 and 622 one stores the operations of 622 given for *P*622 in the order: 1, 7, 8, 9, 4, 10, 11, 12, 2, 3, 5, 6. 622 is found in elements 1 to 12; 32 in 1 to 4 and 9 to 10.

Examples

In the following, the symmetry operations for the point groups are taken from the *Space Group* section of *International Tables for Crystallography* (1983). The full symbol for a symmetry operation is only given where confusion might arise. The sequence of the symmetry operations as given in *International Tables for Crystallography* (1983) needs changing for the use of algorithm *A*. For algorithm *B*, only the first half of all the symmetry operations need be used for centrosymmetric point groups.

α-quartz crystallizes in the trigonal system with non-centrosymmetric space group $P3_121$ and cell dimensions $a = 4{\cdot}913$ and $c = 5{\cdot}404$ Å. The crystal point group is thus $321 = \{1;\ 2\ x,\ x,\ 0;\ 2\ x,\ 0,\ 0;\ 2\ 0,\ y,\ 0;\ 3^+;\ 3^-\}$ and the metric symmetry is $6/mmm = \{1;\ 2\ x,\ x,\ 0;\ 2\ x,\ 0,\ 0;\ 2\ 0,\ y,\ 0;\ 2\ 0,0,\ z;\ 2\ x,\ \bar{x},\ 0;\ 2\ x,\ 2x,\ 0;\ 2\ 2x,\ x,\ 0;\ 3^+;\ 3^-;\ 6^+;\ 6^-;\ \bar{I};\ m\ x,\ \bar{x},\ z;\ m\ x,\ 2x,\ z;\ m\ 2x,\ x,\ z;\ m\ x,\ y,\ 0;\ m\ x,\ x,\ z;\ m\ x,\ 0,\ z;\ m\ 0,\ y,\ z;\ \bar{3}^+;\ \bar{3}^-;\ \bar{6}^+;\ \bar{6}^-\}$ with the group arranged in the sequence ready for use by algorithm *A*. The coset decomposition is thus $6/mmm = \{1;\ 2\ x,\ x,\ 0;\ 2\ x,\ 0,\ 0;\ 2\ 0,\ y,\ 0;\ 3^+;\ 3^-\} + \{2\ 0,\ 0,\ z;\ 2\ x,\ \bar{x},\ 0;\ 2\ x,\ 2x,\ 0;\ 2\ 2x,\ x.\ 0;\ 6^+;\ 6^-\} + \{\bar{I};\ m\ x,\ \bar{x},\ z;\ m\ x,\ 2x,\ z;\ m\ 2x,\ x,\ z;\ \bar{3}^+;\ \bar{3}^-\} + \{m\ x,\ y,\ 0;\ m\ x,\ x,\ z;\ m\ x,\ 0,\ z;\ m\ 0,\ y,\ z;\ \bar{6}^+;\ 6^-\}$ Applying either algorithm *A* or *B* one obtains $\{1;\ 2\ 0,\ 0,\ z;\ \bar{I};\ m\ x,\ y,\ 0\}$ for the system of representatives. The last three representatives correspond respectively to the twin laws for the well known Dauphiné, Brazil and combined twinning. The twin-related reflections are hence hkl, $\bar{h}\bar{k}l$, $\bar{h}k\bar{l}$, $hk\bar{l}$ in agreement with Le Page, Donnay & Donnay (1984).

Nb_3Si and Nb_3As crystallize in the tetragonal Ti_3P structure type with space group $P4_2/n$ with cell dimensions $a = 10{\cdot}224(1)$, $c = 5{\cdot}189$ Å (for Nb_3Si). The crystal point group is thus $4/m = \{1;\ 2\ 0,\ 0,\ z;\ 4^+;\ 4^-;\ \bar{I};\ m\ x,\ y,\ 0;\ \bar{4}^+;\ \bar{4}^-\}$ and the metric symmetry is $4/mmm = \{1;\ 2\ 0,\ 0,\ z;\ 2\ 0,\ y,\ 0;\ 2\ x,\ 0,\ 0;\ 2\ x,\ x,\ 0;\ 2\ x,\ \bar{x},\ 0;\ 4^+;\ 4^-;\ \bar{I};\ m\ x,\ y,\ 0;\ m\ x,\ 0,\ z;\ m\ 0,\ y,\ z;\ m\ x,\ \bar{x},\ z;\ m\ x,\ x,\ z;\ \bar{4}^+;\ \bar{4}^-\}$. Clearly the coset decomposition of $4/mmm$ with respect to $4/m$ is given by $4/mmm = \{1;\ 2\ 0,\ 0,\ z;\ 4^+;\ 4^-;\ \bar{I};\ m\ x,\ y,\ 0;\ \bar{4}^+;\ \bar{4}^-\} + \{2\ 0,\ y,\ 0;\ 2\ x,\ 0,\ 0;\ 2\ x,\ x,\ 0;\ 2\ x,\ \bar{x},\ 0;\ m\ x,\ 0,\ z;\ m\ 0,\ y,\ z;\ m\ x,\ \bar{x},\ z;\ m\ x,\ x,\ z\}$. Either algorithm *A* or *B* would lead to $4/mmm = 1\{4/m\} + (2\ 0,\ y,\ 0)\{4/m\}$ and hence the system of representatives is $\{1, 2\ 0,\ y,\ 0\}$. The twin-related reflections are hence hkl and $\bar{h}k\bar{l}$ in agreement with Le Page, Donnay & Donnay (1984).

As an example of pseudo-merohedry consider a structure in the space group $R3m$ (on rhombohedral axes) but with cubic ($m\bar{3}m$) metric symmetry. The system of representatives chosen by algorithm *B* (algorithm *A* would give the same result) is: $\{1;\ 2\ 0,\ y,\ 0;\ 2\ 0,\ 0,\ z;\ 2\ x,\ 0,\ 0\}$. The twin-related reflections are hkl, $\bar{h}k\bar{l}$, $\bar{h}\bar{k}l$ and $hk\bar{l}$.

Point group m (details in *Basic theory* section) provides an example of different systems of representatives being produced by algorithms *A* and *B*. *A* produces $\{1, 2\}$ with twin-related reflections hkl and $\bar{h}k\bar{l}$ and *B* gives $\{1, \bar{I}\}$ with twin-related reflections hkl and $\bar{h}\bar{k}\bar{l}$.

Concluding remarks

The calculation described above (algorithm *B*) has been implemented into our version of *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) using a slight adaptation of the cell reduction routine of Le Page (1982). Tests have been performed on the 32 crystal point groups and concur with Le Page, Donnay & Donnay (1984). A few tests of pseudo-merohedry (*e.g.* point group m in a cell of cubic symmetry) have also been undertaken.

For an effective implementation of a treatment of possible merohedral twinning in a crystallographic package of programs two ingredients are necessary.

Firstly it must be possible from the ordinary data available at the structure refinement stage (*viz* cell dimensions and space group) to generate the possible twinning operations due to (pseudo-)merohedry. One of the algorithms described in this paper can be used for this purpose. The second ingredient is the capability to refine the volume fractions of the twin components as variables in the least squares. In principle this poses no major difficulties although attention should be paid to such questions as scale-factor refinement, intensity-data structuring, evaluation of Fourier coefficients for electron density calculation and rotation and/or inversion of atomic parameters. These questions will be examined in detail in a future publication. The treatment of twinning resolves not only the problem of twinned crystals but also solves the difficulties of orientation ambiguities when working from a known list of atomic positional parameters. As an illustration, in the refinements of Nb_3Si and Nb_3As undertaken by Waterstrat, Yvon, Flack & Parthé (1975) from published atomic parameters (see second example above), one compound refined immediately to a low R value whilst the second remained at 50%. When the reflection indices were transformed by the above twin law, the R value of the second compound diminished immediately to a low value. An automatic twin-component refinement would have saved some considerable anxiety and immediately resolved this orientation ambiguity.

The problems of twinning and space-group ambiguities with disorder are intimately related. The coset decomposition of the metric symmetry with respect to the crystal point group furnishes the rotation matrices necessary to describe the merohedral twin laws. It is of course possible in practice that, instead of twinning, disorder could arise and that the declared space group is a subgroup of the correct one. The coset decomposition produces the rotational components of the 'missing' symmetry operations. It would remain to find the translational parts by some other technique.

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The Visibility of Phase Indications in *n*-Beam Diffraction Patterns*

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Abstract

[0*k*0] *n*-beam diffraction patterns of germanium have been recorded by rotation of specimens about the diffraction vectors of the vanishingly weak 020 and 060, and the very strong 040 reflections. *N*-beam interactions were displayed clearly in the [020] and [060] scans, and somewhat less clearly in the [040] scan. Unambiguous phase indications, however, were detected only in the [040] scan. The experiments demonstrate that the visibility of *n*-beam *interactions* does not necessarily imply a corresponding visibility of experimental *phase indications*. The geometry of some unusual four- and five-beam interactions detected in the [0*k*0] scans, and the phases shown by those interactions, are also discussed.

I. Introduction

The visibility of *n*-beam interactions in Renninger patterns increases monotonically with decreasing two-beam background intensity, *i.e.* with decreasing intensity of the primary reflection. It is therefore often assumed that only weak primary reflections are suited

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