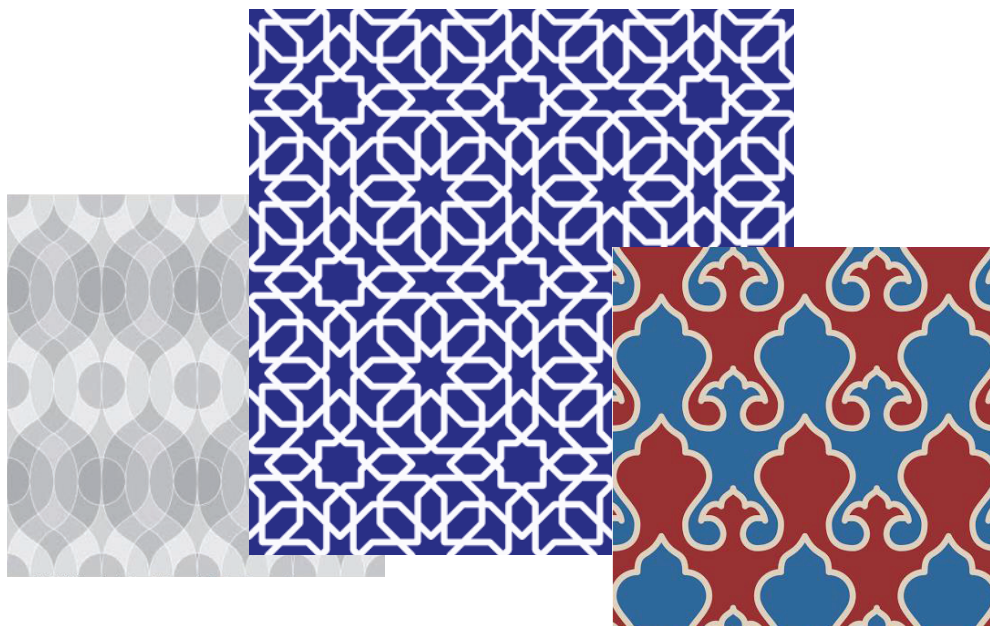


Ivan Červeň

# CRYSTALLOGRAPHIC PLANE GROUPS

Types of symmetry of planar periodic  
structures, their geometric  
and mathematical construction



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Slovak University of Technology in Bratislava

2025

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The symmetry of two-dimensional periodic structures can be seen, for example, on wallpaper, but it is of great importance in crystals, where atoms are regularly arranged in parallel planes. The symmetry of naturally occurring crystals is very diverse, but each crystal in terms of the symmetry of external shapes can be included in one of the 32 types (32 crystal classes), represented by the point groups of symmetry. However, the set of symmetry types of the arrangement of atoms, i.e. the symmetry types of the crystal structure, is much more numerous. Each crystal can be classified into one of 230 types, the so-called *space groups* of symmetry. A group as a mathematical formation represents a set of elements, (with certain rules, given in Appendix D29 on groups), which in the case of crystals and their structure relate to the so-called *symmetry operations*. The elements of such groups are rotations, reflections (mirrorings), inversions (each position vector  $\mathbf{r}$  is transformed into a vector  $-\mathbf{r}$ ) and displacements (translations), including their combinations. Symmetry operations are performed by means of *symmetry elements*, which are rotational axes, reflection planes (mirror planes), or the centre of symmetry. Symmetry operations convert the crystal structure, resp. the whole crystal, to a position which is physically and geometrically indistinguishable from the original position. That is, physical and the geometrical properties of the crystal do not change at any point of the reference system after such an operation.

The above number of space groups was established by *E. S. Fedorov* and *A. Schoenflies* in 1891 after a more extensive mutual correspondence, in the character of only constructive procedure. Consistently, using the theory of groups and matrices, the space groups were derived by *F. Seitz* in the 1930 (a series of articles in the magazine *Zeitschrift für Kristallographie*). Next, using tensors, the derivation was modified by *W. H. Zachariasen* (published just after World War II in a book *Theory of X-Ray Diffraction in Crystals*).

The derivation of 230 space groups is very demanding in scope and content, and so for pedagogical purposes it is more appropriate to document the exact derivation procedure on two-dimensional planar groups of periodic structures, of which there are only 17. And that is the content of the third part of this text (part C). However, this procedure is also for the first contact with space or planar groups very demanding. The geometric construction of possible types of lattices, point groups and plane groups, is therefore more appropriate, and represents the content of the first part of this text (part A). The periodic planar structures can be seen as imprinted patterns on the cloth, but they are also characterized by the arrangement of atoms that appears on a section of a perfect crystal, or on its surface below the electron microscope, or after imaging under an atomic force microscope (AFM). The first part of the text is processed on the basis of A. Fingerland's lecture from 1969 presented

at the Colloquium of Czech and Slovak crystallographers in Smolenice (Slovakia). It was based on the original ideas of A. Bravais from the middle of the 19th century. To understand the essence of the description of symmetry types the geometric construction is completely sufficient, and can be extended to three-dimensional periodic structures.

The third part of this text (part C) is significantly more demanding, it uses group theory and expression of spatial transformations using matrix, or tensor apparatus. It represents the remarkable fact, that it is possible to derive all of the 230 types of symmetry only using simple mathematical principles and the assumption of strict periodicity of the crystal structure. The second part (Part B) serves to better understand part C, and provides information on how to describe symmetry operations using matrices, or tensors. The shapes of matrices and tensors representing rotations and reflections in various crystal systems are given, as well as the method of their application to the transformation of the coordinates of points in space.

Many authors have dealt with the theory of crystal symmetry. Sometimes, as first, is mentioned Johann Kepler's paper on the snowflake from 1611, in which he tried to explain the origin of its hexagonal shape, but also described the tightest arrangement of spheres in plane and space. The constancy of the angles between crystal faces was stated by Nicolas Steno in 1669, and the idea of the structure periodicity in crystals was published by René Just Haüy in 1784. The symmetry of external shapes - its 32 types – was described in 1830 by J. F. Ch. Hessel, and 14 lattice types by A. Bravais in 1848. The search for symmetry types was completed in 1891 by E. S. Fyodorov and A. Schoenflies, who derived 230 symmetry types of crystal structures. The reader can learn more about this search in the book *Symmetry of crystals* [23].

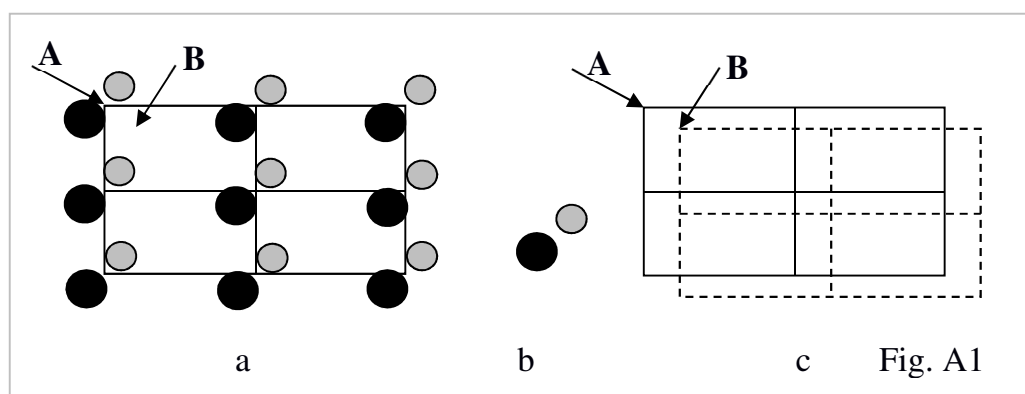
## Part A

### Geometric construction of plane symmetry types

#### A1 Basic terms used in crystal structure description

Due to the periodicity of the crystal structure, a set of points can be found, called **lattice points**, which are characterized by the same neighbourhood. In a two-dimensional example (Fig. A1) such a set of **equivalent points** can be represented by intersections of mutually perpendicular lines. In the crystal structure we can select various sets of points with the same surrounding, periodically distributed in space – more numerous and less numerous sets. The most numerous of them (in other words, with the largest number of points per unit volume) forms a **space lattice**, in connection with crystals, called a **crystal lattice**. For two-dimensional formations it is a **plane lattice**.

When constructing the space lattice of the given structure, it can be assumed from any point in space, the resulting lattice will always be the same, but somewhat shifted. The figure shows two starting points in a planar lattice – point A and point B.



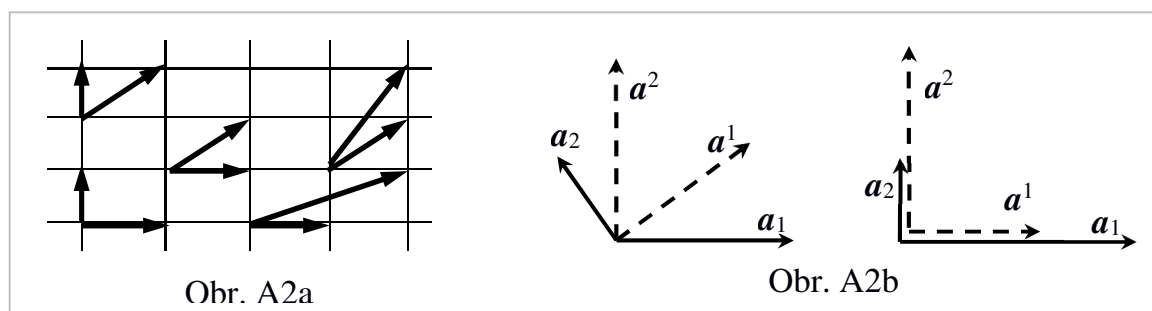
The periodicity of the structure makes it possible to divide the building particles of the crystal (atoms, ions) so that the same group of particles, called a **structural motif**, is assigned to each lattice point (Figure A1b). When selecting a structural motif, it is useful to consider the chemical composition of the substance so that the structural motif consists of, for example, a complete molecule.

The crystal lattice is described by a triplet of non-coplanar vectors  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  (in the plane only pairs) called **basis vectors**, forming the so-called **vector basis**. Their integer linear combinations form a set of **lattice vectors**  $\mathbf{A}_L$ :

$$\mathbf{A}_L = L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2 + L_3 \mathbf{a}_3, \quad (\text{A1.1})$$

whose endpoints form the space lattice of the crystal ( $L_i$  are integers). The set of all lattice vectors forms the **translation group** of the crystal.

With the help of a trio of basis vectors, a lattice is created unambiguously. At however, the choice of basis vectors is not unambiguous for a previously known lattice. The figure A2a shows a selection of several pairs, whose integral linear combination creates the same planar lattice. There were therefore accepted certain conditions for the choose of three vectors, originating from the XIX. century by A. Bravais [1].



These conditions require that the symmetry of the parallelepiped formed by the triple of vectors corresponds to the symmetry of the lattice, the number of right angles between the vectors of the triple is maximal and the volume of the parallelepiped is minimal, i.e., that the vectors of the triple are as short as possible.

The triple thus chosen forms the triple of **basis vectors** of the lattice and the corresponding parallelogram forms the **unit cell**. Successive translations (without rotations) of the unit cell by all lattice vectors fill the entire volume of the crystal without residue. The sizes of the basis vectors and the angles between them are **lattice parameters**.

A line passing through at least two lattice points is a **lattice line**. The direction of a lattice line with respect to a triplet of basis vectors is expressed by the coordinates of the shortest lattice vector that is parallel to the line. The coordinates are put in square brackets, e.g.  $[13\bar{1}]$ , and the fact that the coordinate is negative is expressed by a *minus* sign over the coordinate. In planar structures, only two coordinates are used, of course. The directions of reflection lines in a planar structure may also be denoted in this way, when the symbol  $m$  representing the reflection line to indicate the direction of the reflection line, e.g.  $m_{[\bar{2}1]}$ . Other, abbreviated designations are also used in this text, e.g.  $m_x$  when the reflection line is parallel to the x-axis, or  $m_1$  when it is parallel to the vector  $a_1$ . Given the periodicity of the crystal structure, each lattice line is associated with a set of lattice lines parallel to it that pass through the individual lattice points of the crystal, leaving none of them out. Such a set forms the **set of the lattice lines**.

The **reciprocal lattice** of a crystal is of great importance in the description of the crystal structure, especially in diffraction methods for its determination. It is obtained

by integral linear combinations of a triplet of **reciprocal vectors**,  $\mathbf{a}^1, \mathbf{a}^2, \mathbf{a}^3$  which with respect to a triplet of basis vectors  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  is defined by scalar products:

$$\mathbf{a}_i \cdot \mathbf{a}^j = \delta_{ij} \quad (i, j = 1, 2, 3), \quad (\text{A1.2})$$

where  $\delta_{ij} = 0$  if  $i \neq j$ , and  $\delta_{ij} = 1$  if  $i = j$ .

These relations imply that the vectors  $\mathbf{a}_1, \mathbf{a}^2$  and similarly  $\mathbf{a}_2, \mathbf{a}^1$  are perpendicular to each other. In doing so, vectors with the same indices, e.g.  $\mathbf{a}_2$  and  $\mathbf{a}^2$  need not be parallel. It is true  $\mathbf{a}_2 \cdot \mathbf{a}^2 = a_2 a^2 \cos \alpha = 1$ , so if they are parallel ( $\cos 0^\circ = 1$ ), then the product of their magnitudes equals unity. This is where the name reciprocal vectors comes from, because they have inverse (reciprocal) magnitudes to each other. We do not give further details about reciprocal vectors because they are not needed for planar periodic structures. Figure A2b shows a pair of basis vectors and a pair of corresponding reciprocal vectors in dashed lines. The basis and reciprocal vectors are used to express tensors representing symmetry operations, so their introduction is important.

## A2 Lattices of planar periodic structures

A planar lattice is characterized by two non-collinear vectors  $\mathbf{a}_1, \mathbf{a}_2$  - their sizes and the angle between them, but also by the unit cell formed by these vectors. Since the same planar lattice can be formed by integral linear combinations of different pairs of vectors, for the sake of clarity, the vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  should also be chosen in accordance with the **Bravais conditions** as follows:

the symmetry of the unit cell must be identical to the symmetry of the lattice

a right angle between the basis vectors is to be preferred

the areal content of the unit cell must be minimal.

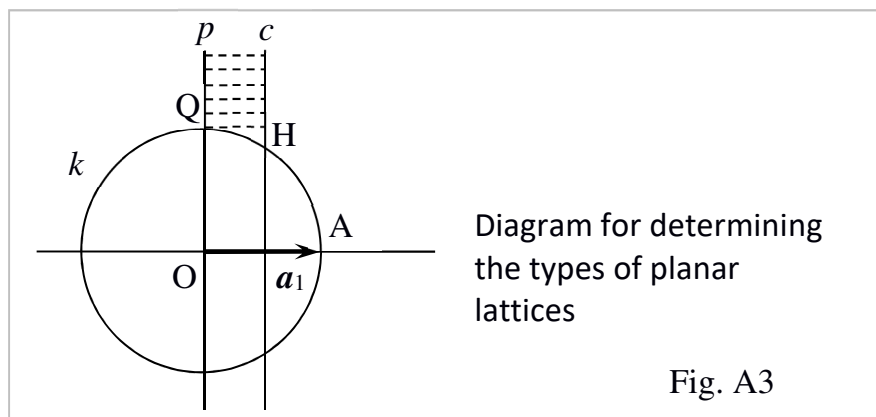
The unit cells, as well as the lattices formed by different pairs of basis vectors, differ from each other in their symmetry. By **symmetry** in this case, we mean the existence of a set of geometric transformations – **symmetry operations** – by which the lattice identifies with itself – gets to an **equivalent position**. The symmetry of a plane lattice is represented by a set of lattice translations, rotational axes - perpendicular to the plane of the lattice, and reflection lines lying in this plane. Unlike translations, reflection and rotation operations do not change the position of at least one point on the lattice, so these operations are called **point symmetry operations**, and this kind of

symmetry **point symmetry**. The set of these operations mathematically forms a group, called a **point group** (→ Appendix D29).

The third Bravais condition can be satisfied by choosing the two shortest lattice vectors. Bravais described his procedure as follows:

In a planar lattice, we choose an arbitrary lattice point O, and among the other lattice points we search for the one closest to it. Let A be that point, then OA is the smallest lattice parameter. Through the points O and A we draw lines Op and Am perpendicular to the line OA, and in the bounded space pOAm we find the next closest lattice point B.

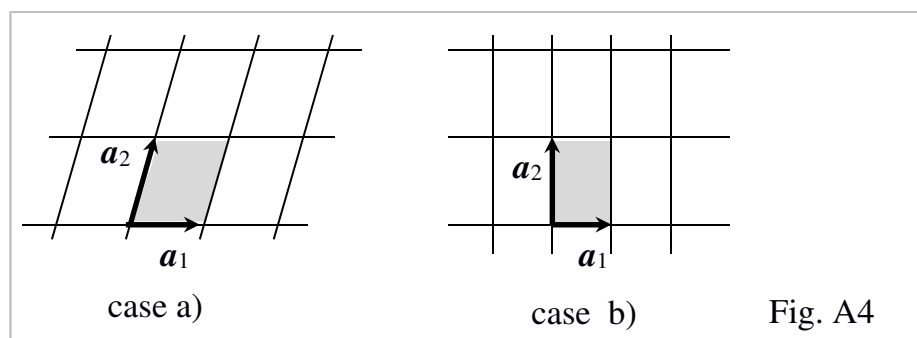
Therefore, we proceed as follows: let vector  $\mathbf{a}_1$  (Fig. A3) be the shortest lattice vector of a given planar lattice. Both the direction and the magnitude of the second shortest vector depend on the lattice type. For example, in a square lattice, we choose the second shortest vector perpendicular to the first one, with both having the same length. To find the second shortest vector in different types of lattices, we will refer to Figure A3. We will show that it suffices to restrict ourselves to the cases where the endpoint of the second shortest vector lies within the hatched region, including its boundaries.



Also, if we plot the vector  $\mathbf{a}_2$  from the point O, its endpoint cannot lie inside the circle bounded by the circle  $k$ , because it would be shorter than  $\mathbf{a}_1$ . Nor can it lie to the right of the line  $c$  (the line passes through the centre of the vector  $\mathbf{a}_1$ ), because it would be closer to point A from there than to point O. Nor will we take into account the endpoints lying to the left of the line  $p$ , because the lattice which would thus be formed would be merely the mirror image of the lattices which are formed when the endpoint lies to the right of the line  $p$ . It would be essentially a top or bottom view of

the same lattice. For the same reason, there is no need to consider the endpoints below the OA line. This leaves only options a) to f), described in detail in the following.

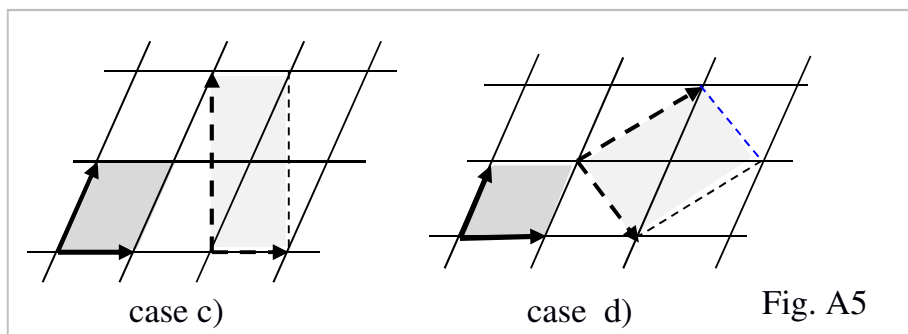
a) The end point of the vector lies inside the hatched region, but not on its boundaries. A **oblique lattice** is then formed, where the sizes of the basis vectors are not equal and the vectors do not take a special angle (meaning angles of  $90^\circ$ ,  $60^\circ$ , or  $120^\circ$ , respectively). The unit cell is in the shape of a parallelogram (Fig. A4a.). Both the cell and the lattice are characterized by twofold axes of symmetry perpendicular to the plane of the lattice; the reflection lines are absent. The twofold axes of symmetry pass through the centre of the unit cell, its vertices, and the centres of the basis vectors, and are thus distributed throughout the lattice. When rotated  $360^\circ$  about the twofold axis, the lattice is twice brought to the equivalent position – identifies itself with itself, hence such a symmetry operation is denoted by the symbol 2. The corresponding point group of the symmetry of the lattice is denoted by the symbol **2** and has two elements  $\{e, 2\}$ , where symbol  $e$  represents the identity (rotation by  $0^\circ$  and  $360^\circ$ , respectively) and symbol 2 the  $180^\circ$  rotation.



b) The end point of the vector  $a_2$  lies on the semi-line  $p$ , but not at the point Q. An **orthogonal lattice** is then formed, the unit cell being **orthogonal** (Fig. A4b.). Both the lattice and the unit cell are characterized by twofold axes of symmetry and two sets of reflection lines perpendicular to each other. The reflection lines are parallel to the basis vectors and are both identical to the sides of the unit cell and pass through the centres of the sides, perpendicular to them. A symmetry of this type is described by a point group **2mm**, which contains the following elements (i.e., symmetry operations):  $\{e, 2, m_{[10]}, m_{[01]}\}$ , where  $m_{[10]}$ , (resp.  $m_{[01]}$ ) represents the reflection in a line perpendicular to the basis vector  $a_1$  (resp.  $a_2$ ). In square brackets next to the symbol  $m$  are the coordinates of the vector perpendicular to the reflection line, expressed in the vector system  $a_1, a_2$ .

c) The end point of the second shortest lattice vector lies on the semi-line  $c$ , but not at the point H. The lattice thus formed has twofold axes of symmetry and two sets of reflection lines perpendicular to each other. It has the same point symmetry as the lattice in the previous case (described by the **2mm** group), but the unit cell formed from the vectors  $\mathbf{a}_1, \mathbf{a}_2$  has only double axes of symmetry, it has no reflection lines (Fig. A5.). Therefore, in accordance with the Bravais conditions, new basis vectors  $\mathbf{b}_1, \mathbf{b}_2$  (drawn in dashed lines) are chosen which are perpendicular to each other and form a unit cell with the same symmetry as the lattice, which is orthogonal. The two sets of reflection lines are parallel to the vectors  $\mathbf{b}_1, \mathbf{b}_2$  respectively. However, a unit cell formed from these vectors also has a lattice point in the middle of its area and is therefore called **centred cell**. The unit cell formed from vectors  $\mathbf{a}_1, \mathbf{a}_2$  is called **primitive** and has lattice points only at its vertices. If a centred cell exists in the lattice, the **lattice** is also called **centred**.

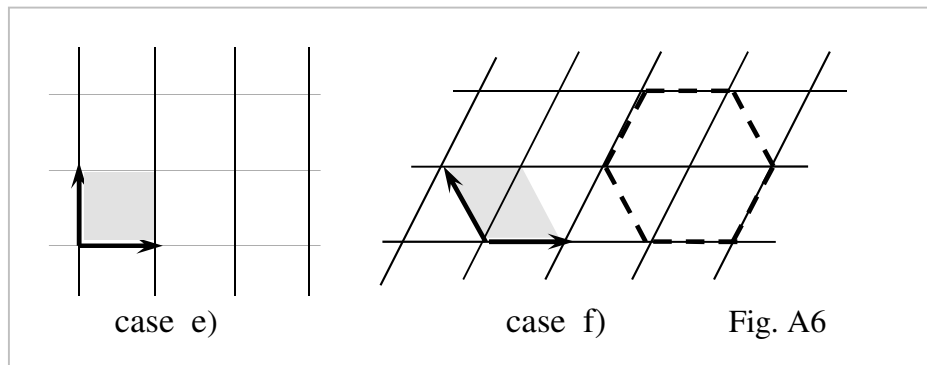
d) The endpoint of the vector  $\mathbf{a}_2$  lies on the circle between Q and H, but not at these points. The vectors  $\mathbf{a}_1, \mathbf{a}_2$  then have the same magnitude, forming a rhombic cell. Both the lattice and the cell are characterized by twofold axes of symmetry and two mutually perpendicular sets of reflection lines, but this time parallel to the diagonals of the rhombus. This lattice represents the same type of symmetry as in case c, is orthogonal. It has the symmetry described by the **2mm** group, and again new basis vectors  $\mathbf{b}_1, \mathbf{b}_2$  can be chosen to form an **orthogonal centred unit cell**. The reflection lines are parallel to the diagonals of the rhombus formed from the vectors  $\mathbf{a}_1, \mathbf{a}_2$ , not to its sides.



e) The end point of the vector  $\mathbf{a}_2$  is identical to the point Q. Both the lattice and the unit cell have the symmetry of a square, i.e., fourfold axes of symmetry and four sets of reflection lines (two parallel to the sides of the square and two parallel to the diagonals of the square). The **lattice** is called **square**. Such a symmetry is described by a point group denoted **4mm**, which has the following elements:  $\{e, 4, 4^2, 4^3, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\bar{1}]}\}$ , where  $m_{[10]}$  and  $m_{[01]}$  represent the reflection lines that are parallel to the basis vectors  $\mathbf{a}_1, \mathbf{a}_2$ , respectively, i.e., the sides of the unit cell,

and  $m_{[11]}$  and  $m_{[1\bar{1}]}$  in lines that are parallel to the diagonals of the unit cell. The symbols  $4$ ,  $4^2$ ,  $4^3$  represent "powers" of  $90^\circ$  rotations, e.g.  $4^3$  represents a  $270^\circ$  rotation.

f) The end point of the vector  $\mathbf{a}_2$  is the point H. The lattice has sixfold axes of symmetry and six sets of reflection lines, successively rotated by  $30^\circ$ . The lattice is called **hexagonal**.



Such a symmetry is described by a point group  **$6mm$** , where the group contains the following elements:

$\{e, 6, 6^2, 6^3, 6^4, 6^5, m_0, m_{30}, m_{60}, m_{90}, m_{120}, m_{150}\}$ . The numeric indices next to the symbol  $m$  represent the angle, expressed in degrees, that the reflection line makes with the basis vector  $\mathbf{a}_1$ .

There are 5 types of planar lattices in total (lattices  $c$  and  $d$  are of the same type). They are summarised in Table TA1. The five lattice types are characterized by only four types of point symmetry. The point symmetry of a lattice determines its membership in one of the four planar **crystal systems** listed in the table. In the rectangular system, two types of unit cells are distinguished, namely primitive (denoted by  $p$ ) and centred (denoted by  $c$ ). In the other systems there are only primitive cells. The five types of planar lattices represent the 5 types of planar translational symmetry, i.e., the 5 types of planar **translation groups**.

**Tab. TA1 Plane lattices, crystal systems and point groups**

| Lattice | Crystal system | Cell type | Basis vectors                        | Point groups            |
|---------|----------------|-----------|--------------------------------------|-------------------------|
| a)      | oblique        | $p$       | $a_1 \neq a_2, \alpha \neq 90^\circ$ | <b>2</b>                |
| b)      | rectangular    | $p$       | $a_1 \neq a_2, \alpha = 90^\circ$    | <b><math>2mm</math></b> |
| c), d)  |                | $c$       |                                      |                         |
| e)      | square         | $p$       | $a_1 = a_2, \alpha = 90^\circ$       | <b><math>4mm</math></b> |
| f)      | hexagonal      | $p$       | $a_1 = a_2, \alpha = 120^\circ$      | <b><math>6mm</math></b> |

### A3 Point groups of planar periodic structures

In the previous section, the symmetries of planar lattices were described. They are characterized by four types of point groups, called **holohedral** (from Greek = complete). In a planar periodic structure repeats a **structural motif** that is the same at each of its lattice points. Also the structural motif has its own point symmetry, which can be higher or lower than the point symmetry of the lattice. Therefore, the point symmetry of a planar periodic structure can also be the same as the symmetry of the lattice, it can also be lower, but not higher. That is, a planar periodic structure can have the same symmetry operations as a lattice, but with less symmetric structural motif the number of them may be smaller. Therefore, a planar periodic structure has a point group identical to point group of lattice, or it is a subgroup of the lattice point group. The four holohedral point groups together with their subgroups form the set of 10 point groups of planar periodic structures. The lattices of planar periodic structures and their point groups are listed in Table TA1, the point groups and their subgroups in the following text and in Table TA2.

The **group  $2mm$**  has four elements:  $2mm \equiv \{e, 2, m_{[10]}, m_{[01]}\}$ , where  $e$  represents the identity,  $2$  the  $180^\circ$  rotation about the twofold axis of symmetry,  $m_{[10]}$  the reflection in a line perpendicular to the basis vector  $\mathbf{a}_1$  and  $m_{[01]}$  the reflection in a line perpendicular to the basis vector  $\mathbf{a}_2$ . The numbers in square brackets (indices) next to the symbols  $m$  represent the coordinates of the vector perpendicular to the reflection lines in the system of basis vectors  $\mathbf{a}_1, \mathbf{a}_2$ . The subgroups of the group  **$2mm$**  are the sets of operations

$\{e, 2\}$ , designation of this group: **2**,  
 $\{e, m_{[10]}\}$ , designation of this group:  **$m$** ,  
 $\{e, m_{[01]}\}$ , designation of this group:  **$m$** ,

unless we also consider the trivial subgroups  $\mathbf{1} \equiv \{e\}$  and  **$2mm$** . The subgroup  $\{e, 2\}$  is denoted by the symbol **2**, the other two by the common symbol  **$m$** , because they represent the same type of symmetry, differing only in the numbering of the basis vectors, which one is considered as  $\mathbf{a}_1$  and which one as  $\mathbf{a}_2$ . If an orthogonal lattice has a symmetry of  **$2mm$** , then a planar structure with such a lattice together with a structure motif may have a symmetry described by the point groups **1, 2,  $m$ ,  $2mm$** . Point groups **1** and **2** also occur in the oblique system, they are characteristic of it, so they are included in the oblique system. Only the  **$m$** , and  **$2mm$**  point groups are included in the rectangular system.

The **group  $4mm$**   $\equiv \{e, 4, 4^2, 4^3, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\bar{1}]}\}$  expresses the point symmetry of the square lattice (the symbol  $m_{[11]}$  represents the reflection in the line dividing the angle between the vectors  $\mathbf{a}_1, \mathbf{a}_2$ , the symbol  $m_{[1\bar{1}]}$  in the line perpendicular to the former). It has the following 8 non-trivial subgroups:

$\{e, 4^2\} \equiv \{e, 2\}$ , group label: **2**,  
 (where  $4^2 \equiv 2$ , because a double  $90^\circ$  rotation is a  $180^\circ$  rotation),  
 $\{e, 4, 4^2, 4^3\}$ , group label: **4**,  
 $\{e, m_{[10]}\}, \{e, m_{[01]}\}, \{e, m_{[11]}\}, \{e, m_{[1\bar{1}]}\}$ , common labeling of groups:  **$m$** ,  
 $\{e, 4^2, m_{[10]}, m_{[01]}\}, \{e, 4^2, m_{[11]}, m_{[1\bar{1}]}\}$  common labelling of groups:  **$2mm$** .

Of these groups, all but the group  $\{e, 4, 4^2, 4^3\}$  are typical of the rectangular system in their nature, so only the groups **4**  $\equiv \{e, 4, 4^2, 4^3\}$  and  **$4mm$**  are included in the square system

The **group  $6mm$**   $\equiv \{e, 6, 6^2, 6^3, 6^4, 6^5, m_0, m_{30}, m_{60}, m_{90}, m_{120}, m_{150}\}$ , expresses the point symmetry of the hexagonal lattice. The notation  $m_{60}$  denotes reflection in a straight line making an angle of  $60^\circ$  with the basis vector  $\mathbf{a}_1$ . It has the following non-trivial subgroups:

$\{e, 6^3\} \equiv \{e, 2\}$ , group label: **2**,  
 $\{e, 6^2, 6^4\} \equiv \{e, 3, 3^2\}$ , group label: **3**,  
 $\{e, 6, 6^2, 6^3, 6^4, 6^5\}$ , group label: **6**,  
 $\{e, m_0\}, \{e, m_{30}\}$ , etc., common label of groups:  **$m$** ,  
 $\{e, 6^2, 6^4, m_0, m_{60}, m_{120}\}, \{e, 6^2, 6^4, m_{30}, m_{90}, m_{150}\}$ , common label:  **$3m$** .

Only the **3,  $3m$ , 6,  $6mm$**  groups are included in the hexagonal system.

## TA2 Affiliation of point groups to the crystal systems

| Crystal system | Point groups belonging to system               | Lattice point group (holohedric group) |
|----------------|------------------------------------------------|----------------------------------------|
| oblique        | <b>1, 2</b>                                    | <b>2</b>                               |
| rectangular    | <b><math>m, 2mm</math></b>                     | <b><math>2mm</math></b>                |
| square         | <b>4, <math>4mm</math></b>                     | <b><math>4mm</math></b>                |
| hexagonal      | <b>3, <math>3m</math>, 6, <math>6mm</math></b> | <b><math>6mm</math></b>                |

According to the point group the belonging of the planar structure to the crystal system is judged. If the lattice has a symmetry higher than required by the crystal system to which the structure belongs, it is said to be **pseudo-symmetric**. For example,

a lattice may have square symmetry, but the structural motif reduces the symmetry to orthogonal. The point groups listed in the last column of the table characterize the symmetry of the lattices belonging to a given crystal system and are called **holohedral groups**.

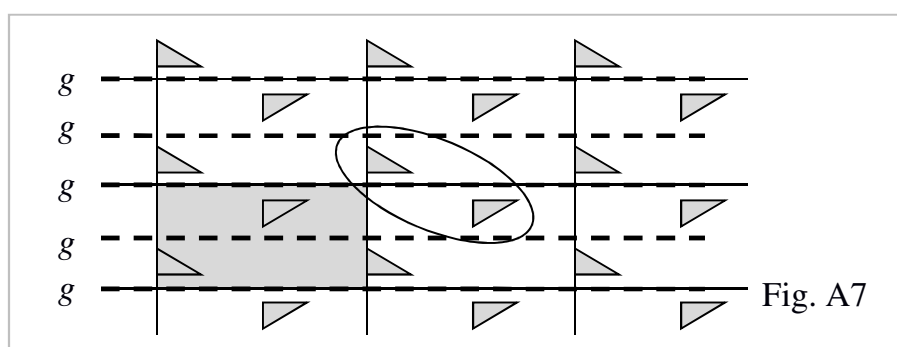
## A4 Plane groups

Plane symmetry represents the periodic distribution of symmetry elements (rotation axes, reflection planes) throughout the plane, the same in each unit cell. Meanwhile, each planar periodic structure is characterized by one of five types of translational symmetry and one of ten types of point symmetry. Combinations of translation groups with point groups give rise to plane groups, but they cannot be combined arbitrarily. For example, the translation group of a hexagonal lattice does not combine with a **4mm** point group. Combinations are only possible within a single crystal system; they are listed in table TA3. The numbers of the plane groups that were formed by direct combination (there are twelve of them) are marked in bold in the table.

TA3 Plane groups

| Group number | Crystal system | Type of unit cell | Point group       | Symbol of plane group |             |
|--------------|----------------|-------------------|-------------------|-----------------------|-------------|
|              |                |                   |                   | full                  | abbreviated |
| 1            | oblique        | <i>p</i>          | 1                 | <i>p1</i>             | <i>p1</i>   |
| 2            |                |                   | 2                 | <i>p211</i>           | <i>p2</i>   |
| 3            | rectangular    | <i>p</i>          | <b><i>m</i></b>   | <i>p1m1</i>           | <i>pm</i>   |
| 4            |                |                   |                   | <i>p1g1</i>           | <i>pg</i>   |
| 5            |                | <i>c</i>          |                   | <i>c1m1</i>           | <i>cm</i>   |
| 6            |                | <i>p</i>          | <b><i>2mm</i></b> | <i>p2mm</i>           | <i>pmm</i>  |
| 7            |                |                   |                   | <i>p2mg</i>           | <i>pmg</i>  |
| 8            |                |                   |                   | <i>p2gg</i>           | <i>pgg</i>  |
| 9            |                | <i>c</i>          |                   | <i>c2mm</i>           | <i>cmm</i>  |
| 10           | square         | <i>p</i>          | 4                 | <i>p4</i>             | <i>p4</i>   |
| 11           |                |                   | <b><i>4mm</i></b> | <i>p4mm</i>           | <i>p4m</i>  |
| 12           |                |                   |                   | <i>p4gm</i>           | <i>p4g</i>  |
| 13           | hexagonal      | <i>p</i>          | 3                 | <i>p3</i>             | <i>p3</i>   |
| 14           |                |                   | <b><i>3m</i></b>  | <i>p3m1</i>           | <i>p3m1</i> |
| 15           |                |                   |                   | <i>p31m</i>           | <i>p31m</i> |
| 16           |                |                   | 6                 | <i>p6</i>             | <i>p6</i>   |
| 17           |                |                   | <b><i>6mm</i></b> | <i>p6mm</i>           | <i>p6m</i>  |

The twelve types do not exhaust the symmetry of planar structures. The structural motif, but also the lattice itself, in some cases induces a special element of symmetry in the structure – a **glide line**. The corresponding operation – **glide reflection** – consists of a reflection in the glide line and a subsequent translation parallel to the glide line. The translational part of this operation does not belong to the translation group, because the magnitude of the displacement (translation) is equal to half the length of the shortest lattice vector parallel to the glide line; therefore, on its own, it cannot represent a symmetry operation. The glide reflection does not belong to the point group either, because it contains the translation – it is a specific element of the plane group. Figure A7 shows part of a planar structure with glide lines.



The structural motif is indicated by an ellipse, the glide lines are dashed and labelled with  $g$ , the unit cell is highlighted in grey. Just by reflection in the glide line, the structural motif does not get to the congruent position, it still has to move by half of the lattice parameter along the glide line. Glide reflections are part of the four types of symmetry of planar structures, denoted in Table TA3 by serial numbers 4, 7, 8 and 12.

In the **oblique system**, glide lines do not occur because there are no reflection lines.

In the **rectangular system**, if the lattice is primitive, glide lines can arise by transformation from reflection lines due to the influence of a structural motif (as seen in Figure A7), so that in addition to the  $pm$  and  $p2mm$  groups, the  $pg$ ,  $p2mg$ , and  $p2gg$  groups also belong to this crystal system. If the lattice is centred, glide lines occur in it even without the influence of the structural motif. Their presence in the structure therefore does not represent a new type of symmetry, so that, for example, the  $c2gg$  type does not appear in Table TA3 because it is identical to the  $p2gg$  type.

In the **square system**, the properties of an orthogonal lattice (orthogonal unit cell) meet those of a lattice whose unit cell is rhombic (at point Q in Figure A3). Both have a point symmetry described by a  $2mm$  group, but differ in the orientation of the

reflection lines. In the orthogonal lattice, the reflection lines are parallel to the sides of the unit cell; in the rhombic lattice, the reflection lines are parallel to the sides of the rhombic cell (Fig. A8.). Therefore, for a rhombic lattice, the typical glide lines are parallel to the diagonals, which then also occur in a square lattice. Therefore, the presence of such glide lines in the square structure does not represent a new type of symmetry. However, a new type can be created by a structural motif that turns the reflection lines parallel to the sides of the square unit cell into glide lines.

In the  $4mm$  symbol, the first  $m$  refers to systems of reflection lines parallel to the sides of the square, the second  $m$  to systems parallel to its diagonals. Therefore, in addition to the symmetry type  $p4mm$ , the type  $p4gm$  can occur as a separate type in the square system, but not the types  $p4mg$  and  $p4gg$ .

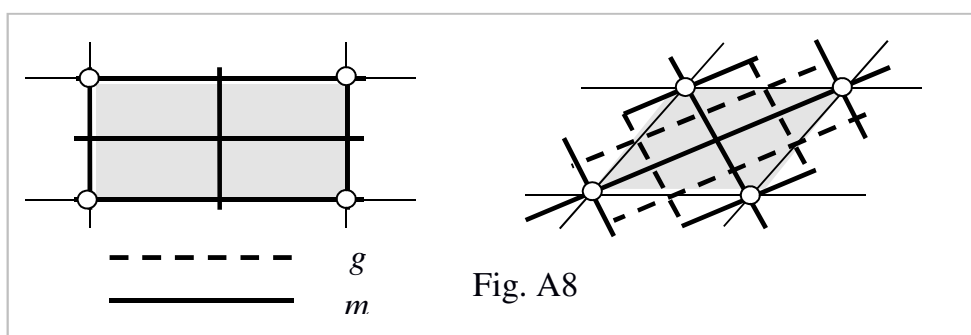


Fig. A8

In the **hexagonal system**, there are no symmetry types in which the presence of glide lines is induced by a structural motif. Also in the hexagonal lattice, the symmetries of two types of lattices - orthogonal centred and rhombic (at point H in Figure A3) – meet. In the orthogonal centred lattice, there are glide lines parallel to both basis vectors, but in the rhombic centred lattice parallel to the diagonals of the rhombus. Therefore, in the hexagonal lattice, their presence does not represent a new type of symmetry.

Particular mention should be made of the plane groups denoted by numbers 14 and 15, which differ in the orientation of the structural motif with trigonal symmetry with respect to the basis vectors of the hexagonal lattice. Therefore, the reflection and glide lines are oriented differently in these groups.

A graphical representation of the 17 types of plane groups is given in the figure part of this book.

## A5 Symmetries of three-dimensional periodic structures

When searching for different types of space lattices differing from each other by their symmetry, it is possible to start from the known five types of planar lattices and proceed by analogy, i.e. search for the third shortest lattice vector. By such a procedure it can be found that there are 14 types of space lattices (so-called **Bravais**

**lattices**), characterized by 14 types of translation groups, which on the basis of their point symmetry are classified into 7 crystal systems. Their point symmetry is characterized by 7 so-called holohedral (i.e. complete) groups, which together with their subgroups form a set of 32 point groups of three-dimensional periodic structures. Structures whose structural motif has symmetry lower than the lattice or is inappropriately oriented with respect to the lattice have symmetry lower than the holohedral symmetry. These 32 point groups characterize the point symmetry of crystals belonging to one of the 32 crystal classes. They determine the macroscopic symmetry - the symmetry of the external shapes of well-developed crystals, but also the symmetry of the physical properties of the crystals, which is manifested by their anisotropy.

| <b>TA4 Lattices and point groups of three-dimensional structures</b> |                                                                                                                                                              |                                |                                                                                         |
|----------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------|-----------------------------------------------------------------------------------------|
| <b>Crystal system</b>                                                | <b>Lattice parameters</b>                                                                                                                                    | <b>Types of lattices</b>       | <b>Point groups</b>                                                                     |
| Triclinic                                                            | $a_1, a_2, a_3$<br>$\alpha_1, \alpha_2, \alpha_3$                                                                                                            | $P$                            | $1, \bar{1}$                                                                            |
| Monoclinic                                                           | $a_1, a_2, a_3$<br>$\alpha_1 = \alpha_3 = 90^\circ, \alpha_2$                                                                                                | $P$<br>$(C_1, C_2, I)$         | $2, m, \frac{2}{m}$                                                                     |
| Orthorombic                                                          | $a_1, a_2, a_3$<br>$\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$                                                                                               | $P, I, F$<br>$(C_1, C_2, C_3)$ | $222, mm2, \frac{2}{m} \frac{2}{m} \frac{2}{m}$                                         |
| Tetragonal                                                           | $a_1 = a_2, a_3$<br>$\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$                                                                                              | $P, I$                         | $4, \bar{4}, \frac{4}{m}, 422$<br>$4mm, \bar{4}2m, \frac{4}{m} \frac{2}{m} \frac{2}{m}$ |
| Trigonal                                                             | $a_1 = a_2 = a_3$<br>$\alpha_1 = \alpha_2 = \alpha_3 \neq 90^\circ$<br><hr/> $a_1 = a_2, a_3$<br>$\alpha_1 = \alpha_2 = 90^\circ,$<br>$\alpha_3 = 120^\circ$ | $R$<br><br>$P$                 | $3, \bar{3}, 32, 3m, \bar{3} \frac{2}{m}$                                               |
| Hexagonal                                                            | $a_1 = a_2, a_3$<br>$\alpha_1 = \alpha_2 = 90^\circ,$<br>$\alpha_3 = 120^\circ$                                                                              | $P$                            | $6, \bar{6}, \frac{6}{m}, 622$<br>$6mm, \bar{6}2m, \frac{6}{m} \frac{2}{m} \frac{2}{m}$ |
| Cubic                                                                | $a_1 = a_2 = a_3$<br>$\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$                                                                                             | $P, I, F$                      | $23, \frac{2}{m} \bar{3}, 432$<br>$\bar{4}3m, \frac{4}{m} \bar{3} \frac{2}{m}$          |

Table TA4 shows the distribution of lattice types and point groups into crystal systems. The membership of a crystal in a crystal system is determined on the basis of its point symmetry, i.e., its point group. The relations between lattice parameters in individual crystal systems (**system metrics**) are also given in the table. In the last column are the symbols of the point groups, while the last in the row is the symbol of the holohedral group, expressing the symmetry of the lattice belonging to the corresponding crystal system.

The table uses the unabbreviated international symbols to denote the point groups. For example, the symbol  $\bar{1}$  represents the inversion,  $\bar{4}$  the fourfold inverse axis (rotation combined with inversion),  $\frac{6}{m}$  the sixfold axis with the plane of symmetry perpendicular to it,  $3m$  the threefold axis lying in the reflection plane. The symbols in the point group labels also have a specified order. For example, in the cubic system, if a symbol consists of three symbols in a row, the first refers to an edge of the cube, the second to a solid, and the third to a wall diagonal. When denoting the angle between two basis vectors, the index of the third one is used. The symbol *P* represents **primitive** unit cell, *I* **body centred** and *F* **face centred** unit cell. When several such symbols are given in parentheses, it means that the corresponding lattice types are equivalent, differing only in the choice of basis vectors. The index (e.g.  $C_1$ ,  $C_2$ ) is assigned according to which of the faces of the unit cell is centred, the same rule for assigning the index as for angles between basis vectors.

The structure of each crystal has a certain translational and point symmetry. Their different combinations, together with the presence of different types of glide planes and screw axes, produce 230 types of symmetry of three-dimensional periodic structures, 230 **space groups**. Their detailed description is given in the international tables [7].

In the following Table TA5 the numbers characterizing the multiplicity of symmetry types of two- and three-dimensional periodic structures are given.

**TA5 Number of groups in planar and space structures**

| Periodic structures | Crystal systems | Lattice types | Point groups | Plane/Space groups |
|---------------------|-----------------|---------------|--------------|--------------------|
| Two dimensional     | 4               | 5             | 10           | 17                 |
| Three dimensional   | 7               | 14            | 32           | 230                |

## Part B

### Representation of symmetry operations by matrices and tensors

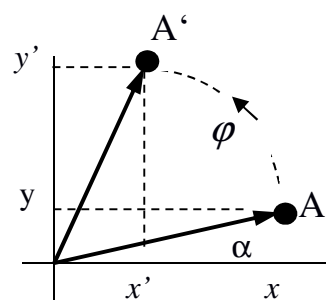
The representation of symmetry operations by matrices (tensors) is understood as such an assignment of a matrix (tensor) to each symmetry operation, which ensures that the result of the successive application of two symmetry operations corresponds to the matrix (tensor) that results from the product of the respective assigned matrices (tensors). The set of symmetry operations in each crystal class forms a group, and, crucially from a representational point of view, the corresponding matrices or tensors also form a group in terms of the multiplication defined between the matrices or tensors, respectively. In other words – if an element  $g$  of the group  $G$  of symmetry operations is assigned the matrix  $M_g$ , and an element  $h$  the matrix  $M_h$ , then the product  $gh$  of these two elements (i.e. their successive application) is assigned the matrix that results from the product of the respective matrices  $M_g M_h$ . The mutually unambiguous assignment of matrices (tensors) to symmetry operations thus gives rise to an isomorphic group of matrices (tensors). The **matrices**, or **tensors**, are then understood as **operators** by means of which the positions of points in space, i.e. their spatial coordinates, are transformed (changed) by appropriate mathematical rules.

#### B1 Representation by matrices

In order to write about the representation of symmetry operations by matrices, it is first necessary to clarify the notion of matrix in the context of spatial transformation of objects. In spatial transformations, such as symmetry operations, individual points of the transformed object are moved to new positions. By relocating a point, its original  $x, y, z$  coordinates in the external coordinate system are changed to  $x', y', z'$ . For example, moving a point by  $x_0$  in the  $x$ -axis direction, changes its coordinates to

$$x' = x + x_0, \quad y' = y, \quad z' = z.$$

If it is a rotation of the body by a certain angle, then such relationships are more complicated. Consider the case of a rotation of a point  $A$  in the plane by an angle  $\varphi$  counter-clockwise about an axis perpendicular to this plane and passing through the



Obr. B1

origin of the coordinate system (Fig. B1). Let point A have coordinates  $x, y$  and hence a distance from the origin of the coordinate system  $r = \sqrt{x^2 + y^2}$ ; after rotation to point  $A'$  it will take on the coordinates  $x', y'$ , the relations being valid:

$$\begin{aligned} x &= r \cos \alpha & y &= r \sin \alpha \\ x' &= r \cos(\alpha + \varphi) & y' &= r \sin(\alpha + \varphi) \end{aligned}$$

or after modification:

$$\begin{aligned} x' &= r \cos(\alpha + \varphi) = r \cos \alpha \cos \varphi - r \sin \alpha \sin \varphi = x \cos \varphi - y \sin \varphi \\ y' &= r \sin(\alpha + \varphi) = r \sin \alpha \cos \varphi + r \cos \alpha \sin \varphi = y \cos \varphi + x \sin \varphi \end{aligned}$$

and after appropriate reordering of members:

$$\begin{aligned} x' &= x \cos \varphi - y \sin \varphi \\ y' &= x \sin \varphi + y \cos \varphi . \end{aligned} \tag{B1.1}$$

This result is written symbolically in the form:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} , \tag{B1.2}$$

in which there are two **column matrices** representing the positions of points (also understood as position vectors) and one **square matrix** representing the transformation of the point position. Only the rotation angle  $\varphi$  appears in the **transformation matrix**, but neither the angle  $\alpha$  of the original position of the point nor its distance  $r$  from the origin of the coordinate system appear in it. Therefore, such a matrix is suitable for calculating the change in coordinates of any point in the plane as it is rotated about the origin of the coordinate system.

The product of the square transformation matrix with the column matrix is indicated on the right-hand side of equation (B1.2), and rules are introduced for their product such that the product returns to the original transformation equations (B1.1). We will state these rules for the case of a square matrix of size  $2 \times 2$ , i.e., a matrix of second degree:

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} , \tag{B1.3}$$

where in the symbol  $a_{ij}$  the first index represents the row number in the matrix, the second the column number. Similarly, using the indices denoting the rows, the coordinates in the column matrices are also expressed, where instead of the symbols  $x$  and  $y$  we use the symbols  $x_1$  and  $x_2$  :

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} , \quad \begin{pmatrix} x'_1 \\ x'_2 \end{pmatrix} .$$

In this notation of both square and column matrices, their product is expressed in the form:

$$\begin{pmatrix} x'_1 \\ x'_2 \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad (\text{B1.4})$$

and rules of their product as follows:

$$x'_1 = a_{11}x_1 + a_{12}x_2 \quad x'_2 = a_{21}x_1 + a_{22}x_2, \quad (\text{B1.5})$$

or more generally:

$$x'_i = \sum_{j=1}^2 a_{ij} x_j. \quad (\text{B1.6})$$

The matrix from equation (B1.2) will be used to determine the shape of the matrices representing the symmetry operations appearing in all the point groups listed in Section A. These are the rotations by  $60^\circ$ ,  $90^\circ$  and their multiplicities, the reflections in different lines, as well as the inversion, which is, however, identical to the rotation by  $180^\circ$  in planar structures. Each of the ten point groups contains a so-called neutral element – identity (denoted by the letter  $e$ ), when the position of the points of the object does not change, i.e. when it is a rotation by  $0^\circ$  (respectively by  $360^\circ$ ), where  $\cos 0 = 1$  and  $\sin 0 = 0$ ; the neutral element thus corresponds to the so-called **unit matrix**

$$\begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \equiv e. \quad (\text{B1.7})$$

In each of the four planar crystal systems there is a holohedral point group, the other point groups belonging to this system being subgroups of it. This also applies to the corresponding matrices. It is therefore sufficient to give the form of the transformation matrices representing the symmetry operations belonging to the holohedral group of the respective system.

In the **oblique system**, the holohedral group is the group with label **2**, which contains only two elements:  $\{e, 2\}$ , i.e. the identity and the rotation by  $180^\circ$  ( $= \pi$  rad). For this angle the relations:  $\sin \pi = 0$ ,  $\cos \pi = -1$  hold, so these two operations are represented by matrices:

$$e \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad 2 \equiv \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (\text{B1.8})$$

We will see that the matrix representing the element with symbol **2** will rotate every position vector to the opposite one if we use the rules of B1.5:

$$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} -x_1 \\ -x_2 \end{pmatrix}. \quad (\text{B1.9})$$

This means that a rotation in the plane by  $180^\circ$  is also an inversion.

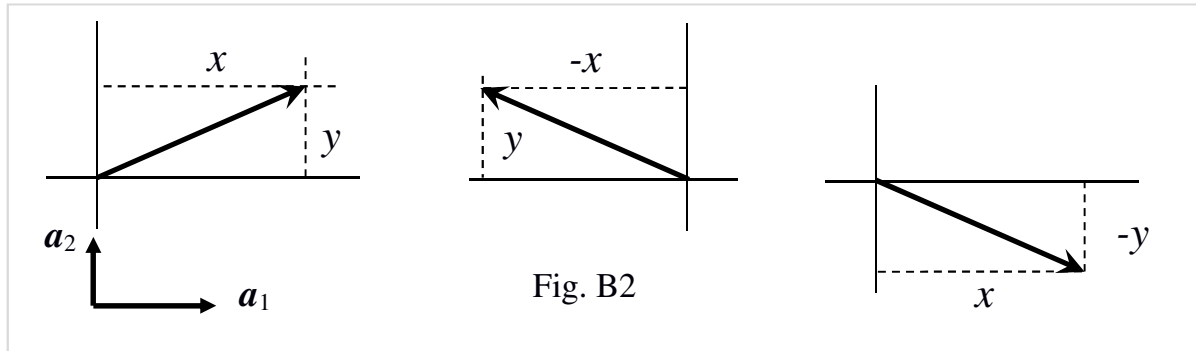
In the **rectangular system** (symmetry of a rectangle), it is a group of **2mm** that contains the following elements (symmetry operations):  $\{e, 2, m_{[10]}, m_{[01]}\}$ , where the symbol  $m_{[10]}$  represents the reflection in a line perpendicular to the basis vector  $\mathbf{a}_1$  and the symbol  $m_{[01]}$  the reflection in a line perpendicular to the vector  $\mathbf{a}_2$ . The matrices representing the elements of this group have the form:

$$e \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad 2 \equiv \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad m_{[10]} \equiv \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad m_{[01]} \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{B1.10})$$

The correctness of the above form of the matrices representing the reflection can be verified by using the rules of B1.5, by applying these matrices to a vector with coordinates  $(a, b)$ :

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} -a \\ b \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ -b \end{pmatrix},$$

from which, as well as from figure B2, it can be seen that the first of the matrices has changed to the opposite first coordinate of the vector, so that it is a reflection in the y-axis (the vertical axis, perpendicular to the vector  $\mathbf{a}_1$ ), the second of the matrices the second coordinate, so that it is a reflection in the x-axis (the axis perpendicular to the vector  $\mathbf{a}_2$ ).



In the **square system**, the holohedral group is the **4mm** group containing eight elements:  $\{e, 4, 4^2, 4^3, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\bar{1}]}\}$ . The symbols  $m_{[11]}$  and  $m_{[1\bar{1}]}$  represent reflections in the diagonals of the square unit cell. The matrices representing the elements of this group have the form:

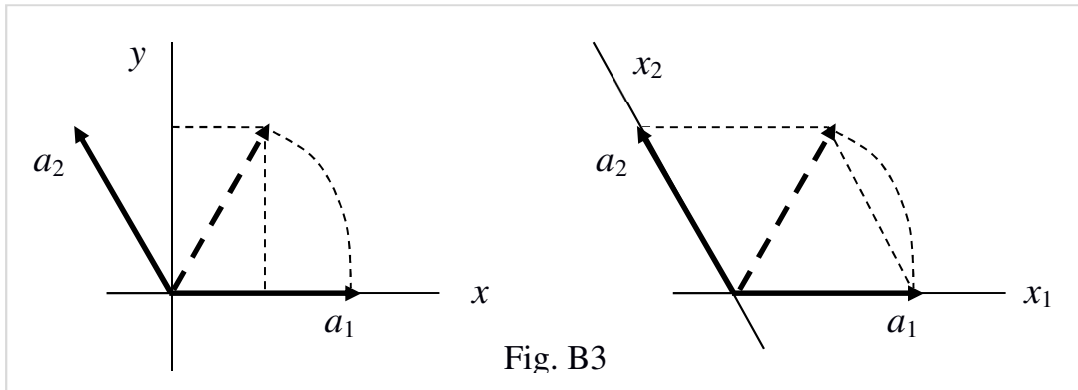
$$e \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad 4 \equiv \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad 4^2 \equiv 2 \equiv \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad 4^3 \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\ m_{[10]} \equiv \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad m_{[01]} \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad m_{[11]} \equiv \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad m_{[1\bar{1}]} \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (\text{B1.11})$$

The **hexagonal** holohedral point group of **6mm**, describing the symmetry of a hexagon, has the largest number of elements:

$\{e, 6, 6^2, 6^3, 6^4, 6^5, m_0, m_{30}, m_{60}, m_{90}, m_{120}, m_{150}\}$ , where the indices at the symbols  $m$  express the angle formed by the reflection line with the basis vector  $\mathbf{a}_1$  and the symbols  $6, 6^2, 6^3 \dots$  represent rotations by  $60^\circ, 120^\circ, 180^\circ \dots$ . The corresponding matrices have the form:

$$\begin{aligned} e &\equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad 6 \equiv \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, \quad 6^2 \equiv 3 \equiv \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \quad 6^3 \equiv 2 \equiv \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \\ 6^4 \equiv 3^2 &\equiv \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \quad 6^5 \equiv \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, \quad m_0 \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad m_{30} \equiv \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\ m_{60} &\equiv \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, \quad m_{90} \equiv \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad m_{120} \equiv \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, \quad m_{150} \equiv \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \end{aligned} \quad (\text{B1.12})$$

In the matrices representing symmetry operations of the oblique, rectangular and square systems, only integers (0, 1, -1) are located; in the hexagonal system, fractions and even irrational numbers are situated. This is a consequence of the use of the Cartesian coordinate system, whose coordinate axes take the angle  $90^\circ$ , although the basis vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , and hence the axes of the so-called natural hexagonal coordinate system, take the angle  $120^\circ$ . When using the natural coordinate system, even in the hexagonal system, only integers are in the transformation matrices. For example, rotating the hexagonal basis vector  $\mathbf{a}_1$  by  $60^\circ$  produces a vector (dashed in Figure B3) that in the Cartesian system (left part of the figure) is projected onto the x-axis at half its magnitude, so that it has a coordinate of  $1/2$ , but its y-coordinate has a



value of  $\sqrt{3}/2$ , which is then reflected in the transformation matrix. If, however, turning is considered in terms of the natural coordinate system (right part of the figure), the projection of the rotated vector in both directions determined by the pair of basis vectors is evaluated by coordinates of magnitude 1. Therefore, even in a transformation matrix expressed in the natural coordinate system, only integers stand out. The transformation matrix of a rotation by  $60^\circ$  then has the form

$$6 \equiv \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}, \quad (\text{B1.13})$$

and its effect on the vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  will be verified. In the natural system, these vectors are written as column matrices:  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ , so we write their transformations as products:

$$\begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}.$$

The result shows that rotating the vector  $\mathbf{a}_1$  by  $60^\circ$  counter-clockwise produces a vector equal to the sum of  $\mathbf{a}_1 + \mathbf{a}_2$ , and rotating the vector  $\mathbf{a}_2$  becomes the vector  $-\mathbf{a}_1$ .

Having given matrices representing the symmetry operations of all four holohedral plane point groups, we can show that the matrices, like the symmetry operations, form a group. This group is isomorphic to the group of symmetry operations of the corresponding crystal class. The set of corresponding matrices forms a group in terms of their multiplication with each other, which, however, needs to be defined. By definition, the product of two square matrices  $A$  and  $B$ , whose elements we denote by the symbols  $a_{ij}$ , and  $b_{ij}$  respectively, gives rise to a new square matrix  $C$ , whose elements  $c_{ij}$  are calculated according to the relation:

$$c_{ij} = \sum_k^n a_{ik} b_{kj}. \quad (\text{B1.14})$$

In two-dimensional space the addition index  $k$  takes only the values 1, 2.

We give an example from the square system, namely the successive application of the rotations by  $90^\circ$  and  $180^\circ$  ( $\rightarrow$  B1.11), which together represent the rotation by  $270^\circ$ :  $4 \cdot 4^2 = 4^3$ . The product of the matrices representing the rotations about  $90^\circ$  and  $180^\circ$  will indeed give the matrix representing the rotation about  $270^\circ$ :

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

which can be verified by using relation (B1.14). Of course, this is also true for other combinations of symmetry operations within a single crystal class. For the set of

matrices representing the symmetry operations of a crystal class to form a group, it must satisfy four conditions.

The product of such two matrices gives a matrix that belongs to this group. This satisfies the closedness condition of the set forming the group.

It can be further verified that the associative law holds for the product of matrices, which the reader can verify for himself. This satisfies the second of the conditions.

Each of the above matrix clusters contains a **unit matrix**  $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ , characterized by the fact that the product with another matrix does not change it. For example:

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

The last condition, is the existence of an inverse element for each of the elements of the group, i.e. in this case the inverse matrix. Here we give an example from the square system, where, say, the inverse element to a rotation by  $90^\circ$  (the element denoted by the symbol 4) is a rotation by  $270^\circ$  (the element denoted by the symbol  $4^3$ ), because their successive application is a rotation by  $360^\circ$ , i.e., a rotation to a position as without rotation. Expressed using the appropriate matrices:

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

This verified all four conditions for the set of matrices representing the symmetry operations to form a group.

An important characteristic of the transformation **matrix** is its **determinant D**. It is a number which, in the case of the matrix  $\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$  is calculated using the formula

$$D = a_{11}a_{22} - a_{12}a_{21}. \quad (\text{B1.15})$$

On the above matrices it can be seen that the determinants of the matrices representing rotations have the value +1, and the determinants of the matrices representing reflections have the value -1. Without proof, we will state that if the absolute value of the determinant of a matrix is equal to 1, it is a transformation in which the distances between any two points of the transformed object are preserved, i.e., there is no deformation of the transformed object. These are so-called **orthogonal matrices**.

Another important characteristic of matrices is their **trace**  $S$ , which is the sum of the members located on the principal diagonal; in the case of a matrix notation of the form B1.3

$$S = a_{11} + a_{22} . \quad (\text{B1.16})$$

In representation theory, the name **character of representation** is used for this number.

## B2 Representation by tensors

The tensor representation is essentially just a modification of the matrix representation. In the matrix representation discussed in Section B1, the transformations were assumed to take place in a Cartesian coordinate system with  $x$  and  $y$  axes. This choice of coordinate system is easily applied in both rectangular and square systems. In other systems (oblique and hexagonal) it is more convenient to adapt the direction of the coordinate axes to the direction of the pair of basis vectors and to consider their lengths as units in the respective directions. While this is possible also in matrix representation, it is not immediately apparent from the notation of the matrices what coordinate system is being used. In the tensor representation, the basis vectors appear explicitly, directly in the notation of the tensors representing the corresponding symmetry operations.

In the **oblique** crystal system, the basis vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  do not have equal lengths and take an angle different from the special angles  $90^\circ$  and  $60^\circ$  typical of the rectangular, square and hexagonal systems ( $\rightarrow$  part A2). The holohedral point group **2** of this system contains only two elements, the identity and the rotation by  $180^\circ$ , represented by the matrices

$$e \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \quad 2 \equiv \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} .$$

The tensor notation of these operators has the form ( $\rightarrow$  table TC2b)

$$\bar{\mathbf{1}} \equiv \mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2 \quad \bar{\mathbf{2}} \equiv -\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2 \quad (\text{B2.1})$$

where  $\mathbf{a}^1$  and  $\mathbf{a}^2$  are a pair of vectors reciprocal to the pair  $\mathbf{a}_1, \mathbf{a}_2$  ( $\rightarrow$  end of section A1).

In the rectangular system, the basis vectors are perpendicular to each other but have different lengths. The holohedral point group has four elements represented by matrices

$$e \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad 2 \equiv \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad m_{[10]} \equiv \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad m_{[01]} \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

or by tensors

$$\begin{aligned} \bar{\bar{1}} &\equiv \mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2, \quad \bar{\bar{2}} \equiv -\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2, \\ \bar{\bar{M}}_{10} &\equiv -\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2, \quad \bar{\bar{M}}_{01} \equiv \mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2. \end{aligned} \quad (\text{B2.2})$$

The tensors representing the two rotations typical of a **hexagonal** system have the shape:

$$\bar{\bar{3}} = \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2, \quad \bar{\bar{6}} = \mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1 \quad (\text{B2.3})$$

From the above examples it can be seen that the tensors also in the hexagonal system contain only integer coefficients for the dyads, which is a consequence of the use of the natural coordinate system.

Starting from relations A1.2 and D30.18, the tensor  $\bar{\bar{2}}$  transforms the vector  $\mathbf{a}_1$  as follows:

$$\mathbf{a}_1 \cdot \bar{\bar{2}} = \mathbf{a}_1 \cdot (-\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2) = -\mathbf{a}_1$$

because  $\mathbf{a}_1 \cdot \mathbf{a}^1 = 1$  and  $\mathbf{a}_1 \cdot \mathbf{a}^2 = 0$ . Tensor  $\bar{\bar{2}}$  has thus changed the direction of the vector  $\mathbf{a}_1$  to the opposite direction.

For matrix multiplication, relation B1.14 applies, and the rule for tensor multiplication is given in Appendix D30, as relation D30.7. As an example, the rotation by  $90^\circ$  applied twice, so it is a rotation by  $180^\circ$ . The rotation by  $90^\circ$  is represented by the tensor  $\bar{\bar{4}} = \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1$ , and the double rotation is expressed as the product of the tensors  $\bar{\bar{4}} \cdot \bar{\bar{4}}$ . This product is to coincide with the tensor  $\bar{\bar{2}} = -\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2$  representing the rotation by  $180^\circ$ :

$$\begin{aligned} \bar{\bar{4}} \cdot \bar{\bar{4}} &= (\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1) \cdot (\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1) = \\ &= \mathbf{a}^1 \mathbf{a}_2 \cdot (\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1) - \mathbf{a}^2 \mathbf{a}_1 \cdot (\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1) = \\ &= \mathbf{a}^1 (\mathbf{a}_2 \cdot \mathbf{a}^1) \mathbf{a}_2 - \mathbf{a}^1 (\mathbf{a}_2 \cdot \mathbf{a}^2) \mathbf{a}_1 - \mathbf{a}^2 (\mathbf{a}_1 \cdot \mathbf{a}^1) \mathbf{a}_2 + \mathbf{a}^2 (\mathbf{a}_1 \cdot \mathbf{a}^2) \mathbf{a}_1 = \\ &= -\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2 = \bar{\bar{2}}, \end{aligned}$$

for  $\mathbf{a}_2 \cdot \mathbf{a}^1 = \mathbf{a}_1 \cdot \mathbf{a}^2 = 0$  and  $\mathbf{a}_1 \cdot \mathbf{a}^1 = \mathbf{a}_2 \cdot \mathbf{a}^2 = 1$ .

An important characteristic is the **scalar of the tensor** ( $\rightarrow$  D30.9), which is equivalent to the trace of the matrix. The **determinant** corresponding to the **tensor** is

obtained by fitting the coordinates of the tensor ( $\rightarrow$  D30.15) to the matrix and then calculating as in the matrix.

All significant tensors are listed in Tables TC2a and TC2b on page 48.

### B3 Elements of representation theory

Representation theory began to develop in the early 20th century. It found wide application not only in mathematics, but also in the consideration of various kinds of physical systems in terms of their symmetry. For example, it has been applied in the classification of quantum states (energy levels) in atoms, molecules and crystals, in the determination of selection rules (allowed and forbidden quantum transitions), which is directly related to the spectra of electromagnetic radiation.

The **trace** of matrices play an important role in representation theory. We give one example – matrices representing the symmetry operations of the **2mm** group ( $\rightarrow$  B1.10):

$$e \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad 2 \equiv \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad m_{[10]} \equiv \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad m_{[01]} \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (\text{B3.1})$$

It has already been mentioned in section B1 that the **determinants** of the matrices representing rotations have the value +1, for reflections the value –1. However, the traces of the matrices, i.e. the sum of the elements in the principal diagonal, have a different meaning. The trace of the matrix representing the identity  $e$  has in this example the value  $S = 2$ , i.e. the same as the number of rows of the square matrix. This is related to the dimension of the space in which the symmetry operations are described. The trace of the matrix representing the rotation by  $180^\circ$  has value  $S = -2$ , and the traces of the matrices representing reflections have value  $S = 0$ . Different trace values correspond to different types of symmetry operations; they can be said to indicate the **character** (nature) of the symmetry **operation**, which probably led to the appropriate naming of this parameter. However, the numerical value of the character also depends on the particular type of representation. The trace values can also be verified on the matrices in the other crystal systems mentioned above.

As mentioned at the beginning of Section B, the matrix representation of symmetry operations is understood as the matrix assignment to each symmetry operation that ensures that the result of the successive application of two symmetry operations corresponds to the matrix obtained by the product of the respective assigned matrices. If a different matrix is assigned to each operation, then the group

of symmetry operations and the group of matrices are isomorphic. The name **faithful representation** is used for such a representation. However, representation theory also considers the so-called homomorphic representation ( $\rightarrow$  Appendix D29), where more symmetry operations are assigned to the same matrix, but keeping the condition stated in the first sentence of this paragraph. This gives rise to different representations, differing also in the characters of the individual operations. A homomorphic representation can be achieved, for example, by assigning one matrix to all symmetry operations belonging to a certain class of associated elements. In doing so, these matrices need not match in size (degree) the dimension of the space in which the symmetry operations are described.

A total trivial homomorphic representation is to assign the number 1 to all symmetry operations. The number 1 can be thought of as an element of a matrix of size  $1 \times 1$ . Such a "set" containing a single element satisfies all the group postulates in terms of multiplication, since it is closed, contains a neutral element which is itself an inverse element, and the associative law holds when multiplying between units. The following table shows three representations of the group **3m** (denoted by a, b, c), which is a subgroup of the above-mentioned group **6mm** ( $\rightarrow$  B1.12) and represents the symmetry operations of an equilateral triangle. In the first line there is a trivial representation in units, the representation in the second line is already richer, it also contains elements  $-1$ , which are assigned to reflections. In the first two rows these are homomorphic representations, one-dimensional representations. Only in the third line are the representations isomorphic, representing the so-called vector representation, which corresponds in degree of matrices to the dimension of the space in which the symmetry operations are described.

|   | <i>e</i>                                       | 3                                                                                                       | 3 <sup>2</sup>                                                                                          | <i>m</i> <sub>0</sub>                           | <i>m</i> <sub>60</sub>                                                                                | <i>m</i> <sub>120</sub>                                                                                 |
|---|------------------------------------------------|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|-------------------------------------------------|-------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
| a | 1                                              | 1                                                                                                       | 1                                                                                                       | 1                                               | 1                                                                                                     | 1                                                                                                       |
| b | 1                                              | 1                                                                                                       | 1                                                                                                       | -1                                              | -1                                                                                                    | -1                                                                                                      |
| c | $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$ | $\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ | $\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$ | $\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$ |

Matrices in different representations have different characters, which are the same for elements belonging to the same class of associated elements. The **3m** group has three classes of associated elements: {*e*}, {3, 3<sup>2</sup>} and {*m*<sub>0</sub>, *m*<sub>60</sub>, *m*<sub>120</sub>}, which can be verified using its multiplication table TC5 (in the tabular part of the text); the characters assigned to them are listed in the following table:

|   | $e$ | $\{3, 3^2\}$ | $\{m_0, m_{60}, m_{120}\}$ |
|---|-----|--------------|----------------------------|
| a | 1   | 1            | 1                          |
| b | 1   | 1            | -1                         |
| c | 2   | -1           | 0                          |

(B3.3)

In two-dimensional space (in the plane), symmetry operations can be represented by "larger" matrices than  $2 \times 2$ , e.g. square matrices of size  $3 \times 3$ , or even larger. This is also true for multidimensional spaces. For example, the matrices (B3.1) can be expanded by both a row and a column, and the number 1 can be written in their intersection. This gives the form:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (\text{B3.4})$$

The set of matrices thus expanded equally well represent the group **2mm**. The above matrices can be expanded in even more complex ways, for example, by repeating the square matrix  $2 \times 2$  in the principal diagonal of the expanded matrix, while leaving the other elements of the matrix zero. The augmented matrices from relation (B3.1) then take the form:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (\text{B3.5})$$

A property of all these particular matrices is that, when transforming a four-dimensional vector with coordinates  $x_1, x_2, x_3, x_4$ , the coordinates  $x'_1$  and  $x'_2$  of the resulting vector are not expressed as a combination of all four coordinates of the original vector, but only the first two, i.e. the coordinates  $x_1$  and  $x_2$ . Similarly, the coordinates  $x'_3$  and  $x'_4$  are expressed as a combination of only the coordinates  $x_3$  and  $x_4$ . This means that the corresponding four-dimensional space in terms of the symmetry operations represented by matrices of the type (B3.5) can be divided into two independent, so-called *invariant* parts. The above statement can be seen well in its general notation:

$$\begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \\ x'_4 \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & a_{44} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} a_{11}x_1 + a_{12}x_2 \\ a_{21}x_1 + a_{22}x_2 \\ a_{33}x_3 + a_{34}x_4 \\ a_{43}x_3 + a_{44}x_4 \end{pmatrix} \quad (\text{B3.6})$$

The extension of the matrices can be even more complex, matrices of different sizes can be inserted into the main diagonal, creating so-called quasidiagonal matrices. Such extended matrices can be reduced to their original "smaller" form, hence they are called **reducible**, and the space in which such matrices act can thus be decomposed into invariant subspaces. Matrices that cannot be reduced are **irreducible**, and such matrices are important in representation theory. The definition of reducible and irreducible matrix representations relies precisely on the possibility of partitioning spaces into invariant subspaces in terms of the action of matrices in these spaces.

One of the important theorems of representation theory states that the number of irreducible representations of any group of symmetry operations is equal to the number of classes of its associated elements. Therefore, the group **3m** has 3 irreducible representations, denoted in Table B3.2 by a, b, c. As the simplest example of a reducible representation, consider the group **2** (the oblique system), which contains only the identity *e* and the rotation by 180°, denoted by the symbol 2. This group has only two elements, so it can have at most two classes of associated elements, and these are {*e*} and {2}, so that there is only one element in each class. By the above theorem, this group can have only two irreducible representations. By relation (B1.8), two elements of this group are represented by matrices:

$$e \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad 2 \equiv \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix},$$

which, when compared to the augmented matrices (B3.5), have a similar structure, they look like augmented quasidiagonal matrices, formed by one-dimensional matrices 1 and −1, respectively. Therefore, this representation is reducible. The two irreducible representations we are looking for, together with a third reducible representation, are listed in the following table, including the characters of the corresponding operations in each representation:

| Representations | <i>e</i>                                       | 2                                                |  | characters |    | (B3.7) |
|-----------------|------------------------------------------------|--------------------------------------------------|--|------------|----|--------|
|                 |                                                |                                                  |  | <i>e</i>   | 2  |        |
| a               | 1                                              | 1                                                |  | 1          | 1  |        |
| b               | 1                                              | −1                                               |  | 1          | −1 |        |
| c               | $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$ |  | 2          | −2 |        |

Group **2** is of great importance in crystallography and theoretical physics because it essentially represents two fundamental operations – identity and changing the value of some parameter to the opposite value. In three-dimensional space it is the reversal of the direction of vectors in the opposite direction, i.e. spatial inversion; when

considering time, it is the reversal of the direction of its passage, i.e. time inversion. This general group is often denoted by the symbol  $C_i$ .

The characters of the representations of the 32-point groups are given, for example, in the Hammermesh monograph [20], but also on the Internet, e.g., at:

<http://staff.ustc.edu.cn/~xjwu/qc/teaching/book/chracter%20table-1.pdf>

There are mathematical relations between the characters of the representations, but we will not state them here. Detailed information on representation theory can be found in many publications; we have listed only a few of them in the reference list: [8], [9], [15], [16], [17].

## Part C

### Derivation of planar symmetry groups

#### C1 The concept of symmetry

By **symmetry** of an object we mean the existence of a set of geometric transformations by which the object under consideration is brought to an equivalent position, it identifies itself with itself. Symmetry is an important characteristic of crystals, referring not only to their external shapes, but especially to the arrangement of atoms, i.e. the crystal structure. It is not a privileged property of crystals, but has a broader application, so it is appropriate to introduce the concept of symmetry more generally.

We place an object in a fixed laboratory (external) coordinate system, and express some selected physical property of the object as a function  $Q(\mathbf{r})$  of its position in this system. With the object we fix a second (internal) coordinate system, whose origin and coordinate axes will be bound to specific points of the object; therefore, this system changes with the object during **transformations** (deformations, motions, rotations) of the object. We then transform the object, limiting ourselves to only those transformations which preserve the distances between any two points of the object (for example, we turn it over). If the values of the function  $Q(\mathbf{r})$  are preserved at all points  $\mathbf{r}$  of the laboratory system after such a transformation, the corresponding transformation is a **symmetry operation** of the object. For example, if a point of the object determined by the position vector  $\mathbf{r}_a$  is transformed to point  $\mathbf{r}_b$  in a symmetry operation, the values of the function  $Q(\mathbf{r})$  at these points must have been the same before the transformation; the corresponding points are referred to as **equivalent**.

Transformations that do not change the distances between points of an object include displacements of the object - translations, rotations, inversions, in-plane reflections, and combinations of these. All such operations represent in the laboratory system transformations of position vectors of specific points of an object into other position vectors. For example, if a point K is moved to a point K' during the transformation, the position vector  $\mathbf{r}$  of point K is transformed into the vector  $\mathbf{r}'$  of point K', which is expressed symbolically by the relation

$$\mathbf{r}' = S \cdot \mathbf{r} \quad (\text{C1.1})$$

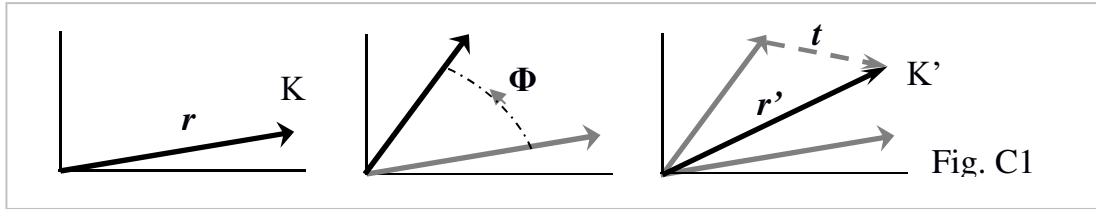
where  $S$  represents the operator of the corresponding transformation. The dot between  $S$  and  $\mathbf{r}$  does not represent an ordinary product, but an application of the operator  $S$  to the vector.

The operator  $S$  generally has two parts - a part related to rotation or reflection, and a part related to translation. The part of the operator representing rotation or reflection is expressed by the matrix, or tensor  $\bar{\Phi}$ , the translation part by the vector  $\mathbf{t}$ . (On representations of symmetry operations, see sections B1, B2, Appendix D30).

The application of the operator  $S$  to the position vector is then written as follows:

$$S \cdot \mathbf{r} = \mathbf{r}' = \mathbf{r} \cdot \bar{\Phi} + \mathbf{t} = \mathbf{r} \cdot [\bar{\Phi}, \mathbf{t}], \quad (\text{C1.2})$$

where  $\mathbf{r} \cdot \bar{\Phi}$  expresses the left scalar product of the tensor  $\bar{\Phi}$  with the position vector  $\mathbf{r}$ .



The use of the left scalar product proves useful when combining multiple transformations. Therefore, it is also convenient to change the symbolic notation of  $S \cdot \mathbf{r}$  to  $\mathbf{r} \cdot S$ . The operator  $S$  in accordance with relation (C1.2) is written in the form:

$$S \equiv [\bar{\Phi}, \mathbf{t}]. \quad (\text{C1.3})$$

This form, introduced by F. Seitz [4], will be used in later sections of the text to more easily formulate multiple uses of the same operator, or in the successive application of different operators.

## C2 Groups of symmetry operations

Every object, including a crystal, has at least one symmetry operation - identity (we denote it by  $E$ ), in which the points of the object transform into themselves. The identity operation is expressed by the relation

$$\mathbf{r} = \mathbf{r} \cdot E \quad (\text{C2.1})$$

valid for every vector  $\mathbf{r}$ . In analogy with relation (C1.3), the identity operation operator is written in the form:

$$E \equiv [\bar{\mathbf{I}}, 0], \quad (\text{C2.2})$$

where  $\bar{\mathbf{I}}$  represents the identity tensor (unit matrix in the matrix representation). By breaking down this operation in more detail, we obtain the relation:

$$\mathbf{r} \cdot \mathbf{E} = \mathbf{r} \cdot [\bar{\mathbf{I}}, 0] = \mathbf{r} \cdot \bar{\mathbf{I}} + \mathbf{0} = \mathbf{r},$$

because the vector is not changed by the scalar product with the identity tensor.

Suppose that the operators  $S_1 \equiv [\bar{\Phi}_1, \mathbf{t}_1]$  and  $S_2 \equiv [\bar{\Phi}_2, \mathbf{t}_2]$  represent two different symmetry operations. If we execute them in sequence, it is logical that the compound operation as a whole is again a symmetry operation. The application of the  $S_1$  operator transforms the vector  $\mathbf{r}$  into the vector  $\mathbf{r}' = \mathbf{r} \cdot S_1$  and this is transformed into the vector  $\mathbf{r}''$  by the  $S_2$  operator:

$$\mathbf{r}'' = \mathbf{r}' \cdot S_2 = (\mathbf{r} \cdot S_1) \cdot S_2 = \mathbf{r} \cdot (S_1 \cdot S_2).$$

Applying the notation of the operations according to relation (C1.2), we obtain the result

$$\begin{aligned} \mathbf{r}'' &= (\mathbf{r} \cdot \bar{\Phi}_1 + \mathbf{t}_1) \cdot S_2 = [(\mathbf{r} \cdot \bar{\Phi}_1 + \mathbf{t}_1) \cdot \bar{\Phi}_2] + \mathbf{t}_2 = \\ &= \mathbf{r} \cdot \bar{\Phi}_1 \cdot \bar{\Phi}_2 + \mathbf{t}_1 \cdot \bar{\Phi}_2 + \mathbf{t}_2, \end{aligned}$$

so that the sequential application of the two operators  $S_1$  and  $S_2$  can be written symbolically as the **product of the operators** and expressed in the form

$$S_1 \cdot S_2 = [\bar{\Phi}_1, \mathbf{t}_1] \cdot [\bar{\Phi}_2, \mathbf{t}_2] = [\bar{\Phi}_1 \cdot \bar{\Phi}_2, \mathbf{t}_1 \cdot \bar{\Phi}_2 + \mathbf{t}_2]. \quad (\text{C2.3})$$

If we reversed the order of the operations, we would get the result

$$S_2 \cdot S_1 = [\bar{\Phi}_2, \mathbf{t}_2] \cdot [\bar{\Phi}_1, \mathbf{t}_1] = [\bar{\Phi}_2 \cdot \bar{\Phi}_1, \mathbf{t}_2 \cdot \bar{\Phi}_1 + \mathbf{t}_1]$$

which shows that swapping the order of operations may not lead to the same result, i.e. the product of symmetry operators may not be commutative.

The product of two operators can be generalized to the product of several operators  $S_1 \cdot S_2 \cdot S_3 \dots$ . A special case is the n-fold application of the same operation (represented by the n-th "power" of the operator:  $S^n$ ). By successive application of relation (C2.3), it can be found ( $\rightarrow$  Appendix D1) to hold:

$$S^n = [\bar{\Phi}^n, \mathbf{t} \cdot \{\bar{\mathbf{I}} + \bar{\Phi} + \bar{\Phi}^2 + \dots + \bar{\Phi}^{n-1}\}], \quad (\text{C2.4})$$

where  $\bar{\bar{\Phi}}^2 = \bar{\bar{\Phi}} \cdot \bar{\bar{\Phi}}$ ,  $\bar{\bar{\Phi}}^3 = \bar{\bar{\Phi}}^2 \cdot \bar{\bar{\Phi}}$ , etc. The sum in the large bracket is symbolic and means that the operators  $\bar{\bar{I}}$ ,  $\bar{\bar{\Phi}}$ ,  $\bar{\bar{\Phi}}^2$ , ... are successively applied to the vector  $\mathbf{t}$ , thus producing a set of vectors to be summed. The result has to be added to the vector produced by applying the operator  $\bar{\bar{\Phi}}^n$  to the initial vector  $\mathbf{r}$ .

To each symmetry operation (operator  $S$ ) there is an inverse operation (operator  $S^{-1}$ ) that returns the object to its original position. Thus, for the inverse operation operator holds:

$$S \cdot S^{-1} = S^{-1} \cdot S = E \quad (C2.5)$$

Using this relation and relations (C2.2) and (C2.3), we obtain the form of the inverse operator:

$$S^{-1} \equiv [\bar{\bar{\Phi}}^{-1}, -\mathbf{t} \cdot \bar{\bar{\Phi}}^{-1}]. \quad (C2.6)$$

For completeness, it is worth recalling that the inverse operation is also a symmetry operation.

#### **In summary, it can be concluded that**

- the set of symmetry operations of a crystal, but also of any other object with respect to their successive application is a closed set, because the combination of even several symmetry operations will bring the object to a physically and geometrically equivalent position; therefore, their combination is also a symmetry operation;
- in the successive application of several symmetry operations, the associative law holds, which follows from the associativity of vector addition and the associativity of tensor (matrix) multiplication;
- in the set of symmetry operations there is always a so-called neutral symmetry operation, which is the identical operation  $E$ . It has the property that in conjunction with another operation, it does not change this one;
- to every symmetry operation there exists an inverse operation with the property that by successive application of the symmetry operation and its inverse to it, an identical operation is produced.

Therefore, the set of symmetry operations of an arbitrary object **forms a group** because it satisfies all the group postulates. Meanwhile, a **binary group operation** is a sequential application of operations ( $\rightarrow$  Appendix D29 on groups).

If the distances between any two points in an object are preserved in its transformation, this means that the lengths of the sides of the triangles are preserved and therefore their angles are preserved. Therefore, the scalar product of the position vectors of any two points of the object is also preserved. This has a significant effect on the tensor part of the symmetry operator because it must hold:

$$\mathbf{r}_1 \cdot \mathbf{r}_2 = \mathbf{r}'_1 \cdot \mathbf{r}'_2 = (\mathbf{r}_1 \cdot \bar{\bar{\Phi}}) \cdot (\mathbf{r}_2 \cdot \bar{\bar{\Phi}}) = (\mathbf{r}_1 \cdot \bar{\bar{\Phi}}) \cdot (\bar{\bar{\Phi}}_C \cdot \mathbf{r}_2) = \mathbf{r}_1 \cdot (\bar{\bar{\Phi}} \cdot \bar{\bar{\Phi}}_C) \cdot \mathbf{r}_2$$

The comparison of the beginning and end of the line implies that the scalar product of the tensor  $\bar{\bar{\Phi}}$  with the conjugate tensor  $\bar{\bar{\Phi}}_C$  must be equal to the identity tensor  $\bar{\bar{I}}$ . But this means that the conjugate tensor  $\bar{\bar{\Phi}}_C$  must simultaneously be an inverse tensor, i.e., it must hold

$$\bar{\bar{\Phi}}_C = \bar{\bar{\Phi}}^{-1}, \text{ resp. } \bar{\bar{\Phi}} = \bar{\bar{\Phi}}_C^{-1}. \quad (\text{C2.7})$$

Tensors (matrices) representing symmetry operations must have this property. The corresponding **matrices** are referred to as rectangular.

### C3 Groups of symmetry operations of crystal structures

In describing the symmetry of the crystal structure (i.e. the symmetry of the arrangement of atoms in the crystal), it is necessary to start from the lattice postulate. This states that any property of a crystal - macroscopic or microscopic - is invariant with respect to a translation by the **lattice vector**  $\mathbf{A}_L$ , the so-called **lattice translation**:

$$\mathbf{A}_L = \sum_{i=1}^3 L_i \mathbf{a}_i = L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2 + L_3 \mathbf{a}_3, \quad (\text{C3.1})$$

where the vectors  $\mathbf{a}_i$  represent the triplet of basis vectors (basis) of the crystal lattice and  $L_i$  are integers. The **lattice postulate** is expressed by the relation

$$Q(\mathbf{r}) = Q(\mathbf{r} + \sum_{i=1}^3 L_i \mathbf{a}_i), \quad (\text{C3.2})$$

where  $Q(\mathbf{r})$  represents a physical property of the crystal (scalar, vector, or tensor) as a function of spatial coordinates in the laboratory coordinate system. For example, the electron density varies periodically in a crystal (with a period at the level of the interatomic distances), so that by shifting the crystal by one or a few lattice vectors, the crystal will reach a physically identical position - at a given point in the laboratory system, all properties of the crystal will have the same value again. Thus translations

of a crystal by a lattice vector are symmetry operations, and given the circumstance that they are related to the lattice postulate, they are **trivial symmetry operations**.

***Note** Effects at the edges of a finite crystal are not accounted for, or the reasoning is quite correct for the case of an infinitely large crystal.*

The **translation operator**  $T_L$  representing translation by a lattice vector  $\mathbf{A}_L$ , according to relation (1.3) is expressed in the form

$$T_L \equiv [\bar{\mathbf{I}}, \mathbf{A}_L] = [\bar{\mathbf{I}}, L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2 + L_3 \mathbf{a}_3] . \quad (\text{C3.3})$$

It is not difficult to see that the set of all lattice translations (there are infinitely many) forms a group, the binary operation being the successive application of two translations, represented by the sum of the lattice vectors. It is called **the translation group** and will be denoted by the symbol  $T$ . Lattice translations form only a part of the symmetry operations of a crystal; they form a subgroup of the group of all symmetry operations, which include various rotations and reflections. The set of rotations and reflections has a finite number of elements. The group of all symmetry operations of a crystal is called the **space group** of the crystal and is referred to as  $G$  in this text.

If  $S \equiv [\bar{\Phi}, \mathbf{t}]$  represents a symmetry operation, then in accordance with relation (C2.3), the product  $S^{-1} \cdot T_L \cdot S$  also represents a symmetry operation. In detailed notation, this product is represented by the expression ( $\rightarrow$  Appendix D2)

$$S^{-1} \cdot T_L \cdot S = [\bar{\mathbf{I}}, \mathbf{A}_L \cdot \bar{\Phi}] , \text{ or } S \cdot T_L \cdot S^{-1} = [\bar{\mathbf{I}}, \mathbf{A}_L \cdot \bar{\Phi}^{-1}] . \quad (\text{C3.4})$$

The identity tensor is in square brackets in the first place, so in both cases the resulting operation is a translation by the rotated lattice vector  $\mathbf{A}_L$ . This means that in addition to the vector  $\mathbf{A}_L$  the rotated vector (i.e., the scalar product  $\mathbf{A}_L \cdot \bar{\Phi}$ ) must also be an element of the translation group of the crystal. The relation (C3.4) can also be written in the form

$$S^{-1} \cdot T_L \cdot S = T_L'$$

while in general the translations corresponding to the operators  $T_L$  and  $T_L'$  are not equal. These considerations hold for any translation belonging to the translation group  $T$ . That is, when the symbol  $S$  represents any element of the space group  $G$  and  $S^{-1}$  its inverse, we can write the group equation

$$S^{-1} \cdot T \cdot S = T , \Rightarrow T \cdot S = S \cdot T . \quad (\text{C3.5})$$

It follows from relation (C3.5) that the translation group  $T$  is an **invariant subgroup** of the space group  $G$  because its left and right cosets  $S \cdot T$  and  $T \cdot S$  respectively, associated to any element  $S = [\bar{\Phi}, t]$  of the space group, are the same. An element of  $S$  is the representative of the corresponding coset. Using additional elements  $S$  of the space group, additional cosets are created and the group  $G$  is thus decomposed into a subgroup  $T$  with representative of  $E = [\bar{I}, 0]$ , and into cosets with representatives  $S_1, S_2, \dots$ , of which there are a finite number. Each coset contains an infinite number of elements, consisting of translation and a point operation, and in all its elements the point operation is the same; the elements of coset differ from each other only by different lattice translations. The location of the corresponding elements of point symmetry (rotation axes, reflection lines) in the crystal lattice is not crucial.

The translational subgroup  $T$  of the space group  $G$  together with its cosets as units form a **factor group**, which is denoted by the symbol  $(G/T)$ . The space group can then be expressed as the direct product of the translation group and the factor group:

$$G = T \cdot (G/T) = (G/T) \cdot T . \quad (C3.6)$$

The elements of a factor group (i.e. a subgroup  $T$  + its cosets) are symbolically denoted by their representatives  $E, S_1, S_2, S_3 \dots$ :

$$(G/T) \leftrightarrow \{E, S_1, S_2, S_3 \dots\} .$$

In doing so, it is important to note that the set of representatives  $E, S_1, S_2, S_3 \dots$  need not form a group. The set of operations  $S_1, S_2, S_3 \dots$ , excluding the operation  $E$ , represents the non-trivial symmetry operations of the crystal structure. If the translational part of these operations is dropped, i.e.,  $[\bar{\Phi}_i, t_i] \rightarrow [\bar{\Phi}_i, 0]$ , what remains are operations that do not shift the crystal, i.e., they leave at least one point at the original location. Therefore, they are called **point operations**. These point operations, together with the identical operation  $E$ , form the **point group** of the crystal structure symmetry.

Among the elements of the point group of a crystal represented by the operators  $[\bar{I}, 0], [\bar{\Phi}_1, 0], [\bar{\Phi}_2, 0], \dots$  and the elements of the factor group, there is a one-unique relationship, therefore

**the factor group and the point group of a crystal are isomorphic.**

The relation (C3.6) is the starting point in the search for possible types of crystal space groups. It implies that all possible translation groups and all factor groups must first be known. However, factor groups are isomorphic to point groups, and so the task of finding all space groups reduces to finding all possible point groups and translation groups. One has to start with the point groups, because the translation groups – as will

be shown later – can be derived from the requirements imposed by the symmetry operations of the individual point groups on the basis vectors  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  of the lattice. And further, point groups can be constructed from the obtained allowed point symmetry operations, which are defined by the periodicity of the crystal structure.

Previous considerations have been concerned with both two- and three-dimensional structures. However, to rigorously derive all point, translation and space groups of three-dimensional periodic structures is a task challenging in content but especially in scope. From a pedagogical point of view, it is therefore appropriate to restrict ourselves to two-dimensional structures. In doing so, the methodology is the same as for three-dimensional structures. It was published by F. Seitz between 1934 and 1936 in a series of articles in the *Zeitschrift für Kristallography* [2 - 5] and methodologically improved by W. H. Zachariasen in the book "Theory of X-Ray Diffraction", published in 1945 [6]. This text is based on Zachariasen's procedure, adapted to two-dimensional periodic structures.

## C4 Symmetry operations of two-dimensional periodic structures

For two-dimensional periodic structures, symmetry operations include translations in the plane of the structure, rotations about axes perpendicular to this plane, and reflections in lines lying in the plane, as well as combinations of these operations. Rotation by  $180^\circ$  coincides with inversion, which is a separate operation only in three-dimensional structures. The symmetry operations of planar structures can thus consist of a rotational part (understood in a broader sense together with reflections) and a translational part, so that the corresponding operators have the general form  $S \equiv [\bar{\Phi}, \mathbf{t}]$ .

In the following sections, the influence of the periodicity of planar structures on the rotation and translation part of the operators  $S$  is described. This is essentially a search for allowed rotations and allowed translations that bring the structure to an equivalent position. For two-dimensional structures, translations are expressed by vectors with only two components; similarly, tensors are only two-dimensional.

### C4.1 Tensor part of the operator S

The tensor, and hence the second degree tensor, is used in this text as the operator that mediates the transformation in space. The transformation of a vector  $\mathbf{r}$  into a vector  $\mathbf{r}'$  is expressed as the scalar product of this vector with the tensor:

$$\mathbf{r}' = \mathbf{r} \cdot \bar{\bar{\Phi}} \quad (\text{C4.1})$$

If a two-dimensional tensor (i.e., a tensor consisting of two linearly independent dyads) transforms a pair of noncolinear vectors  $\mathbf{a}_1, \mathbf{a}_2$  into vectors  $\mathbf{d}_1, \mathbf{d}_2$ , i.e., when

$$\mathbf{a}_1 \cdot \bar{\bar{\Phi}} = \mathbf{d}_1 \quad \text{and} \quad \mathbf{a}_2 \cdot \bar{\bar{\Phi}} = \mathbf{d}_2, \quad (\text{C4.2})$$

then tensor can be written in the form ( $\rightarrow$  Appendix D3)

$$\bar{\bar{\Phi}} = \mathbf{a}^1 \mathbf{d}_1 + \mathbf{a}^2 \mathbf{d}_2, \quad (\text{C4.3})$$

where the vectors  $\mathbf{a}^1, \mathbf{a}^2$  represent a pair of reciprocal vectors to the pair  $\mathbf{a}_1, \mathbf{a}_2$ .

The tensor part of the operator  $S \equiv [\bar{\bar{\Phi}}, \mathbf{t}]$  represents such tensor transformations in which a certain set of points transforms into itself (point symmetry operations). Therefore, there exists a nonempty set of position vectors, for which

$$\mathbf{r} = \mathbf{r} \cdot \bar{\bar{\Phi}},$$

or in another notation

$$\mathbf{r} \cdot \bar{\bar{\Phi}} - \mathbf{r} = \mathbf{0} \Rightarrow \mathbf{r} \cdot (\bar{\bar{\Phi}} - \bar{\bar{I}}) = \mathbf{0},$$

respectively in the designation  $\bar{\bar{T}} = (\bar{\bar{\Phi}} - \bar{\bar{I}})$ :

$$\mathbf{r} \cdot \bar{\bar{T}} = \mathbf{0}. \quad (\text{C4.4})$$

Since the tensor part of the symmetry operator must satisfy condition (C2.7), i.e.  $\bar{\bar{\Phi}}_C = \bar{\bar{\Phi}}^{-1}$ , resp.  $\bar{\bar{\Phi}} = \bar{\bar{\Phi}}_C^{-1}$  the relation ( $\rightarrow$  Appendix D4) holds for the same position vectors

$$\bar{\bar{\Phi}} \cdot \mathbf{r} = \mathbf{r} \rightarrow (\bar{\bar{\Phi}} - \bar{\bar{I}}) \cdot \mathbf{r} = \mathbf{0}, \quad \text{t.j.}$$

$$\bar{\bar{T}} \cdot \mathbf{r} = \mathbf{0}. \quad (\text{C4.5})$$

Equations (C4.4) and (C4.5) are satisfied trivially for  $\mathbf{r} = \mathbf{0}$ , i.e., for the origin of the reference frame, so no restrictions are then placed on the tensor  $\bar{\bar{T}}$ . This is the case for any rotation of the plane about the origin of the reference frame (to avoid confusion - it is a rotation about an axis perpendicular to the plane). If the above equations are to hold for arbitrary  $\mathbf{r} \neq \mathbf{0}$ , the tensor  $\bar{\bar{T}}$  must be incomplete. An incomplete tensor can be either zero or linear (consisting of only one dyad).

If the tensor  $\bar{\bar{\mathbf{T}}}$  is zero, then  $\bar{\bar{\mathbf{T}}} = \bar{\bar{\Phi}} - \bar{\mathbf{I}} = \mathbf{0}$ , which implies

$$\bar{\bar{\Phi}} = \bar{\mathbf{I}},$$

i.e. it is an identical transformation.

If the tensor  $\bar{\bar{\mathbf{T}}}$  is linear, then there is only one dyad

$$\bar{\bar{\mathbf{T}}} = \mathbf{ab}, \quad (\text{C4.6})$$

and according to equations (C4.4) and (C4.5):  $\mathbf{r} \cdot \mathbf{ab} = \mathbf{ab} \cdot \mathbf{r} = 0$ .

For a non-zero vector  $\mathbf{r}$ , both vectors of the dyad  $\mathbf{ab}$  must be perpendicular to vector  $\mathbf{r}$ . This means that the tensor  $\bar{\bar{\mathbf{T}}}$  is convenient to write in the form

$$\bar{\bar{\mathbf{T}}} = s\mathbf{uu}, \quad (\text{C4.7})$$

where  $s$  is a scalar and  $\mathbf{u}$  a unit vector perpendicular to the vector  $\mathbf{r}$ . Recall that the vector  $\mathbf{r}$  points to invariant points when transformed by the tensor

$$\bar{\bar{\Phi}} = \bar{\mathbf{I}} + \bar{\bar{\mathbf{T}}} = \bar{\mathbf{I}} + s\mathbf{uu}.$$

Now we calculate how the vector  $\mathbf{u}$  is transformed by the tensor  $\bar{\bar{\Phi}} = \bar{\mathbf{I}} + s\mathbf{uu}$ :

$$\mathbf{u}' = \mathbf{u} \cdot \bar{\bar{\Phi}} = \mathbf{u} \cdot (\bar{\mathbf{I}} + s\mathbf{uu}) = \mathbf{u} + s\mathbf{u} = (1 + s)\mathbf{u}.$$

We require that the symmetry operation preserves lengths, i.e., it must be the case that  $(1 + s) = \pm 1$ , which implies that the scalar  $s$  can take only two values: 0,  $-2$ .

The case  $s = 0$  leads to  $\bar{\bar{\Phi}} = \bar{\mathbf{I}}$  i.e. to an identity transformation. If  $s = -2$ , the tensor  $\bar{\bar{\mathbf{T}}}$  has the form  $\bar{\bar{\mathbf{T}}} = -2\mathbf{uu}$  and the tensor  $\bar{\bar{\Phi}}$ :

$$\bar{\bar{\Phi}} = \bar{\mathbf{I}} - 2\mathbf{uu}, \quad (\text{C4.8})$$

whereby this tensor ( $\rightarrow$  Appendix D5)

- a) preserves the components of the vectors perpendicular to the vector  $\mathbf{u}$
- b) transforms the components parallel to  $\mathbf{u}$  to the opposite.

It is thus a **reflection** in a line perpendicular to the vector  $\mathbf{u}$ ; the line in question is called the **reflection line (mirror line)** (marker  $m$ ). In the following, these operations are described in more detail.

### C4.1.1 Rotation

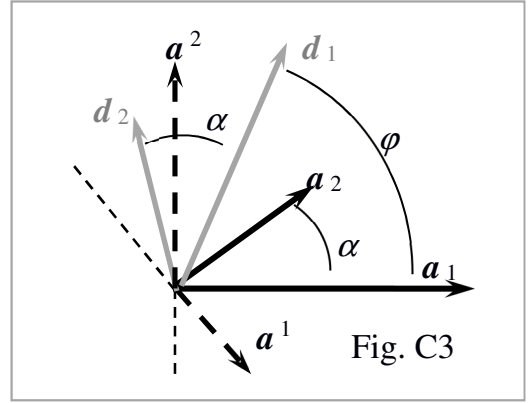
Let the basis of a planar structure be a pair of vectors  $\mathbf{a}_1, \mathbf{a}_2$ , its reciprocal pair being  $\mathbf{a}^1, \mathbf{a}^2$ . Let the vectors  $\mathbf{a}_1, \mathbf{a}_2$  form an angle  $\alpha$ . Let the tensor  $\bar{\Phi}$  represent the rotation of the vectors  $\mathbf{a}_1, \mathbf{a}_2$  by an angle  $\varphi$  such that  $\mathbf{a}_1 \rightarrow \mathbf{d}_1, \mathbf{a}_2 \rightarrow \mathbf{d}_2$ . By relation (C4.3), the tensor  $\bar{\Phi}$  then takes the form:

$$\bar{\Phi} = \mathbf{a}^1 \mathbf{d}_1 + \mathbf{a}^2 \mathbf{d}_2 .$$

We express the vectors  $\mathbf{d}_1, \mathbf{d}_2$  as a linear combination of the original vectors  $\mathbf{a}_1, \mathbf{a}_2$ :

$$\begin{aligned} \mathbf{d}_1 &= p\mathbf{a}_1 + q\mathbf{a}_2 \\ \mathbf{d}_2 &= r\mathbf{a}_1 + s\mathbf{a}_2 , \end{aligned} \quad (\text{C4.9})$$

where the scalar coefficients  $p, q, r, s$  are the coordinates of the vectors  $\mathbf{d}_1, \mathbf{d}_2$  with respect to the basis vectors  $\mathbf{a}_1, \mathbf{a}_2$ . The next task will be to calculate these coordinates.



The scalar product of the first of the equations (C4.9) with the vector  $\mathbf{a}^1$  gives:

$$\mathbf{d}_1 \cdot \mathbf{a}^1 = (p\mathbf{a}_1 + q\mathbf{a}_2) \cdot \mathbf{a}^1 = p(\mathbf{a}_1 \cdot \mathbf{a}^1) + q(\mathbf{a}_2 \cdot \mathbf{a}^1) = p .$$

Similarly, we obtain the other scalar coefficients:

$$p = \mathbf{d}_1 \cdot \mathbf{a}^1, \quad q = \mathbf{d}_1 \cdot \mathbf{a}^2, \quad r = \mathbf{d}_2 \cdot \mathbf{a}^1, \quad s = \mathbf{d}_2 \cdot \mathbf{a}^2 . \quad (\text{C4.10})$$

Calculating the scalar products in relations (C4.10), we obtain the scalar coefficients as functions of the magnitudes of the basis vectors  $\mathbf{a}_1, \mathbf{a}_2$ , and the angles  $\varphi$  and  $\alpha$  ( $\rightarrow$  Appendix D6). After plugging their values into the transformation relations (C4.9), we obtain:

$$\begin{aligned} \mathbf{d}_1 &= \frac{\sin(\alpha - \varphi)}{\sin \alpha} \mathbf{a}_1 + \frac{a_1 \sin \varphi}{a_2 \sin \alpha} \mathbf{a}_2 \\ \mathbf{d}_2 &= -\frac{a_2 \sin \varphi}{a_1 \sin \alpha} \mathbf{a}_1 + \frac{\sin(\alpha + \varphi)}{\sin \alpha} \mathbf{a}_2 . \end{aligned}$$

Finally, we fit the vectors  $\mathbf{d}_1$  and  $\mathbf{d}_2$  to the transformation tensor:

$$\bar{\Phi} = \mathbf{a}^1 \mathbf{a}_1 \frac{\sin(\alpha - \varphi)}{\sin \alpha} + \mathbf{a}^1 \mathbf{a}_2 \frac{a_1 \sin \varphi}{a_2 \sin \alpha} - \mathbf{a}^2 \mathbf{a}_1 \frac{a_2 \sin \varphi}{a_1 \sin \alpha} + \mathbf{a}^2 \mathbf{a}_2 \frac{\sin(\alpha + \varphi)}{\sin \alpha} . \quad (\text{C4.11})$$

This tensor mediates the rotation of the plane defined by the vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  taking an angle  $\alpha$ , by an angle  $\varphi$  measured in the same sense as the deviation of the vector  $\mathbf{a}_2$  from the vector  $\mathbf{a}_1$ . If we require it to represent the symmetry operation of a planar periodic structure, the angle  $\varphi$  cannot be arbitrary. The tensor must transform each lattice vector  $\mathbf{A}_L = L_1\mathbf{a}_1 + L_2\mathbf{a}_2$  ( $L_i$  - integers) into another lattice vector.

For further considerations, it is more convenient to express the tensor (C4.11) more concisely using the scalar coordinates  $\Phi_{ij}$  of the form

$$\bar{\Phi} = \Phi_{11}\mathbf{a}^1\mathbf{a}_1 + \Phi_{12}\mathbf{a}^1\mathbf{a}_2 + \Phi_{21}\mathbf{a}^2\mathbf{a}_1 + \Phi_{22}\mathbf{a}^2\mathbf{a}_2. \quad (\text{C4.12})$$

The transformation of the lattice vector is then written as follows:

$$\begin{aligned} \mathbf{A}'_L &= \mathbf{A}_L \cdot \bar{\Phi} = (L_1\mathbf{a}_1 + L_2\mathbf{a}_2) \cdot \bar{\Phi} = (L_1\Phi_{11} + L_2\Phi_{21})\mathbf{a}_1 + (L_1\Phi_{12} + L_2\Phi_{22})\mathbf{a}_2 = \\ &= L'_1\mathbf{a}_1 + L'_2\mathbf{a}_2. \end{aligned}$$

If the vector  $\mathbf{A}'_L$  is also to be a lattice vector, then the numbers  $L'_1$  and  $L'_2$  must be integers. This condition must be satisfied for arbitrary integers  $L_1$ ,  $L_2$ , which is only possible when the coordinates  $\Phi_{ij}$  of the tensor  $\bar{\Phi}$  are integers, that is, when

$$\Phi_{ij} = \mathbf{a}_i \cdot \bar{\Phi} \cdot \mathbf{a}^j = \text{integer}. \quad (\text{C4.13})$$

If the coordinates of the tensor are integers, then its first scalar, i.e. the sum of the coordinates in the principal diagonal, is also an integer.

For a tensor of the form (C4.11), it follows that the integer  $n$  must equal the sum of

$$\frac{\sin(\alpha - \varphi)}{\sin \alpha} + \frac{\sin(\alpha + \varphi)}{\sin \alpha} = 2 \cos \varphi = n.$$

That is,  $\cos \varphi = n/2$ , so that the cosine function can take on only a few discrete values:  $-1, -0.5, 0, 0.5, 1$ , and hence the angle of rotation  $\varphi$  expressed in degrees only values (if we consider angles less than  $360^\circ$ ):

$$0^\circ, 60^\circ, 90^\circ, 120^\circ, 180^\circ, 240^\circ, 270^\circ, 300^\circ. \quad (\text{C4.14})$$

Substituting  $\varphi = 0$  into relation (C4.11), we obtain a tensor representing the identity operation, i.e. the improper:

$$\bar{\mathbf{I}} = \mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^2\mathbf{a}_2.$$

Substituting  $\varphi = 60^\circ$  ( $= (2\pi/6)\text{rad}$ ) gives a tensor that realizes a  $60^\circ$  rotation, which we denote by  $\bar{\mathbf{6}}$ . If we consider only the rotation operation as an element of the group, not a tensor, we will use the symbol  $\mathbf{6}$ , i.e. without the two commas and written in

plain, not bold, type. Also, multiple applications of the element 6, i.e. its "powers"  $6^2, 6^3, 6^4, 6^5, 6^6$ , are symmetry operations, representing rotations of angles  $120^\circ, 180^\circ, 240^\circ, 300^\circ$  and  $360^\circ$ . A  $360^\circ$  rotation is considered equivalent to a  $0^\circ$  rotation, so it is an identical operation denoted by  $e$ . These rotations (symmetry operations) together as a set, form a group with elements  $\{e, 6, 6^2, 6^3, 6^4, 6^5\}$ . The corresponding group is denoted by the symbol **6**, because the structure gets to the identical position 6 times during  $360^\circ$  rotation. An isomorphic group with group **6** is formed by the corresponding tensors:

$$\bar{\bar{1}}, \bar{\bar{6}}, \bar{\bar{6}}^2, \bar{\bar{6}}^3, \bar{\bar{6}}^4, \bar{\bar{6}}^5, \text{ while } \bar{\bar{1}} \equiv \bar{\bar{6}}^6$$

The group **6** is cyclic and the element 6, whose powers generate all other elements of the group, is the **generating element** of the group.

**Note.** The symmetry operations given in this case form a group, the group operation being the successive application of the operations. With this group is isomorphic the group of the corresponding tensors, the group operation being the scalar product between the tensors.

From the allowed rotations expressed by the angles (C4.14), several cyclic point groups can be constructed, which are listed in Table TC1 below.

| TC1          | Allowed rotations and their groups                                          |                                  |
|--------------|-----------------------------------------------------------------------------|----------------------------------|
| Group symbol | Elements of cyclic groups<br>Marking and corresponding rotations in degrees | Operators of generating elements |
| <b>1</b>     | e<br>0                                                                      | $\bar{\bar{1}}$                  |
| <b>2</b>     | e, 2<br>0, 180                                                              | $\bar{\bar{2}}$                  |
| <b>3</b>     | e, 3, $3^2$<br>0, 120, 240                                                  | $\bar{\bar{3}}$                  |
| <b>4</b>     | e, 4, $4^2$ , $4^3$<br>0, 90, 180, 270                                      | $\bar{\bar{4}}$                  |
| <b>6</b>     | e, 6, $6^2$ , $6^3$ , $6^4$ , $6^5$<br>0, 60, 120, 180, 240, 300            | $\bar{\bar{6}}$                  |

### TC2a Tensors of generating elements of cyclic groups

$$\bar{\bar{1}} = a^1 a_1 + a^2 a_2 .$$

$$\bar{\bar{2}} = -a^1 a_1 - a^2 a_2 = -\bar{\bar{1}} .$$

$$\begin{aligned} \bar{\bar{3}} = a^1 a_1 \left( -\frac{1}{2} - \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \right) + a^1 a_2 \frac{a_1 \sqrt[2]{3}}{a_2} \frac{1}{2 \sin \alpha} - a^2 a_1 \frac{a_2 \sqrt[2]{3}}{a_1} \frac{1}{2 \sin \alpha} \\ + a^2 a_2 \left( -\frac{1}{2} + \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \right) \end{aligned}$$

$$\bar{\bar{4}} = -a^1 a_1 \frac{\cos \alpha}{\sin \alpha} + a^1 a_2 \frac{a_1}{a_2} \frac{1}{\sin \alpha} - a^2 a_1 \frac{a_2}{a_1} \frac{1}{\sin \alpha} + a^2 a_2 \frac{\cos \alpha}{\sin \alpha}$$

$$\begin{aligned} \bar{\bar{6}} = a^1 a_1 \left( +\frac{1}{2} - \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \right) + a^1 a_2 \frac{a_1 \sqrt[2]{3}}{a_2} \frac{1}{2 \sin \alpha} - a^2 a_1 \frac{a_2 \sqrt[2]{3}}{a_1} \frac{1}{2 \sin \alpha} \\ + a^2 a_2 \left( +\frac{1}{2} + \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \right) \end{aligned}$$

In most cases, the size of the vectors is chosen to be the same, i.e.  $a_1 = a_2$ . The angle  $\alpha$  for the  $\bar{\bar{3}}$  and  $\bar{\bar{6}}$  tensors is usually chosen  $\alpha = 120^\circ$  and for the  $\bar{\bar{4}}$  tensor  $\alpha = 90^\circ$ . This simplifies the expression of the tensors considerably and gives the following form:

| TC2b                                                  |
|-------------------------------------------------------|
| $\bar{\bar{1}} = a^1 a_1 + a^2 a_2$                   |
| $\bar{\bar{2}} = -a^1 a_1 - a^2 a_2 = -\bar{\bar{1}}$ |
| $\bar{\bar{3}} = a^1 a_2 - a^2 a_1 - a^2 a_2$         |
| $\bar{\bar{4}} = a^1 a_2 - a^2 a_1$                   |
| $\bar{\bar{6}} = a^1 a_1 + a^1 a_2 - a^2 a_1$         |

### C4.1.2 Reflection

According to relation (C4.8), the tensor representing reflection has the form (for reflection tensor we will use the symbol  $\bar{\bar{\mathbf{M}}}$  instead of  $\bar{\Phi}$ )

$$\bar{\bar{\mathbf{M}}} = \bar{\mathbf{I}} - 2\mathbf{u}\mathbf{u},$$

where  $\mathbf{u}$  is the unit vector perpendicular to the reflection line (lying in the plane of the structure). If reflection is to be a symmetry operation of a periodic structure, an arbitrary lattice vector must transform again into a (generally different) lattice vector. If the vectors  $\mathbf{a}_1, \mathbf{a}_2$  form the basis of a planar lattice, then in such a coordinate system the tensor  $\bar{\bar{\mathbf{M}}}$  must have integer coordinates (relation C4.13). We modify the general form of the tensor  $\bar{\bar{\mathbf{M}}}$  to a binomial:

$$\begin{aligned} \bar{\bar{\mathbf{M}}} &= M_{11} \mathbf{a}^1 \mathbf{a}_1 + M_{12} \mathbf{a}^1 \mathbf{a}_2 + M_{21} \mathbf{a}^2 \mathbf{a}_1 + M_{22} \mathbf{a}^2 \mathbf{a}_2 = \\ &= \mathbf{a}^1 (M_{11} \mathbf{a}_1 + M_{12} \mathbf{a}_2) + \mathbf{a}^2 (M_{21} \mathbf{a}_1 + M_{22} \mathbf{a}_2) = \mathbf{a}^1 \mathbf{A}_1 + \mathbf{a}^2 \mathbf{A}_2, \end{aligned} \quad (\text{C4.15})$$

where  $\mathbf{A}_1, \mathbf{A}_2$  are the right vector coordinates of the tensor  $\bar{\bar{\mathbf{M}}}$ . We also express the tensor  $\bar{\bar{\mathbf{M}}}$  in terms of the left vector coordinates

$$\bar{\bar{\mathbf{M}}} = (M_{11} \mathbf{a}^1 + M_{12} \mathbf{a}^2) \mathbf{a}_1 + (M_{21} \mathbf{a}^1 + M_{22} \mathbf{a}^2) \mathbf{a}_2 = \mathbf{A}^1 \mathbf{a}_1 + \mathbf{A}^2 \mathbf{a}_2. \quad (\text{C4.16})$$

We use these results to modify the tensor  $\bar{\mathbf{T}} = \bar{\bar{\mathbf{M}}} - \bar{\mathbf{I}}$  (label before C4.4):

$$\bar{\mathbf{T}} = \bar{\bar{\mathbf{M}}} - \bar{\mathbf{I}} = \mathbf{a}^1 (\mathbf{A}_1 - \mathbf{a}_1) + \mathbf{a}^2 (\mathbf{A}_2 - \mathbf{a}_2) = (\mathbf{A}^1 - \mathbf{a}^1) \mathbf{a}_1 + (\mathbf{A}^2 - \mathbf{a}^2) \mathbf{a}_2 \quad (\text{C4.17})$$

However, this tensor also has a form (relations C4.7, C4.8 and the text between them)

$$\bar{\mathbf{T}} = -2\mathbf{u}\mathbf{u}.$$

It can be shown ( $\rightarrow$  Appendix D7) that this is only possible when the vector  $\mathbf{u}$  is parallel to the vectors

$$(\mathbf{A}_1 - \mathbf{a}_1), (\mathbf{A}_2 - \mathbf{a}_2), (\mathbf{A}^1 - \mathbf{a}^1), (\mathbf{A}^2 - \mathbf{a}^2).$$

The unit vector  $\mathbf{u}$  is perpendicular to the reflection line, and moreover parallel to some lattice vectors of both the direct and reciprocal lattice. It follows that a reflection line can only be a line with the property that the perpendicular to it has the direction of the lattice vector of the direct and reciprocal lattice at the same time.

Denote the shortest lattice vector parallel to the unit vector  $\mathbf{u}$  as  $\mathbf{b}_1$  and the corresponding reciprocal lattice vector parallel to it as  $\mathbf{b}^1$ . When the vectors  $\mathbf{b}_1$  and  $\mathbf{b}^1$

are parallel to each other, then it can be shown ( $\rightarrow$  Appendix D8) that there exists a pair of vectors  $\mathbf{b}_1$ ,  $\mathbf{b}_2$ , which are perpendicular to each other and form the **orthogonal basis** of the lattice. However, this implies that not only the perpendicular to the reflection line, but also the reflection line itself is parallel to some lattice vector of the direct lattice and simultaneously to some lattice vector of the reciprocal lattice. It follows that reflection lines (i.e. reflections) can only exist in lattices in which orthogonal basis cells can be chosen.

The specific shapes of the tensors are given in the Appendices. Tensors in orthogonal bases are described in Appendix D14, tensors in hexagonal systems in which the basis vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are not perpendicular to each other are described in Appendix D25. Appendix D26 gives the shapes of tensors in orthohexagonal bases.

### C4.1.3 Tensors of multiple rotations and combinations with reflection

When a planar periodic structure is characterized by symmetry operations, which are both rotations and reflections, the symmetry operations are their multiple applications, but also their combinations with each other. The tensors representing rotations are given in Table TC2b, the general form of the tensor representing reflections is given by relation C4.8. In this section the form of the tensors representing multiple rotations, i.e., the "powers" of the tensors given in Table TC2b, as well as the tensors that arise from combinations of rotations with reflections, are justified in detail. The transformations of the lattice vectors mediated by these tensors are also given.

#### Multiple rotations

Rotation about the **twofold** axis occurs in all crystal systems and is expressed by the tensor  $\bar{\bar{2}} = -\bar{\bar{1}} = (-\mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2)$ . In the rectangular crystal system, the basis vectors  $\mathbf{a}_1, \mathbf{a}_2$  make an angle of  $90^\circ$ , while they do not have the same length. However, the preceding relation with these vectors holds even when these vectors are not perpendicular to each other. When rotated by  $180^\circ$ , expressed by the tensor  $-\bar{\bar{1}}$ , each lattice vector  $\mathbf{A}_L$  turns into  $-\mathbf{A}_L$ , i.e., into a vector with the opposite direction.

A double application of such a rotation is assigned a tensor:

$$\bar{\bar{2}} \cdot \bar{\bar{2}} = (-\mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2) \cdot (-\mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2) = (-\bar{\bar{1}}) \cdot (-\bar{\bar{1}}) = \bar{\bar{1}},$$

that is identity tensor. This operation brings the structure back to its original position, since a 180° rotation is itself an inverse operation.

Rotation about the **threefold** axis occurs only in the hexagonal crystal system and is described by the tensor  $\bar{\bar{3}} = (\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2)$ . The vectors  $\mathbf{a}_1, \mathbf{a}_2$  make an angle of 120° and together with the vector  $-(\mathbf{a}_1 + \mathbf{a}_2)$  point from the origin to the vertices of the equilateral triangle whose centre lies at the origin. This tensor transforms the lattice vector  $\mathbf{A}_L = L_1\mathbf{a}_1 + L_2\mathbf{a}_2$  as follows:

$$(L_1\mathbf{a}_1 + L_2\mathbf{a}_2) \cdot (\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2) = L_1\mathbf{a}_2 - L_2\mathbf{a}_1 - L_2\mathbf{a}_2$$

It follows that the point with position vector  $\mathbf{a}_1$  ( $L_1 = 1, L_2 = 0$ ) is transformed to the position occupied (before the transformation) by the point with position vector  $\mathbf{a}_2$ , while the point with position vector  $\mathbf{a}_2$ , is transformed to the position  $-(\mathbf{a}_1 + \mathbf{a}_2)$ . This corresponds to a cyclic change of the positions of the vertices of the equilateral triangle.

The double application of the rotation about the threefold axis is represented by a tensor:

$$\begin{aligned}\bar{\bar{3}}^2 &= \bar{\bar{3}} \cdot \bar{\bar{3}} = (\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2) \cdot (\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2) = \\ &= (-\mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1),\end{aligned}$$

which transforms the lattice vector  $\mathbf{A}_L = L_1\mathbf{a}_1 + L_2\mathbf{a}_2$  as follows:

$$(L_1\mathbf{a}_1 + L_2\mathbf{a}_2) \cdot (-\mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1) = -(L_1\mathbf{a}_1 + L_1\mathbf{a}_2) + L_2\mathbf{a}_1$$

A point with position vector  $\mathbf{a}_1$  is transformed to position  $-(\mathbf{a}_1 + \mathbf{a}_2)$ , and a point with position vector  $\mathbf{a}_2$  is transformed to position  $\mathbf{a}_1$ . Again, this is a cyclic change of the positions of the vertices of the triangle, but by rotation in the opposite direction.

Applying the rotation three times around the threefold axis brings the structure to its original position, so that the tensor representing this transformation coincides with the identity tensor:

$$\begin{aligned}\bar{\bar{3}} \cdot \bar{\bar{3}}^2 &= (\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2) \cdot (-\mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1) = \\ &= \mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^2\mathbf{a}_1 + \mathbf{a}^2\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1 = \mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^2\mathbf{a}_2 = \bar{\bar{1}}.\end{aligned}$$

Rotation about the **fourfold** axis occurs only in the square crystal system and is described by the tensor  $\bar{\bar{4}} = \mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1$ . The vectors  $\mathbf{a}_1, \mathbf{a}_2$  have the same length

and make an angle of  $90^\circ$ . The lattice vector  $\mathbf{A}_L = L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2$  is transformed by this tensor as follows:

$$(L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2) \cdot (\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1) = L_1 \mathbf{a}_2 - L_2 \mathbf{a}_1 .$$

The vector  $\mathbf{a}_1$  is rotated into the direction of the vector  $\mathbf{a}_2$ , and the vector  $\mathbf{a}_2$  into the direction of the vector  $-\mathbf{a}_1$ .

The double application leads to a  $180^\circ$  rotation, which coincides with the rotation about the double axis, as can be seen from the product of tensors:

$$\bar{\bar{\mathbf{4}}} \cdot \bar{\bar{\mathbf{4}}} = (\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1) \cdot (\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1) = -\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2 = -\bar{\bar{\mathbf{1}}} = \bar{\bar{\mathbf{2}}}$$

The triple application will provide a tensor:

$$\bar{\bar{\mathbf{4}}} \cdot \bar{\bar{\mathbf{4}}} \cdot \bar{\bar{\mathbf{4}}} = \bar{\bar{\mathbf{4}}} \cdot (-\bar{\bar{\mathbf{1}}}) = -\bar{\bar{\mathbf{4}}} = -\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1 ,$$

which rotates the vector  $\mathbf{a}_1$  in the direction  $-\mathbf{a}_2$  and the vector  $\mathbf{a}_2$  in the direction of the vector  $\mathbf{a}_1$ .

The rotation about the **sixfold** axis occurs only in the hexagonal crystal system and is represented by the tensor  $\bar{\bar{\mathbf{6}}} = \mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1$ . The vectors  $\mathbf{a}_1, \mathbf{a}_2$  make an angle  $120^\circ$  and together with the vector  $-(\mathbf{a}_1 + \mathbf{a}_2)$  point from the origin of the reference frame to the vertices of the equilateral triangle. This tensor transforms the lattice vector  $\mathbf{A}_L = L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2$  as follows:

$$(L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2) \cdot (\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1) = L_1 \mathbf{a}_1 + L_1 \mathbf{a}_2 - L_2 \mathbf{a}_1 .$$

That is, it rotates vector  $\mathbf{a}_1$  in the direction determined by the sum of vectors  $\mathbf{a}_1 + \mathbf{a}_2$ , that is, in the direction that divides the angle between vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , while rotating vector  $\mathbf{a}_2$  in the direction of vector  $-\mathbf{a}_1$ .

A double application of rotation about the sixfold axis is identical to a single rotation about the threefold axis, hence the corresponding tensor has the same form:  $\bar{\bar{\mathbf{6}}}^2 = \bar{\bar{\mathbf{3}}}$ .

The triple rotation represents a rotation about  $180^\circ$ , so the corresponding tensor coincides with the negatively taken identity tensor:  $\bar{\bar{\mathbf{6}}}^3 = -\bar{\bar{\mathbf{1}}}$ .

The fourfold application of rotation about the sixfold axis coincides with the twofold application of rotation about the threefold axis, i.e.  $\bar{\bar{\mathbf{6}}}^4 = \bar{\bar{\mathbf{3}}}^2$ , so this tensor does not need to be mentioned separately either.

A special form is up to the fivefold application, where the tensor can be obtained as the product of the tensors  $\bar{\bar{\mathbf{6}}} \cdot \bar{\bar{\mathbf{3}}}^2$ , which will give the result:

$$(\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1) \cdot (-\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1) = -\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2 .$$

This tensor rotates the vector  $\mathbf{a}_1$  in the direction of the vector  $-\mathbf{a}_2$  and the vector  $\mathbf{a}_2$  in the direction determined by the sum of the vectors  $\mathbf{a}_1 + \mathbf{a}_2$ .

## Combination of rotation with reflection

Reflection only exists in lattices in which a orthogonal unit cell can be selected, whether primitive or centred; is absent in the oblique crystal system. It should be noted that an orthogonal unit cell (centred) can also be chosen in the hexagonal system, which provides advantages in determining the distribution of symmetry elements in the unit cell (→ section C7).

In Appendix D14, different variations of the shape of the reflection tensor are given. In orthogonal lattices, a pair of mutually perpendicular basis vectors  $\mathbf{a}_1, \mathbf{a}_2$ , are chosen, and in the case of a reflection line parallel to the vector  $\mathbf{a}_1$ , the tensor representing the reflection takes the form:

$$\bar{\bar{\mathbf{M}}}_1 = \bar{\mathbf{I}} - 2\mathbf{a}^2\mathbf{a}_2; \quad (\text{a})$$

when reflection in a line parallel to the vector  $\mathbf{a}_2$ , only the indices change.

In the hexagonal system, the basis vectors  $\mathbf{a}_1, \mathbf{a}_2$  are not perpendicular to each other, and in this case it is convenient to choose an orthohexagonal unit cell and express the tensor in the form (→ appendices D14, D26):

$$\bar{\bar{\mathbf{M}}} = \bar{\mathbf{I}} - 2\mathbf{b}^1\mathbf{b}_1, \quad (\text{b})$$

where the reflection line is perpendicular to the vector  $\mathbf{b}_1$ . In Appendix D25, the tensors representing reflections are also expressed using the basis vectors  $\mathbf{a}_1, \mathbf{a}_2$ .

The tensor representing the combination of rotation with reflection is expressed as the product of the corresponding tensors:  $\bar{\bar{\mathbf{n}}} \cdot \bar{\bar{\mathbf{M}}}$ , where  $\bar{\bar{\mathbf{n}}}$  represents one of the rotation tensors.

The combination of **reflection** with **rotation** about the twofold axis is assigned a tensor:

$$\bar{\bar{\mathbf{2}}} \cdot \bar{\bar{\mathbf{M}}} = (-\bar{\mathbf{I}}) \cdot (\bar{\mathbf{I}} - 2\mathbf{u}\mathbf{u}) = -\bar{\mathbf{I}} + 2\mathbf{u}\mathbf{u}.$$

Reflection is applied in orthogonal lattices where the basis vectors  $\mathbf{a}_1, \mathbf{a}_2$  are perpendicular to each other. Then the tensor  $\bar{\bar{\mathbf{M}}}$  can be written in the form  $\bar{\bar{\mathbf{M}}}_1 =$

$(\bar{\bar{\mathbf{I}}} - 2\mathbf{a}^2\mathbf{a}_2)$ , respectively  $\bar{\bar{\mathbf{M}}}_2 = (\bar{\bar{\mathbf{I}}} - 2\mathbf{a}^1\mathbf{a}_1)$ , depending on whether the reflection line is parallel to vector  $\mathbf{a}_1$  or vector  $\mathbf{a}_2$ , respectively.

The combination of tensor  $\bar{\bar{\mathbf{M}}}_1$  with the rotation tensor  $\bar{\bar{\mathbf{2}}}$  will give the result:

$$\bar{\bar{\mathbf{2}}} \cdot \bar{\bar{\mathbf{M}}}_1 = (-\bar{\bar{\mathbf{I}}}) \cdot (\bar{\bar{\mathbf{I}}} - 2\mathbf{a}^2\mathbf{a}_2) = -\bar{\bar{\mathbf{I}}} + 2\mathbf{a}^2\mathbf{a}_2.$$

This tensor transforms the lattice vector  $\mathbf{A}_L$  as follows:

$$(L_1\mathbf{a}_1 + L_2\mathbf{a}_2) \cdot (\bar{\bar{\mathbf{I}}} - 2\mathbf{a}^1\mathbf{a}_1) = L_1\mathbf{a}_1 + L_2\mathbf{a}_2 - 2L_1\mathbf{a}_1 = -L_1\mathbf{a}_1 + L_2\mathbf{a}_2.$$

The same result is obtained by a separate reflection in a line parallel to the vector  $\mathbf{a}_2$ , which is represented by the tensor  $\bar{\bar{\mathbf{M}}}_2$ :

$$(L_1\mathbf{a}_1 + L_2\mathbf{a}_2) \cdot (\bar{\bar{\mathbf{I}}} - 2\mathbf{a}^1\mathbf{a}_1) = L_1\mathbf{a}_1 + L_2\mathbf{a}_2 - 2L_1\mathbf{a}_1 = -L_1\mathbf{a}_1 + L_2\mathbf{a}_2.$$

That is, the combination of reflection in a line parallel to the vector  $\mathbf{a}_1$  and rotation about the twofold axis leads to the same result as reflection in a line parallel to the vector  $\mathbf{a}_2$ . This is consistent with the multiplication table of the **2mm** group, which is also consistent with the fact that changing the order of rotation and reflection leads to the same result. This statement can also be verified using the product of tensors:

$$\bar{\bar{\mathbf{M}}}_1 \cdot \bar{\bar{\mathbf{2}}} = (\bar{\bar{\mathbf{I}}} - 2\mathbf{a}^2\mathbf{a}_2) \cdot (-\bar{\bar{\mathbf{I}}}) = -\bar{\bar{\mathbf{I}}} + 2\mathbf{a}^2\mathbf{a}_2.$$

This result is also correct in the square system, but in the hexagonal system one has to consider the shape of the tensors given in Appendix D25.

The rotation by  $90^\circ$  about the **fourfold axis** passing through the origin of the reference frame is represented by the tensor  $(\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1)$ . The combination of reflection with this rotation is associated with a tensor whose shape depends on which reflection line it is. If the reflection is in the line in which the vector  $\mathbf{a}_1$  lies, the tensor has the form  $\bar{\bar{\mathbf{M}}}_1 = \mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2$ , so that the product yields the tensor

$$\bar{\bar{\mathbf{4}}} \cdot \bar{\bar{\mathbf{M}}}_1 = (\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1) \cdot (\mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2) = -\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1.$$

The product  $\bar{\bar{\mathbf{4}}}^3 \cdot \bar{\bar{\mathbf{M}}}_1$  gives the tensor

$$(-\mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1) \cdot (\mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2) = \mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1.$$

The second of these two tensors represents the reflection in the diagonal of the square that passes through the origin of the reference frame, the first of two tensors reflection in the second diagonal of the square.

## C4.2 Translational part of operator S

In the previous sections - on rotations and reflections - the tensor part  $\bar{\Phi}$  of the symmetry operator  $S \equiv [\bar{\Phi}, \mathbf{t}]$  has been fully described. When considering the translational part  $\mathbf{t}$  of operator S it is convenient to start from Figure C4. A square lattice is drawn on it. If we rotate it by  $90^\circ$  around point A or around point B, it will identify with itself, i.e. we perform a symmetry operation. However, if we rotate the

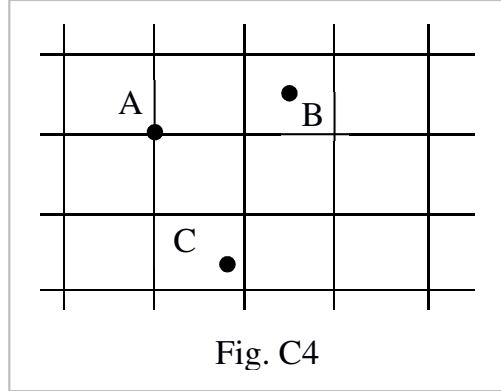


Fig. C4

lattice by the same angle about point C, the lattice will only come to an equivalent position after adding a suitable translation  $\mathbf{t}$ , which is not a lattice translation, i.e., it does not belong to the translation group. In this case, the operator S, if it is to be the operator of the symmetry operation, must have two parts, a rotational and a non-lattice translational one.

There are several translations  $\mathbf{t}$ , which can be used to bring the lattice to an equivalent position after its first rotation about the point C. It can be seen from the figure that the size of the vector  $\mathbf{t}$  need not exceed the dimensions of the unit cell, but any lattice vector  $\mathbf{A}_L$  can be added to it; in doing so, the transformation remains a symmetry operation. The operator representing such a transformation has the form  $S \equiv [\bar{\Phi}, \mathbf{t} + \mathbf{A}_L]$ .

The point symmetry operations, represented by the tensor part of the operator S, are elements of point groups, which in the case of crystals have a finite number of elements. Multiple applications of a point operation after a certain number of steps lead to an identical operation (e.g., a triple application of a  $120^\circ$  rotation, or a double application of reflection). Therefore, there exists a natural number m, for which  $\bar{\Phi}^m = \bar{\mathbf{I}}$  (we assume that m is the smallest such number). For the corresponding operator S, then (relation (C2.4)) holds:

$$S^m \equiv [\bar{\mathbf{I}}, \mathbf{t} \cdot \{\bar{\mathbf{I}} + \bar{\Phi} + \bar{\Phi}^2 + \dots + \bar{\Phi}^{m-1}\}]. \quad (\text{C4.18})$$

If  $S^m$  is to be a symmetry operation, then

$$\mathbf{t} \cdot \{\bar{\mathbf{I}} + \bar{\Phi} + \bar{\Phi}^2 + \dots + \bar{\Phi}^{m-1}\} = \mathbf{A}_L, \quad (\text{C4.19})$$

that is, an m-fold application of the operator S must represent a lattice translation. The expression in the large bracket  $\{\bar{\mathbf{I}} + \bar{\Phi} + \bar{\Phi}^2 + \dots + \bar{\Phi}^{m-1}\}$  has the name

**characteristic tensor** of the operation  $S$ . If we substitute any of the tensors  $\bar{2}$ ,  $\bar{3}$ ,  $\bar{4}$  or  $\bar{6}$  representing the generating elements of the point groups (Table TC2) after the tensor  $\bar{\Phi}$ , the sum of the terms of the characteristic tensor equals zero. Proving this statement by calculation, except for the  $\bar{2}$  tensor, is tedious, but its truth can be quite easily verified graphically ( $\rightarrow$  Appendix D9). That is, in the case of the above tensors,  $S^m = [\bar{I}, \mathbf{0}]$ , whatever  $\mathbf{t}$  might be. In these cases, the constraints on the vector  $\mathbf{t}$  do not follow from relation (C4.19).

Another case is the operation  $S = [\bar{M}, \mathbf{t}]$ , where  $\bar{M} = \bar{I} - 2\mathbf{u}\mathbf{u}$ . For this tensor, the following holds

$$\bar{M}^2 = (\bar{I} - 2\mathbf{u}\mathbf{u}) \cdot (\bar{I} - 2\mathbf{u}\mathbf{u}) = \bar{I} - 2\mathbf{u}\mathbf{u} - 2\mathbf{u}\mathbf{u} + 4\mathbf{u}\mathbf{u} = \bar{I}.$$

We verify that the characteristic tensor  $\{\bar{M}\}$  of this operation is non-zero:

$$\{\bar{M}\} = \bar{I} + \bar{M} = \bar{I} + \bar{I} - 2\mathbf{u}\mathbf{u} = 2(\bar{I} - \mathbf{u}\mathbf{u}),$$

so that equation (C4.19) does not admit an arbitrary vector  $\mathbf{t}$ , which must satisfy the condition

$$\mathbf{t} \cdot \{\bar{M}\} = \mathbf{t} \cdot 2(\bar{I} - \mathbf{u}\mathbf{u}) = 2[\mathbf{t} - (\mathbf{t} \cdot \mathbf{u})\mathbf{u}] = \mathbf{A}_L. \quad (\text{C4.20})$$

The expression  $(\mathbf{t} \cdot \mathbf{u})\mathbf{u}$  represents the component of the vector  $\mathbf{t}$  parallel to the vector  $\mathbf{u}$ , so the expression  $[\mathbf{t} - (\mathbf{t} \cdot \mathbf{u})\mathbf{u}]$  represents the component perpendicular to the vector  $\mathbf{u}$ , i.e. parallel to the reflection line. It follows from equation (4.20) that this component must be equal to half of the lattice vector parallel to the reflection line. As mentioned above, it is sufficient to restrict to vectors  $\mathbf{t}$ , whose size does not exceed the dimensions of the unit cell (for example, the size of the basis vector  $\mathbf{a}_1$ ). Then for vector  $\mathbf{t}$  we can write the relation

$$[\mathbf{t} - (\mathbf{t} \cdot \mathbf{u})\mathbf{u}] = \left(\frac{j}{2}\right)\mathbf{a}_1, \quad (\text{C4.21})$$

in which  $j$  can only take values  $j = 0, \pm 1$ . No constraints are placed on the component perpendicular to the reflection line. The case  $j = 0$  represents ordinary reflection, the case  $j = \pm 1$  corresponds to reflection with a glide. This means that in such an operation, after reflection in a straight line, the whole structure still needs to be shifted along the reflection line by half of the identity period, i.e., a translation that does not belong to the translation group needs to be performed. The operator with a glide then takes the form

$$[\bar{M}_1, \mathbf{a}_1/2], \quad (\text{C4.22})$$

where the index "1" at the tensor  $\bar{\bar{\mathbf{M}}}_1$  denotes the reflection in a line parallel to the vector  $\mathbf{a}_1$ . The location of the glide lines in the lattice is described in C7.5.

### C4.3 Summary of possible symmetry operations

Operators representing symmetry operations of two-dimensional periodic structures are written in the general form  $S \equiv [\bar{\Phi}, \mathbf{t}]$ . Operators of trivial operations include the identity tensor  $\bar{\bar{\mathbf{I}}}$  and the lattice vector  $\mathbf{A}_L$ :  $S \equiv [\bar{\bar{\mathbf{I}}}, \mathbf{A}_L]$ . Non-trivial operations include rotations and reflections, represented by tensors, which we denote by the symbols  $\bar{\bar{2}}, \bar{\bar{3}}, \bar{\bar{4}}, \bar{\bar{6}}$  and  $\bar{\bar{\mathbf{M}}}$ , their powers and combinations with lattice translation, as well as with special non-lattice translations.

Non-trivial symmetry operations are divided into **open** and **closed**. A closed operation with operator  $S \equiv [\bar{\Phi}, \mathbf{t}]$  is said to be one for which ( $\rightarrow$  text before relation C4.18)

$$S^m = [\bar{\bar{\mathbf{I}}}, \mathbf{0}]. \quad (\text{C4.23})$$

The term *closed operation* is related to the fact that (in the laboratory coordinate system) the sum of the vectors

$$\mathbf{r}, \mathbf{r} \cdot S, \mathbf{r} \cdot S^2, \dots, \mathbf{r} \cdot S^{m-1}$$

forms a closed geometric figure (polygon). Closed operations include all rotations and reflections. For planar structures, the only open operation is glide reflection. For closed operations, it is always possible to make the translational part  $\mathbf{t}$  of the operator zero, i.e.,  $S \equiv [\bar{\Phi}, \mathbf{0}]$ , by a suitable choice of the position of the origin of the coordinate system.

According to the value of the determinant of the corresponding tensor, a distinction is made between **proper** and **improper** symmetry operations. If the determinant of the tensor  $|\bar{\Phi}| = +1$ , the operation is proper, if  $|\bar{\Phi}| = -1$ , it is an improper operation. The determinants of all tensors representing rotations  $\bar{\bar{2}}, \bar{\bar{3}}, \bar{\bar{4}}, \bar{\bar{6}}$  have value +1, the determinant of the tensor  $\bar{\bar{\mathbf{M}}}$  representing reflection has value -1 ( $\rightarrow$  Appendix D10).

An overview of possible symmetry operations is given in the following table TC3. The first column lists all operators that represent possible symmetry operations.

| TC3                            | Possible symmetry operation          |                      |                 |
|--------------------------------|--------------------------------------|----------------------|-----------------|
| Operators<br>$[\bar{\Phi}, t]$ | Restriction of<br>translational part | Name of<br>operation | Operation       |
| $[\bar{1}, t]$                 | $t = 0$                              | identity             | closed proper   |
| $[\bar{2}, t]$                 | no                                   | rotation             |                 |
| $[\bar{3}, t]$                 | no                                   | rotation             |                 |
| $[\bar{4}, t]$                 | no                                   | rotation             |                 |
| $[\bar{6}, t]$                 | no                                   | rotation             |                 |
| $[\bar{M}, t]$                 | $t - (t \cdot u)u = 0$               | reflection           | closed improper |
| $[\bar{M}, t]$                 | $t - (t \cdot u)u = \pm a/2$         | glide reflection     | open            |
| $[\bar{1}, t]$                 | $t = A_L \neq 0$                     | lattice translation  |                 |

## C5 Point groups

Table TC3 on the previous page lists the possible symmetry operations of planar periodic structures. If the translational part  $t$  is omitted from their operators, what remains are the operators of the point operations, i.e., the operators representing the elements of the point groups. The operator  $[\bar{6}, 0]$  mediates a rotation of  $60^\circ$ , but the symmetry operations are also rotations of multiples of this angle, i.e., rotations of  $120^\circ$ ,  $180^\circ$ , etc. The operators of these rotations are "powers" of the  $[\bar{6}, 0]$  operator, by which is meant its multiple use. The magnitudes of the rotations that bring the planar periodic structure to equivalent positions are given in C4.1.1, in the line denoted as relation (C4.14). At the end of that article, in Table TC1, these rotations are classified into groups. No rotation combinations other than the above are possible. For example, if we assume that  $90^\circ$  and  $120^\circ$  rotations belong to the same group, the combination of the two, i.e.  $210^\circ$  rotation, would also have to belong to this group. However, the latter is not a symmetry operation of planar periodic structures, so the

two rotations mentioned above cannot belong to the same point group. Proceeding in this way, it is possible to construct five pointgroups of rotations, all of which are cyclic.

The point operations include the reflection represented by the tensor  $\bar{\bar{\mathbf{M}}}$ . A repeated application of reflection returns the object to its initial position, so that the reflection is itself an inverse operation. Therefore, the reflection group  $\mathbf{m}$  has only two elements, the identity  $e$  and the reflection  $m$ :  $\mathbf{m} \equiv \{e, m\}$ . Therefore, the scalar product of the tensor  $\bar{\bar{\mathbf{M}}}$  with itself must be equal to the identity tensor:  $\bar{\bar{\mathbf{M}}} \cdot \bar{\bar{\mathbf{M}}} = \bar{\bar{\mathbf{I}}}$ , because the tensor  $\bar{\bar{\mathbf{M}}}$  must also be an inverse tensor of itself. The tensors  $\bar{\bar{\mathbf{M}}}$  and  $\bar{\bar{\mathbf{I}}}$ , given the scalar product as a binary operation, form an isomorphic group with the point group  $\mathbf{m}$ .

Combining the reflection group with the rotation groups produces four additional point groups. These are no longer cyclic, two generating elements are needed to create them. In total, this amounts to 10 types of point groups, which are listed in Table TC4.

The combination of a cyclic group and reflection group is expressed as their direct product. For example: group  $\mathbf{4mm} = \{e, 4, 4^2, 4^3\} \cdot \{e, m\} \equiv \{4\} \cdot \{m\}$ . The group  $\mathbf{4}$  is an invariant subgroup of the group  $\mathbf{4mm}$ , so its decomposition into cosets is of the form  $\mathbf{4mm} = \{4\} + \{4\} \cdot m$ , where the reflection  $m$  is the representative of a single coset.

| TC4 Point groups                 |                                                                           |                     |
|----------------------------------|---------------------------------------------------------------------------|---------------------|
| Symbols of groups                | Elements of groups (symmetry operations)                                  | Generating elements |
| <b>1</b>                         | $e$                                                                       | $e$                 |
| <b>2</b>                         | $e, 2$                                                                    | $2$                 |
| <b>3</b>                         | $e, 3, 3^2$                                                               | $3$                 |
| <b>4</b>                         | $e, 4, 4^2, 4^3$                                                          | $4$                 |
| <b>6</b>                         | $e, 6, 6^2, 6^3, 6^4, 6^5$                                                | $6$                 |
| <b><math>\mathbf{m}</math></b>   | $e, m$                                                                    | $m$                 |
| <b><math>\mathbf{2mm}</math></b> | $e, 2, m_x, m_y$                                                          | $2, m_x$            |
| <b><math>\mathbf{3m}</math></b>  | $e, 3, 3^2, m_0, m_{60}, m_{120}$                                         | $3, m_0$            |
| <b><math>\mathbf{4mm}</math></b> | $e, 4, 4^2, 4^3, m_x, m_y, m_{xy}, m_{yx}$                                | $4, m_x$            |
| <b><math>\mathbf{6mm}</math></b> | $e, 6, 6^2, 6^3, 6^4, 6^5, m_0, m_{60}, m_{120}, m_{30}, m_{90}, m_{150}$ | $6, m_0$            |

The symbology used in Table TC4 has the following meaning: the symbols  $m_x, m_y$  in the  $\mathbf{2mm}$  group represent the reflections in the lines labeled  $x, y$ , which are perpendicular to each other and parallel to the basis vectors  $\mathbf{b}_1$  (x-direction) and  $\mathbf{b}_2$  (y-direction). The symbols  $m_{xy}, m_{yx}$  in the  $\mathbf{4mm}$  group represent two other

possible reflection operations, namely in the lines that divide the angle between the  $x, y$  lines in half, which are the diagonals of the square. The symbols  $m_{60}$ ,  $m_{120}$ , etc., denote reflections in lines rotated with respect to  $m_0$  by  $60^\circ$ ,  $120^\circ$ , etc. In other parts of the text relating to reflection operators, the indices 1 and 2, representing the directions of the basis vectors, are often used instead of the indices  $x, y$ .

The creation of a group using generating elements is illustrated by the example of a  **$2mm$**  group ( $\rightarrow$  Appendix D11), which has only four elements. This procedure can also be verified using a graphical construction ( $\rightarrow$  Appendix D12).

The following figure shows a graphical representation of point groups. In the circles symbolizing the groups are marked the symmetry elements – the  $n$ -fold axes as  $n$ -polygons and the reflection lines as line segments. Small solid circles are used to mark all the equivalent positions of one point of the plane into which this point is transformed by the symmetry operations of the corresponding group. The more elements a point group contains, the more equivalent points it produces. The number of equivalent points coincides with the number of elements of the group, i.e. the number of symmetry operations in the group.

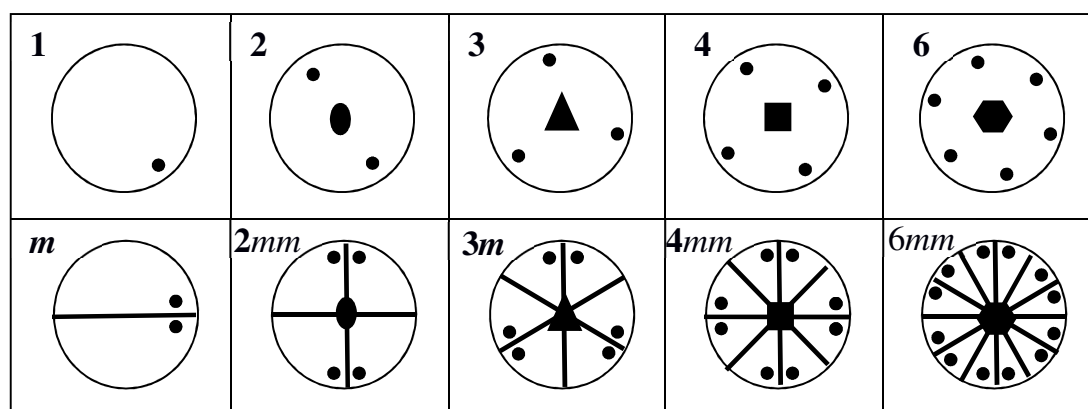


Fig. C5

Among the ten point groups, there are a few that are subgroups of a group with more elements. For example, the group  **$6mm$**  contains subgroups **6**,  **$3m$**  and **3**, if we do not count the trivial subgroup **1**. The group  **$4mm$**  contains the subgroups **4**,  **$2mm$** , **2** and  **$m$** . Subgroups with fewer elements are characterized by structures whose structural motif has lower point symmetry than the lattice.

The successive application of two symmetry operations is referred to as the "product" between two elements of a point group, i.e. as the realization of a group operation between two elements of a point group; the result is another element of the group. The products are compiled into a clear table, called a **multiplication table**. The following table TC5 shows the products in a group  **$2mm$** . The left column shows

the first terms of the product, the top row the second terms, the intersection of column and row shows the result of their product, i.e. the result of their successive application. For example, the product of elements 2 and  $m_x$ , that is, their successive application in the order given, is equivalent to the direct application of element  $m_y$ . The product of the elements  $m_x$  and  $m_y$  is equivalent to a rotation of 2, so that the presence of reflections in two mutually perpendicular directions is inextricably linked to the presence of a rotation about the twofold axis. The table of this group is symmetric with respect to the diagonal, because when the two symmetry operations are applied in this case their order does not matter.

| TC5 Multiplication table<br>of group $2mm$ |       |       |       |       |
|--------------------------------------------|-------|-------|-------|-------|
|                                            | $e$   | 2     | $m_x$ | $m_y$ |
| $e$                                        | $e$   | 2     | $m_x$ | $m_y$ |
| 2                                          | 2     | $e$   | $m_y$ | $m_x$ |
| $m_x$                                      | $m_x$ | $m_y$ | $e$   | 2     |
| $m_y$                                      | $m_y$ | $m_x$ | 2     | $e$   |

From the point of view of the algebra of groups, each point group containing a reflection can be expressed as the direct product ( $\rightarrow$  Appendix D29 on groups) of the corresponding cyclic group and the two-element group of the reflection. This fact is expressed in the algebra of groups by the notation

$$\mathbf{n} \cdot \mathbf{m} \equiv \{n\} \cdot \{m\},$$

where  $\mathbf{n}$  and  $\{n\}$  represent, respectively, the cyclic group with  $n$  elements (related to the  $n$ -fold axis of symmetry) and  $\mathbf{m}$  resp.  $\{m\}$  the two-element group of the reflection.

The point groups and in particular their generating elements will be used in the search for different types of translational symmetry – in determining the set of translation groups.

## C6 Translation groups

The search for types of translational symmetry of planar structures is essentially a matter of determining the possible types of pairs of basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  of planar lattices. There is a relationship between the point symmetry operations of planar structures and the basis vectors, expressed by the condition ( $\rightarrow$  relation C4.13)

$$\Phi_{ij} = \mathbf{a}_i \cdot \bar{\bar{\Phi}} \cdot \mathbf{a}^j = \text{integer}, \quad (\text{C6.1})$$

which requires the scalar coordinates of the tensor to be integers. We exploit the condition by successively inserting the tensors representing the generating elements of the individual point groups into relation (C6.1) (Table TC2). The other elements of the groups that are not generating do not impose new conditions on the choice of the vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ . We go through all the point-groups from table TC4 in turn.

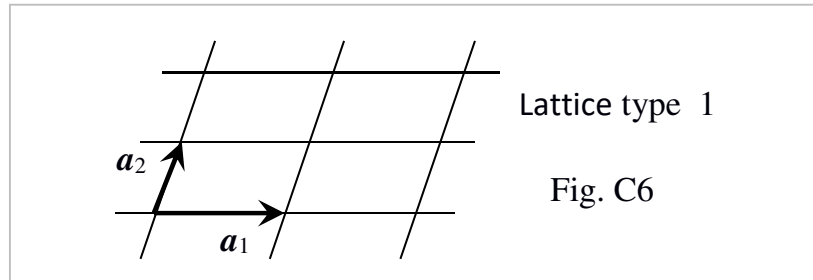
## C6.1 Lattices of structures with point groups 1, 2

### Group 1

The identity tensor  $\bar{\mathbf{I}} = \mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2$  represents the generating element of this group. Its coordinates are integers ( $l_{11} = 1$ ,  $l_{12} = 0$ ,  $l_{21} = 0$ ,  $l_{22} = 1$ ), so condition (6.1) is automatically satisfied, it does not impose any constraints on the basis vectors; the vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  need not be of the same length, nor do they form a special angle.

### Group 2

The generating element is represented by the tensor  $-\bar{\mathbf{I}} = -(\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2)$ . The coordinates of the tensor  $-\bar{\mathbf{I}}$  are again integers, no restrictions on the vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  follow from relation (C6.1). Planar periodic structures with point groups 1 and 2 have the same type of lattice. They may differ by the symmetry of the structural motif embedded to each of its lattice points.



## C6.2 Lattices of structures with point groups 3, 6

The generating elements in these groups correspond to tensors ( $\rightarrow$  TC2)

$$\begin{aligned} \bar{\mathbf{3}} = & \mathbf{a}^1 \mathbf{a}_1 \left( -\frac{1}{2} - \frac{\sqrt[2]{3} \cos \alpha}{2} \right) + \mathbf{a}^1 \mathbf{a}_2 \frac{a_1 \sqrt[2]{3}}{a_2} \frac{1}{2} \frac{1}{\sin \alpha} - \mathbf{a}^2 \mathbf{a}_1 \frac{a_2 \sqrt[2]{3}}{a_1} \frac{1}{2} \frac{1}{\sin \alpha} \\ & + \mathbf{a}^2 \mathbf{a}_2 \left( -\frac{1}{2} + \frac{\sqrt[2]{3} \cos \alpha}{2} \right) \end{aligned}$$

$$\begin{aligned}\bar{\bar{6}} = & \mathbf{a}^1 \mathbf{a}_1 \left( +\frac{1}{2} - \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \right) + \mathbf{a}^1 \mathbf{a}_2 \frac{a_1 \sqrt[2]{3}}{a_2} \frac{1}{2 \sin \alpha} - \mathbf{a}^2 \mathbf{a}_1 \frac{a_2 \sqrt[2]{3}}{a_1} \frac{1}{2 \sin \alpha} + \\ & + \mathbf{a}^2 \mathbf{a}_2 \left( +\frac{1}{2} + \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \right)\end{aligned}$$

or in a more concise general notation

$$\bar{\bar{\Phi}} = \mathbf{a}^1 \mathbf{a}_1 p + \mathbf{a}^1 \mathbf{a}_2 q + \mathbf{a}^2 \mathbf{a}_1 r + \mathbf{a}^2 \mathbf{a}_2 s.$$

The tensor  $\bar{\bar{6}}$  has coordinates

$$p = \frac{1}{2} - \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \quad q = \frac{a_1 \sqrt[2]{3}}{a_2} \frac{1}{2 \sin \alpha} \quad r = -\frac{a_2 \sqrt[2]{3}}{a_1} \frac{1}{2 \sin \alpha} \quad s = \frac{1}{2} + \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha}.$$

The  $q$  and  $r$  coordinates of the  $\bar{\bar{3}}$  and  $\bar{\bar{6}}$  tensors are the same, differing only in the coordinates  $p$  and  $s$ . The coordinates  $p, q, r, s$  are determined by the magnitudes of the basis vectors and the angle  $\alpha$  between them. If all coordinates are to be integers, this places conditions on the ratio of the magnitudes of the basis vectors and on the magnitude of the angle between them. If we subtract the coordinate  $p$  from the coordinate  $s$ , regardless of whether the tensor is  $\bar{\bar{3}}$  or  $\bar{\bar{6}}$ , we get (the number  $n$  is supposed to be integer):

$$s - p = \sqrt{3} \frac{\cos \alpha}{\sin \alpha} = n,$$

from where, after modification, we obtain

$$\sin \alpha = \sqrt{\frac{3}{3 + n^2}}.$$

Next, multiply the coordinates  $q$  and  $r$  with each other, substituting the obtained value after  $\sin \alpha$ . The product  $q \cdot r$  must also be equal to an integer:

$$q \cdot r = \frac{3}{4} \cdot \frac{3 + n^2}{3} = \frac{3 + n^2}{4}.$$

This equation has integer solutions for odd  $n$ , i.e. for  $n = 1, 3, 5, \dots$ . Let us check each option.

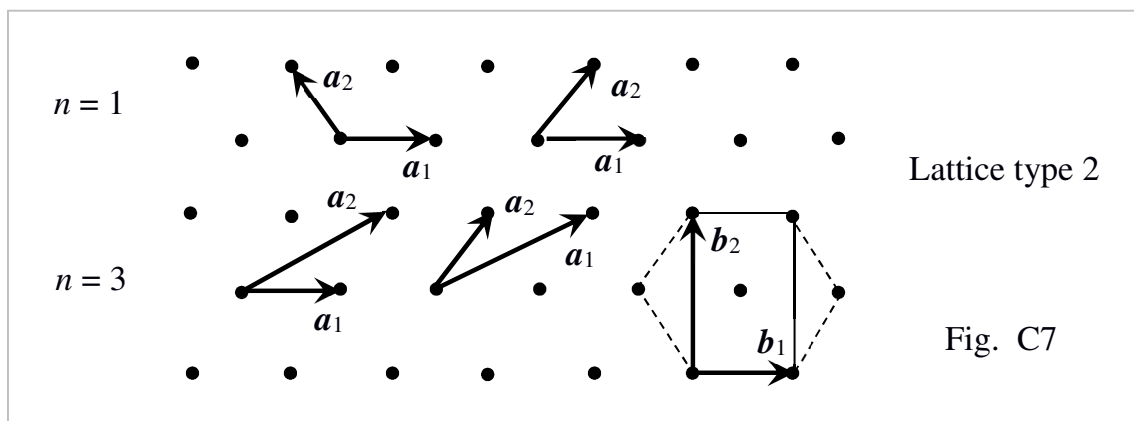
**For  $n = 1$ ,** the product  $q \cdot r = 1$ , and since both  $q$  and  $r$  are integers,  $q = r = 1$  and

$$\sin \alpha = \sqrt{\frac{3}{3 + n^2}} = \sqrt{\frac{3}{3 + 1}} = \frac{\sqrt{3}}{2}, \quad \text{there for } \alpha = 60^\circ, \text{ or } 120^\circ.$$

The result  $q = r = 1$  further implies that the magnitudes of the basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  are the same. The angle between them is  $60^\circ$ , or  $120^\circ$ , however, both choices of angle lead to the same lattice, as can be seen graphically.

**For  $n = 3$**  we get  $\sin \alpha = 1/2$  (i.e.  $\alpha = 30^\circ$ , or  $150^\circ$ ), and  $q \cdot r = 3$ . This means that either  $q = 1, r = 3$ , or conversely,  $q = 3, r = 1$ . Let us choose  $\alpha = 30^\circ$ . If we choose  $q = 1$ , then  $a_2 = a_1\sqrt{3}$ , and the opposite choice, i.e.  $r = 1$ , gives  $a_1 = a_2\sqrt{3}$ . Both cases represent the same type of lattice, as in the case  $n = 1$ .

Examining the remaining choices, i.e.,  $n = 5$ , etc., we would find that they lead again to the same type of lattice as shown in the following Figure C7.



Among all possible pairs of vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , a pair with equal sizes  $a_1 = a_2$ , taking an angle  $\alpha = 120^\circ$ , is chosen by convention in this type of lattice. In doing so,  $\mathbf{a}_2 = \mathbf{a}_1 \cdot \bar{\mathbf{3}}$ , or  $\mathbf{a}_2 = \mathbf{a}_1 \cdot \bar{\mathbf{6}}^2$ . The lattice in the figure has a typical hexagonal symmetry. An **orthogonal cell** with basis vectors  $\mathbf{b}_1$  and  $\mathbf{b}_2$  ( $\rightarrow$  Figure C7), also called **orthohexagonal cell**, may also be chosen in this lattice, on the basis of which the positions of the reflection lines are more easily determined. There are three equivalent choices of orthohexagonal cells, differing in their mutual rotation by  $60^\circ$ .

As mentioned above, due to the similarity of coordinates, the  $\bar{\mathbf{3}}$  tensor generates the same lattice as the  $\bar{\mathbf{6}}$  tensor. Groups **3** and **6**, like groups **1** and **2**, differ in that they describe planar structures with the same lattice but different structural motifs.

### C6.3 Lattices of structures with point group 4

The generating element of the group corresponds to tensor  $\bar{4}$  ( $\rightarrow$  tab. TB2):

$$\bar{4} = -a^1 a_1 \frac{\cos \alpha}{\sin \alpha} + a^1 a_2 \frac{a_1}{a_2} \frac{1}{\sin \alpha} - a^2 a_1 \frac{a_2}{a_1} \frac{1}{\sin \alpha} + a^2 a_2 \frac{\cos \alpha}{\sin \alpha}.$$

We start with the coordinate  $p = \cos \alpha / \sin \alpha$ , which, like the other coordinates, is supposed to be an integer. From here we express  $\sin \alpha$  :

$$\sin \alpha = \frac{1}{\sqrt{1 + p^2}}.$$

By multiplying the second and third coordinates together, after inserting the calculated  $\sin \alpha$ , we get:

$$1 + p^2 = q \cdot r.$$

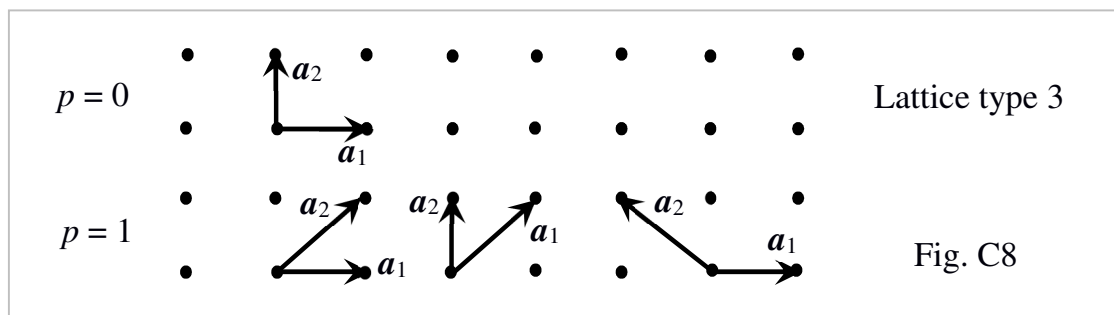
Adding integers after  $p$  gradually gives more possibilities.

With  $p = 0$   $\sin \alpha = 1$ , so  $\alpha = 90^\circ$ , also the product  $q \cdot r = 1$ , so  $a_1 = a_2$ , so the lattice is tetragonal (square).

With  $p = 1$   $\sin \alpha = 1/\sqrt{2}$ , so  $\alpha = 45^\circ$ , or  $135^\circ$ . Then  $q \cdot r = 2$ , so there are two possibilities:

$$a_2 = a_1 \frac{\sqrt{2}}{2}, \quad \text{or} \quad a_1 = a_2 \frac{\sqrt{2}}{2}.$$

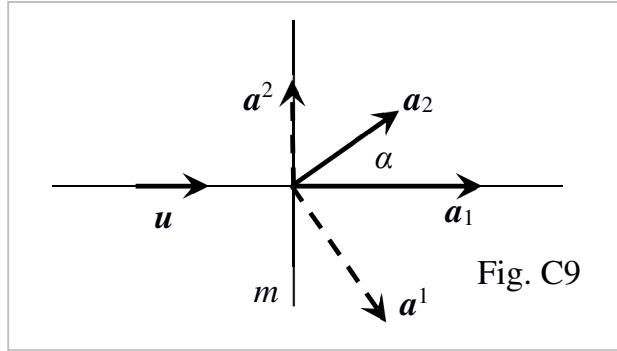
From the set of different pairs, vectors of equal length ( $a_1 = a_2$ ) and perpendicular to each other are selected as the basis. Then  $a_2 = a_1 \cdot \bar{4}$ .



## C6.4 Lattices of structures with point group $m$

The tensor  $\bar{\mathbf{M}} = \bar{\mathbf{I}} - 2\mathbf{u}\mathbf{u}$  corresponds to the generating element in the group  $m$  (Section C4.1.2), where  $\mathbf{u}$  is the unit vector perpendicular to the reflection line  $m$ . That section states that both the reflection line and the direction perpendicular to it are parallel to the directions of the lattice vectors of the direct and reciprocal lattice simultaneously. Thus, we could choose the basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  such that one is parallel to the reflection line and the other is perpendicular to it.

However, let us consider more generally and assume that, for example, vector  $\mathbf{a}_1$  is perpendicular to the reflection line and vector  $\mathbf{a}_2$  makes an angle  $\alpha$  with vector  $\mathbf{a}_1$ . In Fig. C9, the corresponding pair of reciprocal vectors  $\mathbf{a}^1$ ,  $\mathbf{a}^2$  is drawn in dashed lines. Under such assumptions, we will



look for the conditions that must be satisfied for the coordinates of the tensor  $\bar{\mathbf{M}}$  to be integer. We first compute the scalar coordinates of the tensor in the system with the basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  according to relation (C4.13):

$$M_{ij} = \mathbf{a}_i \cdot \bar{\mathbf{M}} \cdot \mathbf{a}^j .$$

That's what we get:

$$\begin{aligned} M_{11} &= \mathbf{a}_1 \cdot \bar{\mathbf{M}} \cdot \mathbf{a}^1 = \mathbf{a}_1 \cdot (\bar{\mathbf{I}} - 2\mathbf{u}\mathbf{u}) \cdot \mathbf{a}^1 = [\mathbf{a}_1 \cdot \bar{\mathbf{I}} - 2(\mathbf{a}_1 \cdot \mathbf{u})\mathbf{u}] \cdot \mathbf{a}^1 = \\ &= [\mathbf{a}_1 - 2a_1 \mathbf{u}] \cdot \mathbf{a}^1 = [\mathbf{a}_1 - 2\mathbf{a}_1] \cdot \mathbf{a}^1 = -\mathbf{a}_1 \cdot \mathbf{a}^1 = -1 \end{aligned}$$

$$M_{12} = \mathbf{a}_1 \cdot \bar{\mathbf{M}} \cdot \mathbf{a}^2 = \mathbf{a}_1 \cdot (\bar{\mathbf{I}} - 2\mathbf{u}\mathbf{u}) \cdot \mathbf{a}^2 = 0$$

$$\begin{aligned} M_{21} &= \mathbf{a}_2 \cdot \bar{\mathbf{M}} \cdot \mathbf{a}^1 = \mathbf{a}_2 \cdot (\bar{\mathbf{I}} - 2\mathbf{u}\mathbf{u}) \cdot \mathbf{a}^1 = [\mathbf{a}_2 \cdot \bar{\mathbf{I}} - 2(\mathbf{a}_2 \cdot \mathbf{u})\mathbf{u}] \cdot \mathbf{a}^1 = \\ &= [\mathbf{a}_2 - 2a_2 \cos \alpha \mathbf{u}] \cdot \mathbf{a}^1 = \\ &= 0 - 2a_2 \cos \alpha a^1 \cos(\pi/2 - \alpha) = -2 \frac{a_2}{a_1} \cos \alpha . \end{aligned}$$

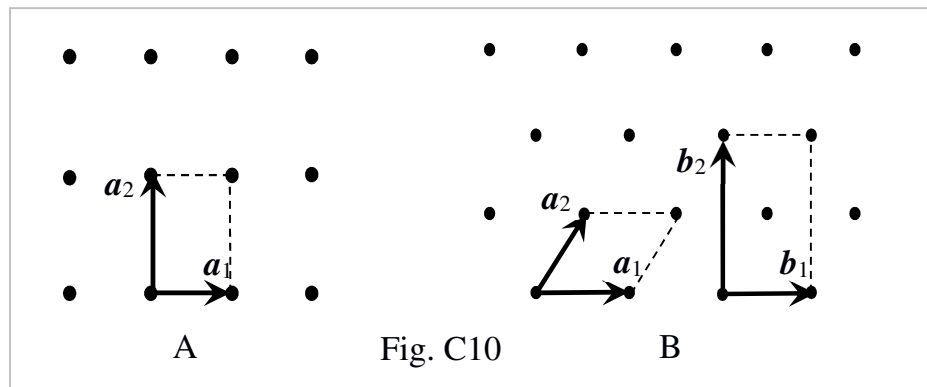
$$M_{22} = \mathbf{a}_2 \cdot \bar{\mathbf{M}} \cdot \mathbf{a}^2 = \mathbf{a}_2 \cdot (\bar{\mathbf{I}} - 2\mathbf{u}\mathbf{u}) \cdot \mathbf{a}^2 = \mathbf{a}_2 \cdot \mathbf{a}^2 - 2(\mathbf{a}_2 \cdot \mathbf{u})(\mathbf{u} \cdot \mathbf{a}^2) = 1 .$$

If we require that the number  $M_{21}$  is also integer, the condition must be satisfied

$$a_2 \cos \alpha = \frac{a_1}{2} n . \quad (\text{C6.2})$$

That is, the magnitude of the projection of the vector  $\mathbf{a}_2$  onto the vector  $\mathbf{a}_1$  should be equal to an integer multiple of half the magnitude of the vector  $\mathbf{a}_1$ . If  $n = 0$ , then the projection is zero and the vector  $\mathbf{a}_2$  is perpendicular to the vector  $\mathbf{a}_1$ , so the lattice is orthogonal. Meanwhile, the ratio of the lengths of these vectors can be arbitrary, so the unit cell is orthogonal (lattice A in Figure C 10).

When  $n = \pm 1$ , the ratio of the sizes of the basis vectors can again be arbitrary, but their orientation relative to each other must be such that the projection of the vector  $\mathbf{a}_2$  onto the vector  $\mathbf{a}_1$  is exactly half its size (in Figure C10 lattice B).



If  $n$  is an even number, an A-type lattice is always produced, if it is odd, a B-type lattice. But even a B-type lattice is orthogonal, although the unit cell constructed from the vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  is not orthogonal. In accordance with the requirement that the symmetry of the unit cell should match the symmetry of the lattice (Bravais conditions), a pair of basis vectors  $\mathbf{b}_1$ ,  $\mathbf{b}_2$ , is introduced in this case to form an orthogonal cell, but with a lattice point also in the middle of the cell. Such a unit cell is called centred, in contrast to the primitive cell formed by the vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , which has a smaller area content but a symmetry not matching the symmetry of the lattice. The name centred lattice is used for a lattice in which an orthogonal centred primitive cell can be chosen. In centred lattices, reflection with glide is applied, i.e. there are glide lines in them ( $\rightarrow$  relations C4.21 and C4.22).

By integer linear combinations of the primitive-cell basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , we obtain the position vectors of all lattice points. The set of all translations of type  $\mathbf{A}_L = L_1\mathbf{a}_1 + L_2\mathbf{a}_2$ , where  $L_i$  are integers, forms the full translation group  $T_p$  of the corresponding lattice, for which we use the name **primitive translation group**. However, the integer linear combination of the vectors  $\mathbf{b}_1$ ,  $\mathbf{b}_2$  cannot be used to obtain the position vectors of lattice points lying in the middle of the cells. Therefore, the group  $T_b$  of analogous linear combinations  $\mathbf{B}_L = L_1\mathbf{b}_1 + L_2\mathbf{b}_2$  is not identical to the full translation group, it is less numerous, forming an invariant subgroup of it. To

obtain the position vectors of all lattice points, we need to add to each translation  $\mathbf{B}_L$  a translation

$$\mathbf{t}_b = \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2 ,$$

thus achieving a match with the full translation group. In this case, the full translation group of the centred lattice, which is identical to the primitive translation group of  $T_p$  , can be written as a sum:

$$T_p = T_b + \mathbf{t}_b \cdot T_b . \quad (\text{C6.3})$$

The second term of the sum represents the coset of the group  $T_p$  with respect to the subgroup  $T_b$ . The dot between translation  $\mathbf{t}_b$  and group  $T_b$  has the meaning of a group operation, in this case the successive applications of an element of group  $T_b$  and translation  $\mathbf{t}_b$ .

### C6.5 Lattices of structures with point groups $2mm$ , $3m$ , $6mm$ , $4mm$

In the  $2mm$  group, the generating elements are  $180^\circ$  rotation and reflection, i.e., the elements represented by the  $\bar{2}$  and  $\bar{M}$  tensors. The  $\bar{2}$  tensor does not impose requirements on the ratio of the sizes of the basis vectors, nor on the angle between them. Therefore, the lattice of a planar periodic structure with symmetry described by the  $2mm$  group must be as required by reflection, i.e., it must be orthogonal. Thus, the  $2mm$  group does not require the existence of another type of lattice symmetry.

In the  $3m$  and  $6mm$  groups, the generating elements are represented by the tensors  $\bar{3}$  and  $\bar{M}$ , respectively,  $\bar{6}$  and  $\bar{M}$  . The planar periodic structure, in which symmetry with generating tensors  $\bar{3}$  or  $\bar{6}$  is enforced, has a hexagonal lattice. Therefore, it is described by a pair of basis vectors  $\mathbf{a}_1$  ,  $\mathbf{a}_2$  of equal size and conventionally taking an angle  $\alpha = 120^\circ$ . It follows that the projection of the magnitude of the vector  $\mathbf{a}_2$  in the direction of the vector  $\mathbf{a}_1$  is equal to its half magnitude:  $a_2 \cos \alpha = a_1/2$ , thus satisfying condition (C6.2) of corollary C6.4 on structures with group  $m$  . Thus, reflection is a natural symmetry operation of these structures. Thus, the requirements of the  $3m$  and  $6mm$  groups do not lead to a new type of lattice symmetry.

Even the  $4mm$  group does not generate a new type of lattice symmetry. Even group  $4$  already requires a tetragonal lattice that satisfies condition C6.2, so the other elements in the group related to reflections no longer impose new conditions on lattice symmetry.

## C6.6 Summary of lattice types, crystal systems

In C6.1 to C6.5, the types of lattices that are compatible with the symmetry operations of the point groups of planar periodic structures have been described. These are 5 types of lattices that are characterized by different metrics and different shapes of the unit cells. These cells are called

oblique,  
rectangular (orthogonal) primitive,  
rectangular (orthogonal) centred,  
square,  
hexagonal.

The two types of orthogonal cells have the same external shape, differing only in that the centred cell has a lattice point at its centre. The two cells - and the corresponding lattices - are therefore classified in the same group. This gives rise to four types of lattices, for which the name **crystal system** is used. Table TC6 below lists the crystal systems, the types of unit cells, the data on the basis vectors (system metrics), and the point groups to which these types are related.

| TC6    | Crystal systems, their metrics and symmetry |              |                                      |                                   |
|--------|---------------------------------------------|--------------|--------------------------------------|-----------------------------------|
|        | Crystal system                              | Type of cell | Basis vectors                        | Point groups                      |
| 1      | oblique                                     | $p$          | $a_1 \neq a_2, \alpha \neq 90^\circ$ | <b>1, 2</b>                       |
| 2<br>3 | rectangular                                 | $p$<br>$c$   | $a_1 \neq a_2, \alpha = 90^\circ$    | <b><math>m, 2mm</math></b>        |
| 4      | square                                      | $p$          | $a_1 = a_2, \alpha = 90^\circ$       | <b>4, <math>4mm</math></b>        |
| 5      | hexagonal                                   | $p$          | $a_1 = a_2, \alpha = 120^\circ$      | <b>3, <math>3m, 6, 6mm</math></b> |

The table lists 4 crystal systems, 5 types of planar lattices (unit cells, translation groups) and 10 types of point groups. At least two point groups are associated with one crystal system. In this connection it should be noted that in each crystal system the symmetry of the lattice corresponds to the point group with the largest number of elements, i.e. it has the maximum possible point symmetry. For example, the lattice of a structure belonging to the hexagonal system always has a point symmetry described by a  **$6mm$**  group. This point group has 12 elements of symmetry, the most compared to the other point groups of the hexagonal system. Groups with fewer elements are characterized by structures with lower symmetry. The symmetry reduction is not induced by a reduction in the symmetry of the lattice, but by the

insertion of a structural motif into the lattice that has a lower symmetry than the lattice. This fact is discussed in more detail in later sections of this text, in the derivation of the 17 types of plane groups. In each of the four crystal systems, the symmetry of the lattice is characterized by the most numerous point group, which is always given at the end of the line corresponding to the system. These groups - **2**, **2mm**, **4mm** and **6mm** are called **holohedral**, which can be translated as **full** or **complete**.

## C7 Positions of symmetry elements in unit cells

At the beginning of C4.2, it is stated that the translational part  $\mathbf{t}$  of the operator  $S \equiv [\bar{\Phi}, \mathbf{t}]$  can be zero only in those cases where the corresponding element of symmetry (rotation axis, reflection line) passes through a lattice point, or other suitably placed point in the plane of the lattice. However, this is only true if we consider this point to be the origin of the reference frame. Otherwise, even if an element of symmetry passes through a lattice point but we consider the operation with respect to another reference point, this may not be true. However, there exists a set of points in the lattice, displaced with respect to the position of the rotation axis (or reflection line), with respect to which the translational part of the symmetry operators is identical to some lattice vector  $\mathbf{A}_L$ , so that it does not contain a non-lattice translation  $\mathbf{t}$ . The positions of such points can be obtained from relation (g) derived in Appendix D13.

The relation (g) of Appendix D13 expresses the condition that must be satisfied by:

the position vector  $\mathbf{r}_0$  of the displacement of the origin of the reference frame, the tensor  $\bar{\Phi}$  representing the rotation, and the translation  $\mathbf{A}_L + \mathbf{t}$ , in order for the total translation term of the symmetry operator to be zero:

$$\mathbf{r}_0 \cdot (\bar{\mathbf{I}} - \bar{\Phi}) + \mathbf{A}_L + \mathbf{t} = \mathbf{0} .$$

In this part of text, we will look for positions  $\mathbf{r}_0$  of the reference points such that only the non-lattice translation  $\mathbf{t}$  is zero. That is, we will look for position vectors  $\mathbf{r}_0$  that satisfy the condition

$$\mathbf{r}_0 \cdot (\bar{\mathbf{I}} - \bar{\Phi}) = \mathbf{A}_L . \quad (\text{C7.1})$$

**Note:** The  $+\mathbf{A}_L$  and  $-\mathbf{A}_L$  vectors are equivalent in this respect.

In this way, we obtain the positions of points in the lattice at which the rotation axes transforming the lattice to the equivalent position can be placed without the need for additional non-lattice translation. The result depends on the particular tensor representing the rotation (or reflection) as well as on the type of lattice, so all individual cases need to be considered.

The translational parts of the operators with the same tensor part, which represent operations with respect to the symmetry elements distributed in the basis cell based on relation (C7.1), differ from each other only by the lattice vectors. **Therefore, when decomposing the plane group, the corresponding symmetry operations belong to one coset.** (C7.1a)

### C7.1 Twofold rotation axis

The twofold axis of rotation is typical of oblique and rectangular crystal systems. The basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  in these systems are of different lengths, whereas in the rectangular system they are perpendicular to each other. However, twofold axes also occur in the square and hexagonal systems.

The tensor representing the rotation about the twofold axis has the form ( $\rightarrow$  tab. TC2b):

$$\bar{2} \equiv -\mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2 = -\bar{1},$$

so after inserting into relation (C7.1) we get

$$\mathbf{r}_o \cdot (2\bar{1}) = \mathbf{A}_L \Rightarrow 2\mathbf{r}_o = \mathbf{A}_L. \quad (\text{C7.2a})$$

We express the position vector  $\mathbf{r}_o$  as a linear combination of the basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  of the corresponding lattice:  $\mathbf{r}_o = r_1\mathbf{a}_1 + r_2\mathbf{a}_2$ , where  $r_1$ ,  $r_2$  are its scalar coordinates. This is also how we express a lattice vector:  $\mathbf{A}_L = L_1\mathbf{a}_1 + L_2\mathbf{a}_2$ , where  $L_i$  can be any positive and negative integers. So we ask to satisfy the condition:

$$2(r_1\mathbf{a}_1 + r_2\mathbf{a}_2) = L_1\mathbf{a}_1 + L_2\mathbf{a}_2. \quad (\text{C7.2b})$$

By comparing the scalar coordinates of the vectors on the two sides of equation we obtain:

$$r_1 = L_1/2, \quad r_2 = L_2/2.$$

If we restrict ourselves to positions in a single unit cell, it is sufficient to consider only positive coordinate values and values less than 1. Thus,  $r_i = 0, 1/2$ . Then only the following combinations of coordinates of the vector  $\mathbf{r}_o$  are possible:

$$(0,0), \left(0, \frac{1}{2}\right), \left(\frac{1}{2}, 0\right), \left(\frac{1}{2}, \frac{1}{2}\right).$$

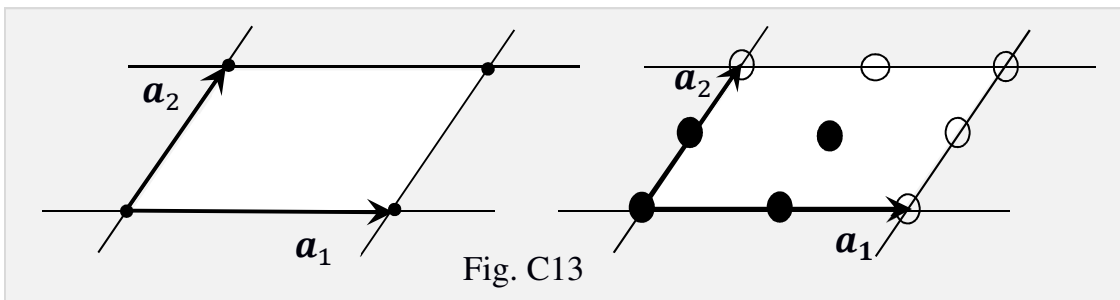
That is, the twofold axis of symmetry can lie at the origin of the reference frame ( $\mathbf{r}_0=0$ ), at the centre of the basis vectors ( $\mathbf{r}_0 = \frac{1}{2}\mathbf{a}_1$  or  $\mathbf{r}_0 = \frac{1}{2}\mathbf{a}_2$ ) and at the centre of the unit cell ( $\mathbf{r}_0 = \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$ ). Larger values of the coordinates  $r_i$  already refer to positions belonging to adjacent unit cells (represented by empty ellipses in Figure C13 on the next page; lattice points in the left part of the figure by small solid circles). It should be noted that the twofold axes are arranged in this way in all types of lattices, hence also in the square and hexagonal lattices. So the rotation operators about axes not passing through the origin of the reference frame, whose position satisfies condition C7.1, have the form ( $\rightarrow$  Appendix D19) :

$$[-\bar{1}, 0], [-\bar{1}, \mathbf{a}_1], [-\bar{1}, \mathbf{a}_2], [-\bar{1}, \mathbf{a}_1 + \mathbf{a}_2]. \quad (\text{C7.2c})$$

For example, the operator  $[-\bar{1}, \mathbf{a}_1]$ , representing a rotation about an axis passing through the centre of the vector  $\mathbf{a}_1$ , moves the point at the end of the vector  $\mathbf{a}_1$  to the origin of the coordinate system, which follows from the transformation relation

$$\mathbf{a}'_1 = \mathbf{a}_1 \cdot [-\bar{1}, \mathbf{a}_1] = \mathbf{a}_1 \cdot (-\bar{1}) + \mathbf{a}_1 = -\mathbf{a}_1 + \mathbf{a}_1 = 0.$$

The symmetry operations represented by these four operators belong to one coset in the decomposition of the plane group, because the translational parts of the operators represent only different lattice vectors, i.e., elements of the translation group.



If it is a centred lattice in which there are lattice points with position vectors  $\mathbf{A}_Q = \mathbf{A}_L + \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$ , then condition (C7.2b) needs to be added:

$$2(r_1\mathbf{a}_1 + r_2\mathbf{a}_2) = L_1\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_1 + L_2\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_2. \quad (\text{C7.2d})$$

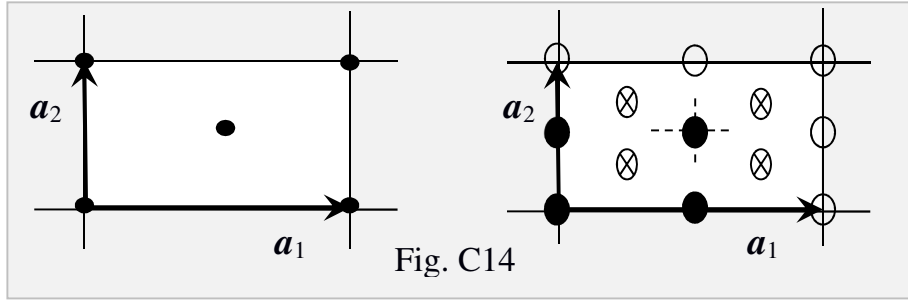
For the coordinates of the vector  $\mathbf{r}_0$  we thus get the conditions:

$$r_1 = \frac{L_1}{2} + \frac{1}{4}, \quad r_2 = \frac{L_2}{2} + \frac{1}{4}.$$

In addition to the above combinations of  $\mathbf{r}_o$  vector coordinates valid for the primitive lattice, the following combinations are also possible in a centred lattice within a single unit cell:

$$\left(\frac{1}{4}, \frac{1}{4}\right), \left(\frac{1}{4}, \frac{3}{4}\right), \left(\frac{3}{4}, \frac{1}{4}\right), \left(\frac{3}{4}, \frac{3}{4}\right),$$

corresponding to the positions shown by the ellipses with a cross in Figure C14.



When the rotation axis is shifted to a point with position vector  $\mathbf{r}_o$ , the corresponding operator has the form  $S_o \equiv [\bar{\Phi}, \mathbf{r}_o \cdot (\bar{\mathbf{I}} - \bar{\Phi})]$  ( $\rightarrow$  relation (h) in Appendix D13). With a twofold axis of symmetry,  $\bar{\Phi} = -\bar{\mathbf{I}}$ , so the operator takes the form  $S_o \equiv [-\bar{\mathbf{I}}, 2\mathbf{r}_o]$ . When the double axis is located, for example, at a position with coordinates  $(1/4, 3/4)$ , then the vector  $\mathbf{r}_o = (1/4)\mathbf{a}_1 + (3/4)\mathbf{a}_2$  and the operator takes the form

$$S \equiv \left[ -\bar{\mathbf{I}}, \frac{1}{2}\mathbf{a}_1 + \frac{3}{2}\mathbf{a}_2 \right]. \quad (\text{C7.2e})$$

As an example, this operator transforms a point with position vector  $\mathbf{r} = \mathbf{0}$  (i.e. a point lying at the origin of the reference frame), into a point with position vector  $\mathbf{r} = (1/2)\mathbf{a}_1 + (3/2)\mathbf{a}_2 = \mathbf{a}_2 + (1/2)\mathbf{a}_1 + (1/2)\mathbf{a}_2$ , i.e., to another lattice point of the centred lattice.

## C 7.2 Fourfold rotation axis

The fourfold axis of rotation is typical of a square crystal system. The basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  in this system are of the same length and perpendicular to each other. We use the same procedure as for the twofold axis. The tensor representing rotation by  $90^\circ$  about the fourfold axis has the form ( $\rightarrow$  tab. TC2b):

$$\bar{\mathbf{4}} \equiv \mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1, \Rightarrow \bar{\mathbf{I}} - \bar{\mathbf{4}} = \mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1 + \mathbf{a}^2\mathbf{a}_2.$$

In the relation (C7.1) we add  $\mathbf{r}_0 = r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2$  and the difference of the tensors  $\bar{\mathbf{I}} - \bar{\mathbf{4}}$ :

$$(r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2) \cdot (+ \mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2) = A_L .$$

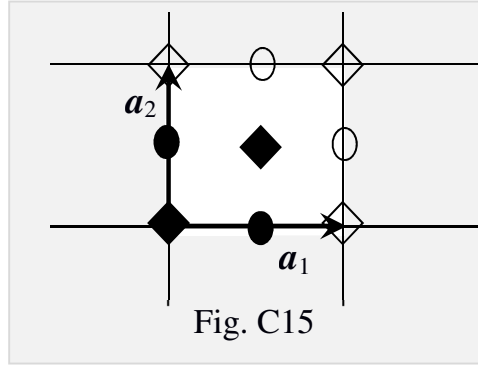
After performing the scalar product of the vector  $\mathbf{r}_0$  with the tensor  $(\bar{\mathbf{I}} - \bar{\mathbf{4}})$ , we get the result:

$$r_1 \mathbf{a}_1 - r_1 \mathbf{a}_2 + r_2 \mathbf{a}_1 + r_2 \mathbf{a}_2 = (L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2) . \quad (\text{C7.3a})$$

By comparing the coordinates at the vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  on the left and right sides of equation:

$$(a) \ r_1 + r_2 = L_1 , \quad (b) \ r_2 - r_1 = L_2 .$$

Adding relations (a) and (b) yields  $2r_2 = L_1 + L_2$ , so that if we restrict to non-negative  $r_2$  we get the values  $0, (1/2), 1, 1(1/2), 2, \dots$ . If  $r_2 = 0$ , then it follows from relation (a) that  $r_1$  can only take integer values. Considering only non-negative values, then  $r_1 = 0, 1, 2, \dots$ . If  $r_2 = 1/2$ , then it follows from relation (a)



that  $r_1$  can also take only half-integer values  $1/2, 3/2, \dots$ . Restricting to values of  $r_1$  and  $r_2$  less than 1, for a vector  $\mathbf{r}_0$  we get only two possibilities:  $\mathbf{r}_0 = \mathbf{0}$  and  $\mathbf{r}_0 = (1/2)\mathbf{a}_1 + (1/2)\mathbf{a}_2$ , i.e. the fourfold axes can only be located at the origin of the reference frame (the unit cell) and in the middle of the unit cell. The other positions, shown by empty squares in the figure, already belong to adjacent cells.

The rotation operators  $90^\circ$  about the axes located at the beginning of the reference frame or in the middle of the unit cell have the form ( $\rightarrow$  Appendix D20):

$$[\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{0}], \text{ resp. } [\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1]. \quad (\text{C7.3b})$$

These two operators represent symmetry operations belonging to the same coset of the plane group, since their translational parts differ only in the lattice vectors.

In the square lattice, the twofold rotation axes are also applied, and the result obtained in the previous article holds for their positions. The two positions overlap

with the positions of the fourfold axes, so that in the square lattice the twofold axes are located as independent only at the centre of the basis vectors. It should be noted, however, that point group **4** contains a subgroup **2**. The distribution of the twofold and fourfold rotational axes in the square lattice is in Figure C15.

### C 7.3 Threefold rotation axis

The threefold axis of rotation is typical of the hexagonal crystal system, but the lattice is also characterized by sixfold axes. The basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  in this system are chosen to be of the same length and to make an angle with the magnitude of  $120^\circ$ . To find the location of the threefold axes, we again use relation (C7.1). The tensor representing the rotation about the threefold axis has the form ( $\rightarrow$  tab. TC2b):

$$\bar{\bar{3}} \equiv \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2, \Rightarrow \bar{\bar{1}} - \bar{\bar{3}} = +\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1 + 2\mathbf{a}^2 \mathbf{a}_2.$$

Substituting  $\mathbf{r}_0 = r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2$  and the difference of the tensors into the relation (C7.1) gives:

$$(r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2) \cdot (+\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1 + 2\mathbf{a}^2 \mathbf{a}_2) = (L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2)$$

and after performing the scalar product:

$$+r_1 \mathbf{a}_1 - r_1 \mathbf{a}_2 + r_2 \mathbf{a}_1 + 2r_2 \mathbf{a}_2 = (L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2). \quad (\text{C7.4})$$

For scalar coordinates the following conditions apply:

$$(a) \ r_1 + r_2 = L_1, \quad (b) \ 2r_2 - r_1 = L_2.$$

From the sum of equations (a) and (b) :  $3r_2 = L_1 + L_2$ , so the coordinate  $r_2$  can take the values 0, 1/3, 2/3, 1, .... Condition (a) then implies the following possibilities for the coordinate combination:

$$(0, 0), (1/3, 2/3), (2/3, 1/3), (1, 0), (0, 1), (1, 1), \dots$$

The rotation operator by  $120^\circ$  about the axis located at position (1/3, 2/3), based on relation (h) from Appendix D13, has the form  $[\bar{\bar{3}}, \mathbf{a}_1 + \mathbf{a}_2]$  and the operator associated with the second position (2/3, 1/3) has the form  $[\bar{\bar{3}}, \mathbf{a}_1]$ .

The location of the threefold axes in the unit cell is shown in the following Figure C16, with the axes belonging to adjacent base cells shown by empty triangles. It is important to note that the hexagonal lattice is also characterized by sixfold axes of symmetry. Threefold axes without the presence of sixfold axes occur in the

structure only when the symmetry of the structure is lower than the symmetry of the lattice, which is caused by the lower symmetry of the structural motif.

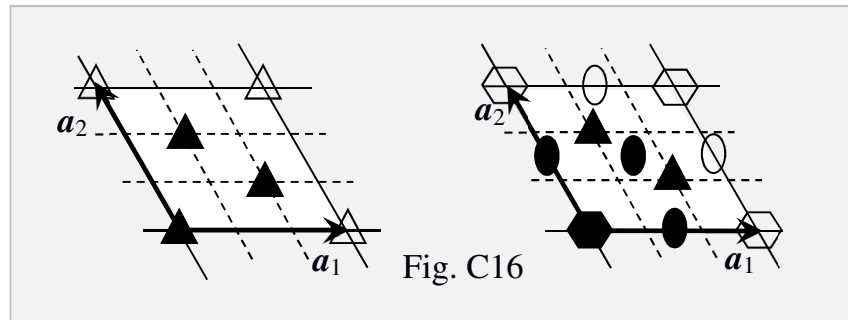


Fig. C16

#### C 7.4 Sixfold rotation axis

The sixfold rotational axis is typical of a hexagonal crystal system. The basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  in this system are conventionally chosen to be of the same length and subtend an angle of magnitude  $120^\circ$ . The tensor representing the rotation about the six-fold axis has the form ( $\rightarrow$  tab. TC2b):

$$\bar{\mathbf{6}} \equiv \mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \Rightarrow \bar{\mathbf{1}} - \bar{\mathbf{6}} = -\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2.$$

Adding the vector  $\mathbf{r}_0 = r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2$  and the difference of the tensors to the relation (C7.1), we get

$$(r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2) \cdot (-\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2) = (L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2)$$

and after performing the scalar product:

$$-r_1 \mathbf{a}_2 + r_2 \mathbf{a}_1 + r_2 \mathbf{a}_2 = (L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2). \quad (\text{C7.5})$$

From here we obtain the conditions for the scalar coordinates:

$$(a) \ r_2 = L_1, \quad (b) \ r_2 - r_1 = L_2,$$

from which the possibilities are:  $r_2 = 0, 1, 2, \dots$  and  $r_1 = 0, 1, 2, \dots$ . This means that there can be a single sixfold axis in the basis cell - at the origin of the reference frame. The other possibilities already correspond to positions in adjacent cells. Figure C16 also shows the positions of the twofold and threefold axes, which are part of the set of symmetry elements of the hexagonal lattice. Fourfold axes do not occur in the hexagonal lattice.

## C 7.5 Reflection line and glide line

**Reflection lines** (mirror lines) occur in all orthogonal lattices, i.e. lattices in which a pair of mutually perpendicular basis vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  can be chosen. This possibility is offered in orthogonal, square as well as hexagonal lattices. The tensors representing reflection in the line in which the basis vectors  $\mathbf{a}_1$ , respectively  $\mathbf{a}_2$ , lie, are of the form

$$\bar{\bar{\mathbf{M}}}_1 = \mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2, \text{ resp. } \bar{\bar{\mathbf{M}}}_2 = -\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2.$$

For the difference of tensors  $\bar{\mathbf{I}} - \bar{\bar{\mathbf{M}}}$  we thus obtain the expressions

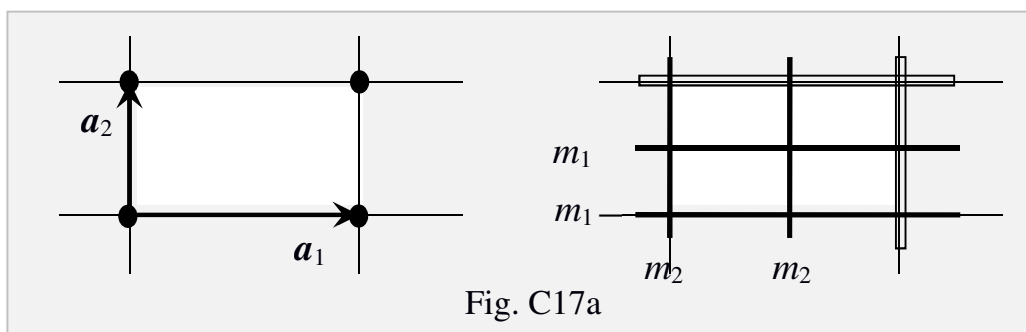
$$\bar{\mathbf{I}} - \bar{\bar{\mathbf{M}}}_1 = 2\mathbf{a}^2 \mathbf{a}_2, \quad \text{resp.} \quad \bar{\mathbf{I}} - \bar{\bar{\mathbf{M}}}_2 = 2\mathbf{a}^1 \mathbf{a}_1.$$

Substituting into equation (C7.1) in the case of tensor  $\bar{\bar{\mathbf{M}}}_1$ , we obtain the relation:

$$(r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2) \cdot (2\mathbf{a}^2 \mathbf{a}_2) = (L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2) \quad (\text{C7.6})$$

and from it the condition for coordinate  $r_2$ :  $2r_2 = L_2$ .

In doing so, no conditions are placed on the  $r_1$  coordinate of the  $\mathbf{r}_0$  vector, which is natural because the mirror line parallel to the  $\mathbf{a}_1$  vector cannot be localized in this direction. However, the coordinate  $r_2$  in the region belonging to the unit cell can take only two values:  $r_2 = 0, 1/2$ . Analogously, for the tensor  $\bar{\bar{\mathbf{M}}}_2$  no conditions are imposed on the coordinate  $r_2$ , the coordinate  $r_1$  can only take on the values  $0, 1/2$ .



Reflection lines complete the set of symmetry elements of orthogonal lattices, occurring along rotational axes. In Figure C17a, they are shown by bold lines and denoted by the letters  $m$ . reflection lines belonging to adjacent cells are shown by empty rectangles.

In a hexagonal lattice, three equivalent orthogonal unit cells can be chosen, rotated by  $60^\circ$  relative to each other, which is related to the distribution of the

reflection lines in the lattice. The distribution of the reflection lines, as well as other elements of symmetry in the unit cells of the seventeen planar groups, is illustrated in the figure section of the text.

The reflection operator in a line parallel to the vector  $\mathbf{a}_1$  and shifted in the direction of the vector  $\mathbf{a}_2$  by the coordinate  $r_2 = 1/2$ , based on relation (h) from Appendix D13, has the form

$$[\bar{\mathbf{M}}_1, \mathbf{a}_2] \equiv [\bar{\mathbf{I}} - 2 \mathbf{a}^2 \mathbf{a}_2, \mathbf{a}_2]. \quad (\text{C7.7})$$

For example, this operator transforms a lattice point  $\mathbf{r} = 0$  to a lattice point with position vector  $\mathbf{a}_2$  and a point with position vector  $\mathbf{a}_2$  back to  $\mathbf{r} = 0$  ( $\rightarrow$  Appendix D14).

When one is dealing with a **centred lattice** in which there are lattice points with position vectors  $\mathbf{A}_Q = \mathbf{A}_L + \mathbf{a}_1/2 + \mathbf{a}_2/2$ , the condition (C7.6) needs to be extended. For a tensor  $\bar{\mathbf{M}}_1$ , this is the case:

$$(r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2) \cdot (2 \mathbf{a}^2 \mathbf{a}_2) = (L_1 \mathbf{a}_1 + \mathbf{a}_1/2 + L_2 \mathbf{a}_2 + \mathbf{a}_2/2), \quad (\text{C7.8})$$

where for the coordinate  $r_2$  of the vector  $\mathbf{r}_0$  we get the condition:  $2 r_2 = L_2 + 1/2$ , while no conditions are imposed on the coordinate  $r_1$ . This means that within a single unit cell, the coordinate  $r_2$  can take values  $1/4$  and  $3/4$ , which are however realized in addition to the values  $0, 1/2$  obtained for the primitive cell, as shown in the following figure.

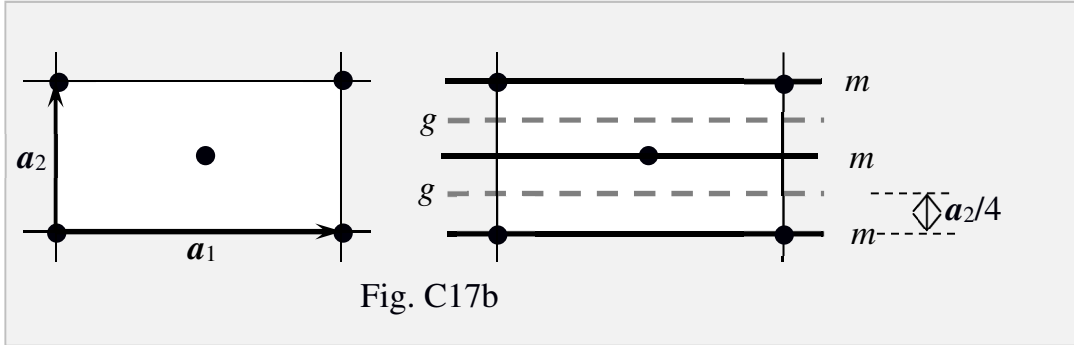


Fig. C17b

However, reflection in such lines, if it is to be a symmetry operation, is associated with a translation of half the length of the basis vector parallel to the reflection line, in accordance with relations (C4.21) and (C4.22), as we will show in the following example. The reflection operator in a line parallel to the vector  $\mathbf{a}_1$  and shifted in the direction of the vector  $\mathbf{a}_2$  to a position with coordinate  $r_2 = 1/4$ , based on relation (h) from Appendix D13, has the form:

$$S \equiv [\bar{\mathbf{I}} - 2 \mathbf{a}^2 \mathbf{a}_2, \mathbf{a}_2/2]. \quad (\text{C7.9})$$

This operator, unlike operator (C7.7), transforms a lattice point with position vector  $\mathbf{r} = 0$  to a point with position vector  $\mathbf{a}_2/2$ , but where the lattice point is not located. Therefore, the operation represented by operator (C7.9) is not a symmetry operation. If this operator is to represent a symmetry operation, it must contain an additional non-lattice translation  $\mathbf{t}$ , which moves the lattice to an equivalent position. Therefore, the condition  $\mathbf{a}_2/2 + \mathbf{t} = \mathbf{A}_Q$  respectively, must be required if the vectors  $\mathbf{t}$  and  $\mathbf{A}_Q$  are expressed in terms of scalar coordinates in the basis  $\mathbf{a}_1, \mathbf{a}_2$ :

$$\mathbf{a}_2/2 + t_1\mathbf{a}_1 + t_2\mathbf{a}_2 = L_1\mathbf{a}_1 + L_2\mathbf{a}_2 + \mathbf{a}_1/2 + \mathbf{a}_2/2, \quad (\text{C7.10})$$

which leads to the conditions:  $t_1 = L_1 + 1/2$  and  $t_2 = L_2$ .

Within a unit cell, it suffices to restrict to the coordinate values  $L_j = 0, 1$ , which yields the coordinate values  $t_i$ , which are shown in the following table:

| $L_1$ | $L_2$ | $t_1$ | $t_2$ |  | $L_1$ | $L_2$ | $t_1$ | $t_2$ |
|-------|-------|-------|-------|--|-------|-------|-------|-------|
| 0     | 0     | 1/2   | 0     |  | 1     | 0     | 3/2   | 0     |
| 0     | 1     | 1/2   | 1     |  | 1     | 1     | 3/2   | 1     |

If  $t_1 = 3/2$ , then there is a displacement of  $(3/2)\mathbf{a}_1$ , which is the sum of the non-lattice translation of  $\mathbf{a}_1/2$  and the lattice translation of  $\mathbf{a}_1$ ; however the lattice translation, as a trivial symmetry operation, can be omitted from the considerations. In doing so, only lattice translations are involved in the direction of the vector  $\mathbf{a}_2$ . Thus, in all cases, a non-lattice translation equal to half of the basis vector  $\mathbf{a}_1$  must be added to the operator (C7.9) if it is to represent the symmetry operation. Therefore, the corresponding symmetry operator has the form

$$S \equiv [\bar{\mathbf{I}} - 2\mathbf{a}^2\mathbf{a}_2, \mathbf{a}_2/2 + \mathbf{a}_1/2] \quad (\text{C7.11})$$

Analogous modifications concern reflection in lines parallel to the vector  $\mathbf{a}_2$ .

**Remark.** If we substitute the vector  $\mathbf{A}_L$  into the relation (C7.10) instead of the vector  $\mathbf{A}_Q$ , then for the values of the coordinates of the vector  $\mathbf{t}$  we would get  $t_1 = 0, 1, t_2 = 1/2, 3/2$ , which, together with the translation  $\mathbf{a}_2/2$ , appearing in the operator, again represent only lattice translations.

### Glide line

This element of symmetry occurs not only in centred lattices, but also in primitive ones, but where it is a consequence of the shape of the structural motif. According to the TC3 table, reflection with glide is represented by the operator

$[\bar{\mathbf{M}}, \mathbf{a}/2]$ , where  $\mathbf{a}$  is one of the basis vectors of the rectangular cell to which the glide line is parallel. If we consider specifically the basis vector  $\mathbf{a}_1$ , the tensor expressing the reflection in the line identical to this vector has the form:

$\bar{\mathbf{M}}_1 = \bar{\mathbf{I}} - 2 \mathbf{a}^2 \mathbf{a}_2$ , and the operator of glide reflection

$$[\bar{\mathbf{I}} - 2 \mathbf{a}^2 \mathbf{a}_2, \mathbf{a}_1/2]$$

This operator expresses a reflection with a shift in the line of vector  $\mathbf{a}_1$ , so the symmetry operation consists of a reflection in this line and a shift represented by the vector  $\mathbf{a}_1/2$ . The tensor part of the operator is the same as in the case of reflection without glide, and so we can use relation (C7.6) to find other positions  $\mathbf{r}_0$  of the glide line in the unit cell. For completeness, we repeat this procedure:

$$\bar{\mathbf{I}} - \bar{\mathbf{M}}_1 = 2 \mathbf{a}^2 \mathbf{a}_2,$$

and after plugging it into equation (C7.1) we get the relation:

$$(r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2) \cdot (2 \mathbf{a}^2 \mathbf{a}_2) = (L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2) \quad (\text{C7.12})$$

and from it the condition for the coordinate  $r_2$ :

$$2 r_2 = L_2$$

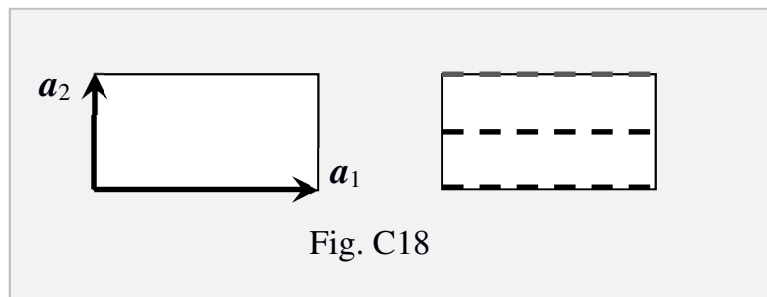
Also in this case, no conditions are placed on the  $r_1$  coordinate of the  $\mathbf{r}_0$  vector. However, the coordinate  $r_2$  in the region belonging to the unit cell can take only two values:  $r_2 = 0, 1/2$ . This means that there are two glide lines belonging to the unit cell, one lying in the vector  $\mathbf{a}_1$ , the other parallel to it and intersecting the vector  $\mathbf{a}_2$  in the middle.

The operator representing the reflection with the glide in the glide line shifted to the centre of the unit cell, in analogy with relation (C6.10), then takes the form

$$[\bar{\mathbf{I}} - 2 \mathbf{a}^2 \mathbf{a}_2, \mathbf{a}_1/2 + \mathbf{a}_2]. \quad (\text{C7.13})$$

This operator transforms, for example, a point with position vector  $\mathbf{a}_2$  to position  $\mathbf{a}_1/2$  and a point with position vector 0 to position  $\mathbf{a}_1/2 + \mathbf{a}_2$ .

The same procedure can be applied to glide lines parallel to vector  $\mathbf{a}_2$ ; glide lines parallel to vector  $\mathbf{a}_1$  are indicated in the figure.



## C 8 Plane groups

In previous considerations of the symmetry of planar periodic structures, all allowed symmetry operations have been found, as well as 10 point groups and 5 translation groups (lattice types), which have been classified into four crystal systems. This created the conditions for determining the set of plane groups. When this condition is considered in terms of the relationship

$$G = T \cdot (G/T) = (G/T) \cdot T , \quad (\text{C8.1})$$

which allows one to construct plane groups ( $\rightarrow$  relation C3.6), it follows that both translation subgroups  $T$  of plane groups  $G$  and their point groups, which are isomorphic to factor groups  $(G/T)$ , are already available. This makes it possible to proceed immediately to the construction of plane groups.

Each plane group  $G$  contains an infinite number of elements representing symmetry operations – translations, rotations, reflections and their combinations. These elements can be divided into cosets with respect to the invariant translation subgroup  $T$  of the group  $G$ . The elements of the translation group are only lattice translations, represented by the **translation operators**  $[\bar{\mathbf{I}}, \mathbf{A}_L]$ . A coset of a planar group  $G$  includes all its elements which are combinations of a particular element of its point group with all elements of the translation group. Thus, it includes the symmetry operations of the group  $G$ , which differ from each other only in the translational part – the different lattice vectors  $\mathbf{A}_L$ . Elements of cosets are then represented by operators  $S \equiv [\bar{\Phi}, \mathbf{t}]$  with the same tensor part  $\bar{\Phi}$ , but with different translational parts  $\mathbf{t}$ . Any of its elements can be chosen to represent a coset, but it is convenient to choose the one whose translational part is zero; the representatives of the cosets are then the elements of the point group. In the case where there is a glide line in the structure, the translational part of the representative of the corresponding coset cannot be zero. According to Table TC3 and relation (C4.22), its operator has the form  $[\bar{\mathbf{M}}, \mathbf{a}/2]$ , where  $\mathbf{a}$  is one of the basis vectors of the orthogonal lattice. This means that the translational part of the coset representative is then not an element of the translation group. However, two elements of the same coset can differ from each other only by a lattice vector, i.e. by an element of the translation group.

The cosets as units are elements of a factor group, but the set of representatives of these cosets – including the neutral element – may not form a group if any one of them contains a nonzero translational part. However, the group is formed by their tensor parts, namely the point group, which is isomorphic to the factor group

( $G/T$ ). This isomorphism makes it possible to apply some important relations valid in point groups to the factor group, specially to the representatives of cosets.

The point groups of planar periodic structures are divided into two sets – groups **1, 2, 3, 4, 6,  $m$**  with one generating element and groups  **$2mm, 3m, 4mm, 6mm$**  with two generating elements. The groups of the second set are formed by the direct product of any of the cyclic groups 2, 3, 4, 6 with the two-element reflection group  **$m$** , i.e. as the product of the groups

$$\mathbf{n} \cdot \mathbf{m}, \text{ resp. } \mathbf{m} \cdot \mathbf{n}, \quad (\text{C8.2})$$

where the symbol  **$n$**  represents one of the cyclic groups. The commutativity of relation (C8.2) can be verified using multiplication tables ( $\rightarrow$  Tables section).

Due to the isomorphism of the factor group with the point group of the planar structure, based on relation (C8.2), the factor group ( $G/T$ ) in relation (C8.1) can be replaced by the direct product  **$n \cdot m$** :

$$G = T \cdot (G/T) \Rightarrow G = T \cdot \mathbf{n} \cdot \mathbf{m}. \quad (\text{C8.3a})$$

The plane group  $G$  expressed by this relation is formed by combining the elements of the point group of a planar structure with all the elements of its translation group. Only symmetry groups of planar periodic structures in which there are no glide lines generated by the structural motif can be expressed in this way. These are the thirteen so-called **symmorphic plane groups**. In doing so, there may be two special cases – when only the group of proper rotations  **$n$**  is involved, e.g., the group **3** with elements  $\{e, 3, 3^2\}$ , or only the reflection group  **$m$**  with elements  $\{e, m\}$ . In these cases, the plane group can be written in the form

$$G = T \cdot \mathbf{n}, \text{ or } G = T \cdot \mathbf{m}. \quad (\text{C8.3b})$$

The representatives of the cosets are then the elements of the point groups, e.g. **3,  $3^2, m$** , to which the operators  $[\bar{\mathbf{3}}, \mathbf{0}]$ ,  $[\bar{\mathbf{3}}^2, \mathbf{0}]$ , resp.  $[\bar{\mathbf{M}}, \mathbf{0}]$  correspond. The operators have such a simple form when the rotation axis is located at the origin of the reference frame, or when the reflection line is identical to some basis vector of the orthogonal lattice. Otherwise, the operators also contain a translational part ( $\rightarrow$  Appendix D13,  $\rightarrow$  part C7), so then they have the more general form  $[\bar{\mathbf{n}}, \mathbf{t}]$  or  $[\bar{\mathbf{M}}, \mathbf{t}]$ , where  **$\bar{\mathbf{n}}$**  symbolizes the rotation tensor belonging to one of the cyclic groups.

In some three-dimensional structures there are screw axes, so that the corresponding symmetry operation has an integral translational part in addition to the rotational part. That is, the symmetry operator must have the form  $S = [\bar{\Phi}, \mathbf{t}]$ , where  **$\mathbf{t}$**  represents the non-lattice translation. However, in planar periodic structures, operations of this kind do not occur, so by placing the origin of the reference frame in

the rotation axis, the translational part of the operator  $S$  can be made equal to zero. The operator  $[\bar{\Phi}, \mathbf{t}]$  is then changed to  $[\bar{\Phi}, \mathbf{0}]$ , or operator  $[\bar{\mathbf{n}}, \mathbf{t}]$  to  $[\bar{\mathbf{n}}, \mathbf{0}]$ . This greatly simplifies further considerations and calculations ( $\rightarrow$  beginning of Section C4.2, or the derivation of the transformation formula in Appendix D13). The possibility of transforming  $[\bar{\mathbf{n}}, \mathbf{t}] \rightarrow [\bar{\mathbf{n}}, \mathbf{0}]$  is regularized by the fact that no constraints are placed on the vector  $\mathbf{t}$  according to Table TC3. If it is not a reflection associated with a glide, the reflection can also be assigned the operator  $[\bar{\mathbf{M}}, \mathbf{0}]$  without a translation term, by a suitable choice of the position of the origin of the reference frame.

The decomposition of the group  $G$  into subclasses is expressed in the above two cases by the relations

$$G = T + T \cdot [\bar{\mathbf{n}}, \mathbf{0}] + T \cdot [\bar{\mathbf{n}}^2, \mathbf{0}] + \dots + T \cdot [\bar{\mathbf{n}}^{n-1}, \mathbf{0}],$$

resp.

$$G = T + T \cdot [\bar{\mathbf{M}}, \mathbf{0}]. \quad (\text{C8.4})$$

where  $[\bar{\mathbf{n}}^i, \mathbf{0}]$  represents the operator belonging to the  $i$ -th element of the cyclic group associated with the  $n$ -fold axis of symmetry. If there are no glide lines in the planar structure, then even combinations of rotations with reflection represent point operations, and the representatives of cosets can be elements of point groups. The number of members of the decomposition into cosets coincides with the number of elements of the point group.

If these are centred lattices (they are all orthogonal and reflection is applied), the decomposition (C8.4) involves the group  $T_c$ , which can be decomposed into two parts according to relation (C6.3):  $T_c = T_b + \mathbf{t}_b \cdot T_b$ . The decomposition of a plane group  $G$  into cosets thus acquires twice the number of members; for example, in the case of a point reflection group:

$$\begin{aligned} G = T_c + T_c \cdot [\bar{\mathbf{M}}, \mathbf{0}] &= (T_b + \mathbf{t}_b \cdot T_b) + (T_b + \mathbf{t}_b \cdot T_b) \cdot [\bar{\mathbf{M}}, \mathbf{0}] = \\ &= T_b + \mathbf{t}_b \cdot T_b + T_b \cdot [\bar{\mathbf{M}}, \mathbf{0}] + T_b \cdot \mathbf{t}_b \cdot [\bar{\mathbf{M}}, \mathbf{0}]. \end{aligned} \quad (\text{C8.5})$$

Thus, if we decompose the group  $G$  into cosets according to the subgroup  $T_b$ , it has up to three cosets instead of one. The translation  $\mathbf{t}_b = (\mathbf{b}_1 + \mathbf{b}_2)/2$  commutes with the operations of the group  $T_b$ , is represented by the operator  $[\bar{\mathbf{I}}, (\mathbf{b}_1 + \mathbf{b}_2)/2]$ , and its product with the operator  $[\bar{\mathbf{M}}, \mathbf{0}]$  yields the result  $[\bar{\mathbf{M}}, (\mathbf{b}_1 + \mathbf{b}_2)/2]$ . The representatives of the three cosets are thus the elements to which the operators are assigned:

$$[\bar{\mathbf{I}}, (\mathbf{b}_1 + \mathbf{b}_2)/2], [\bar{\mathbf{M}}, \mathbf{0}], [\bar{\mathbf{M}}, (\mathbf{b}_1 + \mathbf{b}_2)/2]. \quad (\text{C8.5b})$$

The third of these operators is the product of the first and the second one, which, although they do not commute with each other, swapping their order when transforming an arbitrary lattice point leads to resulting positions whose position vectors differ only by one of the basis vectors of the centred cell. We support the claim by a calculation in the case of reflection in a line parallel to the vector  $\mathbf{b}_1$ , when the reflection tensor has the form  $\bar{\mathbf{M}}_1 = \bar{\mathbf{I}} - 2\mathbf{b}^2\mathbf{b}_2$  ( $\rightarrow$  Appendix D14)

$$[\bar{\mathbf{I}}, \mathbf{b}_1/2 + \mathbf{b}_2/2] \cdot [\bar{\mathbf{M}}_1, \mathbf{0}] = [\bar{\mathbf{M}}_1, \mathbf{b}_1/2 - \mathbf{b}_2/2],$$

$$[\bar{\mathbf{M}}_1, \mathbf{0}] \cdot [\bar{\mathbf{I}}, \mathbf{b}_1/2 + \mathbf{b}_2/2] = [\bar{\mathbf{M}}_1, \mathbf{b}_1/2 + \mathbf{b}_2/2].$$

That is, the representative of the coset of group  $G$  can be anyone of these two products, since the difference of their translational parts is equal to the lattice vector  $\mathbf{b}_2$ , i.e., an element of the translation group. The coset with representative  $[\bar{\mathbf{M}}, \mathbf{0}]$  contains ordinary reflection, the coset with representative  $[\bar{\mathbf{M}}, (\mathbf{b}_1 + \mathbf{b}_2)/2]$  contains reflection with glide in lines that are shifted with respect to the position of the vectors  $\mathbf{b}_1$  and  $\mathbf{b}_2$  ( $\rightarrow$  relations (C4.22), (C7.11)).

The relations (C8.3.a) and (C8.3.b) give rise to 12 planar groups by direct products of translation groups with point groups. This number can be arrived from Table TC6 ( $\rightarrow$  p. 70) by multiplying the number of point groups by the number of translation groups in each crystal system. To these twelve groups one has to add a group that differs from a similar group only by the mutual orientation of the reflection lines of the lattice and the reflection lines of the structural motif ( $\rightarrow$  article C8.4 on the hexagonal system). In total, there are thirteen symmorphic groups.

However, the total number of planar groups is 17, and obtaining four more plane groups, i.e. four more types of symmetry, requires a different procedure. These are the groups that describe the symmetry of structures with primitive lattices in which glide lines occur as a consequence of the specific symmetry of the structural motif ( $\rightarrow$  Appendix D18). The procedure for deriving the aforementioned four types relies on an analogy between two relations – the relation between the elements of the point groups and the relation between the representatives of the cosets of the plane group. There is a relation between the elements of cyclic groups **2, 3, 4, 6** and the reflection operation  $m$ :

$$n \cdot m \cdot n = m,$$

where  $n$  represents an element of one of the groups **2, 3, 4, 6** (for example, the element  $3^2$ ). The relation can be verified using multiplication tables of point groups, ( $\rightarrow$  TC5), and also in the appendices, where it is supported by the relations D15(c),

D16(d) and D17(c). Due to the isomorphism of factor groups with point groups, the validity of the analogous relation is also required for the coset representatives in this case, when the presence of glide lines in the structure is involved:

$$[\bar{n}, 0] \cdot [\bar{M}, t] \cdot [\bar{n}, 0] = [\bar{M}, t + A_L], \quad (C8.6)$$

where  $t$  is one of the allowed translations according to Table TC3. Reflection with glide displaces the entire structure, so that subsequent rotation can no longer bring it to its original position. The relation (C8.6) expresses the requirement that the resulting position of the translated point differs from the original one by a lattice vector. The element with operator  $[\bar{M}, t]$  and the element with operator  $[\bar{M}, t + A_L]$  are equivalent representatives of the same coset, since they differ from each other only by different lattice translations of  $A_L$ . This means that elements with representations  $[\bar{M}, a/2]$  and  $[\bar{M}, -a/2]$  ( $\rightarrow$  tab. TC3), for example, belong to the same coset, because the difference of their translational parts is equal to the basis vector  $a$ , i.e., the shortest lattice vector. The element represented by the operator  $[\bar{M}, t]$  belongs to one of the cosets of the plane group, but is not an element of its point or translation group, since it represents the inseparable union of reflection and translation.

Relation (C8.6), in addition to relation (C4.19), imposes additional conditions on the translational part of the operators  $S \equiv [\bar{\Phi}, t]$ . These two conditions allow us to correctly choose the representatives of the cosets and to construct the factor groups.

### **Influence of the symmetry of the structural motif**

The symmetry of a planar periodic structure depends on both the symmetry of the lattice and the symmetry of the structural motif. The symmetry of the lattice is characterized by both point symmetry and translational symmetry, but we consider the symmetry of the structural motif only locally, i.e., only its point symmetry. For rotations of a certain angle, or for reflections, if these operations are to be symmetry operations of the whole structure, not only the lattice but also the structural motif must be brought to an equivalent position. That is, the corresponding operation must be a joint symmetry operation of both the structural motif and the lattice, it must be an element of both the point group of the lattice and the point group of the motif. This is possible if and only if the point group of the lattice and the point group of the motif share at least one subgroup. Their largest common subgroup then characterizes the point symmetry of the entire planar structure.

For example, if a lattice is characterized by a symmetry described by a point group  $4 \equiv \{e, 4, 4^2, 4^3\}$  and a structural motif by a point group  $6 \equiv \{e, 6, 6^2, 6^3, 6^4, 6^5\}$ , so their only common subgroup is the group  $2 \equiv \{e, 2\}$  related to the  $180^\circ$  rotation represented by the elements  $2 \equiv 4^2 \equiv 6^3$  in these groups.

If a structural motif were characterized by, e.g., a fivefold axis of symmetry, i.e., a group  $5 \equiv \{e, 5, 5^2, 5^3, 5^4\}$ , which (with the exception of the identity  $e$ ) does not share an element with any of the crystallographic point groups, then the symmetry of the structure, irrespective of the type and symmetry of its lattice, would be described by the plane group with the lowest symmetry, i.e., group  $p1$  ( $\rightarrow$  table TA3). Conversely, if a structural motif is, e.g., circularly symmetric, its point symmetry group contains rotations of arbitrary angles, so that a subgroup of this group is any crystallographic point group. The largest common subgroup is then the lattice point group, which determines the point symmetry of the entire planar periodic structure regardless of the high symmetry of the structural motif.

**It follows from the preceding discussion that the point group of the planar periodic structure coincides with the largest common subgroup of the point group of the lattice and the point group of the structural motif.**

(C8.7)

With reflection lines present simultaneously in both the lattice and the structural motif, the mutual parallelism of the respective reflection lines is important so that they can be symmetry elements of the whole structure. This circumstance manifests itself in a special way in the hexagonal crystal system, where the different orientations of the reflection lines of the motif and the lattice lead to two different types of symmetry.

A special case is a structural motif that generates reflection with glide (glide reflection). In centred lattices, such reflections is due to the arrangement of lattice points, but in primitive lattices it is due to the shape of the structural motif ( $\rightarrow$  Figure A7,  $\rightarrow$  Appendix D18). Glide reflections is not a point symmetry operation, so the largest common subgroup rule, as in the case of motif and lattice point groups, does not apply. A glide reflection is an element of a plane group, it belongs neither to the point group nor to the translation group, but it belongs to a separate coset of the plane group, it is a representative of it. Such a structural motif is related to four other types of symmetry, it conditions the existence of four other plane groups.

In the **following parts of text**, the plane groups characterizing different types of symmetries of planar periodic structures are described, successively according to the different crystal systems. The description starts with the oblique system, in which there is the smallest number of symmetry operations.

### C 8.1 Oblique system

Point groups  $\mathbf{1} \equiv \{e\}$  and  $\mathbf{2} \equiv \{e, 2\}$  are included in the oblique crystal system. In this system there exists only the primitive translation group  $T_p$ , so that by its direct product with the point groups we obtain two planar groups denoted by  $p1, p2$ :

$$p1 : \quad G_1 = T_p \cdot \{e\} \equiv T_p$$

$$p2 : \quad G_2 = T_p \cdot \{e, 2\}.$$

The first of these groups has no coset, the decomposition of the second into cosets takes the form:

$$G_2 = T_p + 2 \cdot T_p$$

or by replacing element 2 of point group  $\mathbf{2}$  with the appropriate operator:

$$G_2 = T_p + [\bar{\mathbf{2}}, \mathbf{0}] \cdot T_p. \quad (\text{C8.8})$$

**Note:** The operator representing an element of the point group should be written only as a tensor  $\bar{\mathbf{2}}$ , but the notation with the translational part, in this case zero, allows in the following to distinguish operators representing differently localized symmetry elements and already expresses an element of the planar group.

The symmetry type  $G_2$  is typical for all planar periodic structures characterized by the combination of the translation group  $T_p$  with point group  $\mathbf{2}$ ; they belong to the oblique system no matter how high the symmetry of the lattice is.

The elements of group  $p1$  are only translations, so the operators of all its elements have the form  $[\bar{\mathbf{1}}, \mathbf{A}_L]$ , where  $\mathbf{A}_L$  represents a lattice translation.

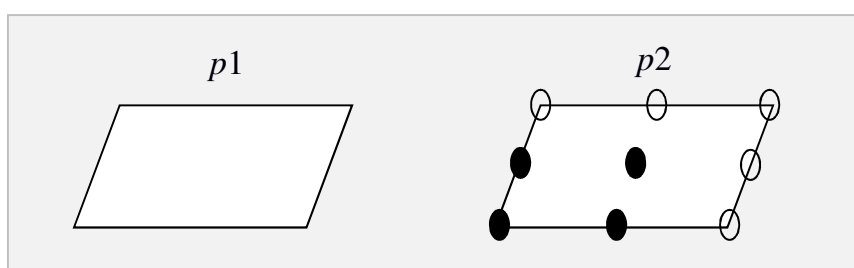
The group  $p2$  contains as a subgroup the group  $p1$ , plus elements which as operators have the form  $[\bar{\mathbf{2}}, \mathbf{A}_L]$ . There are four twofold axes per unit cell, one passing through the origin of the reference frame, and the corresponding operator  $[\bar{\mathbf{2}}, \mathbf{0}]$  has a zero translation term. Operators representing rotations about axes that are

localized away from the origin of the reference frame have a nonzero translational term  $\mathbf{t}$ , which depends on the position of the axis and has the form ( $\rightarrow$  Appendix D19):

$$[\bar{2}, \mathbf{a}_1], [\bar{2}, \mathbf{a}_2] \text{ a } [\bar{2}, \mathbf{a}_1 + \mathbf{a}_2] .$$

The symmetry operations represented by these four operators belong to one coset in the decomposition of the plane group, since the operators differ from each other only by different lattice vectors. The representative of the coset can be any of them, most appropriately the element  $[\bar{2}, \mathbf{0}]$  without a translation term.

The localization of the twofold rotation axes in the unit cell was described in Section C6.7, for completeness we present the corresponding figure:



The oblique system includes two of the 17 plane groups, which we will enter in a table that we will gradually add:

| Plane groups |      |      |    |    |    |    |    |    |   |
|--------------|------|------|----|----|----|----|----|----|---|
| number       | 1    | 2    | 3  | 4  | 5  | 6  | 7  | 8  | 9 |
| symbol       | $p1$ | $p2$ |    |    |    |    |    |    |   |
| number       | 10   | 11   | 12 | 13 | 14 | 15 | 16 | 17 |   |
| symbol       |      |      |    |    |    |    |    |    |   |

## C8.2 Rectangular system

The rectangular crystal system includes two translation groups, the primitive  $T_p$  and the centred  $T_c$ , and two point groups, the **2mm** holohedral group and its subgroup **m**, with its second subgroup **2** belonging to the oblique system. In the first part of this section, the plane groups related to structures with a primitive lattice – the translation group  $T_p$  will be derived, in the second part the plane groups of structures with a centred lattice – the translation group  $T_c$  will be derived.

### C8.2.1 Rectangular system, primitive lattice

An orthogonal lattice that is not centred is characterized by two basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , which are perpendicular to each other, and do not have the same magnitude. The plane groups in this case can be expressed as the direct product of the primitive translation group  $T_p$  with the  $\mathbf{m}$  or  $\mathbf{2mm}$  point groups. For the rectangular system, the presence of reflections – ordinary or with glide – is crucial. If there are glide reflections in lines parallel to one basis vector, then it is a group  $\mathbf{m}$ . The presence of glide reflections in two lines perpendicular to each other is inextricably linked to rotation about the double axis ( $\rightarrow$  multiplication table TB5), so in that case it is already a group  $\mathbf{2mm}$ .

#### Group $\mathbf{m}$

The combination of the translation group  $T_p$  with a simple reflection in the line identical to the vector  $\mathbf{a}_1$ , represented by the operator  $[\bar{\mathbf{M}}_1, \mathbf{0}] \equiv [\bar{\mathbf{I}} - 2\mathbf{a}_2^2 \mathbf{a}_2]$ , yields a planar group:

$$G = T_p \cdot \{e, m\},$$

whose decomposition into cosets has the form

$$G = T_p + T_p \cdot [\bar{\mathbf{M}}_1, \mathbf{0}].$$

The same type of symmetry will be given by reflection in the line identical to the vector  $\mathbf{a}_2$ , represented by the operator  $[\bar{\mathbf{M}}_2, \mathbf{0}] \equiv [\bar{\mathbf{I}} - 2\mathbf{a}_1^2 \mathbf{a}_1]$ , so the index at the tensor  $\bar{\mathbf{M}}$  will be omitted. This gives rise to the third plane group in the sequence, which has label  $\mathbf{pm}$  and decomposition into cosets:

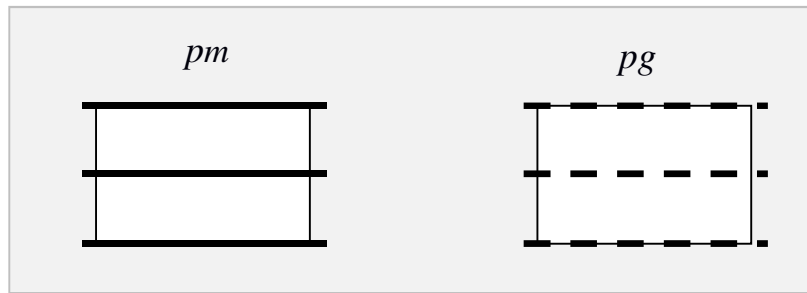
$$\mathbf{pm}: \quad G_3 = T_p + T_p \cdot [\bar{\mathbf{M}}, \mathbf{0}].$$

The combination of the group  $T_p$  and the glide reflection yields another group, with label  $\mathbf{pg}$  and decomposition into cosets

$$\mathbf{pg}: \quad G_4 = T_p + T_p \cdot [\bar{\mathbf{M}}, \mathbf{t}],$$

where  $\mathbf{t}$  represents the translations  $\mathbf{a}_1/2$  and  $\mathbf{a}_2/2$  respectively, depending on whether the tensor is  $\bar{\mathbf{M}}_1$  or  $\bar{\mathbf{M}}_2$ . For a more detailed discussion of the group of this type, see Appendix D18. It should be noted that both cases involve symmetries of structures in which there are reflection lines or glide lines parallel to only one of the basis vectors.

The distribution of symmetry elements in the plane groups  $G_3$  and  $G_4$  is shown in the following figure, where the reflection lines are indicated by continuous



thick lines and the glide lines by dashed lines. Their localization in the unit cell has been justified in section C7. It should be noted that of the three reflection lines, only the two lower ones belong to the unit cell, the third one already belongs to the adjacent higher cell.

### Group $2mm$

The  $2mm$  holohedral group can be expressed as a direct product of its subgroups:

$$2mm = \{2\} \cdot \{m\}.$$

Therefore, the corresponding plane group can also be written as a direct product of the translation group with subgroups  $2$  and  $m$ :

$$G = T_p \cdot \{2\} \cdot \{m\}$$

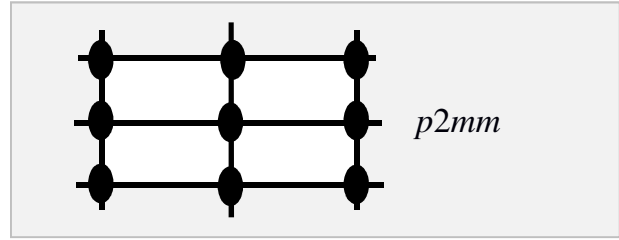
or after explicitly decomposing the elements of the  $2mm$  group:

$$G = T_p \cdot 2mm = T_p \cdot \{e, 2, m_x, m_y\}.$$

The symmetry operations of such a plane group, i.e., its elements, include translations, rotations about twofold axes, reflections in two systems of lines parallel to the basis vectors, and combinations of these operations. The possibility of glide reflection must also be taken into account, as can be seen from both relation (C4.21) and Table TC3.

The symmetry operations in the plane group  $G$  can be represented by the rotation operator  $[\bar{2}, \mathbf{0}]$ , the reflection operators  $[\bar{M}_1, \mathbf{0}]$ ,  $[\bar{M}_2, \mathbf{0}]$ , the glide reflection operators  $[\bar{M}_1, \mathbf{a}_1/2]$  and  $[\bar{M}_2, \mathbf{a}_2/2]$ , the translation operators  $[\bar{I}, \mathbf{A}_L]$  as well as combinations of these operators. An identical operation, which is an integral part of a group, is represented by the operator  $[\bar{I}, \mathbf{0}]$ .

Starting from the above facts, we describe a type of symmetry that is characterized by the presence of rotations  $[\bar{2}, 0]$  and ordinary reflections  $[\bar{M}_1, 0]$  and  $[\bar{M}_2, 0]$  in lines parallel to the basis vectors. A plane group with this symmetry is denoted by the symbol  $p2mm$ , has order number 6, and its decomposition into cosets has the form:



$$p2mm: G_6 = T_p + T_p \cdot [\bar{2}, 0] + T_p \cdot [\bar{M}_1, 0] + T_p \cdot [\bar{M}_2, 0].$$

Another type of symmetry is obtained by replacing one of the ordinary reflection in the  $p2mm$  group by a glide reflection. For example, we replace the  $[\bar{M}_2, 0]$  operator of the reflection in the line identical to the vector  $a_2$  by the  $[\bar{M}_2, a_2/2]$  operator. The product of this operator with the rotation operator gives the result:

$$[\bar{2}, 0] \cdot [\bar{M}_2, a_2/2] = [\bar{M}_1, a_2/2],$$

thus an operator of ordinary reflection in a line parallel to the vector  $a_1$ , but shifted in the direction of the vector  $a_2$  by a quarter of its length ( $\rightarrow$  part C7). In doing so, the glide lines remain in place of the original reflection lines without glide, but the reflection lines perpendicular to them are shifted, as shown in the figure of this plane group. The planar group is denoted by  $p2mg$  and its coset decomposition is of the form:

$$p2mg: G_7 = T_p + T_p \cdot [\bar{2}, 0] + T_p \cdot [\bar{M}_1, a_2/2] + T_p \cdot [\bar{M}_2, a_2/2].$$

Replacing even the second reflection operator by a glide reflection operator will give the last type of symmetry structure with an orthogonal primitive lattice. However, the glide lines cannot lie in the basis vectors, since the combination of glide reflection in such a line with rotation by  $180^\circ$  is equivalent to ordinary reflection, as seen in the previous case. The glide lines must be shifted within one quarter (even three quarters  $\rightarrow$  part C7) of the length of the basis vector. The reflection operator with a glide line parallel to the vector  $a_2$  then has the form  $[\bar{M}_2, a_1/2 + a_2/2]$  ( $\rightarrow$  formula C7.11). The product of this operator with the rotation operator gives the result:

$$[\bar{2}, 0] \cdot [\bar{M}_2, a_1/2 + a_2/2] = [\bar{M}_1, a_1/2 + a_2/2],$$

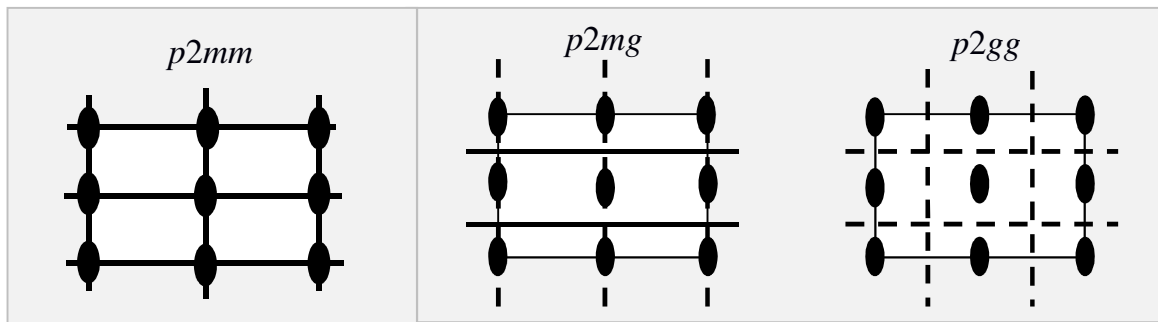
i.e., again glide reflection, but in a line parallel to the vector  $\mathbf{a}_1$  and displaced by  $\mathbf{a}_2/4$ . The corresponding plane group has the symbol  $p2gg$  and its decomposition into cosets has the form:

$$p2gg: G_8 = T_p + T_p \cdot [\bar{\mathbf{2}}, \mathbf{0}] + T_p \cdot [\bar{\mathbf{M}}_1, \mathbf{a}_1/2 + \mathbf{a}_2/2] + T_p \cdot [\bar{\mathbf{M}}_2, \mathbf{a}_1/2 + \mathbf{a}_2/2].$$

The operator representing the glide reflection in a line parallel to the vector  $\mathbf{a}_1$  and shifted to position  $(3/4)\mathbf{a}_2$  has the form  $[\bar{\mathbf{M}}_1, \mathbf{a}_1/2 + (3/2)\mathbf{a}_2]$ , its translational part differs from the operator  $[\bar{\mathbf{M}}_1, \mathbf{a}_1/2 + \mathbf{a}_2/2]$  by the lattice vector  $\mathbf{a}_2$ , so that the corresponding operations belong to one coset of the plane group.

This exhausted all types of symmetries of planar periodic structures with primitive orthogonal lattices, so that five groups were added to the table:

$pm, pg, p2mm, p2mg$  and  $p2gg$ .



| Plane groups |      |      |      |      |    |        |        |        |   |
|--------------|------|------|------|------|----|--------|--------|--------|---|
| number       | 1    | 2    | 3    | 4    | 5  | 6      | 7      | 8      | 9 |
| symbol       | $p1$ | $p2$ | $pm$ | $pg$ |    | $p2mm$ | $p2mg$ | $p2gg$ |   |
| number       | 10   | 11   | 12   | 13   | 14 | 15     | 16     | 17     |   |
| symbol       |      |      |      |      |    |        |        |        |   |

### C8.2.2 Rectangular system, centred lattice

We express the translation group  $T_c$  of a centred lattice by decomposing it into an incomplete translation subgroup  $T_b$  and a coset with respect to this subgroup:

$$T_c = T_b + T_b \cdot \mathbf{t}_b, \quad (\text{C8.9})$$

where  $\mathbf{t}_b = \mathbf{b}_1/2 + \mathbf{b}_2/2$ , and  $\mathbf{b}_1$  and  $\mathbf{b}_2$  are the basis vectors in the centred lattice ( $\rightarrow$  relation C6.3 and the text preceding it,  $\rightarrow$  relation C8.5).

## Group $m$

Also in the centred lattice, these will be combinations of the translation group with the point groups  $m$  and  $2mm$ . We start by combining the group  $m$  with the group  $T_c$ , so we first write the plane group as their direct product:

$$G = T_c \cdot \{e, m\}.$$

The coset breakdown by translational subgroup  $T_c$  looks like this:

$$G = T_c + T_c \cdot m,$$

or by replacing the element  $m$  of the point group by its tensor operator:

$$G = T_c + T_c \cdot [\bar{\bar{\mathbf{M}}}, \mathbf{0}].$$

A better view of the set of symmetry elements and their distribution in the unit cell is obtained by decomposing the plane group  $G$  into cosets according to the incomplete translation group  $T_b$ , i.e. according to relation (C8.9). This allows a better assessment of the symmetry of the centred lattice structure. When we use their tensor operators instead of the group elements, and consider reflections in lines parallel to the vector  $\mathbf{b}_1$ , the decomposition into cosets takes the form ( $\rightarrow$  relation C8.5):

$$G = T_b + T_b \cdot \mathbf{t}_b + T_b \cdot [\bar{\bar{\mathbf{M}}}_1, \mathbf{0}] + T_b \cdot \mathbf{t}_b \cdot [\bar{\bar{\mathbf{M}}}_1, \mathbf{0}].$$

The first of the cosets -  $T_b \cdot \mathbf{t}_b$  - completes the group  $T_b$  to the full translation group  $T_c$ , with the element with operator  $[\bar{\mathbf{I}}, (\mathbf{b}_1 + \mathbf{b}_2)/2]$  as its representative ( $\rightarrow$  relation C8.5b). The representative of the second coset is the element with operator  $[\bar{\bar{\mathbf{M}}}_1, \mathbf{0}]$  representing the ordinary reflection in the line in which the vector  $\mathbf{b}_1$  lies. The representative of the third coset is the operator we obtain as the product:

$$\mathbf{t}_b \cdot [\bar{\bar{\mathbf{M}}}_1, \mathbf{0}] = \left[ \bar{\mathbf{I}}, \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2) \right] \cdot [\bar{\bar{\mathbf{M}}}_1, \mathbf{0}] = \left[ \bar{\bar{\mathbf{M}}}_1, \frac{1}{2}\mathbf{b}_1 - \frac{1}{2}\mathbf{b}_2 \right].$$

By reversing the order in the product of the operators we get:

$$[\bar{\bar{\mathbf{M}}}_1, \mathbf{0}] \cdot \mathbf{t}_b = [\bar{\bar{\mathbf{M}}}_1, \mathbf{0}] \cdot \left[ \bar{\mathbf{I}}, \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2) \right] = \left[ \bar{\bar{\mathbf{M}}}_1, \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2 \right],$$

which implies that the results of the products differ only by the basis vector  $\mathbf{b}_2$ , so that both elements can be representatives of the same coset.

The operator  $[\bar{\bar{\mathbf{M}}}_1, \mathbf{b}_1/2 + \mathbf{b}_2/2]$  represents a glide reflection in a line parallel to the vector  $\mathbf{b}_1$ , but shifted in the direction of the vector  $\mathbf{b}_2$  by a quarter of its length. Details of an operator of this type are given in the text preceding relation (C7.11).

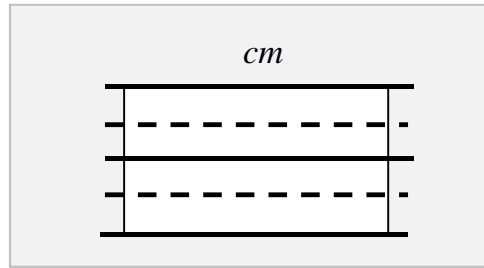
It is worth noting that in addition to the ordinary reflection represented by the operator  $[\bar{\mathbf{M}}_1, \mathbf{0}]$ , there cannot exist a glide reflection in the same line, represented by the operator  $[\bar{\mathbf{M}}_1, \mathbf{b}_1/2]$ . The product of these operators yields the operator  $[\bar{\mathbf{I}}, \mathbf{b}_1/2]$ , which is not a symmetry operator because the translation of  $\mathbf{b}_1/2$  is not itself part of the translation group.

Thus, we obtain another plane group which is a combination of a centred translation group  $T_c$  and a point group  $\mathbf{m}$ , in which both ordinary reflections and glide reflections occur as symmetry operations. The distribution of these symmetry elements in the unit cell is described in Section C7.

The symbol  $cm$  is used for this group and it is listed as the fifth in the order of plane groups:

$$cm : \quad G_5 = T_c \cdot \{e, m\},$$

while the decomposition of the group into cosets has already been discussed above.



### Group $2mm$

We first express the plane group as the direct product of the translation group  $T_c$  and the point group  $2mm$ :

$$G = T_c \cdot \{2mm\} = T_c \cdot \{2\} \cdot \{m\} = T_c \cdot \{e, 2\} \cdot \{e, m\} = T_c \cdot \{e, 2, m_x, m_y\}.$$

The decomposition of the group  $G$  into cosets can be done with respect to the complete translation subgroup  $T_c$ , but also with respect to the incomplete translation subgroup  $T_b$ , as in the case of the group  $\mathbf{m}$ . The latter method will give more information about the symmetry elements and their localization in the unit cell.

The decomposition of the planar group  $G$  by the translation subgroup  $T_c$  has four members, three of which are cosets, similar to the decomposition of the group  $G_6$  for the primitive lattice:

$$G = T_c + [\bar{\mathbf{2}}, \mathbf{0}] \cdot T_c + [\bar{\mathbf{M}}_1, \mathbf{0}] \cdot T_c + [\bar{\mathbf{M}}_2, \mathbf{0}] \cdot T_c.$$

The decomposition by the group  $T_b$  has eight members, seven of which are cosets, and directly expresses all operations or symmetry elements in the structure

$$G = T_b + \mathbf{t}_b \cdot T_b + T_b \cdot [\bar{2}, \mathbf{0}] + \mathbf{t}_b \cdot T_b \cdot [\bar{2}, \mathbf{0}] + \\ + T_b \cdot [\bar{\mathbf{M}}_1, \mathbf{0}] + \mathbf{t}_b \cdot T_b \cdot [\bar{\mathbf{M}}_1, \mathbf{0}] + T_b \cdot [\bar{\mathbf{M}}_2, \mathbf{0}] + \mathbf{t}_b \cdot T_b \cdot [\bar{\mathbf{M}}_2, \mathbf{0}].$$

The eight members of the decomposition can be divided into three sets. The first and second members represent the complete translation group  $T_c$ .

The second set includes the third, fifth and seventh members, represented by operators for which the translation  $\mathbf{t}_b$  does not occur, so they are zero-translation operators. All of them are also part of the group  $G_6$ , denoted  $p2mm$ .

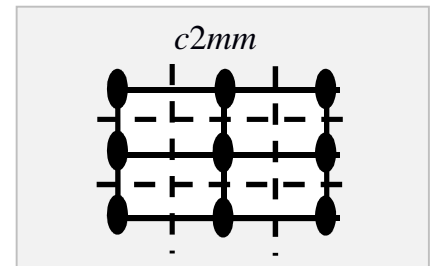
The third set includes three terms in which the  $\mathbf{t}_b$  translation is already present, so we can write them in the general form

$$[\bar{2}, \mathbf{t}], [\bar{\mathbf{M}}_1, \mathbf{t}] \text{ and } [\bar{\mathbf{M}}_2, \mathbf{t}],$$

where according to relation (C8.5b)  $\mathbf{t} = (\mathbf{b}_1 + \mathbf{b}_2)/2$ . Such a combination of symmetry elements does not occur in the symmetry types described so far, so it represents its next type, the ninth planar group  $G_9$ , denoted by  $c2mm$ .

The operator  $[\bar{2}, \mathbf{t}] \equiv [\bar{2}, (\mathbf{b}_1 + \mathbf{b}_2)/2]$  represents a rotation about a twofold axis located at a point with position vector  $(\mathbf{b}_1 + \mathbf{b}_2)/4$ , which is a typical location for a centred lattice ( $\rightarrow$  Fig. C14), while other possible positions of this axis, are given in Section C7. Operators  $[\bar{\mathbf{M}}_1, (\mathbf{b}_1 + \mathbf{b}_2)/2]$  and  $[\bar{\mathbf{M}}_2, (\mathbf{b}_1 + \mathbf{b}_2)/2]$  represent glide reflections in two mutually perpendicular lines, shifted by 1/4 the length of the basis vectors. A more detailed description of these is given in the text before relation (C6.14). Meanwhile, the presence of glide lines in which the basis vectors lie is ruled out, because combining an operator representing a glide reflection, i.e.,  $[\bar{\mathbf{M}}_1, \mathbf{b}_1/2]$ , for example with the operator  $[\bar{\mathbf{M}}_1, (\mathbf{b}_1 + \mathbf{b}_2)/2]$ , yields  $[\bar{1}, \mathbf{b}_1 + \mathbf{b}_2/2]$ , which is a translation that does not belong to the translation group, so it is not a symmetry operation.

Thus, the next planar group is the group  $G_9$ , denoted by the symbol  $c2mm$ , shown in the adjacent figure. However, the glide line markers do not appear in the international symbol of group  $G_9$ , because glide lines are a natural part of structures with centred lattices.



$$c2mm : G_9 = T_c \cdot \{e, 2, m_x, m_y\}$$

Based on the considerations of the centred lattice in the rectangular system, two more groups were added to the table of planar groups:  $cm$  and  $c2mm$ .

| Plane groups |      |      |      |      |      |        |        |        |        |
|--------------|------|------|------|------|------|--------|--------|--------|--------|
| number       | 1    | 2    | 3    | 4    | 5    | 6      | 7      | 8      | 9      |
| symbol       | $p1$ | $p2$ | $pm$ | $pg$ | $cm$ | $p2mm$ | $p2mg$ | $p2gg$ | $c2mm$ |
| number       | 10   | 11   | 12   | 13   | 14   | 15     | 16     | 17     |        |
| symbol       |      |      |      |      |      |        |        |        |        |

### C8.3 Square system

The tetragonal crystal system includes only one type of translation group – the  $T_p$  group representing the primitive lattice, and two point groups: **4**, **4mm**. The unit cell is determined by two basis vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , which are perpendicular to each other and have the same size.

The group **4** is cyclic, with a single generating element represented by the operator  $[\bar{4}, \mathbf{0}] \equiv [\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{0}]$ , and its direct product with the group  $T_p$  yields the first of the plane groups belonging to the square system:

$$p4 : G_{10} = T_p \cdot \{4\} \equiv T_p \cdot \{e, 4, 4^2, 4^3\},$$

or after decomposition into cosets

$$p4 : G_{10} = T_p + [\bar{4}, \mathbf{0}] \cdot T_p + [\bar{4}^2, \mathbf{0}] \cdot T_p + [\bar{4}^3, \mathbf{0}] \cdot T_p, \quad (\text{C8.10})$$

while

$$[\bar{4}^2, \mathbf{0}] \equiv [\bar{2}, \mathbf{0}] \equiv [-\bar{1}, \mathbf{0}] \text{ and } [\bar{4}^3, \mathbf{0}] \equiv [-\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1, \mathbf{0}] \quad (\rightarrow \text{C4.1.3}).$$

There are two fourfold axes per unit cell ( $\rightarrow$  article C7.2), one localized at the origin of the reference frame, the other at the centre of the unit cell. Operations related to the second position are represented by operators ( $\rightarrow$  Appendix D20):

$$[\bar{4}, \mathbf{a}_1], \quad [\bar{4}^2, \mathbf{a}_1 + \mathbf{a}_2], \quad [\bar{4}^3, \mathbf{a}_2]$$

whose translational parts differ from the operators in relation (C8.10) only by different lattice vectors, i.e. different elements of the translation group. This means that the symmetry operations represented, for example, by the operators  $[\bar{4}^3, \mathbf{0}]$  and  $[\bar{4}^3, \mathbf{a}_1]$  belong to one coset of the plane group and each of them can be its representative.

Two twofold axes are also localized in the unit cell of the square lattice, at positions  $(1/2, 0)$ ,  $(0, 1/2)$ , with the corresponding rotations of 2 being identical to the rotations of  $4^2$ . The operators of these rotations have the form ( $\rightarrow$  Appendix D19)

$$[\bar{2}, \mathbf{a}_1] \equiv [\bar{4}^2, \mathbf{a}_1] \text{ resp. } [\bar{2}, \mathbf{a}_2] \equiv [\bar{4}^2, \mathbf{a}_2],$$

and differ from the operator  $[\bar{4}^2, \mathbf{0}]$  only by the translational part augmented by lattice vectors. Therefore, the corresponding operations belong to the same coset of the plane group as the operations represented by the operator  $[\bar{4}^2, \mathbf{0}]$ . The decomposition (C8.10) of the group  $G_{10}$  is thus complete.

The group **4mm** has two generating elements, it can be obtained by the direct product of the group **4** with the reflection group **m**: **4mm** = **4** · **m**  $\equiv$   $\{4\} \cdot \{m\}$ . The plane group is obtained by its direct product with the translation group  $T_p$

$$G = T_p \cdot \{4\} \cdot \{m\} \equiv T_p \cdot \{4\} \cdot \{\bar{\mathbf{M}}\}$$

As shown in Table TC3, there are two variants of reflection in planar structures – ordinary reflection and glide reflection, which must be taken into account. Therefore, when expressing the plane group, we write the direct product in a more general form that takes this into account:

$$G = T_p \cdot \{4\} \cdot \{\bar{\mathbf{M}}, t_1 \mathbf{a}_1 + t_2 \mathbf{a}_2\}.$$

The possible values of the coordinates  $t_1$  and  $t_2$  are obtained from the condition (C8.6) expressed by the relation:  $[\bar{\mathbf{n}}, \mathbf{0}] \cdot [\bar{\mathbf{M}}, \mathbf{t}] \cdot [\bar{\mathbf{n}}, \mathbf{0}] = [\bar{\mathbf{M}}, \mathbf{t} + \mathbf{A}_L]$ , which we modify for this particular case:

$$[\bar{4}, \mathbf{0}] \cdot [\bar{\mathbf{M}}, t_1 \mathbf{a}_1 + t_2 \mathbf{a}_2] \cdot [\bar{4}, \mathbf{0}] = [\bar{\mathbf{M}}, t_1 \mathbf{a}_1 + t_2 \mathbf{a}_2 + \mathbf{A}_L].$$

This equation implies constraints on the values of  $t_i$  ( $\rightarrow$  Appendix D16):

$$t_1 = t_2 = 0, \text{ or } t_1 = t_2 = 1/2, \Rightarrow \mathbf{t} = \mathbf{0}, \text{ or } \mathbf{t} = (\mathbf{a}_1 + \mathbf{a}_2)/2. \quad (\text{C8.11})$$

Thus we get two mutually distinct plane groups, in the first case the group

$$p4mm : G_{11} = T_p \cdot \{4\} \cdot \{\bar{\mathbf{M}}, \mathbf{0}\},$$

in the second case, the group

$$p4gm : G_{12} = T_p \cdot \{4\} \cdot \{\bar{\mathbf{M}}, \mathbf{t}\},$$

or after decomposition into subclasses:

$$p4mm : \quad G_{11} = T_p + [\bar{4}] \cdot T_p + [\bar{4}^2] \cdot T_p + [\bar{4}^3] \cdot T_p + [\bar{\mathbf{M}}_x, \mathbf{0}] \cdot T_p + \\ + [\bar{\mathbf{M}}_y, \mathbf{0}] \cdot T_p + [\bar{\mathbf{M}}_{xy}, \mathbf{0}] \cdot T_p + [\bar{\mathbf{M}}_{yx}, \mathbf{0}] \cdot T_p \quad (C8.12)$$

$$p4gm : \quad G_{12} = T_p + [\bar{4}] \cdot T_p + [\bar{4}^2] \cdot T_p + [\bar{4}^3] \cdot T_p + [\bar{\mathbf{M}}_x, \mathbf{t}] \cdot T_p + \\ + [\bar{\mathbf{M}}_y, \mathbf{t}] \cdot T_p + [\bar{\mathbf{M}}_{xy}, \mathbf{t}] \cdot T_p + [\bar{\mathbf{M}}_{yx}, \mathbf{t}] \cdot T_p \quad (C8.13)$$

We will describe these two groups in more detail, because the brief method given does not point to important details. The **4mm** group has eight elements, and in addition to rotations, it also contains reflection in lines parallel to the sides ( $m_x, m_y$ ) and diagonals ( $m_{xy}, m_{yx}$ ) of the unit cell, so that a more detailed description of the plane group *p4mm* takes the form

$$p4mm: \quad G_{11} = T_p \cdot \{e, 4, 4^2, 4^3, m_x, m_y, m_{xy}, m_{yx}\},$$

while its decomposition into cosets has already been given above.

As in the case of group  $G_{10}$ , it is appropriate to consider all symmetry elements distributed in the unit cell. The distribution of the rotation axes is the same as for group  $G_{10}$ , but in this case the distribution of the reflection lines must also be considered. According to the results presented in C7.5, the reflection lines parallel to the basis vector  $\mathbf{a}_1$  incident to the unit cell are represented by two operators ( $\rightarrow$  relation C8.7):

$$[\bar{\mathbf{M}}_x, \mathbf{0}] \equiv [\bar{\mathbf{M}}_1, \mathbf{0}] \equiv [\bar{\mathbf{I}} - 2 \mathbf{a}^2 \mathbf{a}_2, \mathbf{0}] = [\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2, \mathbf{0}], \\ [\bar{\mathbf{M}}_1, \mathbf{a}_2] \equiv [\bar{\mathbf{I}} - 2 \mathbf{a}^2 \mathbf{a}_2, \mathbf{a}_2] = [\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2, \mathbf{a}_2],$$

and reflections in lines parallel to vector  $\mathbf{a}_2$  by two other operators

$$[\bar{\mathbf{M}}_y, \mathbf{0}] \equiv [\bar{\mathbf{M}}_2, \mathbf{0}] \equiv [\bar{\mathbf{I}} - 2 \mathbf{a}^1 \mathbf{a}_1, \mathbf{0}] = [-\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2, \mathbf{0}], \\ [\bar{\mathbf{M}}_2, \mathbf{a}_1] \equiv [\bar{\mathbf{I}} - 2 \mathbf{a}^1 \mathbf{a}_1, \mathbf{a}_1] = [-\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2, \mathbf{a}_1].$$

The operators  $[\bar{\mathbf{M}}_1, \mathbf{0}]$  and  $[\bar{\mathbf{M}}_1, \mathbf{a}_2]$  differ from each other only in their translational part, namely the elements of the translation group, so the corresponding operations belong to one coset of the plane group. The same is true for the operations represented by the operators  $[\bar{\mathbf{M}}_2, \mathbf{0}]$  and  $[\bar{\mathbf{M}}_2, \mathbf{a}_1]$ .

The reflection operator in the line identical to the diagonal  $xy$  of the unit cell (passing through the origin of the reference frame) has the form ( $\rightarrow$  end of Section C4.1.3):

$$[\bar{\mathbf{M}}_{xy}, \mathbf{0}] \equiv [\bar{\mathbf{M}}_{12}, \mathbf{0}] = [\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1, \mathbf{0}], \quad (C8.14)$$

and the reflection operator in a line perpendicular to it (and also passing through the origin of the reference frame):

$$[\bar{\mathbf{M}}_{yx}, \mathbf{0}] \equiv [\bar{\mathbf{M}}_{21}, \mathbf{0}] = [-\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1, \mathbf{0}].$$

The reflection operators  $[\bar{\mathbf{M}}_x, \mathbf{0}]$ ,  $[\bar{\mathbf{M}}_y, \mathbf{0}]$ ,  $[\bar{\mathbf{M}}_{xy}, \mathbf{0}]$  and  $[\bar{\mathbf{M}}_{yx}, \mathbf{0}]$  act in the decomposition of the plane group  $G_{11}$  as representatives of its cosets. However, glide lines are a natural part of the symmetry of the square lattice ( $\rightarrow$  the figure at the end of this part, or the figure in the appendices), which makes it appear as if the decomposition (C8.12) of the plane group  $G_{11}$  is incomplete. However, operators representing glide reflections can be obtained from operators of ordinary reflections by adding certain lattice translations, i.e., certain elements of the translation group. In terms of operators, the addition of a translation can be realized as the product of the corresponding operator with the translation operator  $[\bar{\mathbf{I}}, \mathbf{A}_L]$ , where  $\mathbf{A}_L$  is an element of the translation group. The operators representing the glide reflections in lines parallel to the  $xy$  diagonal (their labels are in Appendices D21 and D22) are obtained by the following products:

$$M_{12a} : [\mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1, \mathbf{0}] \cdot [\bar{\mathbf{I}}, \mathbf{a}_1] = [\mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1, \mathbf{a}_1],$$

$$M_{12b} : [\mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1, \mathbf{0}] \cdot [\bar{\mathbf{I}}, \mathbf{a}_2] = [\mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1, \mathbf{a}_2].$$

The operators representing the glide reflections in lines parallel to the diagonal  $yx$  have the form:

$$M_{21b} : [-\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1, \mathbf{0}] \cdot [\bar{\mathbf{I}}, \mathbf{a}_1] = [-\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1, \mathbf{a}_1],$$

$$M_{21c} : [-\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1, \mathbf{0}] \cdot [\bar{\mathbf{I}}, \mathbf{a}_2] = [-\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1, \mathbf{a}_2].$$

A more detailed discussion of these operators is given in Appendices D21 and D22. Appendix D21 also gives examples showing that glide reflections is equivalent to a sequential application of ordinary reflection and rotation about one of the axes of symmetry. The above fact implies that the decomposition (C8.12) of the  $p4mm$  group is complete.

**The next plane group**, denoted  $p4gm$ , differs from the previous one by assuming the presence of glide reflections in lines parallel to both the sides and the diagonals of the unit cell. Thus, in the reflection operators of the decomposition (C8.13) of a plane group, the non-lattice translation  $\mathbf{t} = \mathbf{a}_1/2 + \mathbf{a}_2/2$  ( $\rightarrow$  relation

C8.11) comes into play, so that the decomposition of the group into cosets takes the form:

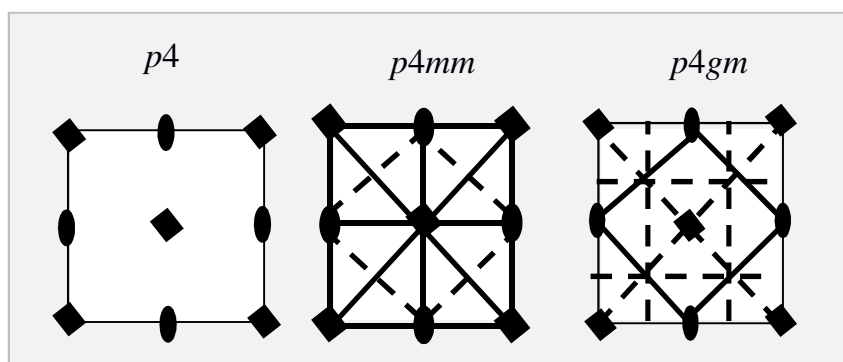
$$\begin{aligned}
 p4gm: \quad G_{12} = & T_p + [\bar{4}] \cdot T_p + [\bar{4}^2] \cdot T_p + [\bar{4}^3] \cdot T_p + \\
 & + [\bar{M}_1, \frac{1}{2}a_1 + \frac{1}{2}a_2] \cdot T_p + [\bar{M}_2, \frac{1}{2}a_1 + \frac{1}{2}a_2] \cdot T_p + \\
 & + [\bar{M}_{12}, \frac{1}{2}a_1 + \frac{1}{2}a_2] \cdot T_p + [\bar{M}_{21}, \frac{1}{2}a_1 + \frac{1}{2}a_2] \cdot T_p .
 \end{aligned}$$

The data in Appendices D23 and D24 show that  $[\bar{M}_1, a_1/2 + a_2/2]$  operator represents a reflection with glide  $a_1/2$  in a line parallel to the vector  $a_1$  and shifted to position  $a_2/4$ , the operator  $[\bar{M}_2, a_1/2 + a_2/2]$  reflection with glide  $a_2/2$  in a line parallel to the vector  $a_2$  and shifted by  $a_1/4$ , and then a third operator  $[\bar{M}_{12}, a_1/2 + a_2/2]$  reflection with glide  $a_1/2 + a_2/2$  in a line identical to diagonal  $xy$  of the unit cell. The fourth operator  $[\bar{M}_{21}, a_1/2 + a_2/2]$  represents an ordinary reflection in a line parallel to the diagonal  $yx$ , while the operator  $[\bar{M}_{21}, a_1/2 - a_2/2]$ , i.e. the operator with the translation part changed by the lattice vector  $-a_2$ , represents a glide reflection in a line identical to the diagonal  $yx$ .

In this group, there are three other reflections without glide within the unit cell that are not visibly represented in its decomposition (C8.13), but, as in the  $p4mm$  group, their operators are formed by adding a lattice translation to the operators representing the glide reflection. Details are given in Appendix D24; a list of the operators of the  $p4gm$  group belonging to the unit cell is given in Appendix D23.

The next table includes three square lattice groups,  $p4$ ,  $p4mm$  and  $p4gm$ .

| Rovinné grupy |      |        |        |      |      |        |        |        |        |
|---------------|------|--------|--------|------|------|--------|--------|--------|--------|
| číslo         | 1    | 2      | 3      | 4    | 5    | 6      | 7      | 8      | 9      |
| značka        | $p1$ | $p2$   | $pm$   | $pg$ | $cm$ | $p2mm$ | $p2mg$ | $p2gg$ | $c2mm$ |
| číslo         | 10   | 11     | 12     | 13   | 14   | 15     | 16     | 17     |        |
| značka        | $p4$ | $p4mm$ | $p4gm$ |      |      |        |        |        |        |



## C8.4 Hexagonal system

In the hexagonal system, only the primitive lattice described by the primitive translation group  $T_p$ , but four point groups apply: **3**, **3m**, **6** and **6mm**, the last one being holohedral. The holohedral group includes the multiplicities of the  $60^\circ$  rotation, denoted by the symbols  $6, 6^2, 6^3, 6^4, 6^5$ , plus the set of reflections in the six lines, which are denoted by the symbols  $m_0, m_{30}, m_{60}, m_{90}, m_{120}, m_{150}$ ; the indices express the angle that these lines take with the basis vector  $\mathbf{a}_1$ .

The unit cell in the hexagonal system is by default determined by the vectors  $\mathbf{a}_1, \mathbf{a}_2$ , which have the same length and conventionally take the angle  $120^\circ$ . Such a unit cell is primitive. An alternative is the centred **orthohexagonal cell** introduced in C6.2. Some of its properties, including the shape of the rotation and reflection operators, are described in Appendix D26, not included in the main text.

**The point group 3** in combination with the translation group  $T_p$  gives rise to the planar group  $p3$  :

$$p3: \quad G_{13} = T_p \cdot \{3\} \equiv T_p \cdot \{e, 3, 3^2\},$$

and after decomposition into cosets:

$$G_{13} = T_p + T_p \cdot [\bar{3}, \mathbf{0}] + T_p \cdot [\bar{3}^2, \mathbf{0}].$$

The tensor representing the  $120^\circ$  rotation, i.e. generating element of the cyclic group  $\{3\}$ , written using the basis vectors  $\mathbf{a}_1, \mathbf{a}_2$ , has the form according to Table TC2b:

$$\bar{3} = \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2.$$

There are 3 threefold axes per unit cell, with localizations  $(0,0)$ ,  $(1/3, 2/3)$  and  $(2/3, 1/3)$ .

The operators representing the respective rotations have the form

$$[\bar{3}, \mathbf{0}], [\bar{3}, \mathbf{a}_1 + \mathbf{a}_2], \text{ resp. } [\bar{3}, \mathbf{a}_1],$$

and differ only in the translational part by different lattice vectors, so that the corresponding elements of the plane group belong to one coset. The operators representing rotations by  $240^\circ$  about the axes localized at these positions have an analogous shape.

**The point group 3m** combined with the translation group  $T_p$  gives rise to two plane groups, denoted by the symbols  $p3m1$  and  $p31m$ , which differ from each other by the orientations of the reflection lines with respect to the basis vector  $\mathbf{a}_1$ . Both

groups are formed by the direct product  $G = T_p \cdot \{3m\}$ , but they differ in the detail of the elements of the point group:

$$p3m1 : G_{14} = T_p \cdot \{e, 3, 3^2, m_{30}, m_{90}, m_{150}\}$$

$$p31m : G_{15} = T_p \cdot \{e, 3, 3^2, m_0, m_{60}, m_{120}\}.$$

The notation of these groups after decomposition into cosets:

$$G_{14} = T_p + T_p \cdot [\bar{3}, \mathbf{0}] + T_p \cdot [\bar{3}^2, \mathbf{0}] + T_p \cdot [\bar{M}_{30}, \mathbf{0}] + T_p \cdot [\bar{M}_{90}, \mathbf{0}] + T_p \cdot [\bar{M}_{150}, \mathbf{0}],$$

$$G_{15} = T_p + T_p \cdot [\bar{3}, \mathbf{0}] + T_p \cdot [\bar{3}^2, \mathbf{0}] + T_p \cdot [\bar{M}_0, \mathbf{0}] + T_p \cdot [\bar{M}_{60}, \mathbf{0}] + T_p \cdot [\bar{M}_{120}, \mathbf{0}].$$

Glide lines also occur in both groups ( $\rightarrow$  images at the end of this article), with glide reflections belonging to the same coset as reflections in a line parallel to these glide lines. Appendix D27 gives a more detailed description of reflections in the  $p31m$  group, Appendix D28 covers reflections in the  $p3m1$  group.

**The point group 6** combined with the translation group  $T_p$  produces a plane group with ordinal number 16, denoted by the symbol  $p6$ :

$$p6: G_{16} = T_p \cdot \{6\} \equiv T_p \cdot \{e, 6, 6^2, 6^3, 6^4, 6^5\},$$

with a breakdown of the cosets:

$$G_{16} = T_p + T_p \cdot [\bar{6}, \mathbf{0}] + T_p \cdot [\bar{6}^2, \mathbf{0}] + T_p \cdot [\bar{6}^3, \mathbf{0}] + T_p \cdot [\bar{6}^4, \mathbf{0}] + T_p \cdot [\bar{6}^5, \mathbf{0}].$$

In this plane group, there are no reflections, but for the unit cell, in addition to one hexagonal axis with localization (0, 0), there are 2 threefold axes with localizations (1/3, 2/3) and (2/3, 1/3), and three twofold axes with localizations (1/2, 0), (0, 1/2) and (1/2, 1/2). The operators of the threefold axes have the same form as for the group  $p3$ , i.e.

$$[\bar{3}, \mathbf{a}_1 + \mathbf{a}_2], \text{ resp. } [\bar{3}, \mathbf{a}_1],$$

differ from each other only by lattice translations, so that the corresponding operations belong to one coset of the plane group  $p6$ .

The twofold axis operators have the same form as in the group  $p2$ , i.e.:

$$[\bar{2}, \mathbf{a}_1], [\bar{2}, \mathbf{a}_2] \text{ and } [\bar{2}, \mathbf{a}_1 + \mathbf{a}_2],$$

and the same is true for them as for operators related to threefold axes of symmetry.

The point group **6mm** combined with the translation group  $T_p$  produces a plane group with the sequence number 17, denoted by the symbol  $p6mm$ ; it is the last of the set of plane groups.

It is written as a direct product:

$$G_{17} = T_p \cdot \{6\} \cdot \{m\},$$

The tensor representing the  $60^\circ$  rotation, i.e. generating element of the cyclic group  $\{6\}$ , written using the basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , has the form according to Table TB2b:

$$\bar{\mathbf{6}} = \mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1$$

and the operator of the corresponding element of the plane group (with zero translation):  $[\bar{\mathbf{6}}, \mathbf{0}]$ . When we choose the generating element of the point group  $\{m\}$  to be a mirror in the line parallel to the vector  $\mathbf{a}_1$ , the tensor of this operation, denoted by the symbol  $\bar{\mathbf{M}}_0$ , has the form ( $\rightarrow$  Appendix D25)

$$\bar{\mathbf{M}}_0 = \mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2$$

and the corresponding operator of the plane group element  $[\bar{\mathbf{M}}_0, \mathbf{0}]$ . Appendix D25 also lists the operators of the other rotations and reflections applied in the  $p6mm$  group.

When we want to include glide lines in the considerations, we write the reflection operator in the form  $[\bar{\mathbf{M}}_0, \mathbf{t}]$ , where the translation  $\mathbf{t}$  must satisfy condition (C8.3):

$$[\bar{\mathbf{6}}, \mathbf{0}] \cdot [\bar{\mathbf{M}}_0, \mathbf{t}] \cdot [\bar{\mathbf{6}}, \mathbf{0}] = [\bar{\mathbf{M}}_0, \mathbf{t} + \mathbf{A}_L],$$

where  $\mathbf{A}_L$  is a lattice vector. According to the result obtained in Appendix D17, within the unit cell, only the translation  $\mathbf{t} = \mathbf{0}$  satisfies this condition. This means that despite the presence of glide reflections, the representatives of all cosets of this plane group can be ordinary reflections, i.e., reflection operators without a translation term:

$$\begin{aligned} G_{17} = & T_p + T_p \cdot [\bar{\mathbf{6}}, \mathbf{0}] + T_p \cdot [\bar{\mathbf{6}}^2, \mathbf{0}] + T_p \cdot [\bar{\mathbf{6}}^3, \mathbf{0}] + T_p \cdot [\bar{\mathbf{6}}^4, \mathbf{0}] + T_p \cdot [\bar{\mathbf{6}}^5, \mathbf{0}] + \\ & + T_p \cdot [\bar{\mathbf{M}}_0, \mathbf{0}] + T_p \cdot [\bar{\mathbf{M}}_{30}, \mathbf{0}] + T_p \cdot [\bar{\mathbf{M}}_{60}, \mathbf{0}] + T_p \cdot [\bar{\mathbf{M}}_{90}, \mathbf{0}] + \\ & + T_p \cdot [\bar{\mathbf{M}}_{120}, \mathbf{0}] + T_p \cdot [\bar{\mathbf{M}}_{150}, \mathbf{0}]. \end{aligned}$$

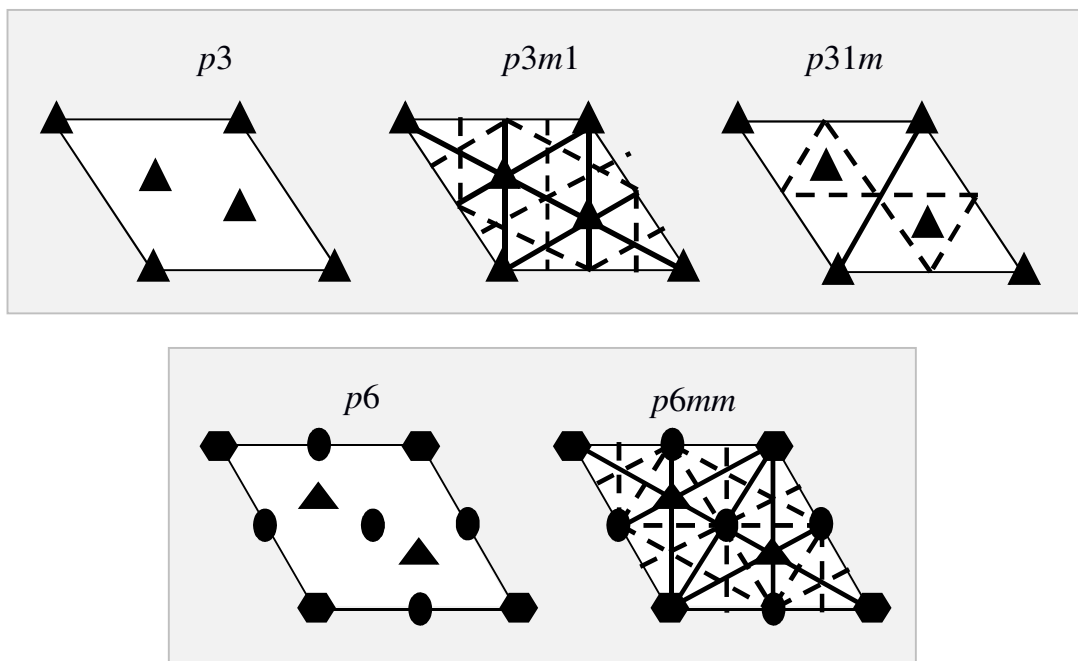
Note that the operator  $[\bar{\mathbf{6}}^2, \mathbf{0}]$  is identical to the operator  $[\bar{\mathbf{3}}, \mathbf{0}]$ , and the operator  $[\bar{\mathbf{6}}^3, \mathbf{0}]$  to the operator  $[\bar{\mathbf{2}}, \mathbf{0}]$ , and that the threefold and twofold axes of

symmetry are also distributed in the hexagonal unit cell, as mentioned above for the group  $p6$ .

Adding translation group elements to the translation members of the reflection operators produces operators representing either a combination of reflection with lattice translation or glide reflections. Due to the circumstance that the set of reflections of the group  $p6mm$  coincides with the sum of the sets of reflections in the groups  $p31m$  and  $p3m1$ , it is not necessary to give further information about them. However, some details are given in Appendices D27 and D28, which refer to groups  $p31m$  and  $p3m1$ .

There are 5 planar groups included in the hexagonal system:

|        |                                             |
|--------|---------------------------------------------|
| $p3$   | $G_{13} = T_p \cdot \{3\}$                  |
| $p3m1$ | $G_{14} = T_p \cdot \{3\} \cdot \{m_{30}\}$ |
| $p31m$ | $G_{15} = T_p \cdot \{3\} \cdot \{m_0\}$    |
| $p6$   | $G_{16} = T_p \cdot \{6\}$                  |
| $p6mm$ | $G_{17} = T_p \cdot \{6\} \cdot \{m\}$      |



The hexagonal system has been used to exhaust the last types of symmetries of planar periodic structures and the corresponding plane groups have been determined. The following table lists the symbols of all 17 planar groups.

| Plane groups  |            |             |             |           |             |             |             |             |             |
|---------------|------------|-------------|-------------|-----------|-------------|-------------|-------------|-------------|-------------|
| <b>number</b> | 1          | 2           | 3           | 4         | 5           | 6           | 7           | 8           | 9           |
| <b>symbol</b> | <i>p1</i>  | <i>p2</i>   | <i>pm</i>   | <i>pg</i> | <i>cm</i>   | <i>p2mm</i> | <i>p2mg</i> | <i>p2gg</i> | <i>c2mm</i> |
| <b>number</b> | 10         | 11          | 12          | 13        | 14          | 15          | 16          | 17          |             |
| <b>symbol</b> | <i>p4m</i> | <i>p4mm</i> | <i>p4gm</i> | <i>p3</i> | <i>p3m1</i> | <i>p31m</i> | <i>p6</i>   | <i>p6mm</i> |             |

An overview of all the plane groups with their assignment to crystal systems is given in Table TA3 in Section A and repeated in the tabular section. In the figure section, the shape and distribution of structural motifs is indicated for each plane group - in addition to the shape of the unit cell. In the figure section you will also find a schematic representation of the wallpaper patterns, with the symmetry belonging to the corresponding plane group. Their author is Edmund Dobročka, the creator of the program for drawing them [24].

## C9 Black-white groups

In addition to the spatial coordinates of the atom expressing its position in the unit cell, another parameter was considered that could characterize some of its physical or chemical properties and take two or more values (e.g., the direction of the magnetic moment). A parameter with two values was already the subject of consideration in 1929 by the German mathematician Heinrich Heesch [25], who in his doctoral thesis gave the name **black–white** to the respective symmetry groups.

The consistent derivation of 58 types of black–white point groups (three-dimensional) is associated with the 1951 work of the Russian crystallographer A. V. Shubnikov [26]. Shubnikov began to use the term *anti-symmetry*, which has its origin in the opposition of states corresponding to two possible values of the *anti-symmetry parameter*. For example, in antiferromagnetics there are two opposite orientations of the magnetic moments of the atoms, which contributed to the use of the threefold naming of these groups - the *black–white*, *magnetic*, and *Shubnikov groups*. The increase in the number of parameters characterizing the atom in the unit cell results in an increase in the number of symmetry types, for example, for crystal point groups from 32 to 58. Black–white groups can be applied, for example, to characterize the symmetry of printed fabrics or wallpapers with periodic alternation of two colours in a structural motif.

A. V. Shubnikov together with N. V. Belov in 1964 published a book entitled *Colored symmetry* [27], in which they considered the case of several possible values of another parameter of the atom, and under the influence of the name black- white groups, the name **colour groups** was coined. These, however, will not be the subject of this text, as it is too difficult a topic in scope. To describe the effect of increasing the number of parameters of an atom on the number of types of symmetry, the example of black-white groups will suffice. This topic is also dealt with, for example, in the book by A. V. Shubnikov, V. A. Koptsik: *Symmetry in Science and Art* [28].

The principle of the construction of black-white groups in the plane will be illustrated by the example of a structural motif whose two possible colours (black – white) alternately change after the application of a certain symmetry operation, such as translation. When a structural motif is translated from a certain position by a symmetry operation to another position (equivalent in terms of spatial symmetry), but in which it should have the opposite colour, the complete identification of the structure is only achieved when the colour of the translated structural motif changes.

From a mathematical point of view, the colour transformation can be expressed symbolically by the number  $-1$ , understood as a colour transformation operator (colour inversion operator, anti-symmetry operator), which is added to the operator representing the corresponding spatial operation (rotation, reflection, or translation). However, another symmetry operation can be used to bring the structural motif to a position in which the same colour is required; colour preservation can be expressed by the application of the operator represented by the number  $+1$ . A pair of numbers (operators)  $-1, +1$ , in terms of the binary multiplication operation forms a group, in this case called the group of inversion and denoted by the symbol  $R \equiv \{1, -1\}$ , or by Shubnikov  $R \equiv \{1, 1'\}$ . The comma over the symbol of the symmetry operation was also used by Shubnikov for other spatial operations associated with the transformation of colour, or more generally – with the change of the value of the anti-symmetry parameter. For example, the rotation by  $90^\circ$  about the fourfold axis of symmetry associated with the change of colour was denoted by the symbol  $4'$ .

**Note** We will use an asterisk instead of a comma in this text:  $4' \rightarrow 4^*$ .

It should be noted that in structures in which there are two alternating colours, only some symmetry operations are combined with a colour change, so they form only part of the corresponding set of symmetry operations – each black-white symmetry group contains both "with asterisk" and "without asterisk" operations.

The black-white groups (we denote them by  $M$ ) related to the group  $G$  of spatial transformations are formed on the basis of its subgroup  $H$  with index 2 ( $H$  has half of the elements of  $G$ ). The elements of subgroup  $H$  are space transformations (rotations, reflections, translations) without combining with a colour change, while all other elements of group  $G$ , i.e., the elements of the coset  $G - H$  they are written in the symbolic form  $(G - H)1^*$  with a colour change. The notation of the black-white group  $M$  thus takes the form:

$$M = H + (G - H)1^*$$

This construction of black-white groups applies directly to both point and translation groups, but for space (and planar) groups, as discussed below, there are two types of black-white groups.

To illustrate the properties of black-white point groups, the following figure will serve.

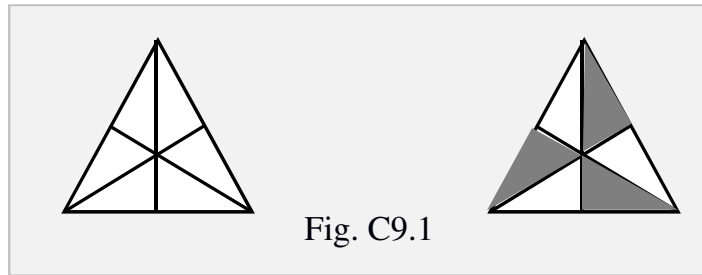


Fig. C9.1

The point group  $G$  of the left object contains the rotations by  $0^\circ$ ,  $120^\circ$  and  $240^\circ$  (symbols  $e, 3, 3^2$ ), associated with the threefold axis of symmetry perpendicular to the plane of the triangle and passing through its centre, and furthermore the reflections with labels  $m_0, m_{60}$  and  $m_{120}$ , in the three planes perpendicular to the plane of the triangle, which make angles  $60^\circ$  to each other. In each of these transformations, the object is identified with itself. Thus, the *one-colour* point group  $G$  contains the following elements:

$$G \equiv \{e, 3, 3^2, m_0, m_{60}, m_{120}\}.$$

The object on the right side of the figure identifies with itself after rotations by  $0^\circ$ ,  $120^\circ$  and  $240^\circ$ , and this set of symmetry operations - without colour change - with the labels  $e, 3, 3^2$ , forms a subgroup with index 2 of the group  $G$ . However, after reflections, the object only reaches the congruent position after the black and white colours have been interchanged. Therefore, the reflection must be combined with the colour inversion, represented by an asterisk. The black-white point group  $M$  then has the following elements:

$$M \equiv \{e, 3, 3^2, m_0^*, m_{60}^*, m_{120}^*\}.$$

The symmetry of the left object in this view represents the symmetry of a monochrome wallpaper, the symmetry of the right object, a two-colour one.

Based on such considerations, we show how point, translation, and even plane black- white symmetry groups of planar periodic structures are formed.

### Black–white point groups

There are 10 types of point groups in planar two-dimensionally periodic singlechrome structures, which are listed in both Tables TA2 and TA3 and illustrated in the figure. These are the groups that have been denoted in the previous text by the symbols

$$1, 2, m, 2mm, 3, 3m, 4, 4mm, 6, 6mm .$$

The following table lists the elements of these groups.

| <b>Table C9.1</b> |                   |                                                                               |
|-------------------|-------------------|-------------------------------------------------------------------------------|
|                   | <b>Symbols</b>    | <b>Elements of groups</b>                                                     |
| 1                 | <b>1</b>          | $\{e\}$                                                                       |
| 2                 | <b>2</b>          | $\{e, 2\}$                                                                    |
| 3                 | <b><i>m</i></b>   | $\{e, m\}$                                                                    |
| 4                 | <b><i>2mm</i></b> | $\{e, 2, m_x, m_y\}$                                                          |
| 5                 | <b>3</b>          | $\{e, 3, 3^2\}$                                                               |
| 6                 | <b><i>3m</i></b>  | $\{e, 3, 3^2, m_0, m_{60}, m_{120}\}$                                         |
| 7                 | <b>4</b>          | $\{e, 4, 4^2, 4^3\}$                                                          |
| 8                 | <b><i>4mm</i></b> | $\{e, 4, 4^2, 4^3, m_x, m_y, m_{xy}, m_{yx}\}$                                |
| 9                 | <b>6</b>          | $\{e, 6, 6^2, 6^3, 6^4, 6^5\}$                                                |
| 10                | <b><i>6mm</i></b> | $\{e, 6, 6^2, 6^3, 6^4, 6^5, m_0, m_{30}, m_{60}, m_{90}, m_{120}, m_{150}\}$ |

We will create black-white groups by finding subgroups with index 2 in each of the given point groups. The other elements of the group, forming a coset of the group, will be associated with a colour change, so we will add the appropriate asterisk to them.

The point group denoted by the symbol **1** has only one element, the identity, so it has no subgroup.

Point group **2** has two elements, with the identity - the element marked  $e$  being its only subgroup with index 2. So the corresponding black-white group has the following composition:  $\{e, 2^*\}$ .

The point group ***m*** also has only two elements, identity and reflection, so the corresponding black-white group consists of the elements  $\{e, m^*\}$ .

There are two subgroups of index 2,  $\{e, 2\}$  and  $\{e, m_x\}$ , (respectively  $\{e, m_y\}$ ) in the ***2mm*** point group, so that two black-white groups can be formed:  $\{e, 2, m_x^*, m_y^*\}$  and  $\{e, m_x, 2^*, m_y^*\}$ . The group  $\{e, m_y, 2^*, m_x^*\}$  is equivalent to the latter; it is just a change of coordinate axis labels, so it does not represent a new type of symmetry.

Point group **3** has an odd number of elements, so it cannot contain a subgroup with index 2.

In the point group **3m** there is only one suitable subgroup, the cyclic group of rotations  $\{e, 3, 3^2\}$ , so the corresponding black-white group consists of elements:  $\{e, 3, 3^2, m_0^*, m_{60}^*, m_{120}^*\}$

Point group **4** has a single subgroup with index 2, namely  $\{e, 4^2\}$ , so the corresponding black-white group has the composition:  $\{e, 4^2, 4^*, 4^{3*}\}$ .

Three subgroups with index 2 are present in the **4mm** point group, and thus the same number of black-white groups:  $\{e, 4, 4^2, 4^3, m_x^*, m_y^*, m_{xy}^*, m_{yx}^*\}, \{e, 4^2, m_x, m_y, 4^*, 4^{3*}, m_{xy}^*, m_{yx}^*\}, \{e, 4^2, m_{xy}, m_{yx}, 4^*, 4^{3*}, m_x^*, m_y^*\}$

The point group **6** has a single subgroup with index 2, the group  $\{e, 6^2, 6^4\}$ , so there is a single black-white group associated with it:  $\{e, 6^2, 6^4, 6^*, 6^{3*}, 6^{5*}\}$ .

There are three suitable subgroups in the **6mm** group, so there are also three black-white groups:

$$\begin{aligned} &\{e, 6, 6^2, 6^3, 6^4, 6^5, m_0^*, m_{30}^*, m_{60}^*, m_{90}^*, m_{120}^*, m_{150}^*\}, \\ &\{e, 6^2, 6^4, m_0, m_{60}, m_{120}, 6^*, 6^{3*}, 6^{5*}, m_{30}^*, m_{90}^*, m_{150}^*\}, \\ &\{e, 6^2, 6^4, m_{30}, m_{90}, m_{150}, 6^*, 6^{3*}, 6^{5*}, m_0^*, m_{60}^*, m_{120}^*\}. \end{aligned}$$

On the next page is a table of black-white groups, followed by a graphical representation of them.

| Table C9.2   |              |                                                                                              |
|--------------|--------------|----------------------------------------------------------------------------------------------|
| Group symbol | Group number | Black-white point groups                                                                     |
| <b>1</b>     |              | No subgroup                                                                                  |
| <b>2</b>     | 1            | $\{e, 2^*\}$                                                                                 |
| <b>m</b>     | 2            | $\{e, m^*\}$                                                                                 |
| <b>2mm</b>   | 3            | $\{e, 2, m_x^*, m_y^*\},$                                                                    |
|              | 4            | $\{e, m_x, 2^*, m_y^*\}$                                                                     |
| <b>3</b>     |              | No subgroup with index 2                                                                     |
| <b>3m</b>    | 5            | $\{e, 3, 3^2, m_0^*, m_{60}^*, m_{120}^*\}$                                                  |
| <b>4</b>     | 6            | $\{e, 4^2, 4^*, 4^{3*}\}$                                                                    |
| <b>4mm</b>   | 7            | $\{e, 4, 4^2, 4^3, m_x^*, m_y^*, m_{xy}^*, m_{yx}^{*'}\}$                                    |
|              | 8            | $\{e, 4^2, m_x, m_y, 4^*, 4^{3*}, m_{xy}^*, m_{yx}^*\}$                                      |
|              | 9            | $\{e, 4^2, m_{xy}, m_{yx}, 4^*, 4^{3*}, m_x^*, m_y^*\}$                                      |
| <b>6</b>     | 10           | $\{e, 6^2, 6^4, 6^*, 6^{3*}, 6^{5*}\}$                                                       |
| <b>6mm</b>   | 11           | $\{e, 6, 6^2, 6^3, 6^4, 6^5, m_0^*, m_{30}^*, m_{60}^*, m_{90}^*, m_{120}^*, m_{150}^*\}$    |
|              | 12           | $\{e, 6^2, 6^4, m_0, m_{60}, m_{120}, 6^*, 6^{3*}, 6^{5*}, m_{30}^*, m_{90}^*, m_{150}^*\}$  |
|              | 13           | $\{e, 6^2, 6^4, m_{30}, m_{90}, m_{150}, 6^*, 6^{3*}, 6^{5*}, m_0^*, m_{60}^*, m_{120}^*\}.$ |

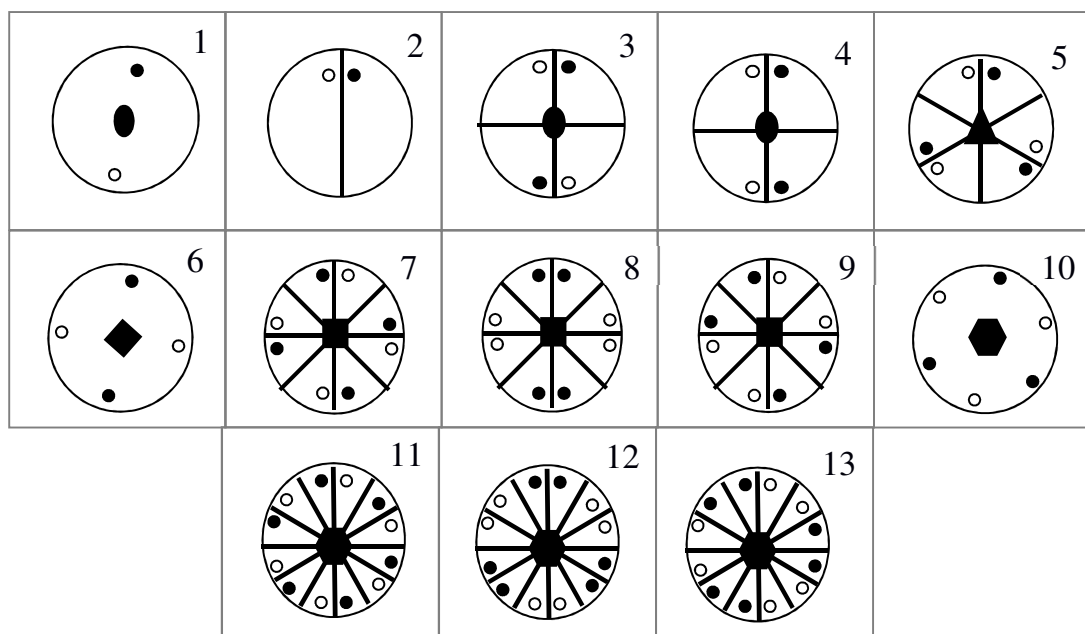


Fig. C9.2

## Translational black–white groups

They are constructed in a similar way to the black–white point groups. That is, a subgroup with index 2 is selected from the translation group  $T$  whose elements will not be associated with a colour change, all other translations - i.e. not belonging to this subgroup - are given a colour change operator. Due to the infinite number of elements of the translation group, this selection is not unambiguous, but it must preserve the two-dimensional periodicity of the structure; the black–white motifs must alternate regularly in both fundamental directions. On the left side of Figure C9.3 is a single-colour structure with a oblique lattice and a simple structural motif, a black ring at the beginning of the unit cell. One unit cell is highlighted in grey. On the right side of the image is a black–white structure in which the colours of the structural motif alternate. It is obtained so that after translation in the direction of the basis vector by one of its length, the colour of the structure motif changes. It can be seen from the figure that the unit cell, coloured grey, representing the smallest regularly repeating object, is then larger. While the original single-colour cell had one structural motif, the black and white unit cell has two black and two white motifs.

The regular alternation of colour imposes conditions on the coordinates  $L_i$  of the lattice vectors  $\mathbf{A}_L = L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2$  determining the position of the black–white structural motifs, respectively. Such a lattice vector simultaneously represents a translation  $\mathbf{t}$  from the origin of the coordinate system to the corresponding lattice point. According to the right part of Figure C9.3, the sum of the coordinates corresponding to the black motifs is an even number, for the white ones an odd number. This distinguishes  $\mathbf{t}$  translations from  $\mathbf{t}^*$  translations. Similarly, the asterisk distinguishes the translation group  $T$  of a single-colour structure from the translation group  $T^*$ , containing half of the translations combined with the colour change. For example, the elements of group  $T$  are translations  $0, \mathbf{a}_1, 2\mathbf{a}_1, 3\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_1 + \mathbf{a}_2, \dots$  and the elements of group  $T^*$  are translations  $\mathbf{a}_1^*, \mathbf{a}_2^*, 3\mathbf{a}_1^*, \dots$

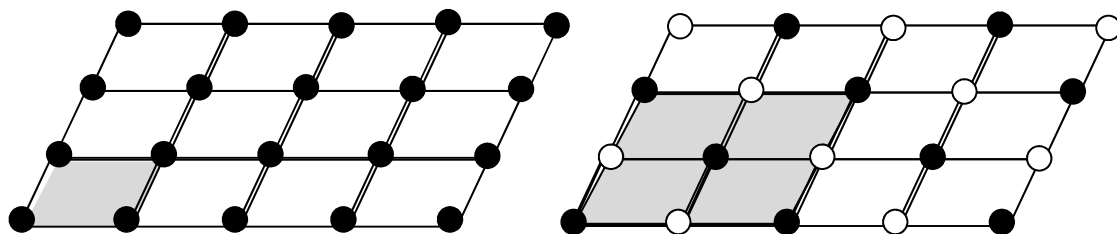


Fig. C9.3

The situation is the same in the rectangular, square and hexagonal lattices, where only primitive unit cells are considered. However, the situation looks different in an orthogonal lattice with a centred unit cell, where two structural motifs – one in the corner and the other in the centre of the unit cell – are attributed to this cell. In

the construction of black-white lattices, two possibilities come into play there. The first option is to proceed similarly to the primitive cells, i.e., the colour of both motifs will change after translation by the length of the basis vector; the second option is to change the colour after translation by  $(1/2)(\mathbf{a}_1 + \mathbf{a}_2)$ , so that the motif in the corner of the cell will be black, for example, and the motif in the centre of the cell will be white. These two options are shown in the following figure, along with the original single-colour structure.

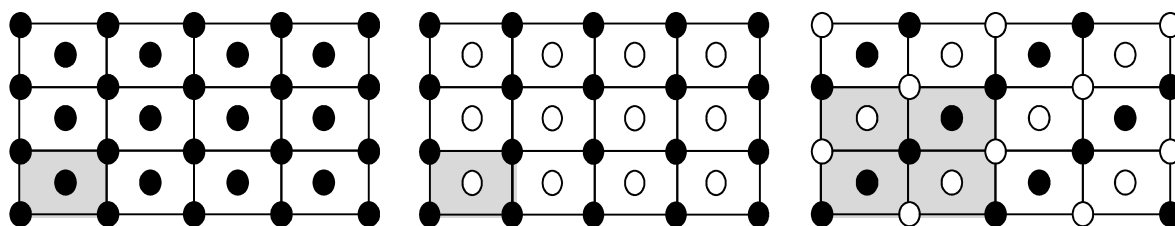


Fig. C9.4

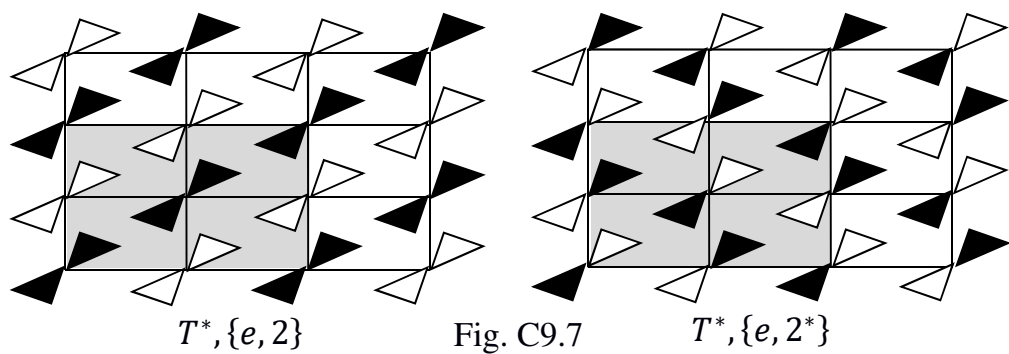
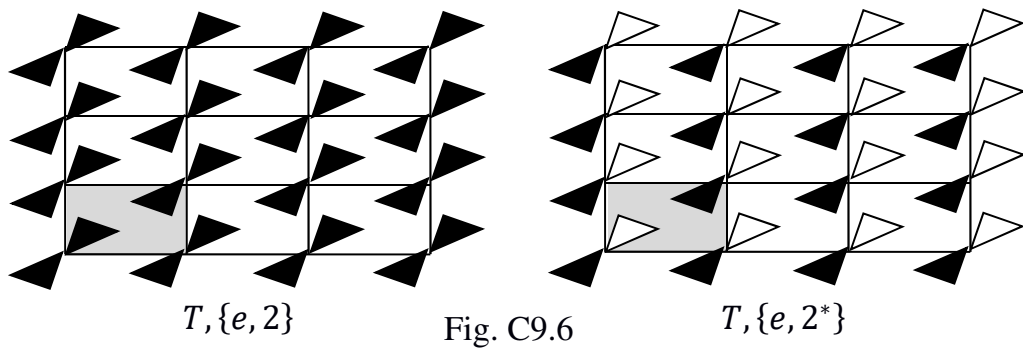
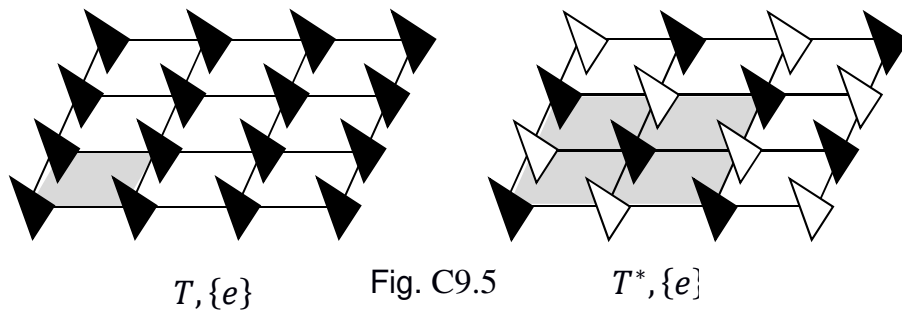
Thus, in planar periodic structures, there are not many possibilities to construct black-white translation groups. The two types exist only in the orthogonal centred lattice, so there is not even a need to summarize them in the resulting table. We do not consider colour alternation in units larger than the unit cell.

### Plane black–white groups

Elements of the plane symmetry groups include translations, forming the translation group, as well as point group operations, i.e. elements of the point group. In doing so, the set of translations forms an invariant subgroup  $T$  of the plane group. Two types of black-white planar groups are distinguished. The groups of the *first kind* are those whose translation subgroup  $T$  does not contain colour-changing translations. The colour change is associated only with operations belonging to the point group. The unit cell of such groups is of the same size as that of the corresponding single-colour group. In plane groups of the *second kind*, the translation group  $T^*$  contains half of the translations combined with colour change; the unit cell is then larger than the corresponding single-colour cell. In these groups there may be cases where the colour change involves only translations, or both translations and point operations.

We will not go into the construction of all black-white plane groups, we will just give some simpler examples to give an indication of how this is done.

Figure C9.5 shows the distribution of the structural motifs (triangles) in the plane group  $p1$  (left part of the figure) and the black-white group derived from it. The group  $p1$  does not contain point symmetry operations, therefore the colour change is only related to translations. After each translation by the basis vector, the colour of the structural motif changes. The grey colour indicates the unit cell of both single-colour and black-white structures. It can be clearly seen that in the black-white structure, the identity period in both directions of the lattice is twice as large as in the single-colour one.



The plane group  $p2$  serves as another example. Its point group  $\{e, 2\}$  contains only two elements, the identity and the  $180^\circ$  rotation, and so does the corresponding black-white point group, the two elements  $\{e, 2^*\}$ . Therefore, there is only one black-white plane group of the first kind. In Figure C9.6, the group  $p2$  and its black-white point group of the first kind are shown side by side. The sizes of their unit cells are the

same. Two black-white groups of the second kind are shown in Figure C9.7. Since these are groups in which the colour change is also associated with translations, their unit cells are larger. In the left part, the colour change is only associated with translation, in the right part, both translation and rotation.

The situation is similar for the plane group  $pm$ , whose point group contains only two elements  $\{e, m\}$ , so there is only one pointwise black-white group  $\{e, m^*\}$ .

For the planar group  $pg$ , a glide line is typical. A glide reflection is an element of symmetry that belongs neither to the point group nor to the translation group, but only to the plane group, because it is a combination of point and translation operations. Having stated this, it will be obvious that the symbol  $\{e, g\}$  that we will use does not represent a point group. It is a representation of a coset in the plane group  $pg$  with respect to the invariant subgroup of translations. The structural motif in the following figures represents two triangles, the first one being identified with the second one after being reflected in the line of the basis vector (vertical in the figure) and shifted by half its length. After this introduction, we can draw four more pictures: a picture of a single-coloured group, one group of the first kind (Fig. C9.8), and two groups of the second kind with a larger unit cell (Fig. C9.9).

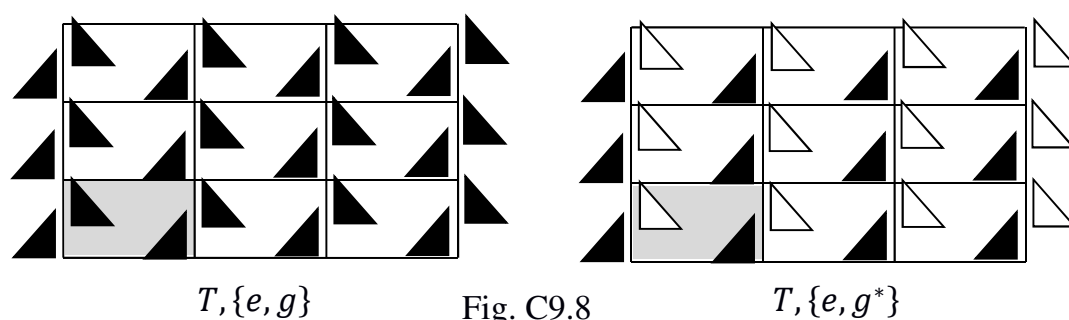


Fig. C9.8

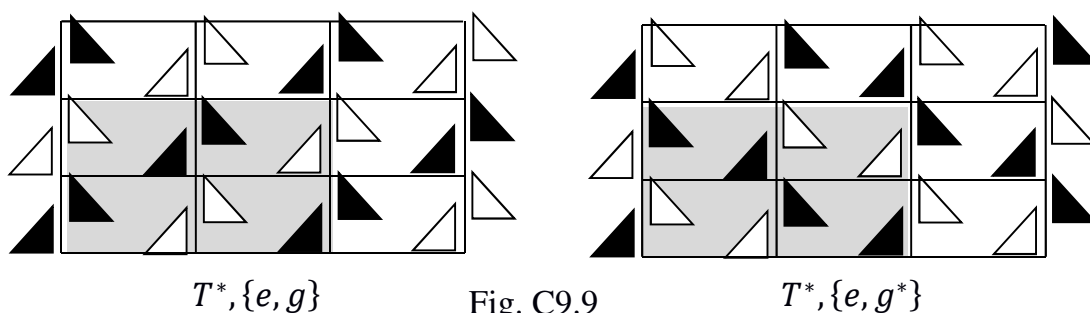
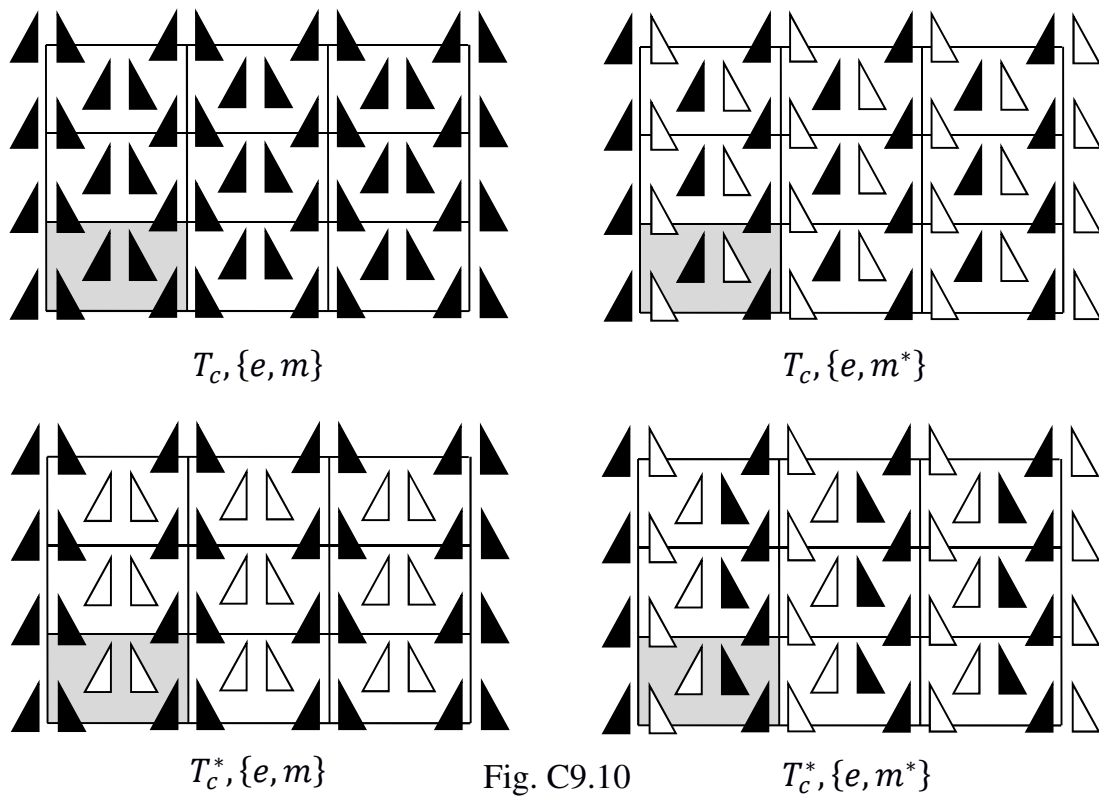


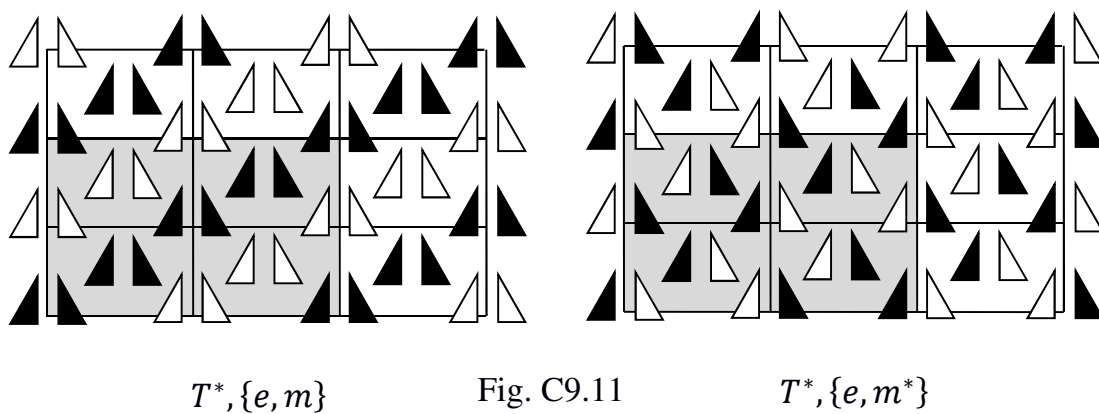
Fig. C9.9

The  $cm$ -group, unlike the previous cases, has a centred lattice, which means that a glide line occurs in it regardless of the symmetry of the structural motif. The corresponding point group also has only two elements  $\{e, m\}$  in this case, but the translation group  $T_c$  also contains translations with half-length basis vectors. As already mentioned in the section on translation black-white groups, when the colour

changes after the translation  $(1/2)(a_1 + a_2)$ , the size of the unit cell does not change when the symmetry is extended to black-white. (Fig. 9.10).



But there is another type of black-white symmetry in plane structures with a centred lattice. when the colour changes after translation by the full length of the basis vector, so that when it is a translation group  $T^*$ . As can be seen from Figure C9.11, the unit cell is four times the size. It can be noticed in the figures that the position of the glide lines, which are a natural part of the centred lattices, is preserved, while in some cases there is a change  $g \rightarrow g^*$ .



The construction of two-colour, i.e., black-white groups (point, translation, and space), is based on the decomposition of the single-colour group into a subgroup with index 2 and the corresponding coset; the anti-symmetry parameter  $s$  then takes two values. All elements of the coset are combined with the anti-symmetry operation, i.e. with the second value of the parameter  $s$ . In the construction of multicolour groups, when the parameter  $s$  can take  $n$  values ( $n$  - "colours"), the decomposition of the single-colour group into an invariant subgroup with index  $n$  and the corresponding  $n - 1$  cosets is used. The elements of the cosets are then successively combined with the operators representing the individual values of the parameter  $s$  and thus other types of symmetry are generated. However, in the case of plane point groups, the set of invariant subgroups with index greater than 2 is not large.

## Appendices

### D1 Multiple operator application

$$\text{Ak } S_1 \cdot S_2 = [\bar{\Phi}_1, t_1] \cdot [\bar{\Phi}_2, t_2] = [\bar{\Phi}_1 \cdot \bar{\Phi}_2, t_1 \cdot \bar{\Phi}_2 + t_2], \text{ tak}$$

$$S \cdot S = [\bar{\Phi}, t] \cdot [\bar{\Phi}, t] = [\bar{\Phi} \cdot \bar{\Phi}, t \cdot \bar{\Phi} + t] = [\bar{\Phi}^2, t \cdot \bar{\Phi} + t],$$

$$\begin{aligned} S \cdot S \cdot S &= [\bar{\Phi}^2, t \cdot \bar{\Phi} + t] \cdot [\bar{\Phi}, t] = [\bar{\Phi}^2 \cdot \bar{\Phi}, (t \cdot \bar{\Phi} + t) \cdot \bar{\Phi} + t] = \\ &= [\bar{\Phi}^3, t \cdot \bar{\Phi}^2 + t \cdot \bar{\Phi} + t] = \\ &= [\bar{\Phi}^3, t \cdot \{\bar{I} + \bar{\Phi} + \bar{\Phi}^2\}] \end{aligned}$$

$$S^n = [\bar{\Phi}^n, t \cdot \{\bar{I} + \bar{\Phi} + \bar{\Phi}^2 + \dots + \bar{\Phi}^{n-1}\}]$$

### D2 Product of operators $S \cdot T_L \cdot S^{-1}$

This product of operators is expressed by (C2.3):

$$S_1 \cdot S_2 = [\bar{\Phi}_1, t_1] \cdot [\bar{\Phi}_2, t_2] = [\bar{\Phi}_1 \cdot \bar{\Phi}_2, t_1 \cdot \bar{\Phi}_2 + t_2] \quad (\text{a})$$

$$\text{Ak } S_1 = S = [\bar{\Phi}, t] \text{ a } S_2 = T_L = [\bar{I}, A_L], \text{ then}$$

$$S \cdot T_L = [\bar{\Phi}, t] \cdot [\bar{I}, A_L] = [\bar{\Phi} \cdot \bar{I}, t \cdot \bar{I} + A_L] = [\bar{\Phi}, t + A_L]. \quad (\text{b})$$

The inverse operation is expressed by writing (C2.6):

$$S^{-1} \equiv [\bar{\Phi}^{-1}, -t \cdot \bar{\Phi}^{-1}]$$

and its product with expression (b) based on (a) gives the result

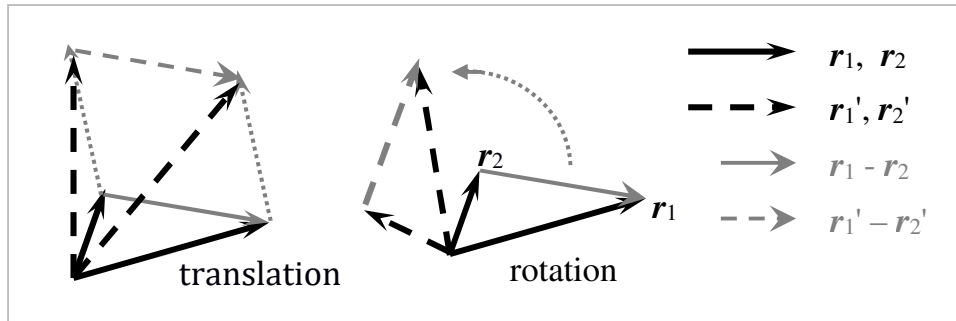
$$\begin{aligned} S \cdot T_L \cdot S^{-1} &= [\bar{\Phi}, t + A_L] \cdot [\bar{\Phi}^{-1}, -t \cdot \bar{\Phi}^{-1}] = \\ &= [\bar{\Phi} \cdot \bar{\Phi}^{-1}, t \cdot \bar{\Phi}^{-1} + A_L \cdot \bar{\Phi}^{-1} - t \cdot \bar{\Phi}^{-1}] = \\ &= [\bar{I}, A_L \cdot \bar{\Phi}^{-1}], \end{aligned} \quad (\text{c})$$

so that the result is an operator representing the translation by the rotated lattice vector.

Applying this combined operator  $S \cdot T_L \cdot S^{-1}$  to the position vectors  $\mathbf{r}_1$  and  $\mathbf{r}_2$  yields the vectors  $\mathbf{r}'_1 = \mathbf{r}_1 + \mathbf{A}_L \cdot \bar{\Phi}^{-1}$ ,  $\mathbf{r}'_2 = \mathbf{r}_2 + \mathbf{A}_L \cdot \bar{\Phi}^{-1}$ . Their difference is equal to the difference of the original vectors, i.e.

$$\mathbf{r}'_2 - \mathbf{r}'_1 = \mathbf{r}_2 - \mathbf{r}_1, \quad (d)$$

which is a confirmation of the fact that the operation  $S \cdot T_L \cdot S^{-1}$  represents a translation. Unlike translation, this result does not hold for rotation, as can be seen in the following figure.



### D3 Transformation tensor

If the transformation tensor has the form  $\bar{\Phi} = \mathbf{a}^1 \mathbf{d}_1 + \mathbf{a}^2 \mathbf{d}_2$ , then the relations apply

$$\mathbf{a}_1 \cdot \bar{\Phi} = \mathbf{a}_1 \cdot (\mathbf{a}^1 \mathbf{d}_1 + \mathbf{a}^2 \mathbf{d}_2) = (\mathbf{a}_1 \cdot \mathbf{a}^1) \mathbf{d}_1 + (\mathbf{a}_1 \cdot \mathbf{a}^2) \mathbf{d}_2 \quad (a)$$

By definition for reciprocal vectors

$$\mathbf{a}_i \cdot \mathbf{a}^j = \delta_{ij}, \text{ resp. } \mathbf{a}^i \cdot \mathbf{a}_j = \delta_{ij},$$

i.e. if  $i = j$ , then  $\delta_{ij} = 1$ , but if  $i \neq j$ , then  $\delta_{ij} = 0$ .

Thus

$$\mathbf{a}_1 \cdot \mathbf{a}^1 = 1, \text{ but } \mathbf{a}_1 \cdot \mathbf{a}^2 = 0,$$

which, when substituted into relation (a), gives the result:

$$\mathbf{a}_1 \cdot \bar{\Phi} = (\mathbf{a}_1 \cdot \mathbf{a}^1) \mathbf{d}_1 + (\mathbf{a}_1 \cdot \mathbf{a}^2) \mathbf{d}_2 = \mathbf{d}_1,$$

which confirms that the tensor transforms the vector  $\mathbf{a}_1$  into the vector  $\mathbf{d}_1$ .

#### D4 Properties of transformation tensor

If the tensor  $\bar{\bar{\Phi}}$  satisfies the conditions (C2.7), i.e.

$$\bar{\bar{\Phi}}_c = \bar{\bar{\Phi}}^{-1}, \text{ resp. } \bar{\bar{\Phi}} = \bar{\bar{\Phi}}_c^{-1},$$

and we know that the definition of the conjugate tensor implies the equality

$$\mathbf{r} \cdot \bar{\bar{\Phi}}_c = \bar{\bar{\Phi}} \cdot \mathbf{r},$$

then we can the equation  $\mathbf{r} \cdot \bar{\bar{\Phi}} = \mathbf{r}$  from relation (C4.4) multiply by the conjugate tensor and make the adjustment

$$\mathbf{r} \cdot \bar{\bar{\Phi}} \cdot \bar{\bar{\Phi}}_c = \mathbf{r} \cdot \bar{\bar{\Phi}}_c \Rightarrow \mathbf{r} \cdot \bar{\bar{\mathbf{I}}} = \mathbf{r} \cdot \bar{\bar{\Phi}}_c \Rightarrow \mathbf{r} = \mathbf{r} \cdot \bar{\bar{\Phi}}_c \Rightarrow \mathbf{r} = \bar{\bar{\Phi}} \cdot \mathbf{r}$$

so

$$\mathbf{r} \cdot \bar{\bar{\Phi}} = \bar{\bar{\Phi}} \cdot \mathbf{r}$$

which means that the tensor, which leaves some points of the space in place during the transformation, is symmetric.

#### D5 Transformation of vector components in reflection

If the tensor mediating the symmetry operation has the form  $\bar{\bar{\Phi}} = \bar{\bar{\mathbf{I}}} - 2\mathbf{u}\mathbf{u}$ , then the scalar product of the vector  $\mathbf{u}$  with this tensor gives the result

$$\mathbf{u} \cdot \bar{\bar{\Phi}} = \mathbf{u} \cdot (\bar{\bar{\mathbf{I}}} - 2\mathbf{u}\mathbf{u}) = \mathbf{u} \cdot \bar{\bar{\mathbf{I}}} - 2(\mathbf{u} \cdot \mathbf{u})\mathbf{u} = \mathbf{u} - 2\mathbf{u} = -\mathbf{u}.$$

If we multiply the tensor  $\bar{\bar{\Phi}}$  by a scalar unit vector  $\mathbf{w}$ , which is perpendicular to the vector  $\mathbf{u}$ , the product with the identity tensor does not change it, and the scalar product  $\mathbf{w} \cdot \mathbf{u} = 0$ . Therefore,  $\mathbf{w} \cdot \bar{\bar{\Phi}} = \mathbf{w}$ .

That is, the vector  $\mathbf{r} = p\mathbf{u} + q\mathbf{w}$  is transformed as follows:

$$\mathbf{r}' = \mathbf{r} \cdot \bar{\bar{\Phi}} = (p\mathbf{u} + q\mathbf{w}) \cdot (\bar{\bar{\mathbf{I}}} - 2\mathbf{u}\mathbf{u}) = (p\mathbf{u} - 2p\mathbf{u}) + q\mathbf{w} = -p\mathbf{u} + q\mathbf{w}$$

so that the component perpendicular to the vector  $\mathbf{u}$  does not change, the component parallel to it changes to the opposite.

## D6 Calculation of scalar coefficients in transformation equations

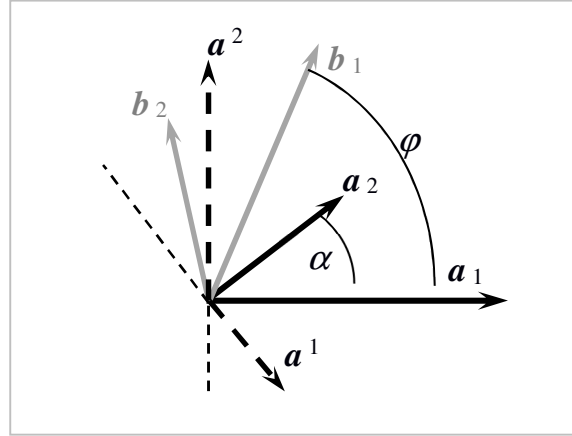
Taking the scalar product of the first of the equations (C4.9) with the vector  $\mathbf{a}^1$ , we get

$$\begin{aligned}\mathbf{b}_1 \cdot \mathbf{a}^1 &= (p\mathbf{a}_1 + q\mathbf{a}_2) \cdot \mathbf{a}^1 = \\ &= p(\mathbf{a}_1 \cdot \mathbf{a}^1) + q(\mathbf{a}_2 \cdot \mathbf{a}^1) = p.\end{aligned}$$

Similarly, we obtain the other scalar coefficients, so that:

$$p = \mathbf{b}_1 \cdot \mathbf{a}^1, \quad q = \mathbf{b}_1 \cdot \mathbf{a}^2, \quad r = \mathbf{b}_2 \cdot \mathbf{a}^1,$$

$$s = \mathbf{b}_2 \cdot \mathbf{a}^2.$$



In further modifications of these formulas, we use the relations between the magnitudes of the vectors:  $b_1 = a_1$ ,  $b_2 = a_2$ , because the vectors  $\mathbf{b}$  are just the rotated vectors of  $\mathbf{a}$ . From the definition of reciprocal vectors, the relations between the magnitudes of the direct and reciprocal vectors hold (see also the figure):

$$(\mathbf{a}_1 \cdot \mathbf{a}^1) = a_1 a^1 \cos\left(\frac{\pi}{2} - \alpha\right) = 1, \quad \Rightarrow \quad a^1 = 1/(a_1 \sin \alpha)$$

$$(\mathbf{a}_2 \cdot \mathbf{a}^2) = a_2 a^2 \cos\left(\frac{\pi}{2} - \alpha\right) = 1, \quad \Rightarrow \quad a^2 = 1/(a_2 \sin \alpha)$$

For the scalar  $p$ , after adding the results, we get

$$p = \mathbf{b}_1 \cdot \mathbf{a}^1 = b_1 a^1 \cos\left(\frac{\pi}{2} + \varphi - \alpha\right) = a_1 \frac{1}{a_1 \sin \alpha} \sin(\alpha - \varphi) = \frac{\sin(\alpha - \varphi)}{\sin \alpha}.$$

Similarly, we obtain relations for the other coefficients:

$$q = \frac{a_1 \sin \varphi}{a_2 \sin \alpha}, \quad r = -\frac{a_2 \sin \varphi}{a_1 \sin \alpha}, \quad s = \frac{\sin(\alpha + \varphi)}{\sin \alpha}.$$

## D7 Vector coordinates of the tensor

We multiply the equality  $(\mathbf{A}^1 - \mathbf{a}^1) \mathbf{a}_1 + (\mathbf{A}^2 - \mathbf{a}^2) \mathbf{a}_2 = -2\mathbf{u}\mathbf{u}$  scalarly from the right-hand side by the vector  $\mathbf{a}^1$ :

$$(\mathbf{A}^1 - \mathbf{a}^1)(\mathbf{a}_1 \cdot \mathbf{a}^1) + (\mathbf{A}^2 - \mathbf{a}^2)(\mathbf{a}_2 \cdot \mathbf{a}^1) = -2\mathbf{u}(\mathbf{u} \cdot \mathbf{a}^1)$$

By the definition of reciprocal vectors ( $\mathbf{a}_1 \cdot \mathbf{a}^1 = 1$  and  $(\mathbf{a}_2 \cdot \mathbf{a}^1) = 0$ , leaving only the difference of the vectors  $(\mathbf{A}^1 - \mathbf{a}^1)$  on the left-hand side. On the right side, the result of the scalar product in parentheses is the scalar, so on the right side is the scalar multiple of the vector  $\mathbf{u}$ . This means that the vectors  $\mathbf{u}$  and  $(\mathbf{A}^1 - \mathbf{a}^1)$  are parallel. By analogy, it can be shown that the vectors  $(\mathbf{A}^2 - \mathbf{a}^2)$ ,  $(\mathbf{A}_1 - \mathbf{a}_1)$ ,  $(\mathbf{A}_2 - \mathbf{a}_2)$ , are parallel to the unit vector  $\mathbf{u}$ .

## D8 Reciprocal vectors of orthogonal basis

For a pair of basis vectors  $\mathbf{b}_1$ ,  $\mathbf{b}_2$  and their reciprocal pair  $\mathbf{b}^1$ ,  $\mathbf{b}^2$  the next relations are valid:

$$\mathbf{b}_1 \cdot \mathbf{b}^1 = 1 \quad (\text{a}) \quad \mathbf{b}_1 \cdot \mathbf{b}^2 = 0 \quad (\text{b})$$

$$\mathbf{b}_2 \cdot \mathbf{b}^1 = 0 \quad (\text{c}) \quad \mathbf{b}_2 \cdot \mathbf{b}^2 = 1 \quad (\text{d})$$

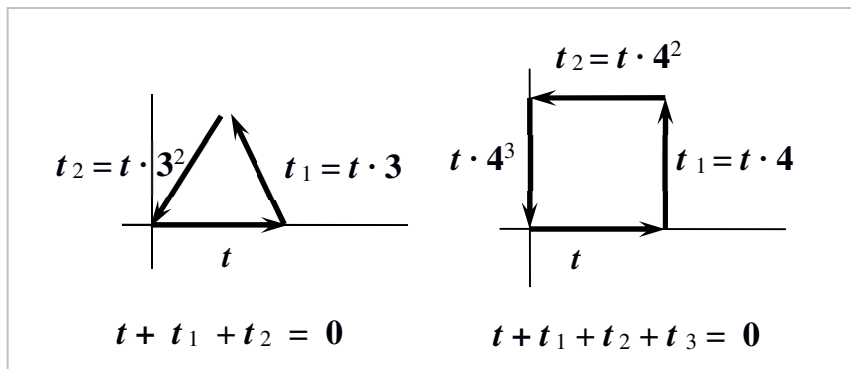
If, by coincidence, the vectors  $\mathbf{b}_1$  and  $\mathbf{b}^1$  are parallel, one of them can be expressed as a scalar multiple of the other, e.g.,  $\mathbf{b}^1 = s \mathbf{b}_1$ , and substituted into relation (c):

$$\mathbf{b}_2 \cdot s \mathbf{b}_1 = 0,$$

which implies that the vectors  $\mathbf{b}_1$  and  $\mathbf{b}_2$  are perpendicular to each other and form an orthogonal basis. Then the reciprocal lattice is also orthogonal, i.e. the vectors  $\mathbf{b}^1$  and  $\mathbf{b}^2$  are perpendicular to each other.

## D9 Property of the characteristic tensor

Applying the characteristic tensor  $\mathbf{t} \cdot \{\bar{\mathbf{I}} + \bar{\Phi} + \bar{\Phi}^2 + \dots + \bar{\Phi}^{m-1}\}$  to any translation  $\mathbf{t}$  prescribes summation of the vectors  $\mathbf{t} = \mathbf{t} \cdot \bar{\mathbf{I}}$ ,  $\mathbf{t}_1 = \mathbf{t} \cdot \bar{\Phi}$ ,  $\mathbf{t}_2 = \mathbf{t} \cdot \bar{\Phi}^2$ , etc. The first is the vector  $\mathbf{t}$  itself, the second is rotated by the first application of the tensor  $\bar{\Phi}$ , the third by two applications, etc. The following figure shows two cases - when we substitute tensors  $\bar{\mathbf{3}}$  and  $\bar{\mathbf{4}}$  in place of  $\bar{\Phi}$ .



If we substitute the tensor  $\bar{\bar{2}} = -\bar{\bar{1}}$  ( $\rightarrow$  tab. TB2), for which the number  $m = 2$ , in place the tensor  $\bar{\bar{\Phi}}$ , the sum of the terms that make up the characteristic tensor gives the result:  $\{\bar{\bar{1}} + \bar{\bar{2}}\} = \{\bar{\bar{1}} - \bar{\bar{1}}\} = 0$ .

## D10 Determinants of tensors – proper and improper operation

Determinant of tensor  $\bar{\bar{4}}$  ( $\rightarrow$  tab. TC2)

$$\bar{\bar{4}} = -\mathbf{a}^1 \mathbf{a}_1 \frac{\cos \alpha}{\sin \alpha} + \mathbf{a}^1 \mathbf{a}_2 \frac{a_1}{a_2} \frac{1}{\sin \alpha} - \mathbf{a}^2 \mathbf{a}_1 \frac{a_2}{a_1} \frac{1}{\sin \alpha} + \mathbf{a}^2 \mathbf{a}_2 \frac{\cos \alpha}{\sin \alpha}$$

is calculated using its coordinates:

$$\begin{vmatrix} -\frac{\cos \alpha}{\sin \alpha} & \frac{a_1}{a_2} \frac{1}{\sin \alpha} \\ -\frac{a_2}{a_1} \frac{1}{\sin \alpha} & \frac{\cos \alpha}{\sin \alpha} \end{vmatrix} = -\frac{\cos^2 \alpha}{\sin^2 \alpha} + \frac{1}{\sin^2 \alpha} = \frac{1 - \cos^2 \alpha}{\sin^2 \alpha} = +1.$$

The determinant of the tensor of reflection  $\bar{\bar{\mathbf{M}}} = \bar{\bar{\mathbf{I}}} - 2\mathbf{u}\mathbf{u}$  can be expressed only after its modification. Reflection occurs only in orthogonal lattices ( $\rightarrow$  article B4.1.2) in which the basis vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are perpendicular to each other. According to Appendix D14, the tensor of reflection in a line identical to the vector  $\mathbf{a}_1$  then takes the form:

$$\bar{\bar{\mathbf{M}}}_1 = \bar{\bar{\mathbf{I}}} - 2\mathbf{a}^2 \mathbf{a}_2 = \mathbf{a}_1 \mathbf{a}^1 - \mathbf{a}_2 \mathbf{a}^2$$

Therefore, the determinant of the tensor  $\bar{\bar{\mathbf{M}}}$  is equal to

$$|\bar{\bar{\mathbf{M}}}| = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} = -1.$$

## D11 Use of generating elements of the group

For groups with one generating element, all its elements can be expressed as "powers" of this element. Such groups are cyclic groups, e.g. group  $\mathbf{4}$ , which has four elements:  $\mathbf{4} \equiv \{e, 4, 4^2, 4^3\}$ , between which the relations hold:

$$4 \cdot 4 = 4^2, \quad 4 \cdot 4 \cdot 4 = 4^3, \quad 4 \cdot 4 \cdot 4 \cdot 4 = e,$$

so that all elements can be expressed as powers of element 4. The elements of the group can be represented by tensor operators between which the same relations hold.

As the simplest example of a group with two generating elements, consider the group **2mm**, which has four elements:  $\mathbf{2mm} \equiv \{e, 2, m_x, m_y\}$ , which will be represented by tensor operators. The group belongs to an rectangular system in which we choose the basis vectors such that the vector  $\mathbf{a}_1$  is parallel to the x-axis and the vector  $\mathbf{a}_2$  is parallel to the y-axis. Between the basis vectors  $\mathbf{a}_1, \mathbf{a}_2$  and the reciprocal vectors  $\mathbf{a}^1, \mathbf{a}^2$  the relations

$$\mathbf{a}^1 \cdot \mathbf{a}_2 = 0, \quad \mathbf{a}^2 \cdot \mathbf{a}_1 = 0, \quad \mathbf{a}^1 \cdot \mathbf{a}_1 = 1, \quad \mathbf{a}^2 \cdot \mathbf{a}_2 = 1.$$

The tensors representing the elements of the **2mm** group have the shape (→ Table TC2b, → Appendix D14):

|                      |                                                                                                         |
|----------------------|---------------------------------------------------------------------------------------------------------|
| identical operation  | $\bar{\mathbf{I}} = \mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2,$                             |
| rotation             | $\bar{\mathbf{2}} \equiv -\bar{\mathbf{I}} = -(\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2),$ |
| reflection in line x | $\bar{\mathbf{M}}_x \equiv \bar{\mathbf{M}}_1 = \mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2,$ |
| reflection in line y | $\bar{\mathbf{M}}_y \equiv \bar{\mathbf{M}}_2 = \mathbf{a}^2 \mathbf{a}_2 - \mathbf{a}^1 \mathbf{a}_1.$ |

The generating elements can be either 2 and  $m_x$ , or 2 and  $m_y$ . We choose the first option and compute products between tensors representing these elements:

$$\bar{\mathbf{2}} \cdot \bar{\mathbf{2}} = (-\bar{\mathbf{I}}) \cdot (-\bar{\mathbf{I}}) = \bar{\mathbf{I}}$$

resulting in an identity tensor representing the neutral element of the group.

$$\begin{aligned} \bar{\mathbf{M}}_x \cdot \bar{\mathbf{M}}_x &= (\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2) \cdot (\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2) = \\ &= \mathbf{a}^1 (\mathbf{a}_1 \cdot \mathbf{a}^1) \mathbf{a}_1 - \mathbf{a}^1 (\mathbf{a}_1 \cdot \mathbf{a}^2) \mathbf{a}_2 - \mathbf{a}^2 (\mathbf{a}_2 \cdot \mathbf{a}^1) \mathbf{a}_1 + \mathbf{a}^2 (\mathbf{a}_2 \cdot \mathbf{a}^2) \mathbf{a}_2 = \\ &= \mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2 = \bar{\mathbf{I}}. \end{aligned}$$

The result is again the neutral element of the group.

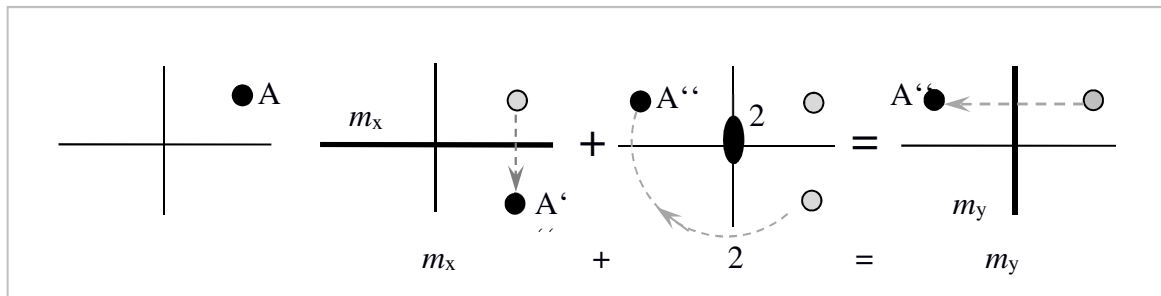
$$\begin{aligned} \bar{\mathbf{M}}_x \cdot \bar{\mathbf{2}} &= (\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2) \cdot [-(\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2)] = \\ &= -[\mathbf{a}^1 (\mathbf{a}_1 \cdot \mathbf{a}^1) \mathbf{a}_1 + \mathbf{a}^1 (\mathbf{a}_1 \cdot \mathbf{a}^2) \mathbf{a}_2 - \mathbf{a}^2 (\mathbf{a}_2 \cdot \mathbf{a}^1) \mathbf{a}_1 - \mathbf{a}^2 (\mathbf{a}_2 \cdot \mathbf{a}^2) \mathbf{a}_2] = \\ &= -(\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2) = -\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2 = \bar{\mathbf{M}}_y. \end{aligned}$$

The product  $\bar{\mathbf{M}}_x \cdot \bar{\mathbf{2}}$  results in the operator  $\bar{\mathbf{M}}_y$  representing the reflection in the line y. The product in reverse order will give the same result:  $\bar{\mathbf{2}} \cdot \bar{\mathbf{M}}_x = \bar{\mathbf{M}}_y$ .

This exhausted all products between the generating elements of the group, and thus obtained all elements of the group, represented by the operators  $\bar{I}, \bar{2}, \bar{M}_x$  and  $\bar{M}_y$ . The result is consistent with the multiplication table ( $\rightarrow$  TC5).  $\bar{M}_y$  can also be used as the generating element, where.  $\bar{M}_y \cdot \bar{2} = \bar{M}_x$ ; also in this case, swapping the order of the operators will give the same result.

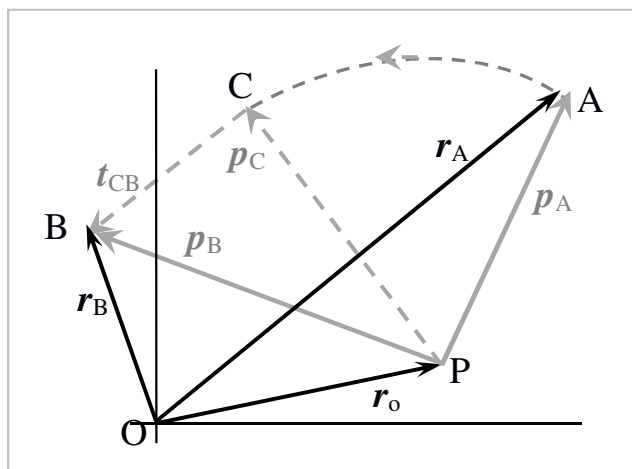
## D12 Graphical representation of the application of two symmetry operations

By reflecting point A in the x-axis, we get point A'. Rotating around the point O by 180°, point A' is transformed into point A''. This was a combination of two operations. We get the same result by applying a single operation - reflection in the y-axis.



Also from the figure it can be seen that reflection and 180° rotation commute.

## D13 Effect of reference frame displacement on the symmetry operator



Let the rotation of the lattice point A about the point P to the point C be represented by the tensor  $\bar{\Phi}$  ( $\rightarrow$  figure). In general, point C need not be a lattice point, so an additional translation, which we denote by  $t_{CB}$ , is required to transform it to lattice point B. The additional translation ensures that the entire transformation is a symmetry operation. Starting from the

labels in the figure, the next relationships apply

$$\mathbf{p}_C = \mathbf{p}_A \cdot \bar{\bar{\Phi}} \quad \mathbf{p}_B = \mathbf{p}_A \cdot \bar{\bar{\Phi}} + \mathbf{t}_{CB} . \quad (a)$$

In general, the size of the translation  $\mathbf{t}_{CB}$  need not exceed the dimensions of the unit cell, but the entire transformation remains a symmetry operation if an arbitrary lattice vector  $\mathbf{A}_L$  is added to it. Therefore, we write the translation of  $\mathbf{t}_{CB}$  as the sum of the lattice translation of  $\mathbf{A}_L$  and the non-lattice translation of  $\mathbf{t}$  :

$$\mathbf{t}_{CB} = \mathbf{A}_L + \mathbf{t} .$$

The second of the relations (a) then takes the form

$$\mathbf{p}_B = \mathbf{p}_A \cdot \bar{\bar{\Phi}} + \mathbf{A}_L + \mathbf{t} . \quad (b)$$

We express this operation with respect to the reference point O, using transformation relations (according to the figure)

$$\mathbf{p}_A = \mathbf{r}_A - \mathbf{r}_o \quad (c)$$

$$\mathbf{p}_B = \mathbf{r}_B - \mathbf{r}_o , \quad (d)$$

in which  $\mathbf{r}_o$  is the position vector of point P with respect to the new reference point O. Substituting transformations (c) and (d) into relation (b), we get

$$\mathbf{r}_B - \mathbf{r}_o = (\mathbf{r}_A - \mathbf{r}_o) \cdot \bar{\bar{\Phi}} + \mathbf{A}_L + \mathbf{t}$$

and after modification

$$\mathbf{r}_B = \mathbf{r}_o + \mathbf{r}_A \cdot \bar{\bar{\Phi}} - \mathbf{r}_o \cdot \bar{\bar{\Phi}} + \mathbf{A}_L + \mathbf{t} ,$$

or

$$\mathbf{r}_B = \mathbf{r}_A \cdot [\bar{\bar{\Phi}} , \mathbf{r}_o \cdot (\bar{\mathbf{I}} - \bar{\bar{\Phi}}) + \mathbf{A}_L + \mathbf{t}] .$$

The result shows that by changing the reference point, the shape of the operator changes. With respect to the point P, the operator has the form  $[\bar{\bar{\Phi}}, \mathbf{t}]$ , but with respect to the point O for the same operation, it has the form

$$S_O = [\bar{\bar{\Phi}}, \mathbf{r}_o \cdot (\bar{\mathbf{I}} - \bar{\bar{\Phi}}) + \mathbf{A}_L + \mathbf{t}] . \quad (f)$$

From relations (e) and (f), it follows that by changing the position of the origin of the reference frame, it is possible to make the translational part of the operator S zero, either the whole or just its non-lattice translation  $\mathbf{t}$ . The whole translational part will be zero if the vector  $\mathbf{r}_o$  is chosen so that the condition

$$\mathbf{r}_o \cdot (\bar{\mathbf{I}} - \bar{\bar{\Phi}}) + \mathbf{A}_L + \mathbf{t} = \mathbf{0} . \quad (g)$$

If we want only the non-lattice part  $\mathbf{t}$  of the translation to be zero, we need to shift the origin of the reference frame by the vector  $\mathbf{r}_0$ , which must satisfy the condition

$$\mathbf{r}_0 \cdot (\bar{\mathbf{I}} - \bar{\Phi}) = \mathbf{A}_L.$$

**Note:** The  $+\mathbf{A}_L$  and  $-\mathbf{A}_L$  vectors are equivalent in this respect because the integer coordinates of the  $\mathbf{A}_L$  vector can be both positive and negative numbers.

That is, if we want the symmetry operator expressed in terms of the new position to have the form  $S \equiv [\bar{\Phi}, \mathbf{A}_L]$ , then the position vector  $\mathbf{r}_0$  must satisfy the modified condition (g) and we can express the operator in the form:

$$S \equiv [\bar{\Phi}, \mathbf{r}_0 \cdot (\bar{\mathbf{I}} - \bar{\Phi})]. \quad (\text{h})$$

## D14 Tensor of reflection

### A) The form of tensor

According to relation (C4.8), the tensor representing reflection in a straight line has the form

$$\bar{\mathbf{M}} = \bar{\mathbf{I}} - 2\mathbf{u}\mathbf{u},$$

where  $\mathbf{u}$  is the unit vector perpendicular to the reflection line. In an rectangular system, where the basis vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are perpendicular to each other, the magnitudes of the basis and reciprocal vectors are reciprocal (inverted). If the vector  $\mathbf{a}_1$  lies in the reflection line, the vectors  $\mathbf{a}_2$  and  $\mathbf{a}^2$  are perpendicular to it, they can be expressed as scalar multiples of the vector  $\mathbf{u}$  :  $\mathbf{a}_2 = a_2\mathbf{u}$  ,  $\mathbf{a}^2 = (1/a_2)\mathbf{u}$ , so the dyad  $\mathbf{u}\mathbf{u}$  can also be written in the form  $\mathbf{a}^2\mathbf{a}_2$  because:

$$\mathbf{a}^2\mathbf{a}_2 = (1/a_2)\mathbf{u}a_2\mathbf{u} = \mathbf{u}\mathbf{u}.$$

Therefore, the tensor  $\bar{\mathbf{M}}$  in this case can be expressed in the form

$$\bar{\mathbf{M}}_1 = \bar{\mathbf{I}} - 2\mathbf{a}^2\mathbf{a}_2,$$

where the index 1 denotes the fact that the reflection line has the direction of the vector  $\mathbf{a}_1$ . If the reflection is in a line parallel to the vector  $\mathbf{a}_2$ , the tensor has the form

$$\bar{\mathbf{M}}_2 = \bar{\mathbf{I}} - 2\mathbf{a}^1\mathbf{a}_1.$$

The tensors of reflection in the hexagonal system have a different shape because the basis vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are not perpendicular to each other; they are given in

Appendix D25. However, in this system it is also possible to choose an orthogonal unit cell that is centred, with the basis vectors  $\mathbf{b}_1$  and  $\mathbf{b}_2$  perpendicular to each other ( $\rightarrow$  Section C6.2), so that the tensors then have the shape ( $\rightarrow$  Appendix D26):

$$\bar{\bar{\mathbf{M}}}_1 = \bar{\bar{\mathbf{I}}} - 2\mathbf{b}^2\mathbf{b}_2, \quad \bar{\bar{\mathbf{M}}}_2 = \bar{\bar{\mathbf{I}}} - 2\mathbf{b}^1\mathbf{b}_1.$$

## B) Effect of reference frame origin displacement on the tensor shape

According to C7.4, the operator of reflection in a line parallel to the vector  $\mathbf{a}_1$  and shifted in the direction of the vector  $\mathbf{a}_2$  to a position with coordinate  $r_2 = 1/2$ , has the form (relation C7.7):

$$[\bar{\bar{\mathbf{I}}} - 2\mathbf{a}^2\mathbf{a}_2, \mathbf{a}_2].$$

This tensor transforms, e.g., a lattice point with position vector  $\mathbf{r} = \mathbf{a}_1 + \mathbf{a}_2$  into a lattice point with position vector  $\mathbf{a}_1$ , which can be verified by the following calculation:

$$\begin{aligned} (\mathbf{a}_1 + \mathbf{a}_2) \cdot [\bar{\bar{\mathbf{I}}} - 2\mathbf{a}^2\mathbf{a}_2, \mathbf{a}_2] &= (\mathbf{a}_1 + \mathbf{a}_2) \cdot \bar{\bar{\mathbf{I}}} - (\mathbf{a}_1 + \mathbf{a}_2) \cdot 2\mathbf{a}^2\mathbf{a}_2 + \mathbf{a}_2 = \\ &= \mathbf{a}_1 + \mathbf{a}_2 - 2\mathbf{a}_1 \cdot \mathbf{a}^2\mathbf{a}_2 - 2\mathbf{a}_2 \cdot \mathbf{a}^2\mathbf{a}_2 + \mathbf{a}_2 = \mathbf{a}_1 + \mathbf{a}_2 - \mathbf{0} - 2\mathbf{a}_2 + \mathbf{a}_2 = \mathbf{a}_1. \end{aligned}$$

Thus, it can be verified that this operator transforms a lattice point with position vector  $\mathbf{r} = \mathbf{0}$  into a lattice point with position vector  $\mathbf{a}_2$  and a point with position vector  $\mathbf{a}_2$  into a lattice point with position vector  $\mathbf{r} = \mathbf{0}$ .

## D15 Product of operators $[\bar{\bar{\mathbf{2}}}, \mathbf{0}] \cdot [\bar{\bar{\mathbf{M}}}, \mathbf{t}] \cdot [\bar{\bar{\mathbf{2}}}, \mathbf{0}]$

For the product of operators, the general relation (C2.3) holds:

$$S_1 \cdot S_2 = [\bar{\bar{\Phi}}_1, \mathbf{t}_1] \cdot [\bar{\bar{\Phi}}_2, \mathbf{t}_2] = [\bar{\bar{\Phi}}_1 \cdot \bar{\bar{\Phi}}_2, \mathbf{t}_1 \cdot \bar{\bar{\Phi}}_2 + \mathbf{t}_2].$$

In this particular case, it is the product of the three operators  $[\bar{\bar{\mathbf{2}}}, \mathbf{0}] \cdot [\bar{\bar{\mathbf{M}}}, \mathbf{t}] \cdot [\bar{\bar{\mathbf{2}}}, \mathbf{0}]$ , which is to be equal to the operator

$$[\bar{\bar{\mathbf{M}}}, \mathbf{t} + \mathbf{A}_L]. \quad (\text{a})$$

In a structure with  $2mm$  point symmetry, there are two orthogonal sets of reflection lines, so there are two operators of reflection  $\bar{\bar{\mathbf{M}}}_x$  and  $\bar{\bar{\mathbf{M}}}_y$ . We will successively compute the product  $[\bar{\bar{\mathbf{2}}}, \mathbf{0}] \cdot [\bar{\bar{\mathbf{M}}}_x, \mathbf{t}] \cdot [\bar{\bar{\mathbf{2}}}, \mathbf{0}]$ , using the multiplication table TC5 of the  $2mm$  group:

$$[\bar{\bar{\mathbf{2}}}, \mathbf{0}] \cdot [\bar{\bar{\mathbf{M}}}_x, \mathbf{t}] = [2 \cdot \bar{\bar{\mathbf{M}}}_x, \mathbf{t}] = [\bar{\bar{\mathbf{M}}}_y, \mathbf{t}]$$

$$[\bar{\bar{\mathbf{M}}}_y, \mathbf{t}] \cdot [\bar{\bar{\mathbf{2}}}, \mathbf{0}] = [\bar{\bar{\mathbf{M}}}_y \cdot \bar{\bar{\mathbf{2}}}, \mathbf{t} \cdot \bar{\bar{\mathbf{2}}} + \mathbf{0}] = [\bar{\bar{\mathbf{M}}}_x, -\mathbf{t}], \quad (\text{b})$$

because the operator  $\mathbf{2}$  rotates each vector in the plane by  $180^\circ$ , so that the vector  $\mathbf{t}$  transforms to the vector  $-\mathbf{t}$ . According to relation (a), this result should be equal to:

$$[\bar{\bar{\mathbf{M}}}_x, -\mathbf{t}] = [\bar{\bar{\mathbf{M}}}_x, \mathbf{t} + \mathbf{A}_L].$$

That is, it must hold  $-\mathbf{t} = \mathbf{t} + \mathbf{A}_L \Rightarrow 2\mathbf{t} = -\mathbf{A}_L = \mathbf{A}'_L$ , resp.

$$2t_1\mathbf{a}_1 + 2t_2\mathbf{a}_2 = L_1\mathbf{a}_1 + L_2\mathbf{a}_2.$$

Based on this result, the coordinates  $t_1$  and  $t_2$  can only take discrete values  $t_1 = 0, 1/2, 1, 3/2, \dots$ ,  $t_2 = 0, 1/2, 1, 3/2, \dots$ , of which only the first two are actual within the unit cell.

In the case when  $\mathbf{t} = 0$ , relations (b) imply:

$$[\bar{\mathbf{2}}, 0] \cdot [\bar{\bar{\mathbf{M}}}_x, 0] \cdot [\bar{\mathbf{2}}, 0] = [\bar{\bar{\mathbf{M}}}_x, 0] \quad (c)$$

#### D16 Product of operators $[\bar{\mathbf{4}}, 0] \cdot [\bar{\bar{\mathbf{M}}}, \mathbf{t}] \cdot [\bar{\mathbf{4}}, 0]$

The translational part of the operator has to fulfil the condition

$$[\bar{\mathbf{4}}, 0] \cdot [\bar{\bar{\mathbf{M}}}, t_1\mathbf{a}_1 + t_2\mathbf{a}_2] \cdot [\bar{\mathbf{4}}, 0] = [\bar{\bar{\mathbf{M}}}, t_1\mathbf{a}_1 + t_2\mathbf{a}_2 + \mathbf{A}_L], \quad (a)$$

where  $\mathbf{A}_L = L_1\mathbf{a}_1 + L_2\mathbf{a}_2$ , and  $L_i$  are integers.

We carry out the products of the operators successively, starting from the formula for the product of the operators

$$S_1 \cdot S_2 = [\bar{\bar{\Phi}}_1, \mathbf{t}_1] \cdot [\bar{\bar{\Phi}}_2, \mathbf{t}_2] = [\bar{\bar{\Phi}}_1 \cdot \bar{\bar{\Phi}}_2, \mathbf{t}_1 \cdot \bar{\bar{\Phi}}_2 + \mathbf{t}_2].$$

$$[\bar{\mathbf{4}}, 0] \cdot [\bar{\bar{\mathbf{M}}}_x, t_1\mathbf{a}_1 + t_2\mathbf{a}_2] = [\bar{\mathbf{4}} \cdot \bar{\bar{\mathbf{M}}}_x, t_1\mathbf{a}_1 + t_2\mathbf{a}_2] = [\bar{\bar{\mathbf{M}}}_{yx}, t_1\mathbf{a}_1 + t_2\mathbf{a}_2], \quad (b)$$

because the combination of a  $90^\circ$  rotation with reflection in the x-axis is identical to reflection in the yx "diagonal" ( $\rightarrow$  multiplication table in the spreadsheet section). The next  $90^\circ$  rotation that follows moves the transformed point to the position as if it had been transformed by the  $\bar{\bar{\mathbf{M}}}_x$  operation alone:

$$\begin{aligned} [\bar{\bar{\mathbf{M}}}_{yx}, t_1\mathbf{a}_1 + t_2\mathbf{a}_2] \cdot [\bar{\mathbf{4}}, 0] &= [\bar{\bar{\mathbf{M}}}_{yx} \cdot \bar{\mathbf{4}}, (t_1\mathbf{a}_1 + t_2\mathbf{a}_2) \cdot \bar{\mathbf{4}}] = \\ &= [\bar{\bar{\mathbf{M}}}_x, -t_2\mathbf{a}_1 + t_1\mathbf{a}_2] \end{aligned} \quad (c)$$

Rotating the vector  $t_1 \mathbf{a}_1 + t_2 \mathbf{a}_2$  by  $90^\circ$  will cause the magnitude of the coordinates to change and the sign of one of them to change. The result of (c) is to be equal to the right hand side of relation (a), so equality is to be satisfied:

$$-t_2 \mathbf{a}_1 + t_1 \mathbf{a}_2 = t_1 \mathbf{a}_1 + t_2 \mathbf{a}_2 + \mathbf{A}_L \Rightarrow -(t_1 + t_2) = L_1, (t_1 - t_2) = L_2$$

Due to the translational symmetry, it is sufficient to restrict to  $L_i = 0, 1$  and not to consider negative values. Then the following alternatives arise:

| $L_1$ | $L_2$ | $t_1$ | $t_2$ |
|-------|-------|-------|-------|
| 0     | 0     | 0     | 0     |
| 0     | 1     | 1/2   | 1/2   |
| 1     | 0     | 1/2   | 1/2   |
| 1     | 1     | 1     | 0     |

The last alternative is not interesting because it represents a lattice translation.

In the case when  $\mathbf{t} = \mathbf{0}$  equality follows from relations (b) and (c):

$$[\bar{4}, 0] \cdot [\bar{M}, 0] \cdot [\bar{4}, 0] = [\bar{M}, 0] \quad (d)$$

### D17 Product of operators $[\bar{6}, 0] \cdot [\bar{M}_0, t] \cdot [\bar{6}, 0]$

We will modify the expression incrementally, using the **6mm** group multiplication table ( $\rightarrow$  spreadsheet):

$$[\bar{6}, 0] \cdot [\bar{M}_0, t] = [\bar{6} \cdot \bar{M}_0, t] = [\bar{M}_{150}, t], \quad (a)$$

$$[\bar{M}_{150}, t] \cdot [\bar{6}, 0] = [\bar{M}_{150} \cdot \bar{6}, t \cdot \bar{6} + 0] = [\bar{M}_0, t \cdot \bar{6}] \quad (b)$$

We still need to compute the transformation of the vector  $\mathbf{t}$  by the operator  $\bar{6}$ , and it is convenient to write it in the component form  $\mathbf{t} = t_1 \mathbf{a}_1 + t_2 \mathbf{a}_2$ :

$$\begin{aligned} \mathbf{t} \cdot \bar{6} &= (t_1 \mathbf{a}_1 + t_2 \mathbf{a}_2) \cdot (\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1) = \\ &= t_1 \mathbf{a}_1 + t_1 \mathbf{a}_2 - t_2 \mathbf{a}_1. \end{aligned}$$

Based on condition (C8.6), this result should equal the sum ( $L_1$  and  $L_2$  are integers)

$$t_1 \mathbf{a}_1 + t_2 \mathbf{a}_2 + L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2$$

i.e. has to pay:

$$t_1 \mathbf{a}_1 + t_1 \mathbf{a}_2 - t_2 \mathbf{a}_1 = t_1 \mathbf{a}_1 + t_2 \mathbf{a}_2 + L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2 ,$$

and after modification

$$-t_2 \mathbf{a}_1 + (t_1 - t_2) \mathbf{a}_2 = L_1 \mathbf{a}_1 + L_2 \mathbf{a}_2 \implies t_2 = L_1, \quad t_1 - t_2 = L_2 .$$

By choosing different combinations of  $L_1$  and  $L_2$  values, we get the possible values of  $t_i$ . When  $L_1 = L_2 = 0$ ,  $t_1 = t_2 = 0$  results. If  $L_1 = 1$ ,  $L_2 = 0$ ,  $t_1 = t_2 = 1$ , i.e. already outside the interval  $0 \leq t_i < 1$ , and similarly for other choices of  $L_i$ . This means that only the vector  $\mathbf{t} = \mathbf{0}$  is relevant within the unit cell, and integer linear combinations of basis vectors are relevant outside it.

In the case that  $\mathbf{t}$  is equal to zero, the equality follows from relations (a) and (b)

$$[\bar{6}, 0] \cdot [\bar{M}, 0] \cdot [\bar{6}, 0] = [\bar{M}, 0] . \quad (c)$$

## D18 Glide reflection in primitive lattice

In the case of the primitive translation group  $\{T_p\}$ , the glide reflection shown in Table TC3 may also occur, which in this case is not due to lattice centration, but is related to the shape of the structural motif ( $\rightarrow$  Fig. A7). If the glide reflection is in a line identical to the basis vector  $\mathbf{a}_1$ , the corresponding operator has the form  $[\bar{M}_1, \mathbf{a}_1/2] \equiv [\bar{I} - 2\mathbf{a}_1^2 \mathbf{a}_2, \mathbf{a}_1/2]$  ( $\rightarrow$  relation C4.22). The double application of glide reflection is then expressed by the operator:

$$[\bar{M}_1, \mathbf{a}_1/2] \cdot [\bar{M}_1, \mathbf{a}_1/2] = [\bar{I}, \mathbf{a}_1] ,$$

triple application:

$$[\bar{I}, \mathbf{a}_1] \cdot [\bar{M}_1, \mathbf{a}_1/2] = [\bar{M}_1, \mathbf{a}_1 + \mathbf{a}_1/2] ,$$

quadruple application:

$$[\bar{M}_1, \mathbf{a}_1 + \mathbf{a}_1/2] \cdot [\bar{M}_1, \mathbf{a}_1/2] = [\bar{I}, 2\mathbf{a}_1] .$$

It follows from relation (C4.21) that in the glide reflection operator, the translation part  $\mathbf{a}_1/2$  can also have a negative sign. Multiple applications of the operator  $[\bar{M}_1, -\mathbf{a}_1/2]$  then lead to another set of operators that differ from the previous ones only by the signs of the translational part. An infinite number of repetitions of such glide reflections yields a set of operations that form a group. In doing so, the neutral element of the group is represented by the operator  $[\bar{I}, \mathbf{0}]$ , which is obtained by the

product of a pair of arbitrary-free two operators differing only by the sign of the translational part, e.g.:

$$[\bar{\bar{\mathbf{M}}}_1, \mathbf{a}_1/2] \cdot [\bar{\bar{\mathbf{M}}}_1, -\mathbf{a}_1/2] = [\bar{\mathbf{I}}, \mathbf{0}] .$$

This means that there is a neutral element in the set of elements, there is an inverse element to each element, the set is closed in terms of the group operation, and since it is a multiplication of tensors and addition of vectors, the associative law holds in the group operation. Thus, all the conditions for a set to form a group are satisfied.

This group, we denote it by  $G_a$ , can be decomposed into two subsets. Elements of type  $[\bar{\mathbf{I}}, n\mathbf{a}_1]$ , i.e., elements without reflection, where  $n$  is an integer (positive, negative, or zero), are elements of the translation group  $T_a$ , the other elements of the set forming a coset of the group  $G_a$  with respect to its subgroup  $T_a$ . The representative of a coset may be an element to which, for example, the operator  $[\bar{\bar{\mathbf{M}}}_1, \mathbf{a}_1/2]$  corresponds. Based on this, we can express the group  $G_a$  in the form:

$$G_a = T_a + [\bar{\bar{\mathbf{M}}}_1, \mathbf{a}_1/2] \cdot T_a .$$

However, the group  $T_a$  is only a subgroup of the full translation group  $T_p$  of the orthogonal lattice, so the group  $G_a$  does not represent all elements of the plane group.

## D19 Operators $[\bar{\bar{\mathbf{2}}}, t]$

There are four double rotation axes per orthogonal unit cell, which according to C7.1 are localized at positions with fractional coordinates:  $(0, 0)$ ,  $(1/2, 0)$ ,  $(0, 1/2)$  and  $(1/2, 1/2)$ . The rotation about the axis located at the origin of the reference frame, i.e., at position  $(0, 0)$ , is represented by the operator  $[\bar{\bar{\mathbf{2}}}, 0]$  with zero translational part, but the operators representing rotations about the other axes have a non-zero translational part.

Starting from the relation  $S \equiv [\bar{\bar{\Phi}}, \mathbf{r}_o \cdot (\bar{\mathbf{I}} - \bar{\bar{\Phi}})]$  ( $\rightarrow$  relation (h) in Appendix D13) and the equality  $\bar{\bar{\Phi}} \equiv \bar{\bar{\mathbf{2}}} = -\bar{\mathbf{I}}$ , the translational part of the operator representing the rotation about the axis shifted to the position  $(1/2, 0)$ , i.e., when  $\mathbf{r}_o = \mathbf{a}_1/2$ , is equal to the product:

$$\frac{1}{2} \mathbf{a}_1 \cdot 2\bar{\mathbf{I}} = \mathbf{a}_1 .$$

At position  $(0, 1/2)$ , the translational part of the operator is equal to the vector  $\mathbf{a}_2$  and in the third case to the vector  $\mathbf{a}_1 + \mathbf{a}_2$ . Based on this, the operators representing the rotations about the twofold axes, incident to the unit cell, have the form:

$$[\bar{\bar{\mathbf{2}}}, 0], [\bar{\bar{\mathbf{2}}}, \mathbf{a}_1], [\bar{\bar{\mathbf{2}}}, \mathbf{a}_2] \text{ and } [\bar{\bar{\mathbf{2}}}, \mathbf{a}_1 + \mathbf{a}_2],$$

or

$$[\bar{\bar{1}}, 0], [\bar{\bar{1}}, \mathbf{a}_1], [\bar{\bar{1}}, \mathbf{a}_2] \text{ and } [\bar{\bar{1}}, \mathbf{a}_1 + \mathbf{a}_2].$$

All operators have the same tensor part, while their translational parts differ from each other only by lattice vectors. Therefore, all symmetry operations represented by these four operators belong to the same coset of the plane group.

The operators of rotation about the twofold axes have the same form in the other crystal systems.

## D20 Operators $[\bar{\bar{4}}, t]$

There are two fourfold rotation axes per unit cell of the square lattice, which, according to C7.2, are localized at positions with fractional coordinates:  $(0, 0)$ , and  $(1/2, 1/2)$ . The rotation about the axis located at the origin of the reference frame, i.e., at position  $(0, 0)$ , is represented by the operator  $[\bar{\bar{4}}, 0]$  with zero translational part, but the operator representing the rotation about the other axis has a nonzero translational part. Starting from the relation  $S \equiv [\bar{\Phi}, \mathbf{r}_o \cdot (\bar{\mathbf{I}} - \bar{\Phi})]$  ( $\rightarrow$  Appendix D13, relation (h)) and the equality  $\bar{\Phi} \equiv \bar{\bar{4}} = \mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1$  ( $\rightarrow$  tab TC2b), the translational part of the operator representing rotation about the axis shifted to the position  $(1/2, 1/2)$ , i.e., when  $\mathbf{r}_o = \mathbf{a}_1/2 + \mathbf{a}_2/2$ , is equal to the product:

$$\left(\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2\right) \cdot (\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2 - \mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1) = \frac{1}{2}\mathbf{a}_1 - \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_1 = \mathbf{a}_1.$$

This means that the operators representing the rotation about the fourfold axes localized at the origin or at the centre of the unit cell have the form

$$[\bar{\bar{4}}, 0] \equiv [\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{0}], \text{ resp. } [\bar{\bar{4}}, \mathbf{a}_1] = [\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1].$$

These two operators have the same tensor part, while their translational parts differ from each other only by the lattice vector, so the symmetry operations represented by them belong to one coset of the plane group.

The repeated rotations by  $90^\circ$  about the axis localized at the centre of the unit cell are assigned to the operators

$$[\bar{\bar{4}}^2, \mathbf{a}_1], \text{ and } [\bar{\bar{4}}^3, \mathbf{a}_1],$$

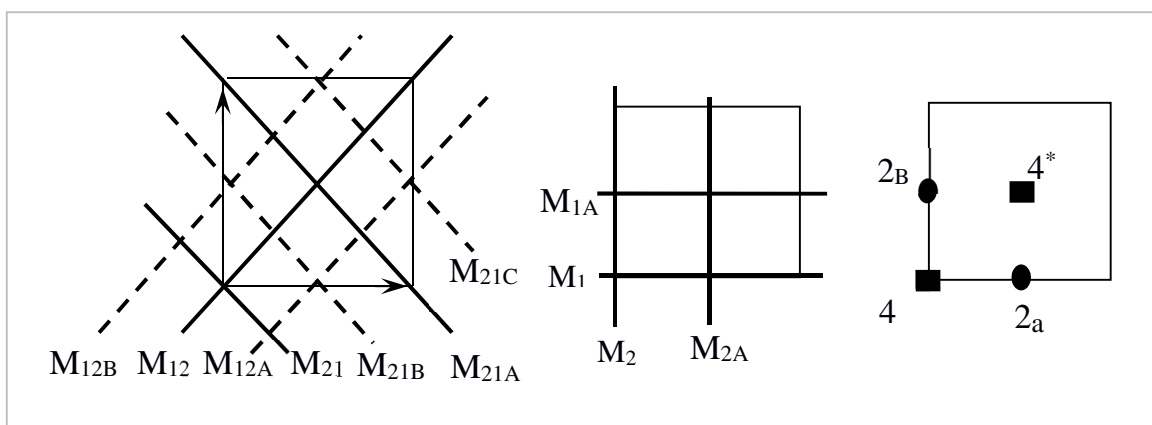
where the elements represented by the operators  $[\bar{\bar{4}}^2, \mathbf{0}], [\bar{\bar{4}}^2, \mathbf{a}_1]$  belong to the same coset, as do the elements with the operators  $[\bar{\bar{4}}^3, \mathbf{0}], [\bar{\bar{4}}^3, \mathbf{a}_1]$ .

## D21 Reflections in plane group $p4mm$

A natural part of the symmetry of the square lattice are the glide lines, which are parallel to, but not identical with, the diagonals of the unit cell ( $\rightarrow$  figure in this appendix). According to C8.3, the plane group  $p4mm$  is formed by combining elements of the point group  $4mm$  with elements of the translation group  $T_p$ , but the glide reflection is not part of either of these groups because it is an element of the plane group only. However, glide reflection in a line parallel to the diagonal of the square is equivalent to successive applications of reflection in a line parallel to some basis vector (i.e., the side of the square) and rotation about a fourfold axis passing through the centre of the unit cell (i.e., the centre of the square; the corresponding axis is indicated by the symbol  $4^*$  in the figure). Such a rotation, expressed with respect to the origin of the reference frame, is represented by the operator  $[\bar{4}, \mathbf{a}_1]$  ( $\rightarrow$  article C7.2), which also has a translational part, so that it is an element of the plane group. The product of this operator with the reflection operator in the line identical to the vector  $\mathbf{a}_2$  :

$$[\bar{4}, \mathbf{a}_1] \cdot [\bar{\mathbf{M}}_2, 0] \equiv [\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1] \cdot [\bar{\mathbf{I}} - 2 \mathbf{a}^1 \mathbf{a}_1, 0] = [\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1],$$

we obtain an operator whose tensor part coincides with the tensor part of the reflection operator  $[\bar{\mathbf{M}}_{12}, 0]$ , but differs from it in the translational part; we write it in the abbreviated form  $[\bar{\mathbf{M}}_{12}, \mathbf{a}_1]$ . The non-zero translational part may be related to the glide, to the localization of an element of symmetry, or even to a combination of these, as in this case. A table of both rotation and reflection operators for this plane group is given in Appendix D22.



We prove that the operator  $[\bar{\mathbf{M}}_{12}, \mathbf{a}_1] \equiv [\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1]$  represents a reflection with glide  $(\mathbf{a}_1 + \mathbf{a}_2)/2$  in the line, which is indicated in the figure by the

symbol  $M_{12A}$ . For example, a point with position vector  $\mathbf{a}_1$  transforms to a point  $\mathbf{a}_1 + \mathbf{a}_2$  :

$$\mathbf{a}_1 \cdot [\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1] = (\mathbf{a}_1 \cdot \mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}_1 \cdot \mathbf{a}^2 \mathbf{a}_1) + \mathbf{a}_1 = \mathbf{a}_2 + \mathbf{0} + \mathbf{a}_1 ,$$

point with position vector  $\mathbf{a}_2$  to position  $2\mathbf{a}_1$  :

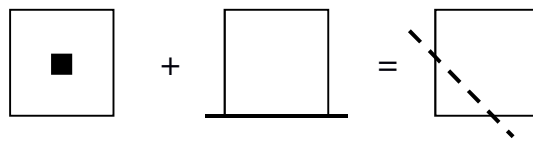
$$\mathbf{a}_2 \cdot [\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1] = (\mathbf{a}_2 \cdot \mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}_2 \cdot \mathbf{a}^2 \mathbf{a}_1) + \mathbf{a}_1 = \mathbf{0} + \mathbf{a}_1 + \mathbf{a}_1 = 2\mathbf{a}_1 ,$$

or point  $\mathbf{0}$  to position  $\mathbf{a}_1$  .

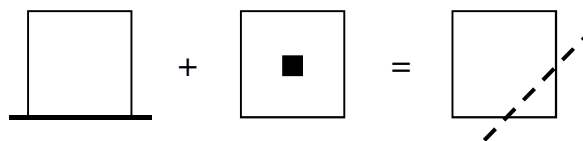
The results of other combinations of rotations with reflections document the fact that the operators representing reflections in mutually parallel lines (ordinary reflections and glide reflections) have the same tensor parts and differ only by translations belonging to the translation group. This fact implies that by changing the zero translation term in the symmetry operator to a nonzero one – by adding an element of the translation group (i.e., a lattice vector), we obtain operators of elements of the plane group belonging to the same coset. Operators with a non-zero translation term represent rotations about axes not passing through the origin of the reference frame and, in the case of reflections, in addition to the displacement of the reflection line, can also represent glide reflections.

To illustrate, the following text show some combinations of symmetry operations in both numerical and graphical form. In the relations, symbols are used in accordance with the figure, e.g., rotation about the fourfold axis placed at the centre of the square by the symbol  $4^*$ .

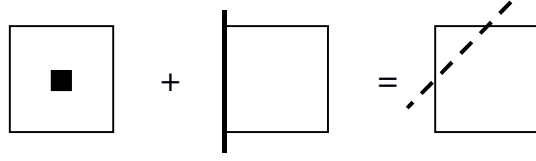
$$4^* \cdot M_1 = [\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1] \cdot [\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2, \mathbf{0}] = [-\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1] = M_{21B}$$



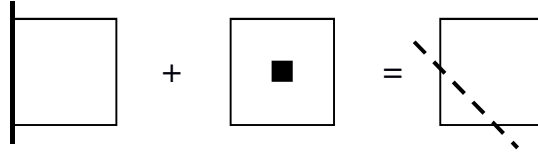
$$M_1 \cdot 4^* = [\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2, \mathbf{0}] \cdot [\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1] = [\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1] = M_{12A}$$



$$4^* \cdot M_2 = [\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1] \cdot [-\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2, \mathbf{0}] = [\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1, -\mathbf{a}_1] = M_{12B}$$



$$\begin{aligned} M_2 \cdot \mathbf{4}^* &= [-\mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2, \mathbf{0}] \cdot [\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1] \\ &= [-\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{a}_1] = M_{21B} \end{aligned}$$



When we note that the operators of reflection in lines parallel to the diagonals and passing through the origin of the reference frame have form

$$[\bar{\mathbf{M}}_{12}, \mathbf{0}] = [\mathbf{a}^1 \mathbf{a}_2 + \mathbf{a}^2 \mathbf{a}_1, \mathbf{0}] \quad \text{and} \quad [\bar{\mathbf{M}}_{21}, \mathbf{0}] = [-\mathbf{a}^1 \mathbf{a}_2 - \mathbf{a}^2 \mathbf{a}_1, \mathbf{0}],$$

so we can write the results of the previous four relations more concisely:

$$\begin{aligned} \mathbf{4}^* \cdot M_1 &= M_{21B} = [\bar{\mathbf{M}}_{21}, \mathbf{a}_1], \\ M_1 \cdot \mathbf{4}^* &= M_{12A} = [\bar{\mathbf{M}}_{12}, \mathbf{a}_1], \\ \mathbf{4}^* \cdot M_2 &= M_{12B} = [\bar{\mathbf{M}}_{12}, -\mathbf{a}_1], \\ M_2 \cdot \mathbf{4}^* &= M_{21B} = [\bar{\mathbf{M}}_{21}, \mathbf{a}_1], \end{aligned}$$

from where it can be better seen that the translational parts of the operators are elements of the translation group.

It can be seen that next relations are also valid

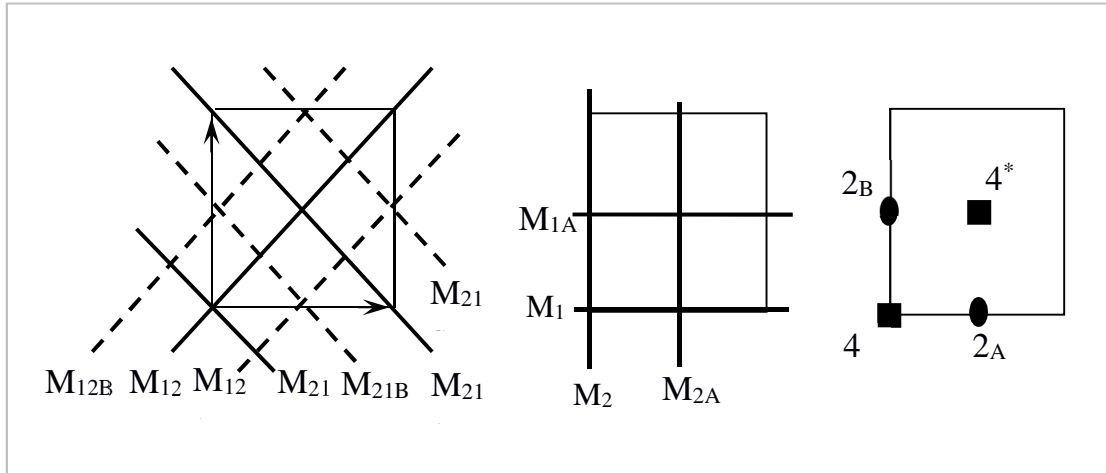
$$\mathbf{4}^* \cdot M_{12} = [\bar{\mathbf{M}}_1, \mathbf{a}_2], \quad M_{12} \cdot \mathbf{4}^* = [\bar{\mathbf{M}}_2, \mathbf{a}_1],$$

which imply reflections in lines parallel to the basis vectors that pass through the centre of the unit cell, as well as relations

$$\mathbf{4}^* \cdot M_{21} = [\bar{\mathbf{M}}_2, \mathbf{0}] \cdot [\bar{\mathbf{I}}, -\mathbf{a}_2], \quad M_{21} \cdot \mathbf{4}^* = [\bar{\mathbf{M}}_1, \mathbf{0}] \cdot [\bar{\mathbf{I}}, \mathbf{a}_1],$$

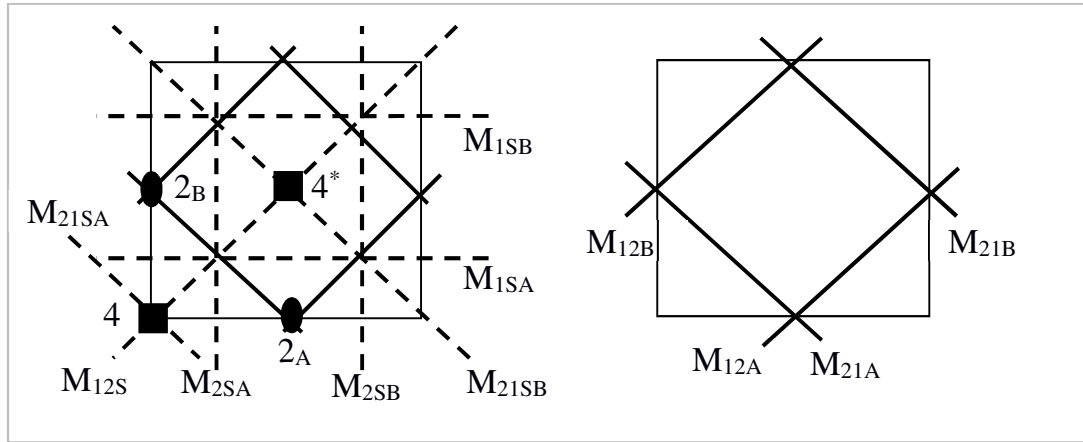
which imply that it is a combination of ordinary reflection with translation by a lattice vector.

## D22 Operators in plane group $p4mm$



|           |                                                                      |
|-----------|----------------------------------------------------------------------|
| $M_1$     | $[\bar{M}_1, 0] \equiv [a^1 a_1 - a^2 a_2, 0]$                       |
| $M_{1A}$  | $[\bar{M}_1, a_2] \equiv [a^1 a_1 - a^2 a_2, a_2]$                   |
| $M_2$     | $[\bar{M}_2, 0] \equiv [-a^1 a_1 + a^2 a_2, 0]$                      |
| $M_{2A}$  | $[\bar{M}_2, a_1] \equiv [-a^1 a_1 + a^2 a_2, a_1]$                  |
| $M_{12}$  | $[\bar{M}_{12}, 0] \equiv [a^1 a_2 + a^2 a_1, 0]$                    |
| $M_{12A}$ | $[\bar{M}_{12}, a_1] \equiv [a^1 a_2 + a^2 a_1, a_1]$                |
| $M_{12B}$ | $[\bar{M}_{12}, a_2] \equiv [a^1 a_2 + a^2 a_1, a_2]$                |
| $M_{21}$  | $[\bar{M}_{21}, 0] \equiv [-a^1 a_2 - a^2 a_1, 0]$                   |
| $M_{21A}$ | $[\bar{M}_{21}, a_1 + a_2] \equiv [-a^1 a_2 - a^2 a_1, a_1 + a_2]$   |
| $M_{21B}$ | $[\bar{M}_{21}, a_1] \equiv [-a^1 a_2 - a^2 a_1, a_1]$               |
| $M_{21C}$ | $[\bar{M}_{21}, 2a_1 + a_2] \equiv [-a^1 a_2 - a^2 a_1, 2a_1 + a_2]$ |
| $4$       | $[\bar{4}, 0] \equiv [a^1 a_2 - a^2 a_1, 0]$                         |
| $4^2$     | $[\bar{4}^2, 0] \equiv [\bar{2}, 0] \equiv [-\bar{1}, 0]$            |
| $4^3$     | $[\bar{4}^3, 0] \equiv [-a^1 a_2 + a^2 a_1, 0]$                      |
| $4^*$     | $[\bar{4}, a_1] \equiv [a^1 a_2 - a^2 a_1, a_1]$                     |
| $2_A$     | $[\bar{2}, a_1] \equiv [-\bar{1}, a_1]$                              |
| $2_B$     | $[\bar{2}, a_2] \equiv [-\bar{1}, a_2]$                              |

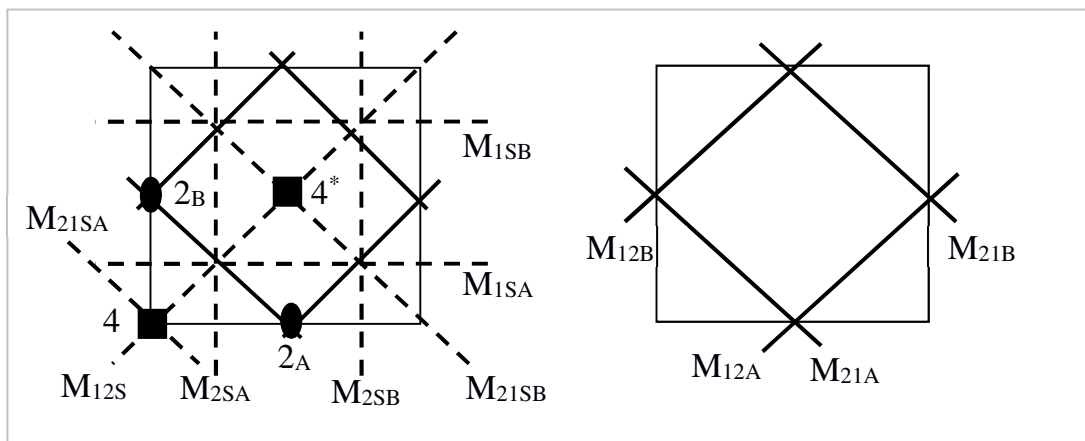
## D23 Operators in plane group $p4gm$



|            |                                                                                      |
|------------|--------------------------------------------------------------------------------------|
| $M_{1SA}$  | $[\bar{\bar{M}}_1, a_1/2 + a_2/2] \equiv [a^1 a_1 - a^2 a_2, a_1/2 + a_2/2]$         |
| $M_{1SB}$  | $[\bar{\bar{M}}_1, a_1/2 + 3a_2/2] \equiv [a^1 a_1 - a^2 a_2, a_1/2 + 3a_2/2]$       |
| $M_{2SA}$  | $[\bar{\bar{M}}_2, a_1/2 + a_2/2] \equiv [-a^1 a_1 + a^2 a_2, a_1/2 + a_2/2]$        |
| $M_{2SB}$  | $[\bar{\bar{M}}_2, 3a_1/2 + a_2/2] \equiv [-a^1 a_1 + a^2 a_2, 3a_1/2 + a_2/2]$      |
| $M_{12S}$  | $[\bar{\bar{M}}_{12}, a_1/2 + a_2/2] \equiv [a^1 a_2 + a^2 a_1, a_1/2 + a_2/2]$      |
| $M_{12A}$  | $[\bar{\bar{M}}_{12}, a_1/2 - a_2/2] \equiv [a^1 a_2 + a^2 a_1, a_1/2 - a_2/2]$      |
| $M_{12B}$  | $[\bar{\bar{M}}_{12}, -a_1/2 + a_2/2] \equiv [a^1 a_2 + a^2 a_1, -a_1/2 + a_2/2]$    |
| $M_{21A}$  | $[\bar{\bar{M}}_{21}, a_1/2 + a_2/2] \equiv [-a^1 a_2 - a^2 a_1, a_1/2 + a_2/2]$     |
| $M_{21B}$  | $[\bar{\bar{M}}_{21}, 3a_1/2 + 3a_2/2] \equiv [-a^1 a_2 - a^2 a_1, 3a_1/2 + 3a_2/2]$ |
| $M_{21SA}$ | $[\bar{\bar{M}}_{21}, a_1/2 - a_2/2] \equiv [-a^1 a_2 - a^2 a_1, a_1/2 - a_2/2]$     |
| $M_{21SB}$ | $[\bar{\bar{M}}_{21}, 3a_1/2 + a_2/2] \equiv [-a^1 a_2 - a^2 a_1, 3a_1/2 + a_2/2]$   |
| 4          | $[\bar{\bar{4}}, 0] \equiv [a^1 a_2 - a^2 a_1, 0],$                                  |
| $4^2$      | $[\bar{\bar{4}}^2, 0] \equiv [\bar{\bar{2}}, 0] \equiv [-\bar{\bar{1}}, 0]$          |
| $4^3$      | $[\bar{\bar{4}}^3, 0] \equiv [-a^1 a_2 + a^2 a_1, 0]$                                |
| $4^*$      | $[\bar{\bar{4}}, a_1] \equiv [a^1 a_2 - a^2 a_1, a_1]$                               |
| $2_A$      | $[\bar{\bar{2}}, a_1] \equiv [-\bar{\bar{1}}, a_1]$                                  |
| $2_B$      | $[\bar{\bar{2}}, a_2] \equiv [-\bar{\bar{1}}, a_2]$                                  |

## D24 Reflections in plane group $p4gm$

In the  $p4gm$  group, only elements representing glide reflections are representative of cosets. However, ordinary reflections are also part of this plane group, and, as in the case of the  $p4mm$  group, these reflections are equivalent to the successive application of two operations belonging to this plane group.



This statement will be verified in several cases, using the table of operators of this group given in Appendix D23.

The reflection in the line marked by the symbol  $M_{21A}$  is equivalent to the successive application of a rotation of  $180^\circ$  about an axis passing through the origin of the reference frame, represented by the operator

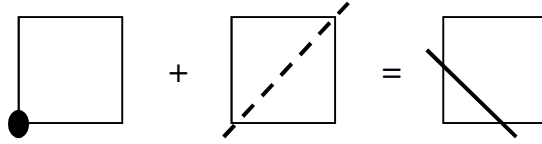
$$[\bar{4}^2, 0] \equiv [\bar{2}, 0] \equiv [-\bar{1}, 0],$$

and glide reflection in the line denoted by the symbol  $M_{12S}$ , represented by the operator

$$[\bar{M}_{12}, a_1/2 + a_2/2] \equiv [a^1 a_2 + a^2 a_1, a_1/2 + a_2/2]:$$

$$[-\bar{1}, 0] \cdot [a^1 a_2 + a^2 a_1, a_1/2 + a_2/2] = [-a^1 a_2 - a^2 a_1, a_1/2 + a_2/2].$$

In abbreviated form:  $[\bar{2}, 0] \cdot M_{12S} = M_{21A}$ , or by using the symbolic figure:

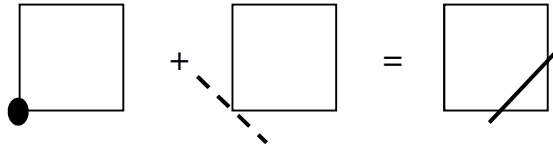


The reflection in the line denoted by the symbol  $M_{12A}$  is equivalent to the successive application of a rotation by  $180^\circ$  about the axis passing through the origin of the reference frame represented by the operator  $[\bar{2}, 0] \equiv [-\bar{1}, 0]$  and glide reflection in the line denoted by the symbol  $M_{21SA}$ , with the operator

$$[-a^1 a_2 - a^2 a_1, a_1/2 - a_2/2]:$$

$$[-\bar{1}, 0] \cdot [-a^1 a_2 - a^2 a_1, a_1/2 - a_2/2] = [a^1 a_2 + a^2 a_1, a_1/2 - a_2/2].$$

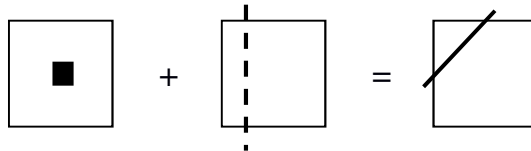
In the abbreviated notation  $[\bar{2}, 0] \cdot M_{21SA} = M_{12A}$  and using the symbolic figure:



The reflection in the line denoted by the symbol  $M_{12B}$  is equivalent to the successive application of a rotation by  $90^\circ$  about an axis passing through the centre of the unit cell represented by the operator  $[\bar{4}, a_1]$  and a glide reflection in the line denoted by the symbol  $M_{2SA}$ , represented by the operator  $[-a^1 a_1 + a^2 a_2, a_1/2 + a_2/2]$ :

$$\begin{aligned} [a^1 a_2 - a^2 a_1, a_1] \cdot \left[ -a^1 a_1 + a^2 a_2, \frac{1}{2} a_1 + \frac{1}{2} a_2 \right] = \\ = \left[ a^1 a_2 + a^2 a_1, -\frac{1}{2} a_1 + \frac{1}{2} a_2 \right]. \end{aligned}$$

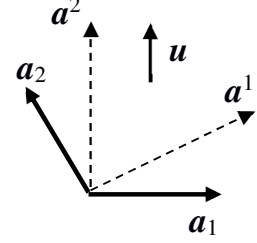
In shorthand notation  $[\bar{4}, a_1] \cdot M_{2SA} = M_{12B}$  and using a symbolic figure:



**Note** The operators  $\bar{4}$  and  $\bar{M}$  do not commute; changing the order of rotation and reflection will give different results.

## D25 Operators of reflection and rotation in hexagonal system

In orthogonal cells whose basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  are perpendicular to each other, the reflection tensors have a relatively simple shape. When reflection in a line identical to the vector  $\mathbf{a}_1$  they have the form  $\bar{\mathbf{M}}_1 = \bar{\mathbf{I}} - 2\mathbf{a}^2\mathbf{a}_2$ , when reflection in a line identical to the vector  $\mathbf{a}_2$  the form  $\bar{\mathbf{M}}_2 = \bar{\mathbf{I}} - 2\mathbf{a}^1\mathbf{a}_1$ . In a hexagonal lattice, one can choose both a primitive unit cell and an orthogonal centred cell. In the primitive cell, the basis vectors have the same size  $|\mathbf{a}_1| = |\mathbf{a}_2|$  but they are not perpendicular to each other, so the tensor needs to be adjusted.



The reflection tensor has the general form ( $\rightarrow$  relation C4.8):

$$\bar{\mathbf{M}} = \bar{\mathbf{I}} - 2\mathbf{u}\mathbf{u},$$

where  $\mathbf{u}$  is the unit vector perpendicular to the reflection line. We modify the tensor by assuming that it is a reflection in the line identical to the vector  $\mathbf{a}_1$  while the goal is to replace the unit vectors  $\mathbf{u}$  by the basis and reciprocal vectors.

The vector  $\mathbf{u}$  ( $\rightarrow$  image) is parallel to both the reciprocal vector  $\mathbf{a}^2$  and the vector  $\mathbf{a}_1 + 2\mathbf{a}_2$ , so we can express it using these vectors, taking their magnitudes into account. According to the definition of reciprocal vectors, the relation

$$1 = \mathbf{a}^2 \cdot \mathbf{a}_2 = |\mathbf{a}^2| \cdot |\mathbf{a}_2| \cos 30^\circ = |\mathbf{a}^2| \cdot |\mathbf{a}_2| \frac{\sqrt{3}}{2},$$

$$|\mathbf{a}^2| = \frac{2}{|\mathbf{a}_2|\sqrt{3}} = \frac{2}{|\mathbf{a}_1|\sqrt{3}}.$$

The size of vector  $\mathbf{a}_1 + 2\mathbf{a}_2$ :

$$|\mathbf{a}_1 + 2\mathbf{a}_2| = 2|\mathbf{a}_2| \cos 30^\circ = 2|\mathbf{a}_1| \frac{\sqrt{3}}{2} = |\mathbf{a}_1| \sqrt{3}.$$

We will use the results to modify the  $2\mathbf{u}\mathbf{u}$  dyad:

$$2\mathbf{u}\mathbf{u} = 2\mathbf{a}^2 \frac{|\mathbf{a}_1|\sqrt{3}}{2} (\mathbf{a}_1 + 2\mathbf{a}_2) \frac{1}{|\mathbf{a}_1|\sqrt{3}} = \mathbf{a}^2\mathbf{a}_1 + 2\mathbf{a}^2\mathbf{a}_2.$$

The reflection tensor thus takes shape:

$$\bar{\mathbf{M}} = \bar{\mathbf{I}} - 2\mathbf{u}\mathbf{u} = \mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^2\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1 - 2\mathbf{a}^2\mathbf{a}_2 = \mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2,$$

$$\bar{\mathbf{M}}_0 = \mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2.$$

In the hexagonal system, this reflection is conventionally denoted by symbol  $m_o$ . It is a reflection in a line identical to the basis vector  $\mathbf{a}_1$ , whose operator, in orthogonal systems, is denoted as  $\bar{\mathbf{M}}_1$ . The operators of the other reflections, i.e.,  $m_{30}$ ,  $m_{90}$ , etc., are obtained by multiplying the operator  $\bar{\mathbf{M}}_0$  by operators representing multiples of the rotation by  $60^\circ$ , where the operator of this rotation is the tensor  $\bar{\mathbf{6}} = \mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1$ .

According to the multiplication table of the  $6mm$  group, the following relations hold:

$$\begin{aligned}\bar{\mathbf{M}}_{30} &= \bar{\mathbf{M}}_0 \cdot \bar{\mathbf{6}}, & \bar{\mathbf{M}}_{60} &= \bar{\mathbf{M}}_0 \cdot \bar{\mathbf{6}}^2, & \bar{\mathbf{M}}_{90} &= \bar{\mathbf{M}}_0 \cdot \bar{\mathbf{6}}^3 = \bar{\mathbf{M}}_0 \cdot (-\bar{\mathbf{I}}), \\ \bar{\mathbf{M}}_{120} &= \bar{\mathbf{M}}_0 \cdot \bar{\mathbf{6}}^4, & \bar{\mathbf{M}}_{150} &= \bar{\mathbf{M}}_0 \cdot \bar{\mathbf{6}}^5.\end{aligned}$$

Based on these relationships, we obtain the results:

$$\begin{aligned}\bar{\mathbf{M}}_{30} &= \mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_2, \\ \bar{\mathbf{M}}_{60} &= \mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^2\mathbf{a}_1, \\ \bar{\mathbf{M}}_{90} &= -\mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^2\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1, \\ \bar{\mathbf{M}}_{120} &= -\mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_2, \\ \bar{\mathbf{M}}_{150} &= -\mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1.\end{aligned}$$

Combinations of these reflections with rotations about axes not passing through the origin of the reference frame give reflections and glide reflections in differently displaced lines.

For completeness, we will also list the rotation operators already expressed in C4.1.3 :

$$\begin{aligned}\bar{\mathbf{6}} &= \mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1, \\ \bar{\mathbf{6}}^2 \equiv \bar{\mathbf{3}} &= \mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1 - \mathbf{a}^2\mathbf{a}_2, \\ \bar{\mathbf{6}}^3 \equiv \bar{\mathbf{2}} &= -\bar{\mathbf{I}}, \\ \bar{\mathbf{6}}^4 \equiv \bar{\mathbf{3}}^2 &= -\mathbf{a}^1\mathbf{a}_1 - \mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1, \\ \bar{\mathbf{6}}^5 &= -\mathbf{a}^1\mathbf{a}_2 + \mathbf{a}^2\mathbf{a}_1 + \mathbf{a}^2\mathbf{a}_2.\end{aligned}$$

## D26 Operators of reflections and rotations in orthohexagonal basis

In the hexagonal system, there are relations between the basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  of the primitive cell and the basis vectors  $\mathbf{b}_1$ ,  $\mathbf{b}_2$  of the orthohexagonal cell:

$$\mathbf{b}_1 \equiv \mathbf{a}_1, \quad \mathbf{b}_2 = \mathbf{a}_1 + 2\mathbf{a}_2$$

and vice-versa

$$\mathbf{a}_1 \equiv \mathbf{b}_1, \quad \mathbf{a}_2 = \frac{1}{2}(\mathbf{b}_2 - \mathbf{b}_1).$$

The following relations hold between the reciprocal vectors of the two bases:

$$\mathbf{a}^1 = \mathbf{b}^1 + \mathbf{b}^2, \quad \mathbf{a}^2 = 2\mathbf{b}^2,$$

and vice-versa

$$\mathbf{b}^1 = \mathbf{a}^1 - \frac{1}{2}\mathbf{a}^2, \quad \mathbf{b}^2 = \frac{1}{2}\mathbf{a}^2.$$

For completeness we also give the magnitudes of these vectors, they are only necessary to derive the relationships between the reciprocal vectors:

$$|\mathbf{a}_2| = |\mathbf{a}_1| = a_1, \quad |\mathbf{b}_1| = a_1, \quad |\mathbf{b}_2| = a_1\sqrt{3}.$$

$$|\mathbf{a}^1| = |\mathbf{a}^2| = \frac{2}{a_1\sqrt{3}}, \quad |\mathbf{b}^1| = \frac{1}{a_1}, \quad |\mathbf{b}^2| = \frac{1}{a_1\sqrt{3}}.$$

We use the relations between the vectors of the direct space and the vectors of the reciprocal space to transform the tensors from the primitive to the orthohexagonal basis.

In the orthohexagonal basis, the tensor of reflection in the line identical to the vector  $\mathbf{b}_1$  has the form

$$\bar{\bar{\mathbf{M}}}_0 = \bar{\bar{\mathbf{I}}} - 2\mathbf{b}^2\mathbf{b}_2 = \mathbf{b}^1\mathbf{b}_1 - \mathbf{b}^2\mathbf{b}_2,$$

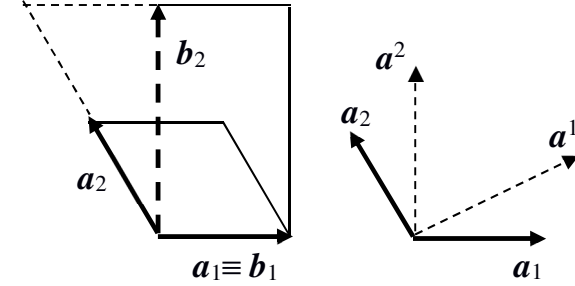
so there is no need to transform it. In particular, the tensor representing the rotation by  $60^\circ$  needs to be transformed. In the primitive basis it has the form:

$$\bar{\bar{\mathbf{G}}} = \mathbf{a}^1\mathbf{a}_1 + \mathbf{a}^1\mathbf{a}_2 - \mathbf{a}^2\mathbf{a}_1,$$

which after transformation takes a more complicated form

$$\bar{\bar{\mathbf{G}}} = \frac{1}{2}\mathbf{b}^1\mathbf{b}_1 + \frac{1}{2}\mathbf{b}^1\mathbf{b}_2 - \frac{3}{2}\mathbf{b}^2\mathbf{b}_1 + \frac{1}{2}\mathbf{b}^2\mathbf{b}_2,$$

and which is the starting point to obtain tensors representing multiple rotations:



$$\bar{\bar{6}}^2 = \bar{\bar{6}} \cdot \bar{\bar{6}} \equiv \bar{\bar{3}} = -\frac{1}{2}b^1b_1 + \frac{1}{2}b^1b_2 - \frac{3}{2}b^2b_1 - \frac{1}{2}b^2b_2 ,$$

$$\bar{\bar{6}}^3 = \bar{\bar{6}} \cdot \bar{\bar{6}} \cdot \bar{\bar{6}} \equiv \bar{\bar{2}} = -\bar{\bar{1}} ,$$

$$\bar{\bar{6}}^4 = -\frac{1}{2}b^1b_1 - \frac{1}{2}b^1b_2 + \frac{3}{2}b^2b_1 - \frac{1}{2}b^2b_2 = -\bar{\bar{6}} ,$$

$$\bar{\bar{6}}^5 = \frac{1}{2}b^1b_1 - \frac{1}{2}b^1b_2 + \frac{3}{2}b^2b_1 + \frac{1}{2}b^2b_2 ,$$

$$\bar{\bar{6}}^6 = \bar{\bar{1}} .$$

The reflection operators  $m_{30}$ ,  $m_{60}$ , etc. can already be obtained by the products that result from the multiplication table of the **6mm** group:

$$\begin{aligned} \bar{\bar{M}}_{30} &= \bar{\bar{M}}_0 \cdot \bar{\bar{6}} = (\bar{\bar{1}} - 2b^2b_2) \cdot \left( \frac{1}{2}b^1b_1 + \frac{1}{2}b^1b_2 - \frac{3}{2}b^2b_1 + \frac{1}{2}b^2b_2 \right) = \\ &= \frac{1}{2}b^1b_1 + \frac{1}{2}b^1b_2 + \frac{3}{2}b^2b_1 - \frac{1}{2}b^2b_2 , \end{aligned}$$

$$\bar{\bar{M}}_{60} = \bar{\bar{M}}_0 \cdot \bar{\bar{6}}^2 = -\frac{1}{2}b^1b_1 + \frac{1}{2}b^1b_2 + \frac{3}{2}b^2b_1 + \frac{1}{2}b^2b_2 ,$$

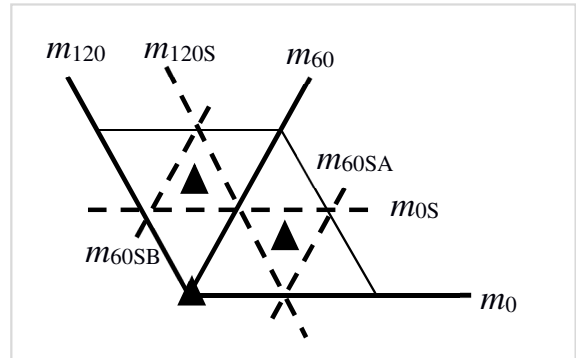
$$\bar{\bar{M}}_{90} = \bar{\bar{M}}_0 \cdot \bar{\bar{6}}^3 = \bar{\bar{M}}_0 \cdot (-\bar{\bar{1}}) = -\bar{\bar{M}}_0 = -b^1b_1 + b^2b_2 ,$$

$$\bar{\bar{M}}_{120} = \bar{\bar{M}}_0 \cdot \bar{\bar{6}}^4 = -\frac{1}{2}b^1b_1 - \frac{1}{2}b^1b_2 - \frac{3}{2}b^2b_1 + \frac{1}{2}b^2b_2 ,$$

$$\bar{\bar{M}}_{150} = \bar{\bar{M}}_0 \cdot \bar{\bar{6}}^5 = \frac{1}{2}b^1b_1 - \frac{1}{2}b^1b_2 - \frac{3}{2}b^2b_1 - \frac{1}{2}b^2b_2 .$$

## D27 Reflections in plane group $p31m$

In this group, ordinary reflections  $m_0, m_{60}$  and  $m_{120}$  are applied in lines passing through the origin of the reference frame, and glide reflections  $m_{0S}$ ,  $m_{60SA}$ ,  $m_{60SB}$ ,  $m_{120S}$  in lines parallel to the reflection lines. Operators representing ordinary reflections were derived in Appendix D25, we list them again for completeness:



$$[\bar{\bar{M}}_0, \mathbf{0}] = [a^1a_1 - a^2a_1 - a^2a_2, \mathbf{0}], \quad [\bar{\bar{M}}_{60}, \mathbf{0}] = [a^1a_1 + a^2a_1, \mathbf{0}],$$

$$[\bar{\bar{M}}_{120}, \mathbf{0}] = [-a^1a_1 + a^1a_2 + a^2a_2, \mathbf{0}].$$

Operators representing reflections in mutually parallel lines are distinguished from each other only by the translation term. The operator of ordinary reflection in a line passing through the origin of the reference frame has zero translation term, the translation term of the operator of glide reflection is a lattice vector, so that the corresponding operations belong to one coset. The operators of glide reflection have the following form:

$$m_{0S} : [\bar{\mathbf{M}}_0, \mathbf{a}_1 + \mathbf{a}_2], \quad m_{60SA} : [\bar{\mathbf{M}}_{60}, \mathbf{a}_1], \quad m_{60SB} : [\bar{\mathbf{M}}_{60}, \mathbf{a}_2],$$

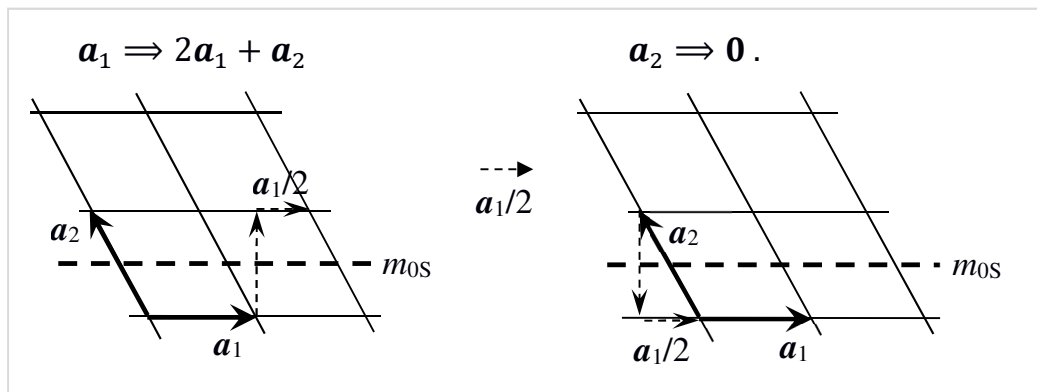
$$m_{120S} : [\bar{\mathbf{M}}_{120}, \mathbf{a}_1 + \mathbf{a}_2].$$

The correctness of these relationships is easily verified by simple examples. We will check how the  $m_{0S}$  reflection transforms the points at the ends of the basis vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$ :

$$\mathbf{a}_1 \cdot [\bar{\mathbf{M}}_0, \mathbf{a}_1 + \mathbf{a}_2] = \mathbf{a}_1 \cdot [\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2, \mathbf{a}_1 + \mathbf{a}_2] = 2\mathbf{a}_1 + \mathbf{a}_2,$$

$$\mathbf{a}_2 \cdot [\mathbf{a}^1 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_1 - \mathbf{a}^2 \mathbf{a}_2, \mathbf{a}_1 + \mathbf{a}_2] = -\mathbf{a}_1 - \mathbf{a}_2 + \mathbf{a}_1 + \mathbf{a}_2 = \mathbf{0}.$$

In both cases it is a reflection with glide  $\mathbf{a}_1/2$  in a line parallel to the vector  $\mathbf{a}_1$ , passing through the centre of the vector  $\mathbf{a}_2$ , i.e. the point with coordinates  $(0, \frac{1}{2})$ , which we document with the following figures:



## D28 Reflections in plane group $p3m1$

The next figure shows the positions of the threefold axes (triangles), the reflection lines (solid lines), and the glide lines (dashed lines) of the plane group  $p3m1$ . We express the operators of some of the reflections that are assigned symbols in the figure. The operator representing the reflection in the line marked in the figure by the symbol  $M_{90A}$ , has the form:

$$[\bar{\bar{M}}_{90}, \mathbf{0}] = [-a^1 a_1 + a^2 a_1 + a^2 a_2, \mathbf{0}],$$

has a zero translation term because the reflection line passes through the origin of the reference frame. The operators of the other reflection lines have translation terms that are elements of the translation group; they are integer linear combinations of the basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ . For a line

$$M_{90B} \equiv [\bar{\bar{M}}_{90}, \mathbf{a}_1] = [-a^1 a_1 + a^2 a_1 + a^2 a_2, \mathbf{a}_1],$$

it is an ordinary reflection (no glide), in other cases it is a glide reflection of  $\frac{1}{2}(\mathbf{a}_1 + 2\mathbf{a}_2)$ , which is half the identity period along the glide line, or half the lattice parameter of the orthohexagonal cell. It is these reflection with glide:

$$M_{90S1} \equiv [\bar{\bar{M}}_{90}, \mathbf{a}_2] = [-a^1 a_1 + a^2 a_1 + a^2 a_2, \mathbf{a}_2],$$

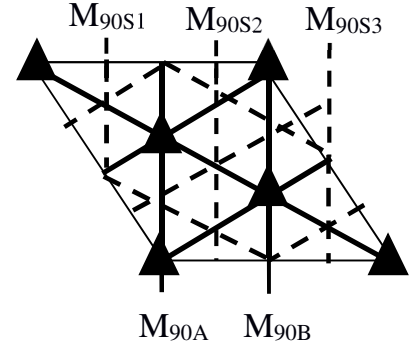
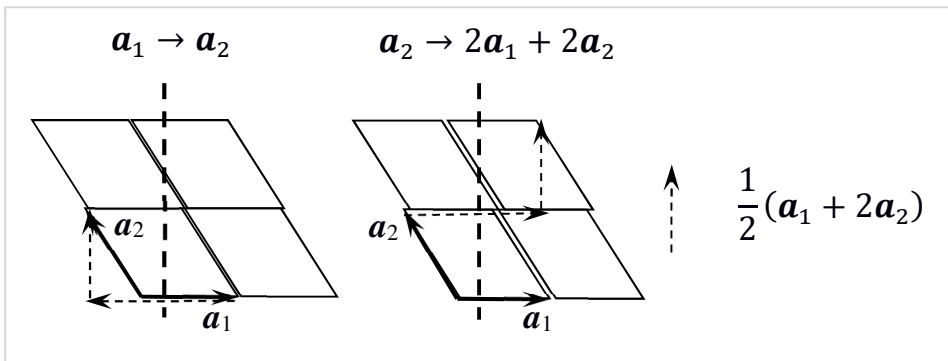
$$M_{90S2} \equiv [\bar{\bar{M}}_{90}, \mathbf{a}_1 + \mathbf{a}_2] = [-a^1 a_1 + a^2 a_1 + a^2 a_2, \mathbf{a}_1 + \mathbf{a}_2],$$

$$M_{90S3} \equiv [\bar{\bar{M}}_{90}, 2\mathbf{a}_1 + \mathbf{a}_2] = [-a^1 a_1 + a^2 a_1 + a^2 a_2, 2\mathbf{a}_1 + \mathbf{a}_2],$$

To verify the correctness of the expressions, we perform a transformation of several points in the glide line  $M_{90S2}$ . We compute how the position vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are transformed and show the transformation graphically:

$$\mathbf{a}_1 \cdot [\bar{\bar{M}}_{90}, \mathbf{a}_1 + \mathbf{a}_2] = \mathbf{a}_1 \cdot [-a^1 a_1 + a^2 a_1 + a^2 a_2, \mathbf{a}_1 + \mathbf{a}_2] = -a_1 + a_1 + a_2 = \mathbf{a}_2$$

$$\begin{aligned} \mathbf{a}_2 \cdot [\bar{\bar{M}}_{90}, \mathbf{a}_1 + \mathbf{a}_2] &= \mathbf{a}_2 \cdot [-a^1 a_1 + a^2 a_1 + a^2 a_2, \mathbf{a}_1 + \mathbf{a}_2] = \\ &= \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_1 + \mathbf{a}_2 = 2\mathbf{a}_1 + 2\mathbf{a}_2. \end{aligned}$$



## D29 Basic information on groups

### Definition

Let  $G$  be a set containing elements  $g_1, g_2, \dots$ , on which a **binary operation** is defined, i.e., an operation that assigns another element to two elements  $g_i, g_j$  with a given order. A set  $G$  with respect to a given operation forms a group if

- a) the set  $G$  is closed with respect to a given operation, i.e.  $g_i, g_j \in G$ , then also  $g_i \cdot g_j = g_k \in G$  (the dot between the elements of the group denotes the corresponding binary operation)
- b) for a given operation, the associative law holds
- c) there exists a **neutral element**  $e$  in the set  $G$  for which  $e \cdot g = g \cdot e = g$  for every  $g \in G$
- d) for each element  $g$  of the set  $G$ , there exists an **inverse element** in  $G$  – denoted  $g^{-1}$  – for which  $g \cdot g^{-1} = e$ .

For a binary operation, the commutative law need not hold.

### A group is, for example

- a) the set of all integers with respect to addition,
- b) the set of all vectors in  $n$ -dimensional space with respect to addition
- c) the set of complex numbers  $\exp(2\pi i \cdot 0/4), \exp(2\pi i \cdot 1/4), \exp(2\pi i \cdot 2/4), \exp(2\pi i \cdot 3/4)$ , with respect to multiplication, if the numbers  $\exp(2\pi i \cdot k/4)$  and  $\exp(2\pi i \cdot (k + 4N)/4)$  are considered equal ( $N$  is an integer)
- d) the set of rotations of the square about the centre by  $90^\circ, 180^\circ$  and  $270^\circ$ , together with the identical transformation, which has the meaning of a neutral element; a binary operation is the execution of two operations in succession.
- e) the set of all tensors (of the same order) with non-zero determinant, with respect to multiplication
- f) the two-element set  $\{1, -1\}$  with respect to multiplication.

The number of elements forming a group is called the **order of the group**. When a binary operation is applied on element itself, we use the notation  $g \cdot g = g^2, g^2 \cdot$

$g = g^3$ , etc., referring to powers of the element, regardless of the nature of the binary operation.

A **cyclic group** consists of all powers of some element of itself:  $a, a^2, a^3, \dots$ . The element whose powers yield the whole group is the **generating element** of the group.

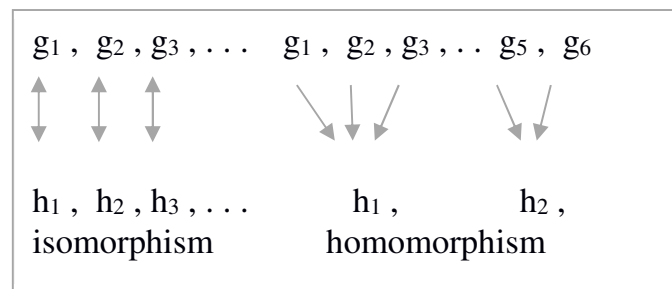
When expressing the elements of a group  $G$  explicitly, we write these in parentheses:

$G \equiv \{e, g_1, g_2, \dots, g_n\}$ , where  $n$  is the order of the group.

## Isomorphism and homomorphism

Two groups  $G$  and  $H$  are *isomorphic* if there exists a simple (mutually unambiguous) mapping of their elements  $g \leftrightarrow h$  such that if  $g_i \leftrightarrow h_i$  and  $g_k \leftrightarrow h_k$ , then  $g_i \cdot g_k \leftrightarrow h_i \cdot h_k$  as well. For example, the groups given as examples c) and d) are isomorphic.

Two groups  $G$  and  $H$  are *homomorphic* if these groups do not have the same number of elements, so that several elements of the more numerous group are associated with one element of the less numerous group, but subject to the condition: if  $g_i \leftrightarrow h_i$  and  $g_k \leftrightarrow h_k$ , then so too is  $g_i \cdot g_k \leftrightarrow h_i \cdot h_k$ . The following diagram shows these two possibilities:



## Subgroup

A subgroup  $H$  of a group  $G$  is any subset of  $G$  that satisfies the group postulates. For example, the group of rotations of  $0^\circ, 180^\circ$  is a subgroup of the group of rotations of  $0^\circ, 90^\circ, 180^\circ$  and  $270^\circ$ . The quotient of the order of the group and the order of the subgroup is called the **subgroup index**. Group  $G$  is a **supergroup** of group  $H$ .

## Cosets

Suppose that  $H \equiv \{e, h_1, h_2, \dots\}$  is a subgroup of group  $G$ . By the symbols  $x \cdot H$  and  $H \cdot x$  we mean the sets of elements

$$\begin{aligned} x \cdot H &= \{x \cdot e, x \cdot h_1, x \cdot h_2, \dots\}, \\ H \cdot x &= \{e \cdot x, h_1 \cdot x, h_2 \cdot x, \dots\} \end{aligned}$$

If an element  $x$  belongs to a subgroup  $H$ , then the above sets are identical to the subgroup  $H$ , which follows from the first group postulate. If  $x$  does not belong to  $H$ , the above sets are called the **right** and **left cosets**, respectively, of the group  $G$  with respect to the subgroup  $H$ . The coset  $x \cdot H$  has the same number of elements as the subgroup  $H$ , and these two sets do not have a single element in common. This means that if there is an element  $y$  in  $G$  that is neither in  $H$  nor in  $x \cdot H$ , there must be another coset of  $y \cdot H$ .

This is how group  $G$  can be decomposed into cosets

$$G = H + x \cdot H + y \cdot H + \dots = [e, x, y, \dots] \cdot H$$

$$G = H + H \cdot v + H \cdot z + \dots = H \cdot [e, v, z, \dots]$$

The elements in square brackets are the **representatives of cosets**; a coset can be represented by any of its elements.

### Conjugated elements and conjugated subgroups

Let us select two elements  $a, b$  from the group  $G$ . If for each element  $x$  of the group  $G$ ,  $x \cdot a = b \cdot x$ , that is,  $b = x \cdot a \cdot x^{-1}$ , then the elements  $a, b$  are called **conjugated**. Each group consists of several **classes of conjugated elements**. For example, for groups of symmetry operations, one class includes all rotations of the same angle.

If  $H$  is a subgroup of  $G$ , then the set of elements  $K = x \cdot H \cdot x^{-1}$  also forms a subgroup, which is called the conjugated subgroup with the subgroup of  $H$ . A subgroup of  $H$  that is conjugated with itself, i.e.,  $x \cdot H \cdot x^{-1} = H$ , is an **invariant subgroup** of  $G$ , or also a **normal divisor**. An invariant subgroup has right and left cosets equal. Therefore, a subgroup with index 2 is always invariant.

### Factor group

The invariant subgroup together with its cosets forms a special group whose elements are the cosets as wholes, with the role of the neutral element being played by the invariant subgroup itself. We call such a special group a **factor group**. The group operation between two cosets is the product of each element of one coset with each element of the other coset. The "product" of the cosets is then another coset, which can be expressed by the relation

$$x \cdot H \cdot y \cdot H = x \cdot y \cdot H \cdot H = z \cdot H,$$

whereby we have exploited the validity of the relations  $x \cdot y = z$ ,  $H \cdot H = H$ .

This procedure can be used to verify that the invariant subgroup, together with its cosets, satisfies all four group postulates. The factor group at the group  $G$ , constructed according to the subgroup  $H$ , is denoted by the symbol  $(G/H)$ .

The invariant subgroup of the space group of a crystal is the translation group. Elements of the point group of a crystal can be chosen as representatives of cosets (but not for all space groups), so that a factor group with a finite number of elements can represent a space group of a crystal that has an infinite number of elements.

### The direct product of groups

If there is the same group operation in the groups  $H$  and  $K$ , if for each  $h \in H$  and  $k \in K$ ,  $h \cdot k = k \cdot h$ , and if the only common element of these groups is the neutral element  $e$ , then the set of all elements  $g_{ij} = h_i \cdot k_j$  forms a group  $G$ , with the groups  $H$  and  $K$  being invariant subgroups of it. The order of the group  $G$  is equal to the product of the orders of the groups  $H$  and  $K$ , which means that no two elements of  $g_{ij}$  are equal. Accordingly, a group  $G$  with an invariant subgroup  $H$  can be expressed as the direct product of a subgroup  $H$  and a factor group  $(G/H)$ :

$$G = H \cdot (G/H) = (G/H) \cdot H.$$

### D30 Basic information on tensors

- The set of ordered pairs of vectors  $A_1 B_1, A_2 B_2, \dots$  called **dyads**, can mediate a linear transformation of the space if we introduce the following operation:

$$\mathbf{r}^* = \mathbf{r} \cdot (A_1 B_1, A_2 B_2, \dots) = (\mathbf{r} \cdot A_1) B_1 + (\mathbf{r} \cdot A_2) B_2 + \dots, \quad (\text{D30.1})$$

where  $\mathbf{r}$  and  $\mathbf{r}^*$  are the original and transformed vectors, and the dot between the vectors represents the scalar product between the vectors. The set of dyads in parentheses is called the tensor and is denoted by the symbol  $\bar{\bar{\mathbf{T}}}$  (bold, standing type, with two lines), so we can write the relation (D30.1) in a more concise form

$$\mathbf{r}^* = \mathbf{r} \cdot \bar{\bar{\mathbf{T}}} \quad (\text{D30.2})$$

- With respect to the definitional relation (D30.1), we write the tensor  $\bar{\bar{\mathbf{T}}}$  in the form

$$\bar{\bar{\mathbf{T}}} = (\mathbf{A}_1\mathbf{B}_1 + \mathbf{A}_2\mathbf{B}_2 + \cdots) = \sum_i \mathbf{A}_i\mathbf{B}_i, \quad (\text{D30.3})$$

where the + sign has only a symbolic meaning, because tensor algebra does not introduce a sum of dyads.

- We call the operation  $\mathbf{r} \cdot \bar{\bar{\mathbf{T}}}$  the **left scalar product** of a vector and a tensor. The **right scalar product** is introduced by the relation

$$\mathbf{r}^{**} = \bar{\bar{\mathbf{T}}} \cdot \mathbf{r} = \mathbf{A}_1(\mathbf{B}_1 \cdot \mathbf{r}) + \mathbf{A}_2(\mathbf{B}_2 \cdot \mathbf{r}) + \dots \quad (\text{D30.4})$$

so that the left and right scalar products of a vector with the same tensor need not be the same.

- If we swap the order of the vectors in all the dyads of the tensor

$$\bar{\bar{\mathbf{T}}} = \sum_i \mathbf{A}_i\mathbf{B}_i, \text{ a } \mathbf{conjugated tensor} \bar{\bar{\mathbf{T}}}_c \text{ is formed}$$

$$\bar{\bar{\mathbf{T}}}_c = \sum_i \mathbf{B}_i\mathbf{A}_i \quad (\text{D30.5})$$

- From relations (D30.1) and (D30.4) it follows that

$$\mathbf{r} \cdot \bar{\bar{\mathbf{T}}} = \bar{\bar{\mathbf{T}}}_c \cdot \mathbf{r} \quad (\text{D30.6})$$

- **Two tensors** are said to **be equal** if their left (or right) scalar products with any vector are equal to each other.
- The **scalar product of tensors**  $\bar{\bar{\mathbf{T}}} \cdot \bar{\bar{\mathbf{U}}}$  is introduced by two transformations in succession:

$$\mathbf{r}^* = \mathbf{r} \cdot \bar{\bar{\mathbf{T}}}$$

$$\mathbf{r}^{**} = \mathbf{r}^* \cdot \bar{\bar{\mathbf{U}}} = (\mathbf{r} \cdot \bar{\bar{\mathbf{T}}}) \cdot \bar{\bar{\mathbf{U}}} = \mathbf{r} \cdot (\bar{\bar{\mathbf{T}}} \cdot \bar{\bar{\mathbf{U}}}).$$

If we write the tensors in the form

$$\bar{\bar{\mathbf{T}}}_c = \sum_i \mathbf{A}_i\mathbf{B}_i, \quad \bar{\bar{\mathbf{U}}} = \sum_j \mathbf{C}_j\mathbf{D}_j$$

then for the product of tensors introduced in this way holds

$$\bar{\bar{\mathbf{T}}}_c \cdot \bar{\bar{\mathbf{U}}} = \sum_i \sum_j \mathbf{A}_i (\mathbf{B}_i \cdot \mathbf{C}_j) \mathbf{D}_j \quad (\text{D30.7})$$

- The unit tensor  $\bar{\bar{\mathbf{I}}}$ , called the **identity tensor**, is introduced by the relation  $\mathbf{r} \cdot \bar{\bar{\mathbf{I}}} = \mathbf{r}$  valid for all vectors.
- The **reciprocal (inverse)** tensor  $\bar{\bar{\mathbf{T}}}^{-1}$  to the tensor  $\bar{\bar{\mathbf{T}}}$  is introduced so that

$$\bar{\bar{\mathbf{T}}}^{-1} \cdot \bar{\bar{\mathbf{T}}} = \bar{\bar{\mathbf{I}}} = \bar{\bar{\mathbf{T}}} \cdot \bar{\bar{\mathbf{T}}}^{-1}. \quad (\text{D30.8})$$

It exists if and only if the determinant of the tensor  $\mathbf{T}$  does not equal zero.

- A tensor  $\bar{\bar{\mathbf{T}}}$  is symmetric if for each vector  $\mathbf{r}$  :  $\mathbf{r} \cdot \bar{\bar{\mathbf{T}}} = \bar{\bar{\mathbf{T}}} \cdot \mathbf{r}$ .
- The scalar  $T_S$  of the tensor  $\bar{\bar{\mathbf{T}}}$  is a number which we obtain using the relation

$$T_S = \sum_i (\mathbf{A}_i \cdot \mathbf{B}_i), \quad (\text{D30.9})$$

that is, by performing a scalar product between the vectors in all dyads. and then summing the scalars.

- The dyad vectors can be expressed in a coordinate system of three non-complanar basis vectors  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ , as their linear combination:

$$\begin{aligned} \bar{\bar{\mathbf{T}}} &= \sum_i (\mathbf{A}_i \mathbf{B}_i) = \sum_i \left( \sum_j A_{ij} \mathbf{a}_j \right) \mathbf{B}_i = \sum_j \mathbf{a}_j \left( \sum_i A_{ij} \mathbf{B}_i \right) = \sum_j \mathbf{a}_j \mathbf{C}_j \\ \bar{\bar{\mathbf{T}}} &= \mathbf{a}_1 \mathbf{C}_1 + \mathbf{a}_2 \mathbf{C}_2 + \mathbf{a}_3 \mathbf{C}_3 . \end{aligned}$$

A tensor consisting of any number of dyads can be reduced to three dyads in three-dimensional space (two dyads in the plane). The vectors  $\mathbf{C}_j$  are the **right vector coordinates** of the tensor.

Similarly, the vectors  $\mathbf{B}_i$ , can be decomposed and the same tensor can be written using the **left vector coordinates**.

$$\bar{\bar{\mathbf{T}}} = \mathbf{D}_1 \mathbf{a}_1 + \mathbf{D}_2 \mathbf{a}_2 + \mathbf{D}_3 \mathbf{a}_3 . \quad (\text{D30.10})$$

- The determinant of a tensor is defined as the product of the mixed products of the basis vectors and the vector coordinates of the tensor:

$$|\bar{\bar{\mathbf{T}}}| = [(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3] [(\mathbf{C}_1 \times \mathbf{C}_2) \cdot \mathbf{C}_3] = [(\mathbf{D}_1 \times \mathbf{D}_2) \cdot \mathbf{D}_3] [(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3] \quad (\text{D30.11})$$

If the determinant of the tensor equals zero, it is an **incomplete tensor**. That is, zero equals the mixed product of vector coordinates, i.e. the vectors  $\mathbf{C}_i$ , respectively  $\mathbf{D}_i$  lie in the same plane (then it is a **planar tensor**), or they are all parallel (a **linear tensor**). A planar tensor can be expressed by a pair of dyads, a linear one by a single dyad.

- The tensor notation can be further modified so that the vector coordinates are also expressed as linear combinations of the basis vectors. This produces a nine-membered

$$\begin{aligned} \bar{\bar{\mathbf{T}}} = & t^{11} \mathbf{a}_1 \mathbf{a}_1 + t^{12} \mathbf{a}_1 \mathbf{a}_2 + t^{13} \mathbf{a}_1 \mathbf{a}_3 + \\ & + t^{21} \mathbf{a}_2 \mathbf{a}_1 + t^{22} \mathbf{a}_2 \mathbf{a}_2 + t^{23} \mathbf{a}_2 \mathbf{a}_3 + \\ & + t^{31} \mathbf{a}_3 \mathbf{a}_1 + t^{32} \mathbf{a}_3 \mathbf{a}_2 + t^{33} \mathbf{a}_3 \mathbf{a}_3 = \sum_{ij} t^{ij} \mathbf{a}_i \mathbf{a}_j \end{aligned} \quad (\text{D30.12})$$

Where  $t^{ij}$  are the so-called **scalar coordinates** of the tensor (inappropriately, the components of the tensor). It is often more convenient to express the left vector coordinates  $\mathbf{D}_i$  as a linear combination of a triple of reciprocal vectors  $\mathbf{a}^1, \mathbf{a}^2, \mathbf{a}^3$ , thus changing the notation of the tensor and expressing it as a symbolic sum of dyads, with *mixed coordinates*:

$$\bar{\bar{\mathbf{T}}} = \sum_{ij} t_{ij}^j \mathbf{a}^i \mathbf{a}_j . \quad (\text{D30.13})$$

The coordinates  $t^{ij}$  and  $t_i^j$  are not the same. In this text only mixed coordinates are used, but for simplicity they are written with subscripts. A tensor using scalar coordinates will be written in the form

$$\bar{\bar{\mathbf{T}}} = \sum_{ij} t_{ij} \mathbf{a}^i \mathbf{a}_j . \quad (\text{D30.14})$$

- When tensor notation of the form (D30.14) is used, some tensors take on a more specific shape.

#### Conjugate tensor

$$\bar{\bar{\mathbf{T}}}_c = \sum_{ij} t_{ij} \mathbf{a}_j \mathbf{a}^i ,$$

#### Identity tensor

$$\bar{\bar{\mathbf{I}}} = \mathbf{a}^1 \mathbf{a}_1 + \mathbf{a}^2 \mathbf{a}_2 + \mathbf{a}^3 \mathbf{a}_3$$

For a **symmetric tensor**

$$t_{ij} = t_{ji} ,$$

and for the **determinant of tensor**

$$|\bar{\bar{\mathbf{T}}}| = \begin{vmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{vmatrix} .$$

The **scalar of tensor** is expressed by the relation

$$T_S = t_{11} + t_{22} + t_{33} .$$

The **tensor coordinates** are obtained by the double scalar product

$$t_{ij} = \mathbf{a}_i \cdot \bar{\bar{\mathbf{T}}} \cdot \mathbf{a}^j \quad (\text{D30.15})$$

- For the product of several tensors, the relations are valid

$$(\bar{\bar{\mathbf{T}}} \cdot \bar{\bar{\mathbf{U}}} \cdot \bar{\bar{\mathbf{V}}} \cdot \dots)_c = \dots \cdot \bar{\bar{\mathbf{V}}}_c \cdot \bar{\bar{\mathbf{U}}}_c \cdot \bar{\bar{\mathbf{T}}}_c ,$$

$$(\bar{\bar{\mathbf{T}}} \cdot \bar{\mathbf{U}} \cdot \bar{\mathbf{V}} \cdot \dots)^{-1} = \dots \cdot \bar{\mathbf{V}}^{-1} \cdot \bar{\mathbf{U}}^{-1} \cdot \bar{\bar{\mathbf{T}}}^{-1} ,$$

and for the determinant of the product of two tensors

$$|\bar{\bar{\mathbf{T}}} \cdot \bar{\mathbf{U}}| = |\bar{\bar{\mathbf{T}}}| |\bar{\mathbf{U}}| \quad (\text{D30.16})$$

- The tensors of symmetry operations must preserve all distances and angles in the linear transformation, i.e. the scalar product of any two vectors

$$\mathbf{r}_1^* \cdot \mathbf{r}_2^* = (\mathbf{r}_1 \cdot \bar{\bar{\mathbf{T}}}) \cdot (\mathbf{r}_2 \cdot \bar{\bar{\mathbf{T}}}) = (\mathbf{r}_1 \cdot \bar{\bar{\mathbf{T}}}) \cdot (\bar{\bar{\mathbf{T}}}_c \cdot \mathbf{r}_2) = \mathbf{r}_1 \cdot \mathbf{r}_2 ,$$

which implies that the equality  $\bar{\bar{\mathbf{T}}} \cdot \bar{\bar{\mathbf{T}}}_c = \bar{\bar{\mathbf{I}}}$  should hold. That is, the conjugate tensor  $\bar{\bar{\mathbf{T}}}_c$  must be simultaneously an inverse tensor:

$$\bar{\bar{\mathbf{T}}}_c = \bar{\bar{\mathbf{T}}}^{-1} .$$

For the product of determinants by (D30.16),  $|\bar{\bar{\mathbf{T}}}| |\bar{\bar{\mathbf{T}}}_c| = |\bar{\bar{\mathbf{I}}}| = 1$ , and since the determinants of the tensor and its conjugate tensor are the same,  $|\bar{\bar{\mathbf{T}}}|^2 = 1$ . This means that the determinant of the tensor, which preserves all lengths and angles in the transformation, is equal to

$$|\bar{\bar{\mathbf{T}}}| = \pm 1 . \quad (\text{D30.17})$$

- In in-plane transformations, the full tensor consists of two dyads and can be written using vector coordinates

$$\bar{\bar{\mathbf{T}}} = \mathbf{D}_1 \mathbf{a}_1 + \mathbf{D}_2 \mathbf{a}_2 ,$$

or by scalar coordinates

$$\bar{\bar{\mathbf{T}}} = t_{11} \mathbf{a}^1 \mathbf{a}_1 + t_{12} \mathbf{a}^1 \mathbf{a}_2 + t_{21} \mathbf{a}^2 \mathbf{a}_1 + t_{22} \mathbf{a}^2 \mathbf{a}_2 .$$

With such a tensor notation, the left scalar product with, e.g., the vector  $\mathbf{a}_1$ , based on relation A1.2, i.e.,  $\mathbf{a}_i \cdot \mathbf{a}^j = \delta_{ij}$ , gives the result:

$$\mathbf{a}_1 \cdot \bar{\bar{\mathbf{T}}} = \mathbf{a}_1 \cdot (t_{11} \mathbf{a}^1 \mathbf{a}_1 + t_{12} \mathbf{a}^1 \mathbf{a}_2 + t_{21} \mathbf{a}^2 \mathbf{a}_1 + t_{22} \mathbf{a}^2 \mathbf{a}_2) = t_{11} \mathbf{a}_1 + t_{12} \mathbf{a}_2 \quad (\text{D30.18})$$

## Tables

| TA1     | Plane lattices, crystal systems and point symmetry |           |                                         |                |
|---------|----------------------------------------------------|-----------|-----------------------------------------|----------------|
| Lattice | Crystal systems                                    | Cell type | Basis vectors                           | Point symmetry |
| a)      | oblique                                            | $p$       | $a_1 \neq a_2$ , $\alpha \neq 90^\circ$ | 2              |
| b)      | rectangular                                        | $p$       | $a_1 \neq a_2$ , $\alpha = 90^\circ$    | $2mm$          |
| c), d)  |                                                    | $c$       |                                         |                |
| e)      | square                                             | $p$       | $a_1 = a_2$ , $\alpha = 90^\circ$       | $4mm$          |
| f)      | hexagonal                                          | $p$       | $a_1 = a_2$ , $\alpha = 120^\circ$      | $6mm$          |

| TA2             | Point groups in crystal systems  |                                           |
|-----------------|----------------------------------|-------------------------------------------|
| Crystal systems | Point groups belonging to system | Point group of lattice (holohedral group) |
| oblique         | 1, 2                             | 2                                         |
| rectangular     | $m$ , $2mm$                      | $2mm$                                     |
| square          | 4, $4mm$                         | $4mm$                                     |
| hexagonal       | 3, $3m$ , 6 , $6mm$              | $6mm$                                     |

| TA3          | Plane symmetry groups |                   |             |             |              |
|--------------|-----------------------|-------------------|-------------|-------------|--------------|
| Group number | Crystal system        | Type of unit cell | Point group | Symbol full | Symbol short |
| 1            | oblique               | $p$               | 1           | $p1$        | $p1$         |
| 2            |                       |                   | 2           | $p211$      | $p2$         |
| 3            | rectangular           | $p$               | $m$         | $p1m1$      | $pm$         |
| 4            |                       |                   |             | $p1g1$      | $pg$         |
| 5            |                       | $c$               |             | $c1m1$      | $cm$         |
| 6            |                       | $p$               | $2mm$       | $p2mm$      | $pmm$        |
| 7            |                       |                   |             | $p2mg$      | $pmg$        |
| 8            |                       |                   |             | $p2gg$      | $pgg$        |
| 9            |                       | $c$               |             | $c2mm$      | $cmm$        |
| 10           | square                | $p$               | 4           | $p4$        | $p4$         |
| 11           |                       |                   | $4mm$       | $p4mm$      | $p4m$        |
| 12           |                       |                   |             | $p4gm$      | $p4g$        |
| 13           | hexagonal             | $p$               | 3           | $p3$        | $p3$         |
| 14           |                       |                   | $3m$        | $p3m1$      | $p3m1$       |
| 15           |                       |                   |             | $p31m$      | $p31m$       |
| 16           |                       |                   | 6           | $p6$        | $p6$         |
| 17           |                       |                   | $6mm$       | $p6mm$      | $p6m$        |

| TA4            | Lattices and point groups of three-dimensional structures                                                                                                     |                                |                                                                                         |
|----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------|-----------------------------------------------------------------------------------------|
| Crystal system | Lattice parameters                                                                                                                                            | Lattice type                   | Point groups                                                                            |
| Triclinic      | $a_1, a_2, a_3$<br>$\alpha_1, \alpha_2, \alpha_3$                                                                                                             | P                              | $1, \bar{1}$                                                                            |
| Monoclinic     | $a_1, a_2, a_3$<br>$\alpha_1 = \alpha_3 = 90^\circ, \alpha_2$                                                                                                 | P<br>( $C_1, C_3, I$ )         | $2, m, \frac{2}{m}$                                                                     |
| Orthorhombic   | $a_1, a_2, a_3$<br>$\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$                                                                                                | P, I, F<br>( $C_1, C_2, C_3$ ) | $222, mm2, \frac{2}{m} \frac{2}{m} \frac{2}{m}$                                         |
| Tetragonal     | $a_1 = a_2, a_3$<br>$\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$                                                                                               | P, I                           | $4, \bar{4}, \frac{4}{m}, 422$<br>$4mm, \bar{4}2m, \frac{4}{m} \frac{2}{m} \frac{2}{m}$ |
| Trigonal       | $a_1 = a_2 = a_3$<br>$\alpha_1 = \alpha_2 = \alpha_3 \neq 90^\circ$<br>or:<br>$a_1 = a_2, a_3$<br>$\alpha_1 = \alpha_2 = 90^\circ,$<br>$\alpha_3 = 120^\circ$ | R<br><br>P                     | $3, \bar{3}, 32, 3m, \bar{3} \frac{2}{m}$                                               |
| Hexagonal      | $a_1 = a_2, a_3$<br>$\alpha_1 = \alpha_2 = 90^\circ,$<br>$\alpha_3 = 120^\circ$                                                                               | P                              | $6, \bar{6}, \frac{6}{m}, 622$<br>$6mm, \bar{6}2m, \frac{6}{m} \frac{2}{m} \frac{2}{m}$ |
| Cubic          | $a_1 = a_2 = a_3$<br>$\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$                                                                                              | P, I, F                        | $23, \frac{2}{m} \bar{3}, 432$<br>$\bar{4}3m, \frac{4}{m} \bar{3} \frac{2}{m}$          |

| TA5        | Numbers in planar and spatial structures |               |              |                    |
|------------|------------------------------------------|---------------|--------------|--------------------|
| Structures | Crystal systems                          | Lattice types | Point groups | Plane/Space groups |
| planar     | 4                                        | 5             | 10           | 17                 |
| spatial    | 7                                        | 14            | 32           | 230                |

| TC1          | Allowed rotations and their groups           |                                  |
|--------------|----------------------------------------------|----------------------------------|
| Group symbol | Elements of groups<br>(rotations in degrees) | Generating elements<br>(tensors) |
| 1            | 0                                            | $I (\bar{1})$                    |
| 2            | 0, 180                                       | $2 (\bar{2})$                    |
| 3            | 0, 120, 240                                  | $3 (\bar{3})$                    |
| 4            | 0, 90, 180, 270                              | $4 (\bar{4})$                    |
| 6            | 0, 60, 120, 180, 240, 300                    | $6 (\bar{6})$                    |

| TC2a      | Tensors of generating elements of cyclic point groups                                                                                                                                                                                                                                                               |
|-----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $\bar{1}$ | $\bar{1} = a^1 a_1 + a^2 a_2 .$                                                                                                                                                                                                                                                                                     |
| $\bar{2}$ | $\bar{2} = -a^1 a_1 - a^2 a_2 = -\bar{1} .$                                                                                                                                                                                                                                                                         |
| $\bar{3}$ | $\bar{3} = a^1 a_1 \left( -\frac{1}{2} - \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \right) + a^1 a_2 \frac{a_1 \sqrt[2]{3}}{a_2} \frac{1}{2 \sin \alpha} - a^2 a_1 \frac{a_2 \sqrt[2]{3}}{a_1} \frac{1}{2 \sin \alpha}$ $+ a^2 a_2 \left( -\frac{1}{2} + \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \right)$ |
| $\bar{4}$ | $\bar{4} = -a^1 a_1 \frac{\cos \alpha}{\sin \alpha} + a^1 a_2 \frac{a_1}{a_2} \frac{1}{\sin \alpha} - a^2 a_1 \frac{a_2}{a_1} \frac{1}{\sin \alpha} + a^2 a_2 \frac{\cos \alpha}{\sin \alpha}$                                                                                                                      |
| $\bar{6}$ | $\bar{6} = a^1 a_1 \left( +\frac{1}{2} - \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \right) + a^1 a_2 \frac{a_1 \sqrt[2]{3}}{a_2} \frac{1}{2 \sin \alpha} - a^2 a_1 \frac{a_2 \sqrt[2]{3}}{a_1} \frac{1}{2 \sin \alpha}$ $+ a^2 a_2 \left( +\frac{1}{2} + \frac{\sqrt[2]{3} \cos \alpha}{2 \sin \alpha} \right)$ |

| TC2b                                      |
|-------------------------------------------|
| $\bar{1} = a^1 a_1 + a^2 a_2$             |
| $\bar{2} = -a^1 a_1 - a^2 a_2 = -\bar{1}$ |
| $\bar{3} = a^1 a_2 - a^2 a_1 - a^2 a_2$   |
| $\bar{4} = a^1 a_2 - a^2 a_1$             |
| $\bar{6} = a^1 a_1 + a^1 a_2 - a^2 a_1$   |

| TC3               | Possible symmetry operations   |                     |                 |
|-------------------|--------------------------------|---------------------|-----------------|
| $[\bar{\Phi}, t]$ | Restrictions on translation    | Name of operation   | Operations      |
| $[\bar{1}, t]$    | $t = 0$                        | identity            | closed proper   |
| $[\bar{2}, t]$    | no                             | rotation            |                 |
| $[\bar{3}, t]$    | no                             | rotation            |                 |
| $[\bar{4}, t]$    | no                             | rotation            |                 |
| $[\bar{6}, t]$    | no                             | rotation            |                 |
| $[\bar{M}, t]$    | $t - (t \cdot u)u = 0$         | reflection          | closed improper |
| $[\bar{M}, t]$    | $t - (t \cdot u)u = \pm b_1/2$ | glide reflection    | open operations |
| $[\bar{1}, t]$    | $t = A_L \neq 0$               | lattice translation |                 |

| TC4                     | Point groups and their elements                                           |                     |
|-------------------------|---------------------------------------------------------------------------|---------------------|
| Group symbols           | Group elements                                                            | Generating elements |
| <b>1</b>                | $e$                                                                       | $e$                 |
| <b>2</b>                | $e, 2$                                                                    | $2$                 |
| <b>3</b>                | $e, 3, 3^2$                                                               | $3$                 |
| <b>4</b>                | $e, 4, 4^2, 4^3$                                                          | $4$                 |
| <b>6</b>                | $e, 6, 6^2, 6^3, 6^4, 6^5$                                                | $6$                 |
| <b><math>m</math></b>   | $e, m$                                                                    | $m$                 |
| <b><math>2mm</math></b> | $e, 2, m_x, m_y$                                                          | $2, m$              |
| <b><math>3m</math></b>  | $e, 3, 3^2, m_0, m_{60}, m_{120}$                                         | $3, m$              |
| <b><math>4mm</math></b> | $e, 4, 4^2, 4^3, m_x, m_y, m_{xy}, m_{yx}$                                | $4, m$              |
| <b><math>6mm</math></b> | $e, 6, 6^2, 6^3, 6^4, 6^5, m_0, m_{60}, m_{120}, m_{30}, m_{90}, m_{150}$ | $6, m$              |

| Table C9.2              |              |                                                                                              |
|-------------------------|--------------|----------------------------------------------------------------------------------------------|
| Group symbols           | Group number | Black-white point groups                                                                     |
| <b>1</b>                |              | has no subgroup                                                                              |
| <b>2</b>                | 1            | $\{e, 2^*\}$                                                                                 |
| <b><math>m</math></b>   | 2            | $\{e, m^*\}$                                                                                 |
| <b><math>2mm</math></b> | 3            | $\{e, 2, m_x^*, m_y^*\},$                                                                    |
|                         | 4            | $\{e, m_x, 2^*, m_y^*\}$                                                                     |
| <b>3</b>                |              | has no subgroup with index 2                                                                 |
| <b><math>3m</math></b>  | 5            | $\{e, 3, 3^2, m_0^*, m_{60}^*, m_{120}^*\}$                                                  |
| <b>4</b>                | 6            | $\{e, 4^2, 4^*, 4^{3*}\}$                                                                    |
| <b><math>4mm</math></b> | 7            | $\{e, 4, 4^2, 4^3, m_x^*, m_y^*, m_{xy}^*, m_{yx}^{*'}\}$                                    |
|                         | 8            | $\{e, 4^2, m_x, m_y, 4^*, 4^{3*}, m_{xy}^*, m_{yx}^*\}$                                      |
|                         | 9            | $\{e, 4^2, m_{xy}, m_{yx}, 4^*, 4^{3*}, m_x^*, m_y^*\}$                                      |
| <b>6</b>                | 10           | $\{e, 6^2, 6^4, 6^*, 6^{3*}, 6^{5*}\}$                                                       |
| <b><math>6mm</math></b> | 11           | $\{e, 6, 6^2, 6^3, 6^4, 6^5, m_0^*, m_{30}^*, m_{60}^*, m_{90}^*, m_{120}^*, m_{150}^*\}$    |
|                         | 12           | $\{e, 6^2, 6^4, m_0, m_{60}, m_{120}, 6^*, 6^{3*}, 6^{5*}, m_{30}^*, m_{90}^*, m_{150}^*\}$  |
|                         | 13           | $\{e, 6^2, 6^4, m_{30}, m_{90}, m_{150}, 6^*, 6^{3*}, 6^{5*}, m_0^*, m_{60}^*, m_{120}^*\}.$ |

### TC5 Multiplication tables

| Group 2mm |       |       |       |       |
|-----------|-------|-------|-------|-------|
|           | $e$   | 2     | $m_x$ | $m_y$ |
| $e$       | $e$   | 2     | $m_x$ | $m_y$ |
| 2         | 2     | $e$   | $m_y$ | $m_x$ |
| $m_x$     | $m_x$ | $m_y$ | $e$   | 2     |
| $m_y$     | $m_y$ | $m_x$ | 2     | $e$   |

| Group 3m  |           |           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|           | $e$       | 3         | $3^2$     | $m_0$     | $m_{60}$  | $m_{120}$ |
| $e$       | $e$       | 3         | $3^2$     | $m_0$     | $m_{60}$  | $m_{120}$ |
| 3         | 3         | $3^2$     | $e$       | $m_{120}$ | $m_0$     | $m_{60}$  |
| $3^2$     | $3^2$     | $e$       | 3         | $m_{60}$  | $m_{120}$ | $m_0$     |
| $m_0$     | $m_0$     | $m_{60}$  | $m_{120}$ | $e$       | 3         | $3^2$     |
| $m_{60}$  | $m_{60}$  | $m_{120}$ | $m_0$     | $3^2$     | $e$       | 3         |
| $m_{120}$ | $m_{120}$ | $m_0$     | $m_{60}$  | 3         | $3^2$     | $e$       |

| Group 4mm |          |          |          |          |          |          |          |          |
|-----------|----------|----------|----------|----------|----------|----------|----------|----------|
|           | $e$      | 4        | $4^2$    | $4^3$    | $m_x$    | $m_{xy}$ | $m_y$    | $m_{yx}$ |
| $e$       | $e$      | 4        | $4^2$    | $4^3$    | $m_x$    | $m_{xy}$ | $m_y$    | $m_{yx}$ |
| 4         | 4        | $4^2$    | $4^3$    | $e$      | $m_{yx}$ | $m_x$    | $m_{xy}$ | $m_y$    |
| $4^2$     | $4^2$    | $4^3$    | $e$      | 4        | $m_y$    | $m_{yx}$ | $m_x$    | $m_{xy}$ |
| $4^3$     | $4^3$    | $e$      | 4        | $4^2$    | $m_{xy}$ | $m_y$    | $m_{yx}$ | $m_x$    |
| $m_x$     | $m_x$    | $m_{xy}$ | $m_y$    | $m_{yx}$ | $e$      | 4        | $4^2$    | $4^3$    |
| $m_{xy}$  | $m_{xy}$ | $m_y$    | $m_{yx}$ | $m_x$    | $4^3$    | $e$      | 4        | $4^2$    |
| $m_y$     | $m_y$    | $m_{yx}$ | $m_x$    | $m_{xy}$ | $4^2$    | $4^3$    | $e$      | 4        |
| $m_{yx}$  | $m_{yx}$ | $m_x$    | $m_{xy}$ | $m_y$    | 4        | $4^2$    | $4^3$    | $e$      |

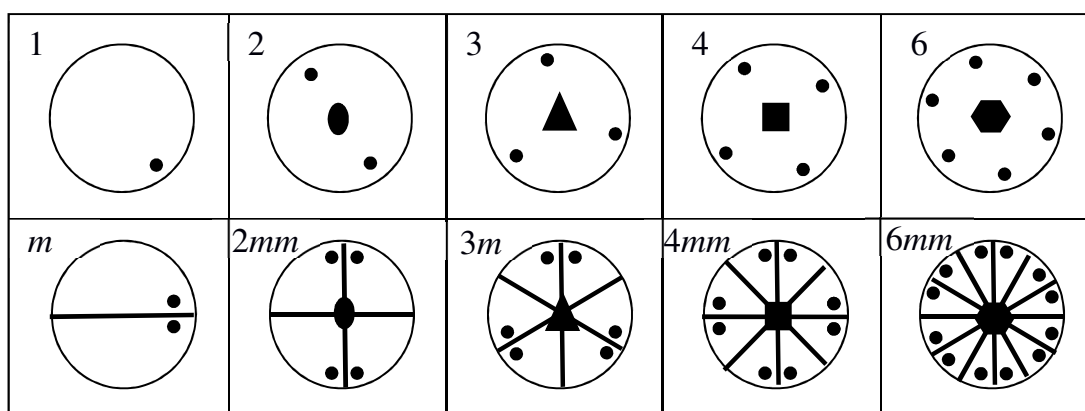
| Group 6mm |           |           |           |           |           |           |           |           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|           | $e$       | 6         | $6^2$     | $6^3$     | $6^4$     | $6^5$     | $m_0$     | $m_{30}$  | $m_{60}$  | $m_{90}$  | $m_{120}$ | $m_{150}$ |
| $e$       | $e$       | 6         | $6^2$     | $6^3$     | $6^4$     | $6^5$     | $m_0$     | $m_{30}$  | $m_{60}$  | $m_{90}$  | $m_{120}$ | $m_{150}$ |
| 6         | 6         | $6^2$     | $6^3$     | $6^4$     | $6^5$     | $e$       | $m_{150}$ | $m_0$     | $m_{30}$  | $m_{60}$  | $m_{90}$  | $m_{120}$ |
| $6^2$     | $6^2$     | $6^3$     | $6^4$     | $6^5$     | $e$       | 6         | $m_{120}$ | $m_{150}$ | $m_0$     | $m_{30}$  | $m_{60}$  | $m_{90}$  |
| $6^3$     | $6^3$     | $6^4$     | $6^5$     | $e$       | 6         | $6^2$     | $m_{90}$  | $m_{120}$ | $m_{150}$ | $m_0$     | $m_{30}$  | $m_{60}$  |
| $6^4$     | $6^4$     | $6^5$     | $e$       | 6         | $6^2$     | $6^3$     | $m_{60}$  | $m_{90}$  | $m_{120}$ | $m_{150}$ | $m_0$     | $m_{30}$  |
| $6^5$     | $6^5$     | $e$       | 6         | $6^2$     | $6^3$     | $6^4$     | $m_{30}$  | $m_{60}$  | $m_{90}$  | $m_{120}$ | $m_{150}$ | $m_0$     |
| $m_0$     | $m_0$     | $m_{30}$  | $m_{60}$  | $m_{90}$  | $m_{120}$ | $m_{150}$ | $e$       | 6         | $6^2$     | $6^3$     | $6^4$     | $6^5$     |
| $m_{30}$  | $m_{30}$  | $m_{60}$  | $m_{90}$  | $m_{120}$ | $m_{150}$ | $m_0$     | $6^5$     | $e$       | 6         | $6^2$     | $6^3$     | $6^4$     |
| $m_{60}$  | $m_{60}$  | $m_{90}$  | $m_{120}$ | $m_{150}$ | $m_0$     | $m_{30}$  | $6^4$     | $6^5$     | $e$       | 6         | $6^2$     | $6^3$     |
| $m_{90}$  | $m_{90}$  | $m_{120}$ | $m_{150}$ | $m_0$     | $m_{30}$  | $m_{60}$  | $6^3$     | $6^4$     | $6^5$     | $e$       | 6         | $6^2$     |
| $m_{120}$ | $m_{120}$ | $m_{150}$ | $m_0$     | $m_{30}$  | $m_{60}$  | $m_{90}$  | $6^2$     | $6^3$     | $6^4$     | $6^5$     | $e$       | 6         |
| $m_{150}$ | $m_{150}$ | $m_0$     | $m_{30}$  | $m_{60}$  | $m_{90}$  | $m_{120}$ | 6         | $6^2$     | $6^3$     | $6^4$     | $6^5$     | $e$       |

## Figures

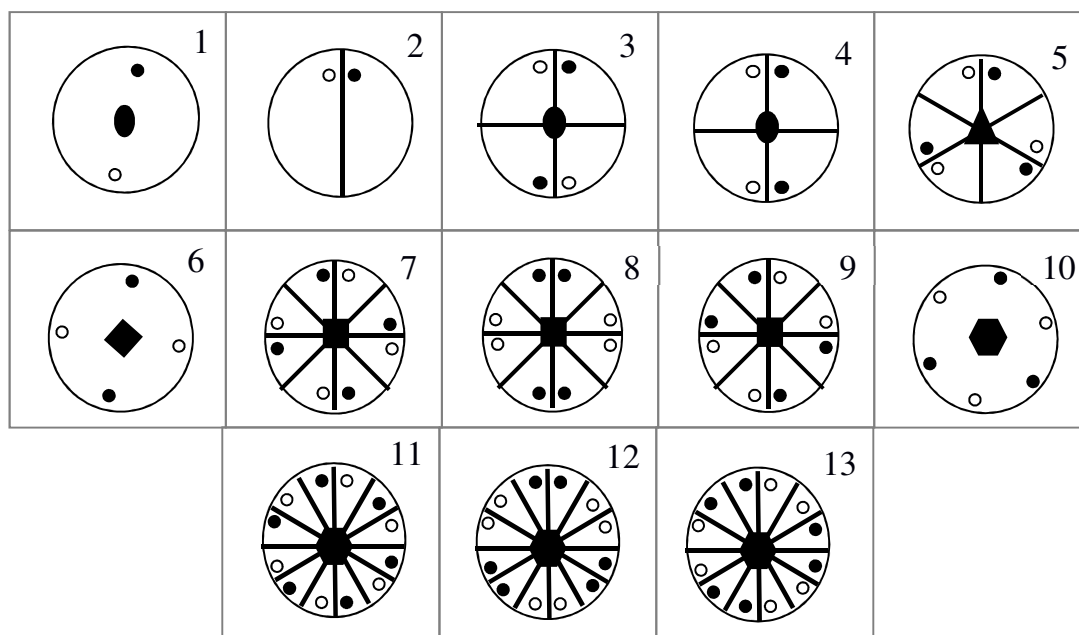
### Označenie prvkov súmernosti

|                                                                                   |                   |                                                                                   |                 |
|-----------------------------------------------------------------------------------|-------------------|-----------------------------------------------------------------------------------|-----------------|
|  | zrkadlová priamka |  | trojnásobná os  |
|  | sklzná priamka    |  | štvornásobná os |
|  | dvojnásobná os    |  | šesťnásobná os  |

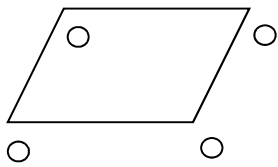
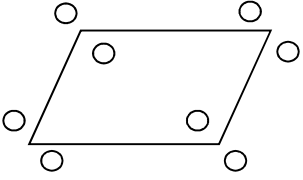
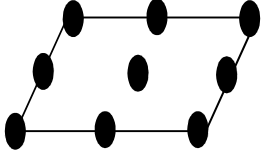
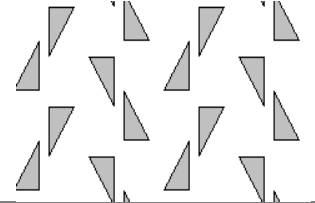
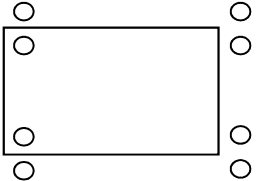
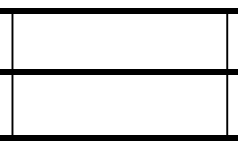
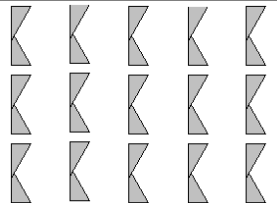
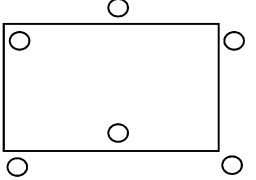
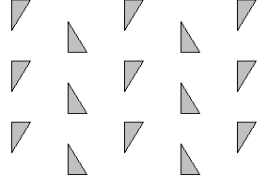
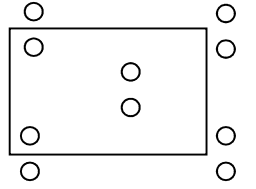
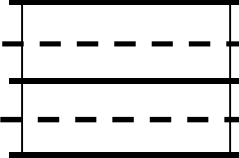
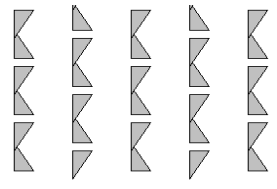
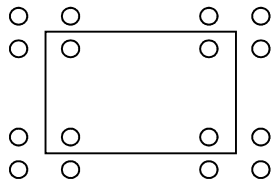
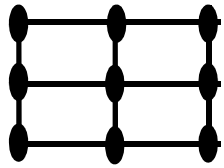
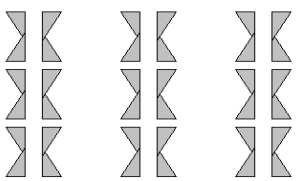
## Single-chrome point groups

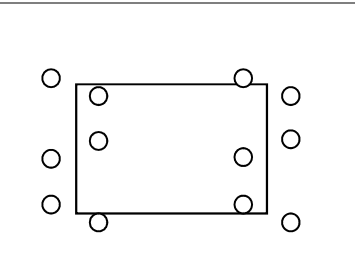
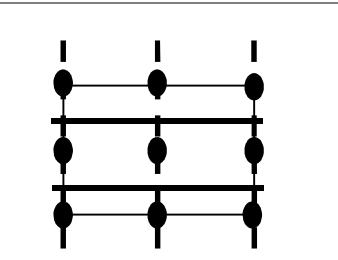
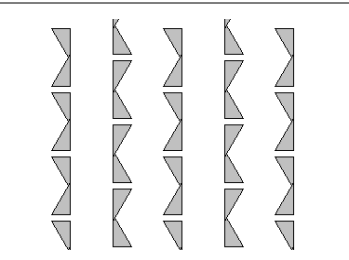
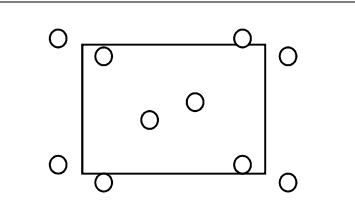
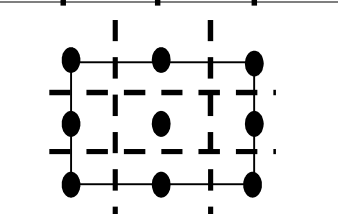
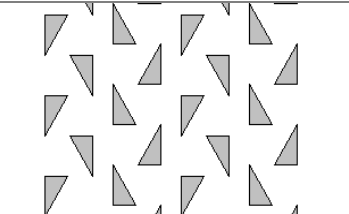
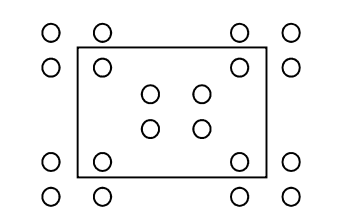
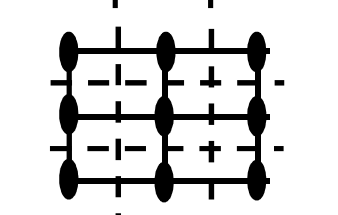
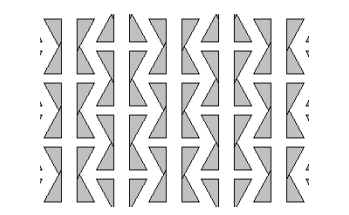
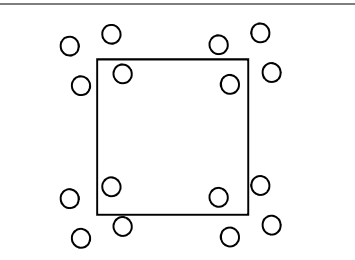
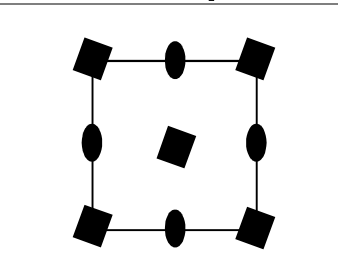
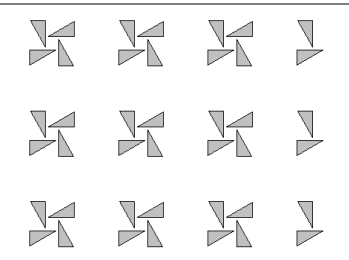
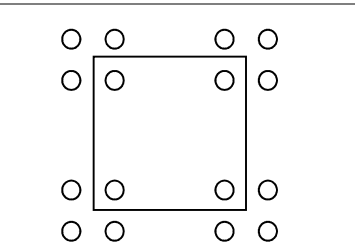
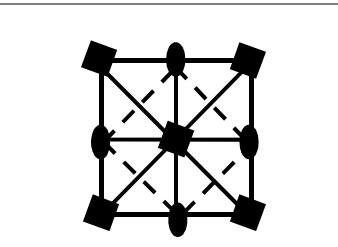
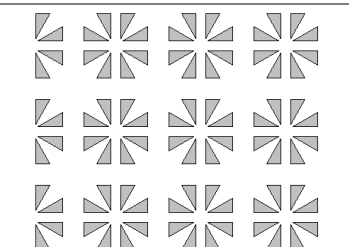
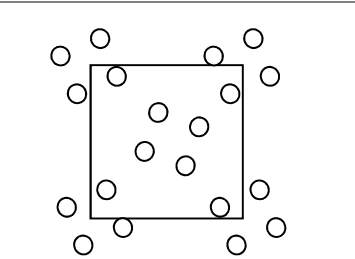
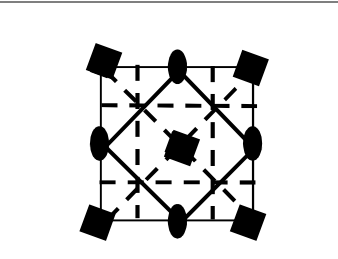
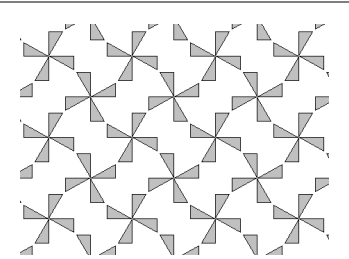
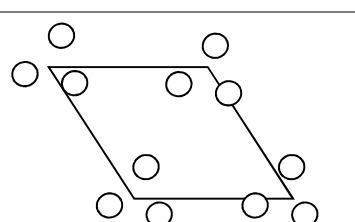
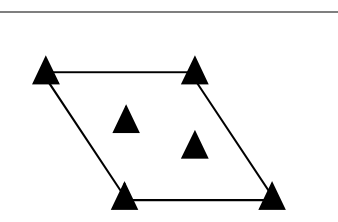
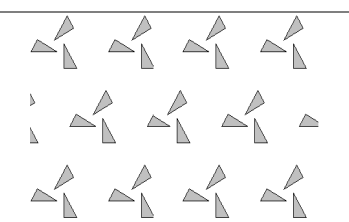


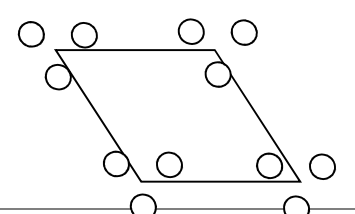
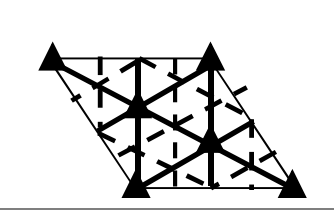
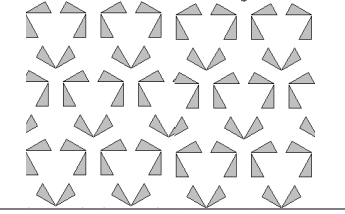
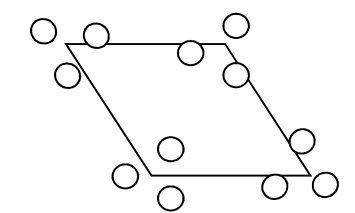
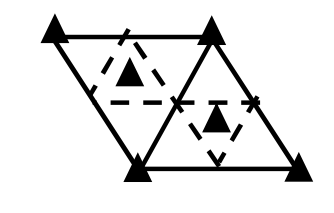
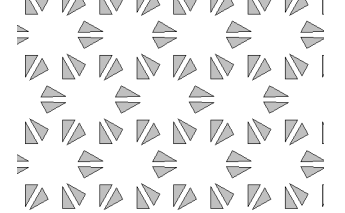
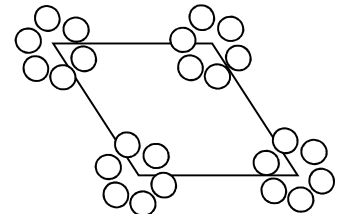
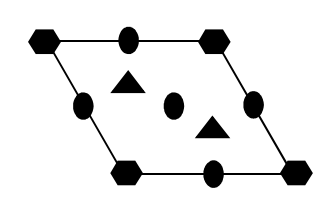
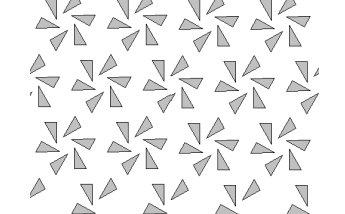
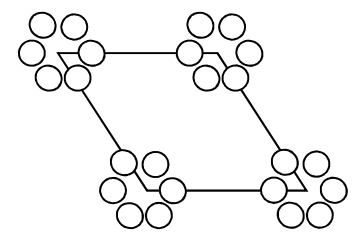
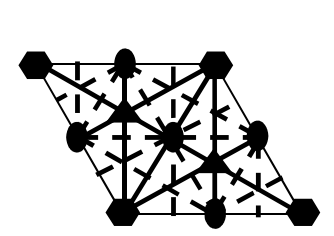
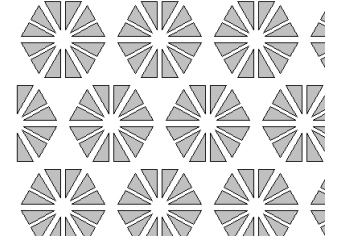
## Black-white point groups



**Plane groups - placement of structural motif, positions of symmetry elements in unit cells and wallpaper pattern schemes**

| Group symbol | Structural motif in unit cell                                                       | Arrangement of symmetry elements in the unit cell                                   | Scheme of the wallpaper patterns                                                      |
|--------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| $p1$         |    |   |    |
| $p2$         |   |  |   |
| $pm$         |  |  |  |
| $pg$         |  |  |  |
| $cm$         |  |  |  |
| $p2mm$       |  |  |  |

|        |                                                                                     |                                                                                      |                                                                                       |
|--------|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| $p2mg$ |    |    |    |
| $p2gg$ |    |    |    |
| $c2mm$ |    |    |    |
| $p4$   |   |   |   |
| $p4mm$ |  |  |  |
| $p4gm$ |  |  |  |
| $p3$   |  |  |  |

|        |                                                                                    |                                                                                     |                                                                                      |
|--------|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
| $p3m1$ |   |   |   |
| $p31m$ |   |   |   |
| $p6$   |   |   |   |
| $p6mm$ |  |  |  |

## Designations used

|                                 |                                                          |
|---------------------------------|----------------------------------------------------------|
| scalar quantities, coordinates  | $s, p, A, n, x, y, r_1, t_2$                             |
| vector quantities               | $\mathbf{a}, \mathbf{r}, \mathbf{t}, \mathbf{A}_L$       |
| basis vectors of primitive cell | $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}$                 |
| basis vectors of centred cell   | $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}$                 |
| reciprocal vectors              | $\mathbf{a}^1, \mathbf{a}^2, \mathbf{b}^1, \mathbf{b}^2$ |
| tensors                         | $\bar{\bar{\mathbf{T}}}, \bar{\bar{\mathbf{M}}}$         |
| symmetry operators              | $[\bar{\Phi}, t]$                                        |
| group of operators              | $\{\bar{\Phi}, t\}$                                      |
| plane groups                    | $G, G_7,$                                                |
| translation groups              | $T, T_p$                                                 |
| point groups                    | <b><math>2mm, m</math></b>                               |
| elements of point groups        | $2, m, 6^4, m_{60}$                                      |
| set of group elements           | $\{e, 2, m_x, m_y\} \equiv \{2mm\}$                      |

\*) In the international tables (7), the symbols for groups are in plain, not bold, type. However, the same font is also used for the elements of the groups, which may lead to misunderstandings. Therefore, in this text, group symbols are in bold and their elements in regular type. For example, if the group is  **$2mm$** , its elements are:  $e, 2, m_x, m_y$ . The set of all elements forming the group is written in parentheses:  $\{e, 2, m_x, m_y\}$ .

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## Register

|                           |            |                           |             |
|---------------------------|------------|---------------------------|-------------|
| allowed rotations         | 47         | dyad                      | 150         |
| anti-symmetry             | 106        | equivalent points         | 7           |
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