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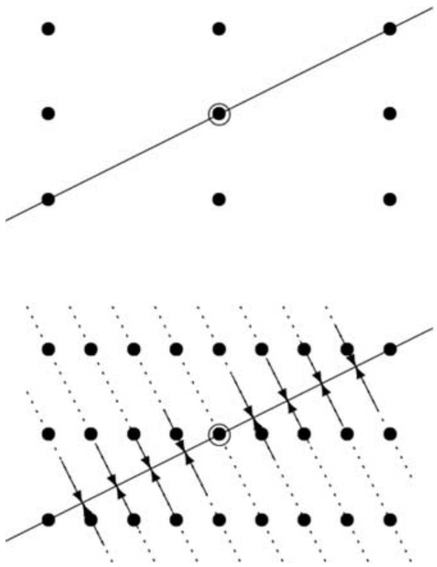

Figure 1.4.5.1
Duality between section and projection.

(i) If a symmetry operation of the slice maps its upper side to the upper side, a vector normal to the slice is fixed.

(ii) If a symmetry operation of the slice maps the upper side to the lower side, a vector normal to the slice is mapped to its opposite and the slice is turned upside down.

Therefore, the symmetries of two-dimensional rational sections are described by *layer groups*, *i.e.* subgroups of space groups with a two-dimensional translation lattice. Layer groups are *subperiodic groups* and for their elaborate discussion we refer to Chapter 1.7 and *IT* E (2010).

Analogous to two-dimensional sections of a crystal pattern, one can also consider the penetration of crystal patterns by a straight line, which is the idealization of a one-dimensional section taking out a rod of the crystal pattern. If the penetration line is along the direction of a translational symmetry of the crystal pattern, the rod has one-dimensional translational symmetry and its group of symmetries is a *rod group*, *i.e.* a subgroup of a space group with a one-dimensional translation lattice. Rod groups are also subperiodic groups, *cf.* *IT* E for their detailed treatment and listing.

A projection along a direction **d** into a plane maps a point of a crystal pattern to the intersection of the plane with the line along **d** through the point. If the projection direction is not along a rational lattice direction, the projection of the crystal pattern will contain points with arbitrarily small distances and additional restrictions are required to obtain a discrete pattern (*e.g.* the cut-and-project method used in the context of quasicrystals). We avoid any such complication by assuming that **d** is along a rational lattice direction. Furthermore, one is usually only interested in *orthogonal* projections in which the projection direction is perpendicular to the projection plane. This has the effect that spheres in three-dimensional space are mapped to circles in the projection plane.

Although it is also possible to regard the projection plane as a two-sided plane by taking into account from which side of the plane a point is projected into it, this is usually not done. Therefore, the symmetries of projections are described by ordinary plane groups.

Sections and projections are related by the *projection–slice theorem* (Bracewell, 2003) of Fourier theory: A section in reciprocal space containing the origin (the so-called zero layer) corresponds to a projection in direct space and *vice versa*. The projection direction in the one space is normal to the slice in the other space. This correspondence is illustrated schematically in Fig. 1.4.5.1. The top part shows a rectangular lattice with $b/a = 2$ and a slice along the line defined by $2x + y = 0$. Normalizing $a = 1$, the distance between two neighbouring lattice points in the slice is $\sqrt{5}$. If the pattern is restricted to this slice, the points of the corresponding diffraction pattern in reciprocal space must have distance $1/\sqrt{5}$ and this is precisely obtained by projecting the lattice points of the reciprocal lattice onto the slice.

The different, but related, viewpoints of sections and projections can be stated in a simple way as follows: For a section perpendicular to the c axis, only those points of a crystal pattern are considered which have z coordinate equal to a fixed value z_0 or in a small interval around z_0. For a projection along the c axis, all points of the crystal pattern are considered, but their z coordinate is simply ignored. This means that all points of the crystal pattern that differ only by their z coordinate are regarded as the same point.

1.4.5.2. Sections

For a space group $\mathcal{G}$ and a point X in the three-dimensional point space $\mathbb{E}^3$, the site-symmetry group of X is the subgroup of operations of $\mathcal{G}$ that fix X. Analogously, one can also look at the subgroup of operations fixing a one-dimensional line or a two-dimensional plane. If the line is along a rational direction, it will be fixed at least by the translations of $\mathcal{G}$ along that direction. However, it may also be fixed by a symmetry operation that reverses the direction of the line. The resulting subgroup of $\mathcal{G}$ that fixes the line is a *rod group*.

Similarly, a plane having a normal vector along a rational direction is fixed by translations of $\mathcal{G}$ corresponding to a two-dimensional lattice. Again, the plane may also be fixed by additional symmetry operations, *e.g.* by a twofold rotation around an axis lying in the plane, by a rotation around an axis normal to the plane or by a reflection in the plane.

Definition

A *rational planar section* of a crystal pattern is the intersection of the crystal pattern with a plane containing two linearly independent translation vectors of the crystal pattern. The intersecting plane is called the *section plane*.

A *rational linear section* of a crystal pattern is the intersection of the crystal pattern with a line containing a translation vector of the crystal pattern. The intersecting line is called the *penetration line*.

A planar section is determined by a vector **d** which is perpendicular to the section plane and a continuous parameter s, called the *height*, which gives the position of the plane on the line along **d**.

A linear section is specified by a vector **d** parallel to the penetration line and a point in a plane perpendicular to **d** giving the intersection of the line with that plane.

Definition

(i) The symmetry group of a planar section of a crystal pattern is the subgroup of the space group $\mathcal{G}$ of the crystal pattern that leaves the section plane invariant as a whole.

If the section is a rational section, this symmetry group is a *layer group*, *i.e.* a subgroup of a space group which contains translations only in a two-dimensional plane.

(ii) The symmetry group of a linear section of a crystal pattern is the subgroup of the space group $\mathcal{G}$ of the crystal pattern that leaves the penetration line invariant as a whole.

If the section is a rational section, this symmetry group is a *rod group*, *i.e.* a subgroup of a space group which contains translations only along a one-dimensional line.

From now on we will only consider rational sections and omit this attribute. Moreover, we will concentrate on the case of planar sections, since this is by far the most relevant case for crystallographic applications. The treatment of one-dimensional sections is analogous, but in general much easier.

Let $\mathbf{d}$ be a vector perpendicular to the section plane. In most cases, $\mathbf{d}$ is chosen as the shortest lattice vector perpendicular to the section plane. However, in the triclinic and monoclinic crystal family this may not be possible, since the translations of the crystal pattern may not contain a vector perpendicular to the section plane. In that case, we assume that $\mathbf{d}$ captures the periodicity of the crystal pattern perpendicular to the section plane. This is achieved by choosing $\mathbf{d}$ as the shortest non-zero projection of a lattice vector to the line through the origin which is perpendicular to the section plane. Because of the periodicity of the crystal pattern along $\mathbf{d}$, it is enough to consider heights s with $0 \le s < 1$, since for an integer m the sectional layer groups at heights s and $s + m$ are conjugate subgroups of $\mathcal{G}$. This is a consequence of the orbit–stabilizer theorem in Section 1.1.7, applied to the group $\mathcal{G}$ acting on the planes in $\mathbb{E}^3$. The layer at height s is mapped to the layer at height $s + m$ by the translation through $m\mathbf{d}$. Thus, the two layers lie in the same orbit under $\mathcal{G}$. According to the orbit–stabilizer theorem, the corresponding stabilizers, being just the layer groups at heights s and $s + m$, are then conjugate by the translation through $m\mathbf{d}$.

Since we assume a rational section, the sectional layer group will always contain translations along two independent directions $\mathbf{a}'$, $\mathbf{b}'$ which, we assume, form a crystallographic basis for the lattice of translations fixing the section plane. The points in the section plane at height s are then given by $x\mathbf{a}' + y\mathbf{b}' + s\mathbf{d}$. In order to determine whether the sectional layer group contains additional symmetry operations which are not translations, the following simple remark is crucial:

Let g be an operation of a sectional layer group. Then the rotational part of g maps $\mathbf{d}$ either to $+\mathbf{d}$ or to $-\mathbf{d}$. In the former case, g is side-preserving, in the latter case it is side-reversing. Moreover, since the section plane remains fixed under g, the vectors $\mathbf{a}'$ and $\mathbf{b}'$ are mapped to linear combinations of $\mathbf{a}'$ and $\mathbf{b}'$ by the rotational part of g. Therefore, with respect to the (usually non-conventional) basis $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$ of three-dimensional space and some choice of origin, the operation g has an augmented matrix of the form

$$\left(\begin{array}{ccc|c} r_{11} & r_{12} & 0 & t_1 \\ r_{21} & r_{22} & 0 & t_2 \\ 0 & 0 & r_{33} & t_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

Here, $r_{33} = \pm 1$. Moreover, if $r_{33} = 1$, *i.e.* g is side-preserving, then t_3 is necessarily zero, since otherwise the plane is shifted along $\mathbf{d}$. On the other hand, if $r_{33} = -1$, *i.e.* g is side-reversing, then a plane situated at height s along $\mathbf{d}$ is only fixed if $t_3 = 2s$.

Table 1.4.5.1

Coset representatives of $Pmn2_1$ (31) relative to its translation subgroup

Seitz symbol	Coordinate triplet	Description
$\{1\|0\}$	x, y, z	Identity
$\{2_{001}\|\frac{1}{2}, 0, \frac{1}{2}\}$	$\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	Twofold screw rotation with axis along [001]
$\{m_{010}\|\frac{1}{2}, 0, \frac{1}{2}\}$	$x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	*n*-glide reflection with normal vector along [010]
$\{m_{100}\|0\}$	$\bar{x}, y, z$	Reflection with normal vector along [100]

From these considerations it is straightforward to determine the conditions under which a space-group operation belongs to a certain sectional layer group (excluding translations):

The side-preserving operations will belong to the sectional layer groups for all planes perpendicular to $\mathbf{d}$, independent of the height s:

(i) rotations with axis parallel to $\mathbf{d}$;
(ii) reflections with normal vector perpendicular to $\mathbf{d}$;
(iii) glide reflections with normal vector and glide vector perpendicular to $\mathbf{d}$.

Side-reversing operations will only occur in the sectional layer groups for planes at special heights along $\mathbf{d}$:

(i) inversion with inversion point in the section plane;
(ii) twofold rotations or twofold screw rotations with rotation axis in the section plane;
(iii) reflections or glide reflections through the section plane with glide vector perpendicular to $\mathbf{d}$;
(iv) rotoinversions with axis parallel to $\mathbf{d}$ and inversion point in the section plane.

Note that, because of the periodicity along $\mathbf{d}$, a side-reversing operation that occurs at height s gives rise to a side-reversing operation of the same type occurring at height $s + \frac{1}{2}$: if g is a side-reversing symmetry operation fixing a layer at height s, then g maps a point in the layer at height $s + \frac{1}{2}$ with coordinates $x, y, s + \frac{1}{2}$ (with respect to the layer-adapted basis $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$) to a point with coordinates $x', y', s - \frac{1}{2}$ and hence the composition $t_{\mathbf{d}}g$ of g with the translation by $\mathbf{d}$ maps $x, y, s + \frac{1}{2}$ to $x', y', s + \frac{1}{2}$, *i.e.* it fixes the layer at height $s + \frac{1}{2}$. This shows that the composition with the translation by $\mathbf{d}$ provides a one-to-one correspondence between the side-reversing symmetry operations in the layer group at height s with those at height $s + \frac{1}{2}$.

If a section allows any side-reversing symmetry at all, then the side-preserving symmetries of the section form a subgroup of index 2 in the sectional layer group. Since the side-preserving symmetries exist independently of the height parameter s, the full sectional layer group is always generated by the side-preserving subgroup and either none or a single side-reversing symmetry.

Summarizing, one can conclude that for a given space group the interesting sections are those for which the perpendicular vector $\mathbf{d}$ is parallel or perpendicular to a symmetry direction of the group, *e.g.* an axis of a rotation or rotoinversion or the normal vector of a reflection or glide reflection.

Example

Consider the space group $\mathcal{G}$ of type $Pmn2_1$ (31). In its standard setting, the cosets of $\mathcal{G}$ relative to the translation subgroup are represented by the operations given in Table 1.4.5.1.

Since this is an orthorhombic group, it is natural to consider sections along the coordinate axes. The space-group diagrams displayed in Fig. 1.4.5.2, which show the orthogonal projections of the symmetry elements along these directions, are very helpful.

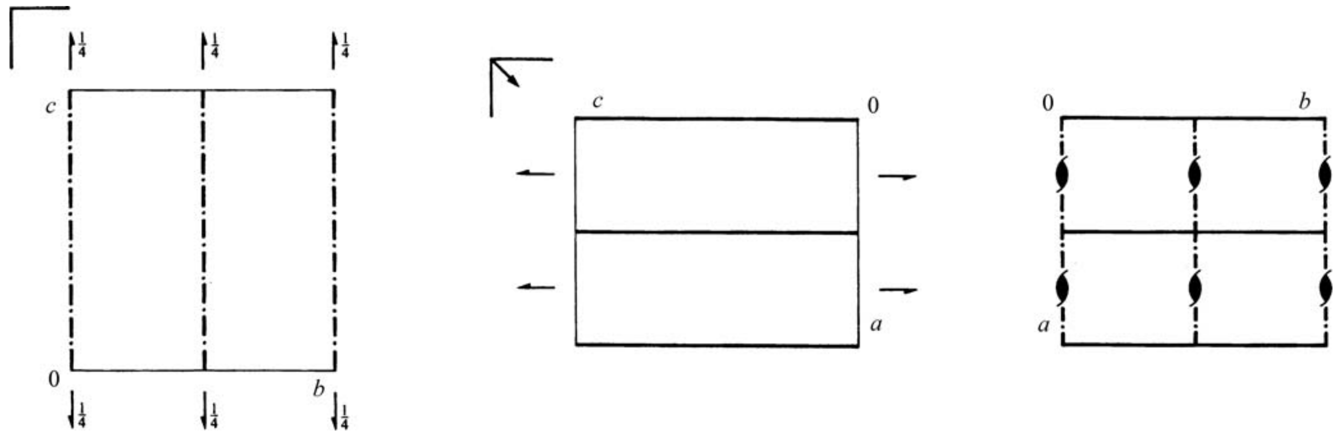

Figure 1.4.5.2
Symmetry-element diagrams for the space group $Pmn2_1$ (31) for orthogonal projections along [100] (left), [010] (middle) and [001] (right).

d *along* [100]: A point x, y, z in a plane perpendicular to the coordinate axis along [100] is mapped to a point x', y', z' in the same plane if $x' = x$, *i.e.* if $x' - x = 0$.

A general operation from the coset of $\{2_{001}|\frac{1}{2}, 0, \frac{1}{2}\}$ maps a point with coordinates x, y, z to a point with coordinates $x' = \bar{x} + \frac{1}{2} + u_1, y' = \bar{y} + u_2, z' = z + \frac{1}{2} + u_3$ for integers u_1, u_2, u_3. One has $x' - x = -2x + \frac{1}{2} + u_1$ which becomes zero for $x = \frac{1}{4}$ (and $u_1 = 0$) and $x = \frac{3}{4}$ (and $u_1 = 1$), thus operations from the coset of $\{2_{001}|\frac{1}{2}, 0, \frac{1}{2}\}$ fix planes at heights $s = \frac{1}{4}$ and $\frac{3}{4}$. In the left-hand diagram in Fig. 1.4.5.2, the symmetry elements to which these operations belong are indicated by the half-arrows, the label $\frac{1}{4}$ indicating that they are at level $x = \frac{1}{4}$ and $x = \frac{3}{4}$.

An operation from the coset of $\{m_{010}|\frac{1}{2}, 0, \frac{1}{2}\}$ maps x, y, z to $x' = x + \frac{1}{2} + u_1, y' = \bar{y} + u_2, z' = z + \frac{1}{2} + u_3$ and one has $x' - x = \frac{1}{2} + u_1$. Since this is never zero, no operation from this coset fixes a plane perpendicular to [100].

Finally, an operation from the coset of $\{m_{100}|0\}$ maps x, y, z to $x' = \bar{x} + u_1,\ y' = y + u_2,\ z' = z + u_3$ and one has $x' - x = -2x + u_1$, which becomes zero for $x = 0$ (and $u_1 = 0$) and $x = \frac{1}{2}$ (and $u_1 = 1$). Thus, operations from the coset of $\{m_{100}|0\}$ fix planes at heights $s = 0$ and $\frac{1}{2}$. The symmetry elements of these reflections with mirror plane parallel to the projection plane are indicated by the right-angle symbol in the upper left corner of the left-hand diagram in Fig. 1.4.5.2.

The sectional layer groups are thus layer groups of type $pm11$ (layer group No. 4 with symbol $p11m$ in a non-standard setting) for $s = 0$ and $s = \frac{1}{2}$, of type $p112_1$ (layer group No. 9 with symbol $p2_111$ in a non-standard setting) for $s = \frac{1}{4}$ and $s = \frac{3}{4}$ and of type $p1$ (layer group No. 1) for all other s between 0 and 1. The side-preserving operations are in all cases just the translations.

It is worthwhile noting that in many cases most of the information about the sectional layer groups can be read off the space-group diagrams. In the present example, the left-hand diagram in Fig. 1.4.5.2 displays the twofold screw rotation at height $s = \frac{1}{4}$ (and thus also at $s = \frac{3}{4}$) and the reflection at height $s = 0$ (and thus also at $s = \frac{1}{2}$). On the other hand, the n glide, indicated by the dashed-dotted lines in the diagram, does not give rise to an element of the sectional layer group, because its glide vector has a component along the [100] direction and can thus not fix any layer along this direction.

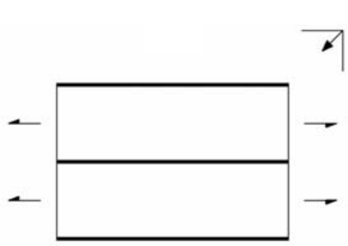

Figure 1.4.5.3
Symmetry-element diagram for the layer group $pm2_1n$ (32).

d *along* [010]: A point x, y, z in a plane perpendicular to the coordinate axis along [010] is mapped to a point x', y', z' in the same plane if $y' = y$, *i.e.* if $y' - y = 0$.

From the calculations above one sees that for operations in the coset of $\{m_{100}|0\}$ one has $y' - y = u_2$, hence operations in this coset fix the plane for any value of s and are side-preserving operations. In the middle diagram in Fig. 1.4.5.2 the symmetry elements for these reflections are indicated by the horizontal solid lines.

For the operations in the coset of $\{2_{001}|\frac{1}{2}, 0, \frac{1}{2}\}$ one has $y' - y = -2y + u_2$, and so these operations fix planes only for $s = 0$ and $s = \frac{1}{2}$. The same is true for the operations in the coset of $\{m_{010}|\frac{1}{2}, 0, \frac{1}{2}\}$, because here one also has $y' - y = -2y + u_2$. The symmetry elements to which the screw rotations belong are indicated by the half arrows in the middle diagram of Fig. 1.4.5.2, and the symmetry elements for the glide reflections are symbolized by the right angle with diagonal arrow in the upper left corner, indicating that the geometric element is a diagonal glide plane.

The sectional layer groups are thus of type $pmn2_1$ (layer group No. 32 with symbol $pm2_1n$ in a non-standard setting) for $s = 0, \frac{1}{2}$ and of type $pm11$ (layer group No. 11) for all other s. The group of side-preserving operations is in all cases of type $pm11$.

In Fig. 1.4.5.3 the diagram of the symmetry elements for the layer group $pm2_1n$ (layer group No. 32) is displayed. It coincides with the middle diagram in Fig. 1.4.5.2 (up to the placement of the symbol for the diagonal glide plane), showing that in this case the sectional layer groups can also be read off directly from the space-group diagrams.

d *along* [001]: A point x, y, z in a plane perpendicular to the coordinate axis along [001] is mapped to a point x', y', z' in the same plane if $z' = z$, *i.e.* if $z' - z = 0$.

As in the case of **d** along [010], operations in the coset of $\{m_{100}|0\}$ fix such a plane for any value of s, since $z' - z = u_3$.

Again, these are side-preserving operations. The symmetry elements to which these reflections belong are indicated by the horizontal solid lines in the right-hand diagram in Fig. 1.4.5.2. For the operations in the cosets of $\{2_{001}|\frac{1}{2}, 0, \frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2}, 0, \frac{1}{2}\}$ one has $z' - z = \frac{1}{2} + u_3$, which is never zero (for an integer u_3), and so operations in these cosets never fix a plane perpendicular to [001].

Thus, for any value of s the sectional layer group is of type $pm11$ (layer group No. 11) and contains only side-preserving operations.

1.4.5.3. Projections

As we have seen, a section of a crystal pattern is determined by a vector **d** and a height s along this vector. Choosing two vectors $\mathbf{a}'$ and $\mathbf{b}'$ perpendicular to **d**, the points of the section plane at height s are precisely given by the vectors $x\mathbf{a}' + y\mathbf{b}' + s\mathbf{d}$. In contrast to that, a *projection* of a crystal pattern along **d** is obtained by mapping an arbitrary point $x\mathbf{a}' + y\mathbf{b}' + z\mathbf{d}$ to the point $x\mathbf{a}' + y\mathbf{b}'$ of the plane spanned by $\mathbf{a}'$ and $\mathbf{b}'$, thereby ignoring the coordinate along the **d** direction.

Definition

In a *projection* of a crystal pattern along the *projection direction* **d**, a point X of the crystal pattern is mapped to the intersection of the line through X along **d** with a fixed plane perpendicular to **d**.

One may think of the projection plane as the plane perpendicular to **d** and containing the origin, but every plane perpendicular to **d** will give the same result.

Let L be the line along **d**. If a symmetry operation g of a space group $\mathcal{G}$ maps L to a line parallel to L, then g maps every plane perpendicular to **d** again to a plane perpendicular to **d**. This means that points that are projected to a single point (*i.e.* points on a line parallel to L) are mapped by g to points that are again projected to a single point and thus the operation g gives rise to a symmetry of the projection of the crystal pattern. Conversely, an operation g that maps L to a line that is inclined to L does not result in a symmetry of the projection, since the points on L are projected to a single point, whereas the image points under g are projected to a line. In summary, the operations of $\mathcal{G}$ that map L to a line parallel to L give rise to symmetries of the projection forming a *plane group*, sometimes called a wallpaper group.

Let $\mathcal{H}$ be the subgroup of $\mathcal{G}$ consisting of those $g \in \mathcal{G}$ mapping the line L to a line parallel to L, then $\mathcal{H}$ is called the *scanning group along* **d**. The scanning group $\mathcal{H}$ can be read off a coset decomposition $\mathcal{G} = g_1\mathcal{T} \cup \cdots \cup g_s\mathcal{T}$ relative to the translation subgroup $\mathcal{T}$ of $\mathcal{G}$. Since translations map lines to parallel lines, one only has to check whether a coset representative g_i maps L to a line parallel to L. This is precisely the case if the linear part of g_i maps **d** to **d** or to $-$**d**. Therefore, $\mathcal{H}$ is the union of those cosets $g_i\mathcal{T}$ relative to $\mathcal{T}$ for which the linear part of g_i maps **d** to **d** or to $-$**d**.

If the operations of a space group $\mathcal{G}$ are written as augmented matrices with respect to a (usually non-conventional) basis $\mathbf{a}'$, $\mathbf{b}'$, **d** such that $\mathbf{a}'$ and $\mathbf{b}'$ are perpendicular to **d**, then an operation g of the scanning group $\mathcal{H}$ is of the form

$$g = \left(\begin{array}{ccc|c} r_{11} & r_{12} & 0 & t_1 \\ r_{21} & r_{22} & 0 & t_2 \\ 0 & 0 & r_{33} & t_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

with $r_{33} = \pm 1$ (just as for planar sections). Then the action of g on the projection along **d** is obtained by ignoring the z coordinate, *i.e.* by cutting out the upper 2×2 block of the linear part and the first two components of the translation part. This gives rise to the plane-group operation

$$g' = \left(\begin{array}{cc|c} r_{11} & r_{12} & t_1 \\ r_{21} & r_{22} & t_2 \\ \hline 0 & 0 & 1 \end{array}\right).$$

The mapping that assigns to each operation g of the scanning group its action g' on the projection is in fact a homomorphism from $\mathcal{H}$ to a plane group and the kernel $\mathcal{K}$ of this homomorphism are the operations of the form

$$\left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & r_{33} & t_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

i.e. translations along **d** and reflections with normal vector parallel to **d**.

Definition

The symmetry group of the projection along the projection direction **d** is the plane group of actions on the projection of those operations of $\mathcal{G}$ that map the line L along **d** to a line parallel to L.

This group is isomorphic to the quotient group of the scanning group $\mathcal{H}$ along **d** by the group $\mathcal{K}$ of translations along **d** and reflections with normal vector parallel to **d**.

Example

We consider again the space group $\mathcal{G}$ of type $Pmn2_1$ (31) for which the augmented matrices of the coset representatives with respect to the translation subgroup (in the standard setting) are given by

$$\{1|0\} = \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

$$\{2_{001}|\tfrac{1}{2}, 0, \tfrac{1}{2}\} = \left(\begin{array}{ccc|c} -1 & 0 & 0 & \frac{1}{2} \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

$$\{m_{010}|\tfrac{1}{2}, 0, \tfrac{1}{2}\} = \left(\begin{array}{ccc|c} 1 & 0 & 0 & \frac{1}{2} \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

$$\{m_{100}|0\} = \left(\begin{array}{ccc|c} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$