International Tables for Crystallography (2016). Vol. A, Section 1.4.5.3, pp. 71–73.

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 $r_{33}=\pm1$ (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

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

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

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

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

Since the linear parts of all four matrices are diagonal matrices, the scanning group for projections along the coordinate axes is always the full group $\mathcal{G}$.

For the projection along the direction [100], one has to cut out the lower 2×2 part of the linear parts and the second and third component of the translation part, thus choosing $\mathbf{a}' = \mathbf{b}, \mathbf{b}' = \mathbf{c}$ as a basis for the projection plane. This gives as matrices for the projected operations

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

in which the third and fourth operations are clearly redundant and which is thus a plane group of type *p*1*g*1 (plane group No. 4 with short symbol *pg*).

The projection along the direction [010] gives for the basis $\mathbf{a}' = \mathbf{a}, \mathbf{b}' = \mathbf{c}$ of the projection plane (thus picking out the first and third rows and columns) the matrices

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

where the second matrix is the product of the third and fourth. The third operation is a centring translation, the fourth a reflection, thus the resulting plane group is of type *c*1*m*1 (plane group No. 5 with short symbol *cm*).

Finally, the projection along the direction [001] results for the basis $\mathbf{a}' = \mathbf{a}, \mathbf{b}' = \mathbf{b}$ of the projection plane in the matrices

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

where again the second matrix is the product of two others. The third operation is a glide reflection and the fourth is a reflection, thus the corresponding plane group is of type *p*2*mg* (plane group No. 7). Note that in order to obtain the plane group *p*2*mg* in its standard setting, the origin has to be shifted to $\frac{1}{4}, 0$ (with respect to the plane basis $\mathbf{a}', \mathbf{b}'$).

As for the sectional layer groups, the typical projection directions considered are symmetry directions of the space group $\mathcal{G}$, *i.e.* directions along rotation or screw axes or normal to reflection or glide planes. In order to relate the coordinate system of the plane group to that of the space group, not only the basis vectors $\mathbf{a}', \mathbf{b}'$ perpendicular to the projection direction $\mathbf{d}$ have to be given, but also the origin for the plane group. This is done by specifying a line parallel to the projection direction which is projected to the origin of the plane group in its conventional setting. The space-group tables list the plane groups for the projections along symmetry directions of the group in the block 'Symmetry of special projections'.

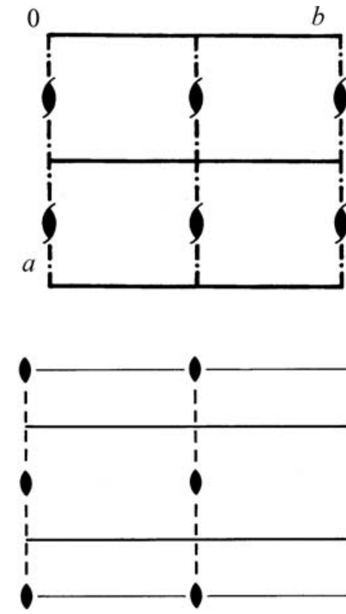

Figure 1.4.5.4
Orthogonal projection along [001] of the symmetry-element diagram for $Pmn2_1$ (31) (top) and the diagram for plane group *p*2*mg* (7) (bottom).

It is not hard to determine the corresponding types of plane-group operations for the different types of space-group operations, as is shown by the following list of simple rules:

(i) a translation becomes a translation (possibly the identity);
(ii) an inversion becomes a twofold rotation;
(iii) a *k*-fold rotation or screw rotation with axis parallel to $\mathbf{d}$ becomes a *k*-fold rotation;
(iv) a three-, four- or sixfold rotoinversion with axis parallel to $\mathbf{d}$ becomes a six-, four- or threefold rotation, respectively;
(v) a reflection or glide reflection with normal vector parallel to $\mathbf{d}$ becomes a translation (possibly the identity);
(vi) a twofold rotation and a screw rotation with axis perpendicular to $\mathbf{d}$ become a reflection and glide reflection, respectively;
(vii) a reflection or a glide reflection with normal vector perpendicular to $\mathbf{d}$ becomes a reflection or glide reflection depending on whether there is a glide component perpendicular to $\mathbf{d}$ or not.

The relationship between the symmetry operations in three-dimensional space and the corresponding symmetry operations of a projection as listed above can be seen directly in the diagrams of the corresponding groups. In Fig. 1.4.5.4, the top diagram shows the orthogonal projection of the symmetry-element diagram of $Pmn2_1$ along the [001] direction and the bottom diagram shows the diagram for the plane group *p*2*mg*, which is precisely the symmetry group of the projection of $Pmn2_1$ along [001]. Firstly, one sees immediately that in order to match the two diagrams, the origin in the projection plane has to be shifted to $\frac{1}{4}, 0$ (as already noted in the example above). Secondly, keeping in mind that the projection direction $\mathbf{d}$ is perpendicular to the drawing plane, one sees the correspondence between the twofold screw rotations in $Pmn2_1$ with the twofold rotations in *p*2*mg* [rule (iii)], the correspondence between the reflections with normal vector perpendicular to **d** in $Pmn2_1$ and the reflections in $p2mg$ [rule (vii)] and the correspondence between the diagonal glide reflections in $Pmn2_1$ (indicated by the dot-dash lines) and the glide reflections in $p2mg$ {rule (vii); note that the diagonal glide vector has a component perpendicular to the projection direction [001]}.

Example

Let $\mathcal{G}$ be a space group of type $P\bar{4}b2$ (117), then the interesting projection directions (*i.e.* symmetry directions) are [100], [010], [001], [110] and [$\bar{1}$10]. However, the directions [100] and [010] are symmetry-related by the fourfold rotoinversion and thus result in the same projection. The same holds for the directions [110] and [$\bar{1}$10]. The three remaining directions are genuinely different and the projections along these directions will be discussed in detail below. The corresponding information given in the space-group tables under the heading 'Symmetry of special projections' is reproduced in Fig. 1.4.5.5 for $P\bar{4}b2$.

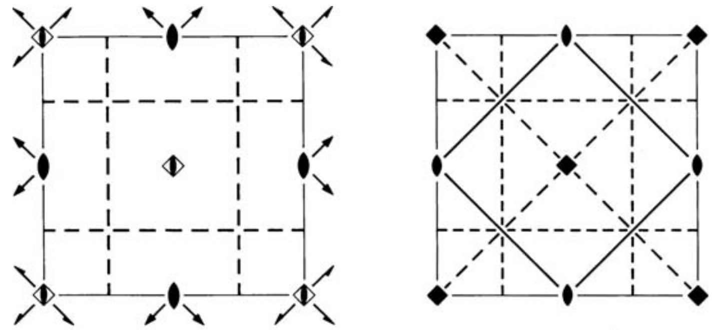

Figure 1.4.5.6
Orthogonal projection along [001] of the symmetry-element diagram for $P\bar{4}b2$ (117) (left) and the diagram for plane group $p4gm$ (12) (right).

Symmetry of special projections

Along [001] $p4gm$	Along [100] $p1m1$	Along [110] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$	$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $0, 0, z$	Origin at $x, 0, 0$	Origin at $x, x, 0$

Figure 1.4.5.5
'Symmetry of special projections' block of $P\bar{4}b2$ (117) as given in the space-group tables.

Coset representatives of $\mathcal{G}$ relative to its translation subgroup can be extracted from the general-positions block in the space-group tables of $P\bar{4}b2$ and are given in Table 1.4.5.2.

d *along* [001]: The linear parts of all coset representatives map [001] to ±[001], and therefore the scanning group $\mathcal{H}$ is the full group $\mathcal{G}$. A conventional basis for the translations of the projection is $\mathbf{a}' = \mathbf{a}$ and $\mathbf{b}' = \mathbf{b}$. The operation g_3 acts as a fourfold rotation, g_5 acts as a glide reflection with normal vector $\mathbf{b}'$ and g_8 as a reflection with normal vector $\mathbf{a}' + \mathbf{b}'$. Thus, the resulting plane group has type $p4gm$ (plane group No. 12). The line parallel to the projection direction [001] which is projected to the origin of $p4gm$ in its conventional setting is the line 0, 0, z.

Again, it is instructive to look at the symmetry-element diagrams for the respective space and plane groups, as displayed in Fig. 1.4.5.6. The twofold rotations and fourfold rotoinversions with axis along [001] are turned into twofold rotations and fourfold rotations, respectively [rules (iii) and (iv)]. The glide reflections with both normal vector and glide vector perpendicular to [001] (dashed lines) result in glide reflections [rule (vii)]. The twofold rotations (full arrows) and screw rotations (half arrows) with rotation axis perpendicular to [001] give reflections and glide reflections, respectively [rule (vi)]. Note that the two diagrams can be matched directly, because the line 0, 0, z which is projected to the origin of $p4gm$ runs through the origin of $P\bar{4}b2$.

Table 1.4.5.2
Coset representatives of $P\bar{4}b2$ (117) relative to its translation subgroup

	Coordinate triplet	Description
g_1:	x, y, z	Identity
g_2:	$\bar{x}, \bar{y}, z$	Twofold rotation with axis along [001]
g_3:	$y, \bar{x}, \bar{z}$	Fourfold rotoinversion with axis along [001]
g_4:	$\bar{y}, x, \bar{z}$	Fourfold rotoinversion with axis along [001]
g_5:	$x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$	Glide reflection with normal vector [010] and glide component along [100]
g_6:	$\bar{x}+\frac{1}{2}, y+\frac{1}{2}, z$	Glide reflection with normal vector [100] and glide component along [010]
g_7:	$y+\frac{1}{2}, x+\frac{1}{2}, \bar{z}$	Twofold screw rotation with axis parallel to [110]
g_8:	$\bar{y}+\frac{1}{2}, \bar{x}+\frac{1}{2}, \bar{z}$	Twofold rotation with axis parallel to [1$\bar{1}$0]

d *along* [100]: Only the linear parts of the coset representatives g_1, g_2, g_5 and g_6 map [100] to ±[100], thus these four cosets form the scanning group $\mathcal{H}$ (which is of index 2 in $\mathcal{G}$). The operation g_6 acts as a translation by $\frac{1}{2}\mathbf{b}$, thus a conventional basis for the translations of the projection is $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ and $\mathbf{b}' = \mathbf{c}$. The operation g_2 acts as a reflection with normal vector $\mathbf{a}'$ and g_5 acts as the same reflection composed with the translation $\mathbf{a}'$. The resulting plane group is thus of type $p1m1$ (plane group No. 3 with short symbol pm). The line which is mapped to the origin of $p1m1$ in its conventional setting is x, 0, 0.

d *along* [110]: Only the linear parts of the coset representatives g_1, g_2, g_7 and g_8 map [110] to ±[110], thus these four cosets form the scanning group $\mathcal{H}$ (of index 2 in $\mathcal{G}$). The translation by $\mathbf{b}$ is projected to a translation by $\frac{1}{2}(-\mathbf{a}+\mathbf{b})$, thus a conventional basis for the translations of the projection is $\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ and $\mathbf{b}' = \mathbf{c}$. The operation g_2 acts as a reflection with normal vector $\mathbf{a}'$, g_7 acts as a twofold rotation and g_8 acts as a reflection with normal vector $\mathbf{b}'$. The resulting plane group is thus of type $p2mm$ (plane group No. 6). The line parallel to the projection direction [110] that is mapped to the origin of $p2mm$ (in its conventional setting) is x, x, 0.

Note that for directions different from those considered above, additional non-trivial plane groups may be obtained. For example, for the projection direction $\mathbf{d} = [1\bar{1}1]$, the scanning group consists of the cosets of g_1 and g_7. The operation g_7 acts as a glide reflection and the resulting plane group is of type $c1m1$ (plane group No. 5).

References

Bracewell, R. N. (2003). *Fourier Analysis and Imaging*. New York: Springer Science+Business Media.

Bradley, C. J. & Cracknell, A. P. (1972). *The Mathematical Theory of Symmetry in Solids*. Oxford University Press.