International Tables for Crystallography (2016). Vol. A, Section 1.4.5, pp. 67–73.

$a = b$, then the eigensymmetry group of an orbit can belong to the tetragonal family.

Note: A space group $\mathcal{G}$ is equal to the intersection of the eigensymmetry groups of the orbits of all its positions. If none of the positions of a space group $\mathcal{G}$ gives rise to a characteristic orbit, this means that each single orbit under $\mathcal{G}$ does not have $\mathcal{G}$ as its symmetry group, but a larger group that contains $\mathcal{G}$ as a proper subgroup. It may thus be necessary to have the union of at least two orbits under $\mathcal{G}$ to obtain a structure that has precisely $\mathcal{G}$ as its group of symmetry operations.

Examples

(1) For the group $\mathcal{G}$ of type *Pmmm* (47) all Wyckoff positions with no further special values of the coordinates give rise to characteristic orbits, because the point group of $\mathcal{G}$ is a holohedry and the general coordinates allow no further translations. However, there are various 'specializations' of the positions that give rise to extraordinary orbits. For example, setting x to the special value $\frac{1}{4}$ for the general position introduces the additional translation $t(\frac{1}{2}, 0, 0)$. In fact, for all positions in which the first coordinate has no specified value (positions 2*i*–2*l*, 4*w*–4*z*, 8α), setting $x = \frac{1}{4}$ introduces the translation $t(\frac{1}{2}, 0, 0)$ and thus gives rise to an extraordinary orbit. In all these cases, the resulting eigensymmetry group is of type *Pmmm* with primitive lattice basis $\frac{1}{2}\mathbf{a}, \mathbf{b}, \mathbf{c}$.

(2) For the group $\mathcal{G}$ of type *Pmm*2 (25) no Wyckoff position gives rise to a characteristic orbit, because this is a polar group (with respect to the c axis). Any orbit of a point with third coordinate z allows an additional mirror plane normal to the c axis and located at $0, 0, z$. For example, the general position gives rise to a non-characteristic orbit with eigensymmetry group *Pmmm* (47). Since the general coordinates allow no additional translation, this is not an extraordinary orbit. However, setting $x = \frac{1}{4}$ for the general position introduces the translation $t(\frac{1}{2}, 0, 0)$ (as in the above example) and thus gives rise to an extraordinary orbit. The eigensymmetry group is *Pmmm* with primitive lattice basis $\frac{1}{2}\mathbf{a}, \mathbf{b}, \mathbf{c}$.

On the other hand, the special positions $x, 0, z$ (Wyckoff position 2*e*) and $x, \frac{1}{2}, z$ (Wyckoff position 2*f*) both have the same eigensymmetry group as the general position and setting $x = \frac{1}{4}$ for each, giving $\frac{1}{4}, 0, z$ and $\frac{1}{4}, \frac{1}{2}, z$, results in these positions having the same eigensymmetry group as the $\frac{1}{4}, y, z$ case of the general position.

(3) For a group $\mathcal{G}$ of type $P\bar{4}c2$ (116) the general-position coordinates are

(1) x, y, z	(2) $\bar{x}, \bar{y}, z$	(3) $y, \bar{x}, \bar{z}$	(4) $\bar{y}, x, \bar{z}$
(5) $x, \bar{y}, z + \frac{1}{2}$	(6) $\bar{x}, y, z + \frac{1}{2}$	(7) $y, x, \bar{z} + \frac{1}{2}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$

A point x, y, z in a general position does not give rise to an extraordinary orbit because, owing to the general coordinates, there can not be any additional translation. Furthermore, the point group $\bar{4}m2$ of $\mathcal{G}$ has index 2 in the holohedry $4/mmm$. Thus, in order to have a non-characteristic orbit one would require an inversion in some point as an additional operation. But an inversion in p_1, p_2, p_3 would map x, y, z to $\bar{x} + 2p_1, \bar{y} + 2p_2, \bar{z} + 2p_3$ and no such point is contained in the orbit for generic x, y, z. The point x, y, z therefore gives rise to a characteristic orbit.

However, if the point in a general position is chosen with $x = y$, one indeed obtains an additional inversion at $0, 0, \frac{1}{4}$ which maps x, x, z to the orbit point $\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$ (general position point No. 8). This orbit thus is non-characteristic, but it is not extraordinary, since no additional translation is introduced. The eigensymmetry group obtained is $P4_2/mcm$ (132).

On the other hand, if the general position is chosen with $y = 0$, no additional inversion is obtained, but the translation by $\frac{1}{2}\mathbf{c}$ maps $x, 0, z$ to $x, 0, z + \frac{1}{2}$ (general-position point No. 5). The position $x, 0, z$ therefore gives rise to an extraordinary orbit with eigensymmetry group $P\bar{4}m2$ (115).

Knowledge of the eigensymmetry groups of the different positions for a group is of utmost importance for the analysis of diffraction patterns. Atoms in positions that give rise to non-characteristic orbits, in particular extraordinary orbits, may cause systematic absences that are not explained by the space-group operations. These absences are specified as *special reflection conditions* in the space-group tables of this volume, but only as long as no specialization of the coordinates is involved. For the latter case, the possible existence of systematic absences has to be deduced from the tables of noncharacteristic orbits. Reflection conditions are discussed in detail in Chapter 1.6.

Example

For the group $\mathcal{G}$ of type *Pccm* (49) the special position $\frac{1}{2}, 0, z$ (Wyckoff position 4*p*) gives rise to an extraordinary orbit, since it allows the additional translation $\frac{1}{2}\mathbf{c}$. The special reflection condition corresponding to this additional translation is the integral reflection condition *hkl*: $l = 2n$. However, if the z coordinate in position 4*p* is set to $z = \frac{1}{8}$, the eigensymmetry group also contains the translation $\frac{1}{4}\mathbf{c}$. In this case, the special reflection condition becomes *hkl*: $l = 4n$.

1.4.5. Sections and projections of space groups

By B. Souvignier

In crystallography, two-dimensional sections and projections of crystal structures play an important role, *e.g.* in structure determination by Fourier and Patterson methods or in the treatment of twin boundaries and domain walls. Planar sections of three-dimensional scattering density functions are used for finding approximate locations of atoms in a crystal structure. They are indispensable for the location of Patterson peaks corresponding to vectors between equivalent atoms in different asymmetric units (the Harker vectors).

1.4.5.1. Introduction

A two-dimensional section of a crystal pattern takes out a slice of a crystal pattern. In the mathematical idealization, this slice is regarded as a two-dimensional plane, allowing one, however, to distinguish its upper and lower side. Depending on how the slice is oriented with respect to the crystal lattice, the slice will be invariant by translations of the crystal pattern along zero, one or two linearly independent directions. A section resulting in a slice with two-dimensional translational symmetry is called a *rational section* and is by far the most important case for crystallography.

Because the slice is regarded as a two-sided plane, the symmetries of the full crystal pattern that leave the slice invariant fall into two types:

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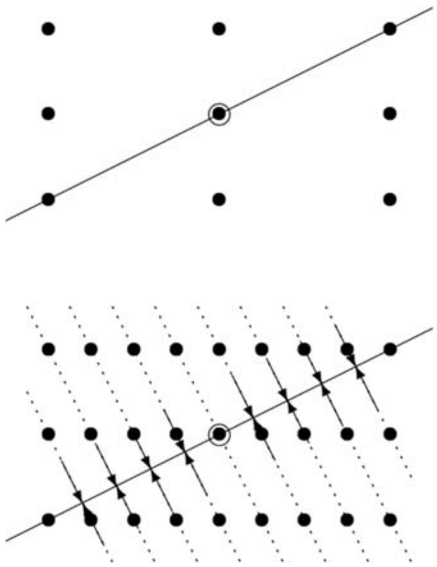

Figure 1.4.5.1
Duality between section and projection.

(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.

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 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 **d** be a vector perpendicular to the section plane. In most cases, **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 **d** captures the periodicity of the crystal pattern perpendicular to the section plane. This is achieved by choosing **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 **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**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**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 **d** either to +**d** or to −**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 $\mathbf{a}'$, $\mathbf{b}'$, **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 **d**. On the other hand, if $r_{33} = -1$, *i.e.* g is side-reversing, then a plane situated at height s along **d** is only fixed if $t_3 = 2s$.

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 **d**, independent of the height s:

(i) rotations with axis parallel to **d**;
(ii) reflections with normal vector perpendicular to **d**;
(iii) glide reflections with normal vector and glide vector perpendicular to **d**.

Side-reversing operations will only occur in the sectional layer groups for planes at special heights along **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 **d**;
(iv) rotoinversions with axis parallel to **d** and inversion point in the section plane.

Note that, because of the periodicity along **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 $\mathbf{a}'$, $\mathbf{b}'$, **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 **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 **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 **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.

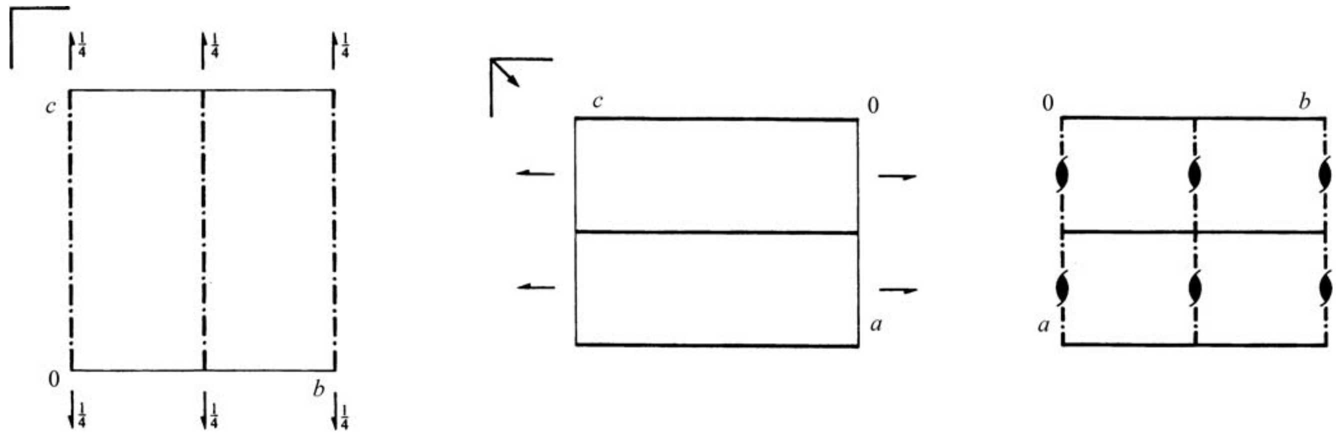

Figure 1.4.5.2
Symmetry-element diagrams for the space group $Pmn2_1$ (31) for orthogonal projections along [100] (left), [010] (middle) and [001] (right).

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.

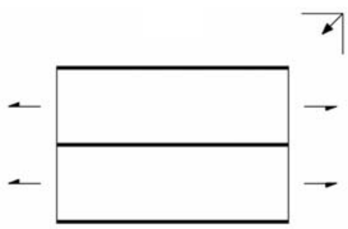

Figure 1.4.5.3
Symmetry-element diagram for the layer group $pm2_1n$ (32).

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 $r_{33}=\pm1$ (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 $p1g1$ (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 $c1m1$ (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 $p2mg$ (plane group No. 7). Note that in order to obtain the plane group $p2mg$ 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'.

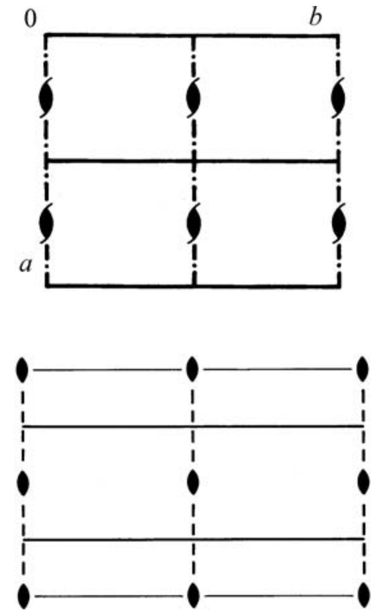

Figure 1.4.5.4
Orthogonal projection along [001] of the symmetry-element diagram for $Pmn2_1$ (31) (top) and the diagram for plane group $p2mg$ (7) (bottom).

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 $p2mg$, 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 $p2mg$ [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 $P\bar{4}b2$.

Symmetry of special projections

Along [001] $p4gm$	Along [100] $p1m1$	Along [110] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\quad \mathbf{b}' = \mathbf{b}$	$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\quad \mathbf{b}' = \mathbf{c}$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}' = \mathbf{c}$
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 $\pm$[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]

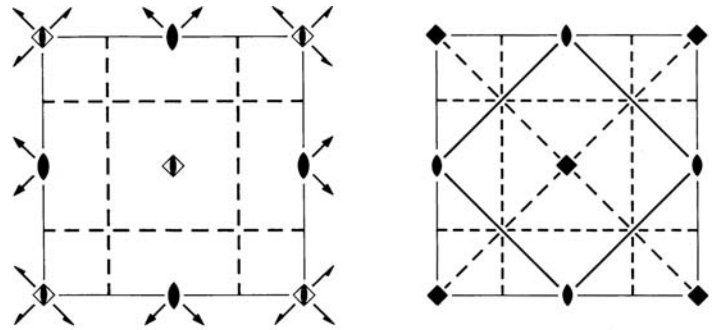

Figure 1.4.5.6
Orthogonal projection along [001] of the symmetry-element diagram for $P\bar{4}b2$ (117) (left) and the diagram for plane group $p4gm$ (12) (right).

d *along* [100]: Only the linear parts of the coset representatives g_1, g_2, g_5 and g_6 map [100] to $\pm$[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 $\pm$[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).

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