

1.4. SPACE GROUPS AND THEIR DESCRIPTIONS

(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 $0 \leq s < 1$, 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.