International Tables for Crystallography (2016). Vol. A, Figure 1.4.5.1, p. 68.

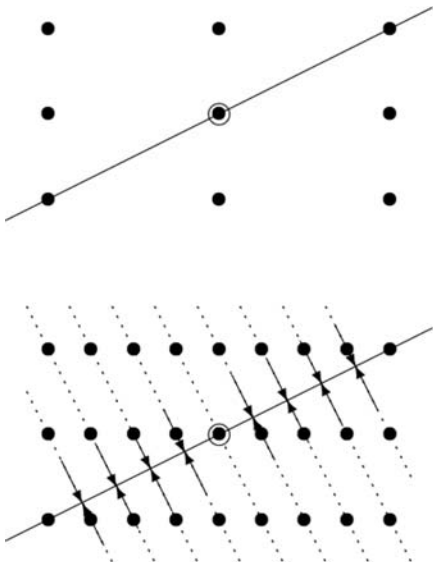

Figure 1.4.5.1
Duality between section and projection.

(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.

