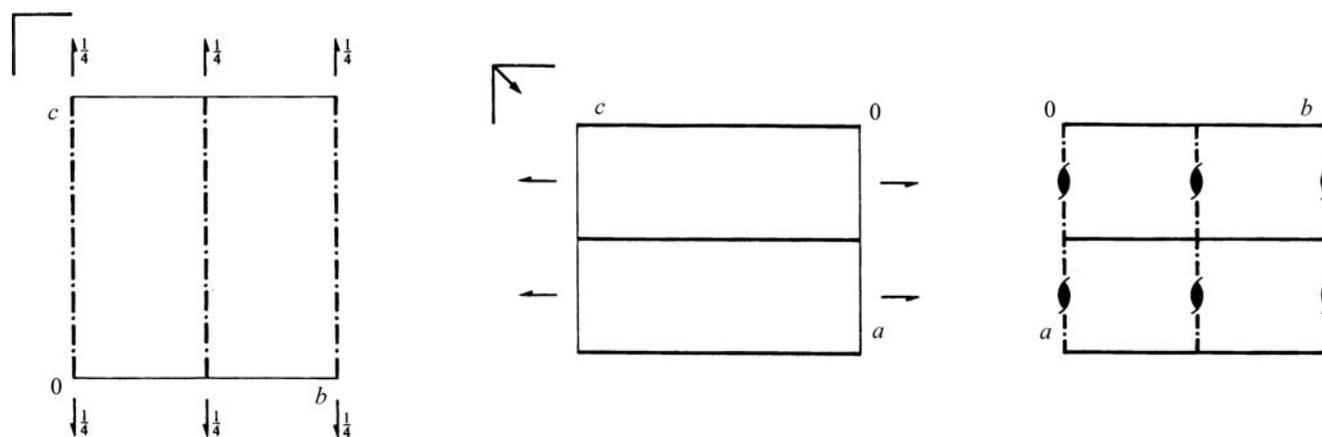1. INTRODUCTION TO SPACE-GROUP SYMMETRY

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
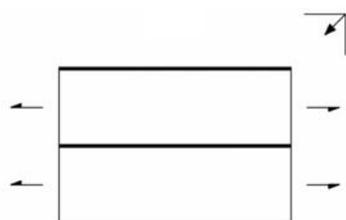
space-group diagrams. In the present example, the left-hand diagram in Fig. 1.4.5.2 displays the twofold screw rotation at height $s = \frac{1}{4}$ (and thus also at $s = \frac{3}{4}$) and the reflection at height $s = 0$ (and thus also at $s = \frac{1}{2}$). On the other hand, the n glide, indicated 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.

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 $z' - z = 0$.

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

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 $z' - z = u_3$.