

1.4. SPACE GROUPS AND THEIR DESCRIPTIONS

reflections with normal vector perpendicular to \mathbf{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

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at x, 0, 0

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 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.

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 $P\bar{4}b2$.

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

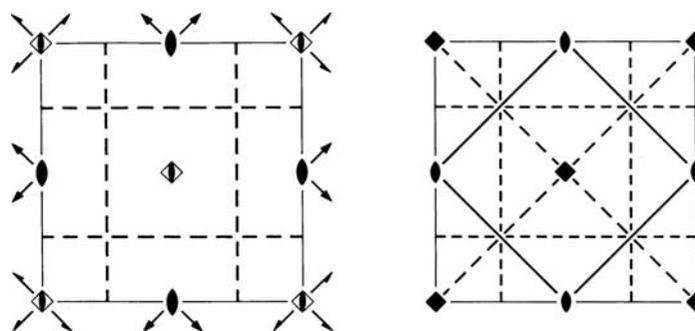


Figure 1.4.5.6

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).

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 $P\bar{4}b2$.

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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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 $[\bar{1}10]$

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

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