1.4. SPACE GROUPS AND THEIR DESCRIPTIONS

reflections with normal vector perpendicular to **d** in *Pmn*2$_1$ and the reflections in *p*2*mg* [rule (vii)] and the correspondence between the diagonal glide reflections in *Pmn*2$_1$ (indicated by the dot-dash lines) and the glide reflections in *p*2*mg* {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

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 *p*4*gm* (12) (right).

Symmetry of special projections

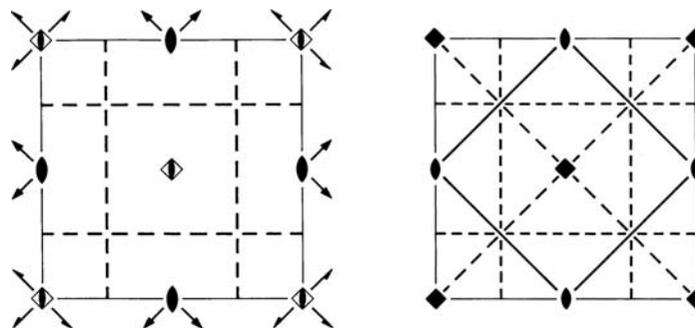| Along [001] $p\,4\,g\,m$	Along [100] $p\,1\,m\,1$	Along [110] $p\,2\,m\,m$
$\mathbf{a}' = \mathbf{a}$ $\quad$ $\mathbf{b}' = \mathbf{b}$	$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\quad$ $\mathbf{b}' = \mathbf{c}$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad$ $\mathbf{b}' = \mathbf{c}$
Origin 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.

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 ±[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 *p*4*gm* (plane group No. 12). The line parallel to the projection direction [001] which is projected to the origin of *p*4*gm* 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 *p*4*gm* 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 ±[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 *p*1*m*1 (plane group No. 3 with short symbol *pm*). The line which is mapped to the origin of *p*1*m*1 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 ±[110], thus these four cosets form the scanning group $\mathcal{H}$ (of index 2 in $\mathcal{G}$). The translation by **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 *p*2*mm* (plane group No. 6). The line parallel to the projection direction [110] that is mapped to the origin of *p*2*mm* (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 *c*1*m*1 (plane group No. 5).

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]

References

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Bradley, C. J. & Cracknell, A. P. (1972). *The Mathematical Theory of Symmetry in Solids*. Oxford University Press.