International Tables for Crystallography (2016). Vol. A, Figure 1.4.2.3, p. 56.

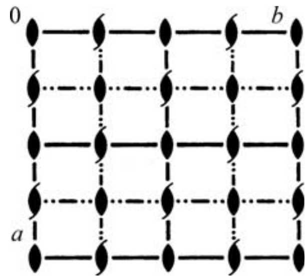

Figure 1.4.2.3
Symmetry-element diagram for space group *Fmm*2 (42) (orthogonal projection along [001]).

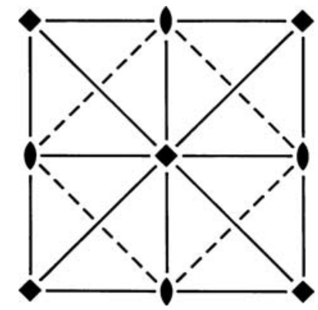

Figure 1.4.2.5
Symmetry-element diagram for space group *P*4*mm* (99) (orthogonal projection along [001]).

in the plane forming the geometric element of W_4. The geometric element of the resulting symmetry operation $\bar{x}, y+\frac{1}{2}, z+\frac{1}{2}$ is still the plane $0, y, z$, but the symmetry operation is now an n glide, *i.e.* a glide reflection with diagonal glide vector.

(ii) $(\frac{1}{2}, 0, \frac{1}{2})$: Analogous to the first centring translation, the composition of W_2 with $t(\frac{1}{2}, 0, \frac{1}{2})$ results in a twofold screw rotation with screw axis $\frac{1}{4}, 0, z$ as geometric element. The roles of the reflections W_3 and W_4 are interchanged, because the translation vector now lies in the plane forming the geometric element of W_3. Therefore, the composition of W_3 with $t(\frac{1}{2}, 0, \frac{1}{2})$ is an n glide with the plane $x, 0, z$ as geometric element, whereas the composition of W_4 with $t(\frac{1}{2}, 0, \frac{1}{2})$ is a c glide with the plane $\frac{1}{4}, y, z$ as geometric element.

(iii) $(\frac{1}{2}, \frac{1}{2}, 0)$: Because this translation vector lies in the plane perpendicular to the rotation axis of W_2, the composition of W_2 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ is still a twofold rotation, *i.e.* a symmetry operation of the same type, but the rotation axis is shifted by $\frac{1}{4}, \frac{1}{4}, 0$ in the xy plane to become the axis $\frac{1}{4}, \frac{1}{4}, z$. The composition of W_3 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ results in the symmetry operation $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$, which is an a glide with the plane $x, \frac{1}{4}, z$ as geometric element, *i.e.* shifted by $\frac{1}{4}$ along the b axis relative to the geometric element of W_3. Similarly, the composition of W_4 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ is a b glide with the plane $\frac{1}{4}, y, z$ as geometric element.

In this example, all additional symmetry operations are listed in the symmetry-operations block of the space-group tables of *Fmm*2 because they are due to compositions of the coset representatives with centring translations.

The additional symmetry operations can easily be recognized in the symmetry-element diagrams (*cf.* Section 1.4.2.5). Fig. 1.4.2.3 shows the symmetry-element diagram of *Fmm*2 for the projection along the c axis. One sees that twofold rotation axes alternate with twofold screw axes and that mirror planes alternate with 'double' or e-glide planes, *i.e.* glide planes with two glide vectors. For example, the dot–dashed lines at $x = \frac{1}{4}$ and $x = \frac{3}{4}$ in Fig. 1.4.2.3 represent the b and c glides with normal vector along the a axis [for a discussion of e-glide notation, see Sections 1.2.3 and 2.1.2, and de Wolff *et al.*, 1992].

Example 2

In a space group of type *P*4*mm* (99), representatives of the space group with respect to the translation subgroup are the powers of a fourfold rotation and reflections with normal vectors along the a and the b axis and along the diagonals [110] and $[1\bar{1}0]$ (*cf.* Fig. 1.4.2.4).

In this case, additional symmetry operations occur although there are no centring translations. Consider for example the reflection W_8 with the plane x, x, z as geometric element. Composing this reflection with the translation $t(1, 0, 0)$ gives rise to the symmetry operation represented by $y+1, x, z$. This operation maps a point with coordinates $x+\frac{1}{2}, x, z$ to $x+1, x+\frac{1}{2}, z$ and is thus a glide reflection with the plane $x+\frac{1}{2}, x, z$ as geometric element and $(\frac{1}{2}, \frac{1}{2}, 0)$ as glide vector. In a similar way, composing the other diagonal reflection with translations yields further glide reflections.

These glide reflections are symmetry operations which are not listed in the symmetry-operations block, although they are clearly of a different type to the operations given there. However, in the symmetry-element diagram as shown in Fig. 1.4.2.5, the corresponding symmetry elements are displayed as diagonal dashed lines which alternate with the solid diagonal lines representing the diagonal reflections.

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*g*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) m $x,0,z$	(6) m $0,y,z$	(7) m $x,\bar{x},z$	(8) m x,x,z

Figure 1.4.2.4
General-position and symmetry-operations blocks as given in the space-group tables for space group *P*4*mm* (99).

1.4.2.5. Space-group diagrams

In the space-group tables of Chapter 2.3, for each space group there are at least two diagrams displaying the symmetry (there are more diagrams for space groups of low symmetry). The *symmetry-element* diagram displays the location and orientation of the symmetry elements of the space group. The *general-position* diagrams show the arrangement of a set of symmetry-equivalent points of the general position. Because of the periodicity of the arrangements, the presentation of the contents of one unit cell is sufficient. Both types of diagrams are orthogonal projections of the space-group unit cell onto the plane of projection along a basis vector of the conventional crystallographic coordinate system. The symmetry elements of triclinic, monoclinic and orthorhombic groups are shown in three different projections along the basis vectors.