

1.2. CRYSTALLOGRAPHIC SYMMETRY

- (c) Similarly, in $Cmme$ (67) with an a -glide reflection $x + 1/2, y, \bar{z}$, the b -glide reflection $x, y + 1/2, \bar{z}$ also occurs. The geometric element is the plane $x, y, 0$ and the symmetry element is an e -glide plane.
In fact, all vectors $(u + \frac{1}{2})\mathbf{a} + v\mathbf{b} + \frac{1}{2}k(\mathbf{a} + \mathbf{b})$, u, v, k integers, are glide vectors of glide reflections through the (001) plane of a space group with a C -centred lattice. Among them one finds a glide reflection b with a glide vector $\frac{1}{2}\mathbf{b}$ related to $\frac{1}{2}\mathbf{a}$ by the centring translation; an a -glide reflection and a b -glide reflection share the same plane as a geometric element. Their symmetry element is thus an e -glide plane.
- (d) In general, the e -glide planes are symmetry elements characterized by the existence of two glide reflections through the same plane with perpendicular glide vectors and with the additional requirement that at least one glide vector is along a crystal axis (de Wolff *et al.*, 1992). The e -glide designation of glide planes occurs only when a centred cell represents the choice of basis (*cf.* Table 2.1.2.2). The ‘double’ e -glide planes are indicated by special graphical symbols on the symmetry-element diagrams of the space groups (*cf.* Tables 2.1.2.3 and 2.1.2.4). For example, consider the space group $I4cm$ (108). The symmetry operations (8) $y, x, z + 1/2$ [*General position* (0, 0, 0) block] and (8) $y + 1/2, x + 1/2, z$ [*General position* (1/2, 1/2, 1/2) block] are glide reflections through the same x, x, z plane, and their glide vectors $\frac{1}{2}\mathbf{c}$ and $\frac{1}{2}(\mathbf{a} + \mathbf{b})$ are related by the centring (1/2, 1/2, 1/2) translation. The corresponding symmetry element is an e -glide plane and it is easily recognized on the symmetry-element diagram of $I4cm$ shown in Chapter 2.3.
- (2) *Screw and rotation axes.* The element set of a screw axis is formed by a screw rotation of angle $2\pi/N$ with a screw vector \mathbf{u} , its $(N - 1)$ powers and all its co-axial equivalents, *i.e.* screw rotations around the same axis, with the same angle and sense of rotation, with screw vectors obtained by adding a lattice-translation vector parallel to \mathbf{u} .
- (a) Twofold screw axis $\parallel [001]$ in a primitive cell: the element set is formed by all twofold screw rotations around the same axis with screw vectors of the type $(u + \frac{1}{2})\mathbf{c}$, *i.e.* screw components as $\frac{1}{2}\mathbf{c}, -\frac{1}{2}\mathbf{c}, \frac{3}{2}\mathbf{c}$ *etc.*
- (b) The symmetry operation $4 - x, -2 - y, z + 5/2$ is a screw rotation of space group $P222_1$ (17). Its geometric element is the line $2, -1, z$ and its symmetry element is a screw axis.
- (c) The determination of the complete element set of a geometric element is important for the correct designation of the corresponding symmetry element. For example, the symmetry element of a twofold screw rotation with an axis through the origin is a twofold screw axis in the space group $P222_1$ but a fourfold screw axis in $P4_1$ (76).
- (3) *Special case.* In point groups $6/m, 6/mmm$ and space groups $P6/m$ (175), $P6/mmm$ (191) and $P6/mcc$ (192) the geometric elements of the defining operations $\bar{6}$ and $\bar{3}$ are the same. To make the element sets unique, the geometric elements should not be given just by a line and a point on it, but should be labelled by these operations. Then the element sets and thus the symmetry element are unique (Flack *et al.*, 2000).

References

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