

11. SYMMETRY OPERATIONS

Example

$4^-(0, 0, \frac{3}{4}) \frac{1}{4}, -\frac{1}{4}, z$ tetragonal system

$$4^- 0, 0, z \Rightarrow \mathbf{W} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ from Table 11.2.2.1.}$$

$x_0 = \frac{1}{4}, y_0 = -\frac{1}{4}, z_0 = 0$ is a fixed point of $4^- \frac{1}{4}, -\frac{1}{4}, z$, i.e. a point on the screw axis.

$$\begin{aligned} \mathbf{w}_l &= (\mathbf{I} - \mathbf{W}) \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} \\ \Rightarrow \mathbf{w}_l &= \begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{4} \\ -\frac{1}{4} \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}; \end{aligned}$$

$$\mathbf{w} = \mathbf{w}_g + \mathbf{w}_l$$

$$\Rightarrow \mathbf{w} = \begin{pmatrix} 0 \\ 0 \\ \frac{3}{4} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{3}{4} \end{pmatrix}$$

$$\Rightarrow \tilde{x} = y + \frac{1}{2}, \quad \tilde{y} = -x, \quad \tilde{z} = z + \frac{3}{4}.$$

References

Wondratschek, H. & Neubüser, J. (1967). *Determination of the symmetry elements of a space group from the 'general positions' listed in International Tables for X-ray Crystallography, Vol. I. Acta Cryst.* **23**, 349–352.