5.2. Transformations of symmetry operations (motions)

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5.2.1. Transformations

Symmetry operations are transformations in which the coordinate system, *i.e.* the basis vectors **a**, **b**, **c** and the origin O, are considered to be at rest, whereas the object is mapped onto itself. This can be visualized as a 'motion' of an object in such a way that the object before and after the 'motion' cannot be distinguished.

A symmetry operation W transforms every point X with the coordinates x, y, z to a symmetrically equivalent point $\tilde{X}$ with the coordinates $\tilde{x}, \tilde{y}, \tilde{z}$. In matrix notation, this transformation is performed by

$$\begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\end{pmatrix} = \begin{pmatrix}W_{11} & W_{12} & W_{13}\\ W_{21} & W_{22} & W_{23}\\ W_{31} & W_{32} & W_{33}\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} + \begin{pmatrix}w_1\\ w_2\\ w_3\end{pmatrix}$$

$$= \begin{pmatrix}W_{11}x + W_{12}y + W_{13}z + w_1\\ W_{21}x + W_{22}y + W_{23}z + w_2\\ W_{31}x + W_{32}y + W_{33}z + w_3\end{pmatrix}.$$

The(3×3) matrix $\boldsymbol{W}$ is the rotation part and the (3×1) column matrix $\boldsymbol{w}$ the translation part of the symmetry operation W. The pair $(\boldsymbol{W}, \boldsymbol{w})$ characterizes the operation uniquely. Matrices $\boldsymbol{W}$ for point-group operations are given in Tables 11.2.2.1 and 11.2.2.2.

Again, we can introduce the augmented (4×4) matrix (*cf.* Chapter 8.1)

$$\mathbb{W} = \begin{pmatrix}\boldsymbol{W} & \boldsymbol{w}\\ \boldsymbol{o} & 1\end{pmatrix} = \begin{pmatrix}W_{11} & W_{12} & W_{13} & w_1\\ W_{21} & W_{22} & W_{23} & w_2\\ W_{31} & W_{32} & W_{33} & w_3\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

The coordinates $\tilde{x}, \tilde{y}, \tilde{z}$ of the point $\tilde{X}$, symmetrically equivalent to X with the coordinates x, y, z, are obtained by

$$\begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\\ 1\end{pmatrix} = \begin{pmatrix}W_{11} & W_{12} & W_{13} & w_1\\ W_{21} & W_{22} & W_{23} & w_2\\ W_{31} & W_{32} & W_{33} & w_3\\ 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}x\\ y\\ z\\ 1\end{pmatrix}$$

$$= \begin{pmatrix}W_{11}x + W_{12}y + W_{13}z + w_1\\ W_{21}x + W_{22}y + W_{23}z + w_2\\ W_{31}x + W_{32}y + W_{33}z + w_3\\ 1\end{pmatrix},$$

or, in short notation,

$$\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}.$$

A sequence of symmetry operations can be obtained as a product of (4×4) matrices $\mathbb{W}$.

An affine transformation of the coordinate system transforms the coordinates $\mathbb{x}$ of the starting point

$$\mathbb{x}' = \mathbb{Q}\mathbb{x}$$

as well as the coordinates $\tilde{\mathbb{x}}$ of a symmetrically equivalent point

$$\begin{aligned}\tilde{\mathbb{x}}' &= \mathbb{Q}\tilde{\mathbb{x}}\\ &= \mathbb{Q}\mathbb{W}\mathbb{x}\\ &= \mathbb{Q}\mathbb{W}\mathbb{P}\mathbb{Q}\mathbb{x} \qquad (\text{with } \mathbb{P} = \mathbb{Q}^{-1})\\ &= \mathbb{Q}\mathbb{W}\mathbb{P}\mathbb{x}'.\end{aligned}$$

Thus, the affine transformation transforms also the symmetry-operation matrix $\mathbb{W}$ and the new matrix $\mathbb{W}'$ is obtained by

$$\mathbb{W}' = \mathbb{Q}\mathbb{W}\mathbb{P}.$$

Example

Space group $P4/n$ (85) is listed in the space-group tables with two origins; origin choice 1 with $\bar{4}$, origin choice 2 with $\bar{1}$ as point symmetry of the origin. How does the matrix $\mathbb{W}$ of the symmetry operation $\bar{4}^+$ 0, 0, z; 0, 0, 0 of origin choice 1 transform to the matrix $\mathbb{W}'$ of symmetry operation $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, 0$ of origin choice 2?

In the space-group tables, origin choice 1, the transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z} = y, \bar{x}, \bar{z}$ are listed. The translation part is zero, *i.e.* $\boldsymbol{w} = (0/0/0)$. In Table 11.2.2.1, the matrix $\boldsymbol{W}$ can be found. Thus, the (4×4) matrix $\mathbb{W}$ is obtained:

$$\mathbb{W} = \begin{pmatrix}\boldsymbol{W} & \boldsymbol{w}\\ \boldsymbol{o} & \mathbf{1}\end{pmatrix} = \begin{pmatrix}0 & 1 & 0 & 0\\ \bar{1} & 0 & 0 & 0\\ 0 & 0 & \bar{1} & 0\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

The transformation to origin choice 2 is accomplished by a shift vector **p** with components $\frac{1}{4}, -\frac{1}{4}, 0$. Since this is a pure shift, the matrices $\boldsymbol{P}$ and $\boldsymbol{Q}$ are the unit matrix $\boldsymbol{I}$. Now the shift vector $\boldsymbol{q}$ is derived: $\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p} = -\boldsymbol{I}\boldsymbol{p} = -\boldsymbol{p}$. Thus, the matrices $\mathbb{P}$ and $\mathbb{Q}$ are

$$\mathbb{P} = \begin{pmatrix}1 & 0 & 0 & \frac{1}{4}\\ 0 & 1 & 0 & \frac{\bar{1}}{4}\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}, \quad \mathbb{Q} = \begin{pmatrix}1 & 0 & 0 & \frac{\bar{1}}{4}\\ 0 & 1 & 0 & \frac{1}{4}\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

By matrix multiplication, the new matrix $\mathbb{W}'$ is obtained:

$$\mathbb{W}' = \mathbb{Q}\mathbb{W}\mathbb{P} = \begin{pmatrix}0 & 1 & 0 & \frac{\bar{1}}{2}\\ \bar{1} & 0 & 0 & 0\\ 0 & 0 & \bar{1} & 0\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

If the matrix $\mathbb{W}'$ is applied to x', y', z', the coordinates of the starting point in the new coordinate system, we obtain the transformed coordinates $\tilde{x}', \tilde{y}', \tilde{z}'$,

$$\begin{pmatrix}\tilde{x}'\\ \tilde{y}'\\ \tilde{z}'\\ 1\end{pmatrix} = \begin{pmatrix}0 & 1 & 0 & \frac{\bar{1}}{2}\\ \bar{1} & 0 & 0 & 0\\ 0 & 0 & \bar{1} & 0\\ 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}x'\\ y'\\ z'\\ 1\end{pmatrix} = \begin{pmatrix}y' - \frac{1}{2}\\ \bar{x}'\\ \bar{z}'\\ 1\end{pmatrix}.$$

By adding a lattice translation **a**, the transformed coordinates $y + \frac{1}{2}, \bar{x}, \bar{z}$ are obtained as listed in the space-group tables for origin choice 2.

5.2.2. Invariants

A crystal structure and its physical properties are independent of the choice of the unit cell. This implies that invariants occur, *i.e.* quantities which have the same values before and after the transformation. Only some important invariants are considered in this section. Invariants of higher order (tensors) are treated by Altmann & Herzig (1994), second cumulant tensors, *i.e.* anisotropic temperature factors, are given in *International Tables for Crystallography* (2004), Vol. C.