1.5.2.2. Metric tensors of direct and reciprocal lattices

The metric tensor of a crystal lattice with a basis **a**, **b**, **c** is the (3 × 3) matrix

$$\boldsymbol{G} = \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix},$$

which can formally be described as

$$\boldsymbol{G} = (\mathbf{a},\mathbf{b},\mathbf{c})^T \cdot (\mathbf{a},\mathbf{b},\mathbf{c}) = \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix} \cdot (\mathbf{a},\mathbf{b},\mathbf{c})$$

(*cf.* Section 1.3.2). The transformation of the metric tensor under the coordinate transformation $(\boldsymbol{P},\boldsymbol{p})$ follows directly from its definition:

$$\begin{aligned} \boldsymbol{G}' &= (\mathbf{a}',\mathbf{b}',\mathbf{c}')^T \cdot (\mathbf{a}',\mathbf{b}',\mathbf{c}') = [(\mathbf{a},\mathbf{b},\mathbf{c})\boldsymbol{P}]^T \cdot (\mathbf{a},\mathbf{b},\mathbf{c})\boldsymbol{P} \\ &= \boldsymbol{P}^T(\mathbf{a},\mathbf{b},\mathbf{c})^T \cdot (\mathbf{a},\mathbf{b},\mathbf{c})\boldsymbol{P} = \boldsymbol{P}^T\boldsymbol{G}\boldsymbol{P}, \end{aligned} \qquad (1.5.2.4)$$

where $\boldsymbol{P}^T$ is the transposed matrix of $\boldsymbol{P}$. The transformation behaviour of $\boldsymbol{G}$ under $(\boldsymbol{P},\boldsymbol{p})$ is determined by the matrix $\boldsymbol{P}$, *i.e.* $\boldsymbol{G}$ is not affected by an origin shift $\boldsymbol{p}$.

The volume V of the unit cell defined by the basis vectors **a**, **b**, **c** can be obtained from the determinant of the metric tensor, $V^2 = \det(\boldsymbol{G})$. The transformation behaviour of V under a coordinate transformation follows from the transformation behaviour of the metric tensor [note that $\det(\boldsymbol{P}) = \det(\boldsymbol{P}^T)$]: $(V')^2 = \det(\boldsymbol{G}')$ $= \det(\boldsymbol{P}^T\boldsymbol{G}\boldsymbol{P}) = \det(\boldsymbol{P})\det(\boldsymbol{P}^T)\det(\boldsymbol{G}) = \det(\boldsymbol{P})^2V^2$, *i.e.*

$$V' = |\det(\boldsymbol{P})|V, \qquad (1.5.2.5)$$

which is reduced to $V' = \det(\boldsymbol{P})V$ if $\det(\boldsymbol{P}) > 0$.

Similarly, the metric tensor $\boldsymbol{G}^*$ of the reciprocal lattice and the volume V^* of the unit cell defined by the basis vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ transform as

$$\boldsymbol{G}^{*\prime} = \boldsymbol{Q}\boldsymbol{G}^*\boldsymbol{Q}^T, \qquad (1.5.2.6)$$

$$V^{*\prime} = |\det(\boldsymbol{Q})|V^* \text{ or } V^{*\prime} = \det(\boldsymbol{Q})V^* = [1/\det(\boldsymbol{P})]V^* \text{ if } \det(\boldsymbol{Q}) > 0. \qquad (1.5.2.7)$$

Again, it is only the linear part $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ that determines the transformation behaviour of $\boldsymbol{G}^*$ and V^* under coordinate transformations.

1.5.2.3. Transformation of matrix–column pairs of symmetry operations

The *matrix–column pairs for the symmetry operations* are changed by a change of the coordinate system (see Section 1.2.2 for details of the matrix description of symmetry operations). A symmetry operation $\mathcal{W}$ that maps a point X to an image point $\tilde{X}$ is described in the 'old' (unprimed) coordinate system by the system of equations

$$\begin{aligned} \tilde{x}_1 &= W_{11}x_1 + W_{12}x_2 + W_{13}x_3 + w_1 \\ \tilde{x}_2 &= W_{21}x_1 + W_{22}x_2 + W_{23}x_3 + w_2 \\ \tilde{x}_3 &= W_{31}x_1 + W_{32}x_2 + W_{33}x_3 + w_3, \end{aligned} \qquad (1.5.2.8)$$

i.e. by the matrix–column pair $(\boldsymbol{W},\boldsymbol{w})$:

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w} = (\boldsymbol{W},\boldsymbol{w})\boldsymbol{x}. \qquad (1.5.2.9)$$

In the new (primed) coordinate system, the symmetry operation $\mathcal{W}$ is described by the pair $(\boldsymbol{W}',\boldsymbol{w}')$:

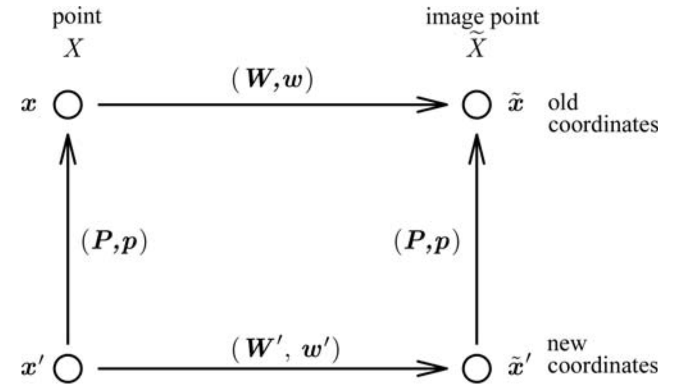

Figure 1.5.2.1
Illustration of the transformation of symmetry operations $(\boldsymbol{W},\boldsymbol{w})$, also called a 'mapping of mappings'.

$$\tilde{\boldsymbol{x}}' = (\boldsymbol{W}',\boldsymbol{w}')\boldsymbol{x}' = \boldsymbol{W}'\boldsymbol{x}' + \boldsymbol{w}'. \qquad (1.5.2.10)$$

The relation between $(\boldsymbol{W},\boldsymbol{w})$ and $(\boldsymbol{W}',\boldsymbol{w}')$ is derived *via* the transformation matrix–column pair $(\boldsymbol{P},\boldsymbol{p})$, which specifies the change of the coordinate system. The successive application of equations (1.5.1.7), (1.5.2.9) and again (1.5.1.7) results in $\tilde{\boldsymbol{x}}' = (\boldsymbol{P},\boldsymbol{p})^{-1}\tilde{\boldsymbol{x}} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})\boldsymbol{x} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p})\boldsymbol{x}'$, which compared with equation (1.5.2.10) gives

$$(\boldsymbol{W}',\boldsymbol{w}') = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p}). \qquad (1.5.2.11)$$

The result indicates that the change of the matrix–column pairs of symmetry operations $(\boldsymbol{W},\boldsymbol{w})$ under a coordinate transformation described by the matrix–column pair $(\boldsymbol{P},\boldsymbol{p})$ is realized by the conjugation of $(\boldsymbol{W},\boldsymbol{w})$ by $(\boldsymbol{P},\boldsymbol{p})$. The multiplication of the matrix–column pairs on the *right-hand side* of equation (1.5.2.11), namely $(\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p}) = (\boldsymbol{P}^{-1},-\boldsymbol{P}^{-1}\boldsymbol{p})(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p}) = (\boldsymbol{P}^{-1}\boldsymbol{W},\boldsymbol{P}^{-1}\boldsymbol{w} - \boldsymbol{P}^{-1}\boldsymbol{p})(\boldsymbol{P},\boldsymbol{p}) = (\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P},\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{p} + \boldsymbol{P}^{-1}\boldsymbol{w} - \boldsymbol{P}^{-1}\boldsymbol{p})$, results in the factorization of the relation (1.5.2.11) into a pair of equations for the rotation and translation parts of $(\boldsymbol{W}',\boldsymbol{w}')$:

$$\boldsymbol{W}' = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} = \boldsymbol{Q}\boldsymbol{W}\boldsymbol{P} \qquad (1.5.2.12)$$

and

$$\begin{aligned} \boldsymbol{w}' &= \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{p} + \boldsymbol{P}^{-1}\boldsymbol{w} - \boldsymbol{P}^{-1}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{w} + \boldsymbol{W}\boldsymbol{p} - \boldsymbol{p}) \\ &= \boldsymbol{Q}(\boldsymbol{w} + \boldsymbol{W}\boldsymbol{p} - \boldsymbol{p}) = \boldsymbol{Q}(\boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}). \end{aligned} \qquad (1.5.2.13)$$

The whole formalism described above can be visualized by means of an instructive diagram, Fig. 1.5.2.1, displaying the transformation of the matrix–column pairs of symmetry operations under coordinate transformations, the so-called *mapping of mappings*.

The points X (left) and $\tilde{X}$ (right), and the corresponding columns of coordinates $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$, and $\boldsymbol{x}'$ and $\tilde{\boldsymbol{x}}'$, are referred to the old and to the new coordinate systems, respectively. The transformation matrices of each step are indicated next to the edges of the diagram, while the arrows indicate the direction, *e.g.* $\boldsymbol{x} = (\boldsymbol{P},\boldsymbol{p})\boldsymbol{x}'$ but $\boldsymbol{x}' = (\boldsymbol{P},\boldsymbol{p})^{-1}\boldsymbol{x}$. From $\boldsymbol{x}'$ to $\tilde{\boldsymbol{x}}'$ it is possible to proceed in two different ways:

(i) $\tilde{\boldsymbol{x}}' = (\boldsymbol{W}',\boldsymbol{w}')\boldsymbol{x}'$,

(ii) $\tilde{\boldsymbol{x}}' = (\boldsymbol{P},\boldsymbol{p})^{-1}\tilde{\boldsymbol{x}} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})\boldsymbol{x} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p})\boldsymbol{x}'$.

The comparison of (i) and (ii) yields equation (1.5.2.11).

1.5.2.4. Augmented-matrix formalism

The augmented-matrix formalism (*cf.* Section 1.2.2) simplifies the equations of the coordinate transformations discussed above.