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:

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

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.*

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

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

$$\boldsymbol{G}^{*\prime} = \boldsymbol{Q}\boldsymbol{G}^*\boldsymbol{Q}^T, \tag{1.5.2.6}$$

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

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 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

$$\begin{aligned}\tilde{x_1} &= W_{11}x_1 + W_{12}x_2 + W_{13}x_3 + w_1\\ \tilde{x_2} &= W_{21}x_1 + W_{22}x_2 + W_{23}x_3 + w_2\\ \tilde{x_3} &= W_{31}x_1 + W_{32}x_2 + W_{33}x_3 + w_3,\end{aligned} \tag{1.5.2.8}$$

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

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

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

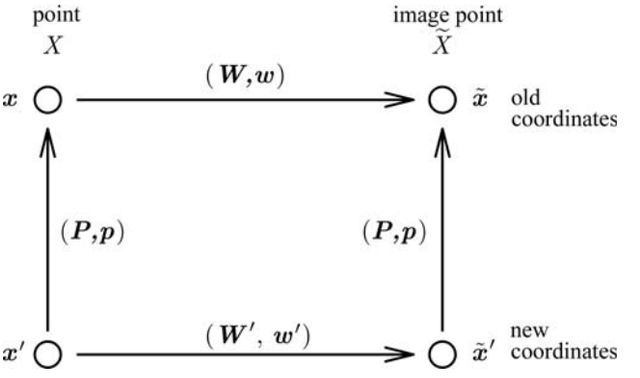

Figure 1.5.2.1
Illustration of the transformation of symmetry operations $(\boldsymbol{W},\boldsymbol{w})$, also called a 'mapping of mappings'.

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

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

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

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 $(\boldsymbol{W}',\boldsymbol{w}')$:

$$\boldsymbol{W}' = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} = \boldsymbol{Q}\boldsymbol{W}\boldsymbol{P} \tag{1.5.2.12}$$

and

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

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.

The matrices $\boldsymbol{P}$, $\boldsymbol{Q}$ may be combined with the corresponding columns $\boldsymbol{p}$, $\boldsymbol{q}$ to form (4×4) matrices:

$$\mathbb{P} = \left(\begin{array}{c|c} \boldsymbol{P} & \boldsymbol{p} \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{Q} = \mathbb{P}^{-1} = \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{q} \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \qquad (1.5.2.14)$$

where $\boldsymbol{0}$ is a 1×3 row with zero coefficients. As already indicated in Section 1.2.2, the horizontal and vertical lines in the augmented matrices have no mathematical meaning; they serve as guide to the eye so that the coefficients can be recognized more easily.

Analogously, the (3×1) columns $\boldsymbol{x}$ and $\boldsymbol{x}'$ are augmented to (4×1) columns by adding '1' as fourth coordinate in order to enable matrix multiplication with the augmented matrices: $\mathbb{x} = \begin{pmatrix} x_1 \\ x_2 \\ \underline{x_3} \\ 1 \end{pmatrix}$; $\mathbb{x}' = \begin{pmatrix} x'_1 \\ x'_2 \\ \underline{x'_3} \\ 1 \end{pmatrix}$. Using the augmented matrices, the transformation behaviour of point coordinates [*cf.* equation (1.5.1.7)] takes the form

$$\begin{aligned} \mathbb{x}' = \mathbb{P}^{-1}\mathbb{x} = \mathbb{Q}\mathbb{x} &= \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{q} \\ \hline \boldsymbol{0} & 1 \end{array}\right) \begin{pmatrix} x_1 \\ x_2 \\ \underline{x_3} \\ 1 \end{pmatrix} \\ &= \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \begin{pmatrix} x_1 \\ x_2 \\ \underline{x_3} \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} Q_{11}x_1 + Q_{12}x_2 + Q_{13}x_3 + q_1 \\ Q_{21}x_1 + Q_{22}x_2 + Q_{23}x_3 + q_2 \\ \underline{Q_{31}x_1 + Q_{32}x_2 + Q_{33}x_3 + q_3} \\ 1 \end{pmatrix}. \end{aligned} \qquad (1.5.2.15)$$

The difference in the transformation behaviour of point coordinates and vector coefficients under coordinate transformations becomes obvious if the augmented-matrix formalism is applied. The (3×1) column of coefficients of a vector between points X and Y,

$$\boldsymbol{r} = \boldsymbol{y} - \boldsymbol{x} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ y_3 - x_3 \end{pmatrix},$$

is augmented by adding *zero* as fourth coefficient:

$$\mathbb{r} = \mathbb{y} - \mathbb{x} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ \underline{y_3 - x_3} \\ 0 \end{pmatrix},$$

and this specific form of $\mathbb{r}$ reflects its specific transformation properties, namely that it is unaffected by origin shifts:

$$\begin{aligned} \mathbb{r}' = \mathbb{P}^{-1}\mathbb{r} = \mathbb{Q}\mathbb{r} &= \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{q} \\ \hline \boldsymbol{0} & 1 \end{array}\right) \begin{pmatrix} r_1 \\ r_2 \\ \underline{r_3} \\ 0 \end{pmatrix} \\ &= \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \begin{pmatrix} r_1 \\ r_2 \\ \underline{r_3} \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} Q_{11}r_1 + Q_{12}r_2 + Q_{13}r_3 \\ Q_{21}r_1 + Q_{22}r_2 + Q_{23}r_3 \\ \underline{Q_{31}r_1 + Q_{32}r_2 + Q_{33}r_3} \\ 0 \end{pmatrix}. \end{aligned} \qquad (1.5.2.16)$$

The Miller indices (hkl) are coefficients of vectors in reciprocal space (plane normals). Therefore, the (1×3) rows (hkl) are augmented by 0: $(hkl|0)$. Thus, only the linear part $\boldsymbol{P}$ of the general coordinate transformation $(\boldsymbol{P}, \boldsymbol{p})$ acts on the Miller indices while the origin shift has no effect, *cf.* equation (1.5.2.2).

The augmented-matrix formulation of transformation of symmetry operations (1.5.2.11) is straightforward if the matrices $\boldsymbol{W}$ and $\boldsymbol{W}'$ are combined with the corresponding columns $\boldsymbol{w}$ and $\boldsymbol{w}'$ to form (4×4) matrices:

$$\mathbb{W} = \left(\begin{array}{c|c} \boldsymbol{W} & \boldsymbol{w} \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{W}' = \left(\begin{array}{c|c} \boldsymbol{W}' & \boldsymbol{w}' \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} W'_{11} & W'_{12} & W'_{13} & w'_1 \\ W'_{21} & W'_{22} & W'_{23} & w'_2 \\ W'_{31} & W'_{32} & W'_{33} & w'_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

Thus, equation (1.5.2.11) is replaced by its (4×4) analogue:

$$\begin{aligned} \mathbb{W}' = \mathbb{P}^{-1}\mathbb{W}\mathbb{P} = \mathbb{Q}\mathbb{W}\mathbb{P} &= \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \cdot \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \\ &\cdot \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \end{aligned} \qquad (1.5.2.17)$$

where $\mathbb{P}$ and $\mathbb{Q}$ are defined according to equation (1.5.2.14). [Note that to avoid any confusion that might result from equation (1.5.2.17) being displayed over more than one line, the matrix multiplication is explicitly indicated by centred dots between the matrices.] In analogy to equation (1.5.2.11), the change of the augmented matrices of symmetry operations $\mathbb{W}$ under coordinate transformations represented by the augmented matrices $\mathbb{P}$ is described by the conjugation of $\mathbb{W}$ with $\mathbb{P}$.

The transformation behaviour of the vector coefficients becomes apparent if the (distance) vector $\mathbf{v}$ is treated as a

translation vector and the transformation behaviour of the translation is considered. The corresponding translation is then described by $(\boldsymbol{I}, \boldsymbol{v})$, *i.e.* $\boldsymbol{W} = \boldsymbol{I}$, $\boldsymbol{w} = \boldsymbol{v}$. Equation (1.5.2.13) shows that the translation and thus the translation vector are not changed under an origin shift, $(\boldsymbol{P}, \boldsymbol{p}) = (\boldsymbol{I}, \boldsymbol{p})$, because $(\boldsymbol{I}, \boldsymbol{v})' = (\boldsymbol{I}, \boldsymbol{v})$ holds. For the same reason, under a general coordinate transformation the origin shift has no effect on the vector coefficients, *cf.* equation (1.5.2.16).

1.5.2.5. Example: paraelectric-to-ferroelectric phase transition of GeTe

Coordinate transformations are essential in the study of structural relationships between crystal structures. Consider as an example two phases **A** (*basic* or *parent* structure) and **B** (*derivative* structure) of the same compound. Let the space group $\mathcal{H}$ of **B** be a proper subgroup of the space group $\mathcal{G}$ of **A**, $\mathcal{H} < \mathcal{G}$. The relationship between the two structures is characterized by a global distortion that, in general, can be decomposed into a homogeneous strain describing the distortion of the lattice of **B** relative to that of **A** and an atomic displacement field representing the displacements of the atoms of **B** from their positions in **A**. In order to facilitate the comparison of the two structures, first the coordinate system of structure **A** is transformed by an appropriate transformation $(\boldsymbol{P}, \boldsymbol{p})$ to that of structure **B**. This new description of **A** will be called the *reference description* of structure **A** relative to structure **B**. Now, the metric tensors $\boldsymbol{G}_{\mathbf{A}}$ of the reference description of **A** and $\boldsymbol{G}_{\mathbf{B}}$ are of the same type and are distinguished only by the values of their parameters. The adaptation of structure **A** to structure **B** can be performed in two further steps. In the first step the parameter values of $\boldsymbol{G}_{\mathbf{A}}$ are adapted to those of $\boldsymbol{G}_{\mathbf{B}}$ by an affine transformation which determines the metric deformation (spontaneous strain) of structure **B** relative to structure **A**. The result is a hypothetical structure which still differs from structure **B** by atomic displacements. In the second step these displacements are balanced out by shifting the individual atoms to those of structure **B**. In other words, if $\mathbf{a}, \mathbf{b}, \mathbf{c}$ represents the basis of the parent phase, then its image under the transformation $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$ should be similar to the basis of the derivative phase $\mathbf{a}_{\mathcal{H}}, \mathbf{b}_{\mathcal{H}}, \mathbf{c}_{\mathcal{H}}$. The difference between $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ and $\mathbf{a}_{\mathcal{H}}, \mathbf{b}_{\mathcal{H}}, \mathbf{c}_{\mathcal{H}}$ determines the metric deformation (spontaneous strain) accompanying the transition between the two phases. Similarly, the differences between the images X' of the atomic positions X of the basic structure under the transformation $(\boldsymbol{P}, \boldsymbol{p})$ and the atomic positions $X_{\mathcal{H}}$ of the derivative structure give the atomic displacements that occur during the phase transition.

As an example we will consider the structural phase transition of GeTe, which is of displacive type, *i.e.* the phase transition is accomplished through small atomic displacements. The room-temperature ferroelectric phase belongs to the rhombohedral space group *R*3*m* (160). At about 720 K a structural phase transition takes place to a high-symmetry paraelectric cubic phase of the NaCl type. The following descriptions of the two phases of GeTe are taken from the ICSD:

(*a*) Wiedemeier & Siemers (1989), ICSD No. 56037. The symmetry of the high-temperature phase is described by the space group $Fm\bar{3}m$ (225) with cell parameters a_c = 6.009 Å and atomic coordinates listed as
Ge: 4*a* 0, 0, 0
Te: 4*b* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

(*b*) Chattopadhyay *et al.* (1987), ICSD No. 56038. The structure is described with respect to the hexagonal-axes setting of *R*3*m* (160) (*cf.* Section 1.5.3.1) with cell parameters $a_{\rm hex}$ = 4.164 (2) Å, $c_{\rm hex}$ = 10.69 (4) Å. The coordinates of the atoms in the asymmetric unit are given as
Ge: 3*a* 0, 0, 0.2376
Te: 3*a* 0, 0, 0.7624

The relation between the basis $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ of the *F*-centred cubic lattice and the basis $\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c$ of the reference description can be obtained by inspection. The $\mathbf{c}'_c$ axis of the reference hexagonal basis must be one of the cubic threefold axes, say [111]. The axes $\mathbf{a}'_c$ and $\mathbf{b}'_c$ must be lattice vectors of the *F*-centred lattice, perpendicular to the rhombohedral axis. They must have equal length, form an angle of 120°, and together with $\mathbf{c}'_c$ define a right-handed basis. For example, the vectors $\mathbf{a}'_c = \frac{1}{2}(-\mathbf{a}_c + \mathbf{b}_c)$, $\mathbf{b}'_c = \frac{1}{2}(-\mathbf{b}_c + \mathbf{c}_c)$ fulfil these conditions.

The transformation matrix $\boldsymbol{P}$ between the bases $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ and $\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c$ can also be derived from the data listed in Table 1.5.1.1 in two steps:

(i) A cubic *F* cell can be considered as a primitive rhombohedral cell with $a_p = a_c \frac{1}{2}\sqrt{2}$ and α = 60°. The relation between the two cells is described by the transformation matrix $\boldsymbol{P}_1$ (*cf.* Table 1.5.1.1 and Fig. 1.5.1.4):

$$(\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p) = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\boldsymbol{P}_1 = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}. \tag{1.5.2.18}$$

(ii) The transformation matrix $\boldsymbol{P}_2$ between the rhombohedral primitive cell and the triple hexagonal cell (obverse setting) of the reference description is read from Table 1.5.1.1 (*cf.* Fig. 1.5.1.6):

$$(\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c) = (\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p)\boldsymbol{P}_2 = (\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p)\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}. \tag{1.5.2.19}$$

Combining equations (1.5.2.18) and (1.5.2.19) gives the orientational relationship between the *F*-centred cubic cell and the rhombohedrally centred hexagonal cell $(\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c) = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\boldsymbol{P}$, where

$$\boldsymbol{P} = \boldsymbol{P}_1\boldsymbol{P}_2 = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & 0 & 1 \\ \frac{1}{2} & -\frac{1}{2} & 1 \\ 0 & \frac{1}{2} & 1 \end{pmatrix}. \tag{1.5.2.20}$$

Formally, the lattice parameters of the reference unit cell can be extracted from the metric tensor $\boldsymbol{G}'_c$ obtained from the metric tensor $\boldsymbol{G}_c$ transformed by $\boldsymbol{P}$, *cf.* equation (1.5.2.4):

$$\begin{aligned} \boldsymbol{G}'_c &= \boldsymbol{P}^T\boldsymbol{G}_c\boldsymbol{P} \\ &= \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} \\ 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} a_c^2 & 0 & 0 \\ 0 & a_c^2 & 0 \\ 0 & 0 & a_c^2 \end{pmatrix}\begin{pmatrix} -\frac{1}{2} & 0 & 1 \\ \frac{1}{2} & -\frac{1}{2} & 1 \\ 0 & \frac{1}{2} & 1 \end{pmatrix} \\ &= a_c^2\begin{pmatrix} \frac{1}{2} & -\frac{1}{4} & 0 \\ -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & 0 & 3 \end{pmatrix}, \end{aligned} \tag{1.5.2.21}$$

which gives $a'_c = a_c \frac{1}{2}\sqrt{2}$ = 4.249 Å and $c'_c = a_c\sqrt{3}$ = 10.408 Å. The comparison of these values with the experimentally deter-