

5.2. TRANSFORMATIONS OF SYMMETRY OPERATIONS

The orthogonality of the basis vectors \mathbf{a} , \mathbf{b} , \mathbf{c} of direct space and the basis vectors \mathbf{a}^* , \mathbf{b}^* , \mathbf{c}^* of reciprocal space,

$$\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} (\mathbf{a}, \mathbf{b}, \mathbf{c}) = \begin{pmatrix} \mathbf{a}^* \cdot \mathbf{a} & \mathbf{a}^* \cdot \mathbf{b} & \mathbf{a}^* \cdot \mathbf{c} \\ \mathbf{b}^* \cdot \mathbf{a} & \mathbf{b}^* \cdot \mathbf{b} & \mathbf{b}^* \cdot \mathbf{c} \\ \mathbf{c}^* \cdot \mathbf{a} & \mathbf{c}^* \cdot \mathbf{b} & \mathbf{c}^* \cdot \mathbf{c} \end{pmatrix} = \mathbf{I},$$

is invariant under a general (affine) transformation. Since both sets of basis vectors are transformed, \mathbf{a}^* is always perpendicular to the plane defined by \mathbf{b} and \mathbf{c} and $\mathbf{a}^{*'}$ perpendicular to \mathbf{b}' and \mathbf{c}' etc.

5.2.2.1. Position vector

The position vector \mathbf{r} in direct space,

$$\mathbf{r} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c},$$

is invariant if the origin of the coordinate system is not changed in the transformation (see example in Section 5.1.3).

5.2.2.2. Modulus of position vector

The modulus r of the position vector \mathbf{r} gives the distance of the point x, y, z from the origin. Its square is obtained by the scalar product

$$\begin{aligned} \mathbf{r}^t \cdot \mathbf{r} = r^2 &= (x, y, z) \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix} (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} x \\ y \\ z \end{pmatrix} \\ &= (x, y, z) \mathbf{G} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \\ &= x^2 a^2 + y^2 b^2 + z^2 c^2 + 2yzbc \cos \alpha \\ &\quad + 2xzac \cos \beta + 2xyab \cos \gamma, \end{aligned}$$

with \mathbf{r}^t the transposed representation of \mathbf{r} ; a, b, c the moduli of the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ (lattice parameters); \mathbf{G} the metric matrix of direct space; and α, β, γ the angles of the unit cell.

The same considerations apply to the vector \mathbf{r}^* in reciprocal space and its modulus r^* . Here, \mathbf{G}^* is applied. Note that \mathbf{r}^* and r^* are independent of the choice of the origin in direct space.

5.2.2.3. Metric matrix

The metric matrix \mathbf{G} of the unit cell in the direct lattice

$$\mathbf{G} = \begin{pmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{a} \cdot \mathbf{b} & \mathbf{a} \cdot \mathbf{c} \\ \mathbf{b} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{b} \cdot \mathbf{c} \\ \mathbf{c} \cdot \mathbf{a} & \mathbf{c} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \end{pmatrix} = \begin{pmatrix} aa & ab \cos \gamma & ac \cos \beta \\ ba \cos \gamma & bb & bc \cos \alpha \\ ca \cos \beta & cb \cos \alpha & cc \end{pmatrix}$$

changes under a linear transformation, but \mathbf{G} is invariant under a symmetry operation of the lattice. The volume of the unit cell V is obtained by

$$V^2 = \det(\mathbf{G}).$$

The same considerations apply to the metric matrix \mathbf{G}^* of the unit cell in the reciprocal lattice and the volume V^* of the reciprocal-lattice unit cell. Thus, there are two invariants under an affine transformation, the product

$$VV^* = 1$$

and the product

$$\mathbf{G}\mathbf{G}^* = \mathbf{I}.$$

5.2.2.4. Scalar product

The scalar product

$$\mathbf{r}^* \cdot \mathbf{r} = hx + ky + lz$$

of the vector \mathbf{r}^* in reciprocal space with the vector \mathbf{r} in direct space is invariant under a linear transformation but not under a shift of origin in direct space.

A vector \mathbf{r} in direct space can also be represented as a product of augmented matrices:

$$\mathbf{r} = (\mathbf{a}, \mathbf{b}, \mathbf{c}, 0) \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}.$$

As stated above, the basis vectors are transformed only by the linear part, even in the case of a general affine transformation. Thus, the transformed position vector \mathbf{r}' is obtained by

$$\mathbf{r}' = (\mathbf{a}, \mathbf{b}, \mathbf{c}, 0) \begin{pmatrix} \mathbf{P} & \mathbf{o}^t \\ \mathbf{o} & 1 \end{pmatrix} \begin{pmatrix} \mathbf{Q} & \mathbf{q} \\ \mathbf{o} & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}.$$

The shift \mathbf{p} is set to zero. The shift of origin is contained in the matrix \mathbf{Q} only.

Similarly, a vector in reciprocal space can be represented by

$$\mathbf{r}^* = (h, k, l, 1) \begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \\ 0 \end{pmatrix} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*.$$

The coordinates h, k, l in reciprocal space transform also only linearly. Thus,

$$\mathbf{r}^{*'} = (h, k, l, 1) \begin{pmatrix} \mathbf{P} & \mathbf{o}^t \\ \mathbf{o} & 1 \end{pmatrix} \begin{pmatrix} \mathbf{Q} & \mathbf{q} \\ \mathbf{o} & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \\ 0 \end{pmatrix}.$$

The reader can see immediately that the scalar product $\mathbf{r}^* \cdot \mathbf{r}$ transforms correctly.

5.2.3. Example: low cristobalite and high cristobalite

The positions of the silicon atoms in the low-cristobalite structure (Nieuwenkamp, 1935) are compared with those of the high-cristobalite structure (Wyckoff, 1925; cf. Megaw, 1973). At low temperatures, the space group is $P4_12_12$ (92). The four silicon atoms are located in Wyckoff position $4(a)$..2 with the coordinates $x, x, 0; \bar{x}, \bar{x}, \frac{1}{2} - x, \frac{1}{2} + x, \frac{1}{4}, \frac{1}{4} + x, \frac{1}{2} - x, \frac{3}{4}; x = 0.300$. During the phase transition, the tetragonal structure is transformed into a cubic one with space group $Fd\bar{3}m$ (227). It is listed in the space-group tables with two different origins. We use 'Origin choice 1' with point symmetry $43m$ at the origin. The silicon atoms occupy the position $8(a)$ $43m$ with the coordinates $0, 0, 0; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ and those related by the face-centring translations. In the diamond structure, the carbon atoms occupy the same position.

In order to compare the two structures, the conventional P cell of space group $P4_12_12$ (92) is transformed to an unconventional C cell (cf. Section 4.3.4), which corresponds to the F cell of $Fd\bar{3}m$ (227). The P and the C cells are shown in Fig. 5.2.3.1. The coordinate system $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ with origin O' of the C cell is obtained from that of