International Tables for Crystallography (2006). Vol. A, Section 5.2.2.3, p. 87.

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

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

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 **b** and **c** and $\mathbf{a}^{*\prime}$ perpendicular to $\mathbf{b}'$ and $\mathbf{c}'$ *etc.*

5.2.2.1. *Position vector*

The position vector **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 **r** gives the distance of the point x, y, z from the origin. Its square is obtained by the scalar product

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

with $\mathbf{r}^{t}$ the transposed representation of **r**; a, b, c the moduli of the basis vectors **a**, **b**, **c** (lattice parameters); $\boldsymbol{G}$ 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, $\boldsymbol{G}^*$ 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 $\boldsymbol{G}$ of the unit cell in the direct lattice

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

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

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

The same considerations apply to the metric matrix $\boldsymbol{G}^*$ 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

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

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 **r** in direct space is invariant under a linear transformation but not under a shift of origin in direct space.

A vector **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

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

The shift $\boldsymbol{p}$ is set to zero. The shift of origin is contained in the matrix $\mathbb{Q}$ 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,

$$\mathbf{r}^{*\prime} = (h,k,l,1)\begin{pmatrix}\boldsymbol{P} & \boldsymbol{o}^t\\ \boldsymbol{o} & 1\end{pmatrix}\begin{pmatrix}\boldsymbol{Q} & \boldsymbol{q}\\ \boldsymbol{o} & 1\end{pmatrix}\begin{pmatrix}\mathbf{a}^*\\ \mathbf{b}^*\\ \mathbf{c}^*\\ 0\end{pmatrix}.$$

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 $x, x, 0$; $\bar{x}, \bar{x}, \frac{1}{2}$; $\frac{1}{2}-x, \frac{1}{2}+x, \frac{1}{4}$; $\frac{1}{2}+x, \frac{1}{2}-x, \frac{3}{4}$; $x = 0.300$. 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 $\bar{4}3m$ 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

references