$$\mathbf{v}\cdot\mathbf{w} = (x_1\, y_1\, z_1)\cdot \boldsymbol{G}\cdot\begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}.$$

From this it follows how the metric tensor transforms under a basis transformation $\boldsymbol{P}$. If $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$, then the metric tensor $\boldsymbol{G}'$ of $\mathbf{L}$ with respect to the new basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ is given by

$$\boldsymbol{G}' = \boldsymbol{P}^{\mathrm{T}}\cdot\boldsymbol{G}\cdot\boldsymbol{P}.$$

An alternative way to specify the geometry of a lattice in $\mathbb{V}^3$ is using the *cell parameters*, which are the lengths of the lattice basis vectors and the angles between them.

Definition

For a lattice $\mathbf{L}$ in $\mathbb{V}^3$ with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ the *cell parameters* (also called *lattice parameters*, *lattice constants* or *metric parameters*) are given by the lengths

$$a = |\mathbf{a}| = \sqrt{\mathbf{a}\cdot\mathbf{a}}, \quad b = |\mathbf{b}| = \sqrt{\mathbf{b}\cdot\mathbf{b}}, \quad c = |\mathbf{c}| = \sqrt{\mathbf{c}\cdot\mathbf{c}}$$

of the basis vectors and by the interaxial angles

$$\alpha = \measuredangle(\mathbf{b}, \mathbf{c}), \quad \beta = \measuredangle(\mathbf{c}, \mathbf{a}), \quad \gamma = \measuredangle(\mathbf{a}, \mathbf{b}).$$

Owing to the relation $\mathbf{v}\cdot\mathbf{w} = |\mathbf{v}|\,|\mathbf{w}|\cos\measuredangle(\mathbf{v}, \mathbf{w})$ for the scalar product of two vectors, one can immediately write down the metric tensor in terms of the cell parameters:

$$\boldsymbol{G} = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}.$$

1.3.2.3. Unit cells

A lattice $\mathbf{L}$ can be used to subdivide $\mathbb{V}^3$ into cells of finite volume which all have the same shape. The idea is to define a suitable subset $\mathbf{C}$ of $\mathbb{V}^3$ such that the translates of $\mathbf{C}$ by the vectors in $\mathbf{L}$ cover $\mathbb{V}^3$ without overlapping. Such a subset $\mathbf{C}$ is called a *unit cell* of $\mathbf{L}$, or, in the more mathematically inclined literature, a *fundamental domain* of $\mathbb{V}^3$ with respect to $\mathbf{L}$. Two standard constructions for such unit cells are the *primitive unit cell* and the *Voronoï domain* (which is also known by many other names).

Definition

Let $\mathbf{L}$ be a lattice in $\mathbb{V}^3$ with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

(i) The set $\mathbf{C} := \{x\mathbf{a} + y\mathbf{b} + z\mathbf{c} \mid 0 \le x, y, z < 1\}$ is called the *primitive unit cell* of $\mathbf{L}$ with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$. The primitive unit cell is the parallelepiped spanned by the vectors of the given basis.

(ii) The set $\mathbf{C} := \{\mathbf{w} \in \mathbb{V}^3 \mid |\mathbf{w}| \le |\mathbf{w} - \mathbf{v}| \text{ for all } \mathbf{v} \in \mathbf{L}\}$ is called the *Voronoï domain* or *Dirichlet domain* or *Wigner–Seitz cell* or *Wirkungsbereich* or *first Brillouin zone* (for the case of reciprocal lattices in dual space, see Section 1.3.2.5) of $\mathbf{L}$ (around the origin).

The Voronoï domain consists of those points of $\mathbb{V}^3$ that are closer to the origin than to any other lattice point of $\mathbf{L}$.

See Fig. 1.3.2.2 for examples of these two types of unit cells in two-dimensional space.

It should be noted that the attribute 'primitive' for a unit cell is often omitted. The term 'unit cell' then either denotes a primitive unit cell in the sense of the definition above or a slight generalization of this, namely a cell spanned by vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ which are not necessarily a lattice basis. This will be discussed in detail in the next section. If a unit cell in the even more general sense of a cell whose translates cover the whole space without overlap (thus including *e.g.* Voronoï domains) is meant, this should be indicated by the context.

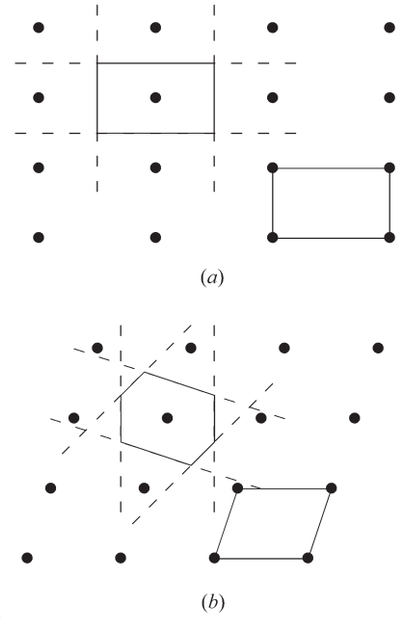

Figure 1.3.2.2
Voronoï domains and primitive unit cells for a rectangular lattice (*a*) and an oblique lattice (*b*).

The construction of the Voronoï domain is independent of the basis of $\mathbf{L}$, as the Voronoï domain is bounded by planes bisecting the line segment between the origin and a lattice point and perpendicular to this segment. In two-dimensional space, the Voronoï domain is simply bounded by lines, in three-dimensional space it is bounded by planes and more generally it is bounded by $(n-1)$-dimensional hyperplanes in n-dimensional space.

The boundaries of the Voronoï domain and its translates overlap, thus in order to get a proper fundamental domain, part of the boundary has to be excluded from the Voronoï domain.

The volume V of the unit cell can be expressed both *via* the metric tensor and *via* the cell parameters. One has

$$\begin{aligned} V^2 &= \det \boldsymbol{G} \\ &= a^2b^2c^2(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma) \end{aligned}$$

and thus

$$V = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}.$$

Although the cell parameters depend on the chosen lattice basis, the volume of the unit cell is not affected by a transition to a different lattice basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$. As remarked in Section 1.3.2.1, two lattice bases are related by an integral basis transformation $\boldsymbol{P}$ of determinant ±1 and therefore $\det \boldsymbol{G}' = \det(\boldsymbol{P}^{\mathrm{T}}\cdot\boldsymbol{G}\cdot\boldsymbol{P}) = \det \boldsymbol{G}$, *i.e.* the determinant of the metric tensor is the same for all lattice bases.

Assuming that the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ form a *right-handed* system, the volume can also be obtained *via*

$$V = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = \mathbf{b}\cdot(\mathbf{c}\times\mathbf{a}) = \mathbf{c}\cdot(\mathbf{a}\times\mathbf{b}).$$

1.3.2.4. Primitive and centred lattices

The definition of a lattice as given in Section 1.3.2.1 states that a lattice consists precisely of the integral linear combinations of the vectors in a lattice basis. However, in crystallographic

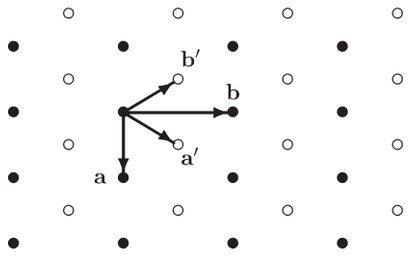

Figure 1.3.2.3
Primitive rectangular lattice (only the filled nodes) and centred rectangular lattice (filled and open nodes).

applications it has turned out to be convenient to work with bases that have particularly nice metric properties. For example, many calculations are simplified if the basis vectors are perpendicular to each other, *i.e.* if the metric tensor has all non-diagonal entries equal to zero. Moreover, it is preferable that the basis vectors reflect the symmetry properties of the lattice. By a case-by-case analysis of the different types of lattices a set of rules for convenient bases has been identified and bases conforming with these rules are called *conventional bases*. The conventional bases are chosen such that in all cases the integral linear combinations of the basis vectors are lattice vectors, but it is admitted that not all lattice vectors are obtained as integral linear combinations.

To emphasize that a basis has the property that the vectors of a lattice are precisely the integral linear combinations of the basis vectors, such a basis is called a *primitive basis* for this lattice.

If the conventional basis of a lattice is not a primitive basis for this lattice, the price to be paid for the transition to the conventional basis is that in addition to the integral linear combinations of the basis vectors one requires one or more *centring vectors* in order to obtain all lattice vectors. These centring vectors have non-integral (but rational) coordinates with respect to the conventional basis. The name *centring* vectors reflects the fact that the additional vectors are usually the centres of the unit cell or of faces of the unit cell spanned by the conventional basis.

Definition

Let $\mathbf{a}, \mathbf{b}, \mathbf{c}$ be linearly independent vectors in $\mathbb{V}^3$.

(i) A lattice $\mathbf{L}$ is called a *primitive lattice* with respect to a basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ if $\mathbf{L}$ consists precisely of all integral linear combinations of $\mathbf{a}, \mathbf{b}, \mathbf{c}$, *i.e.* if $\mathbf{L} = \mathbf{L}_P = \{l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \mid l, m, n \in \mathbb{Z}\}$.

(ii) A lattice $\mathbf{L}$ is called a *centred lattice* with respect to a basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ if the integral linear combinations $\mathbf{L}_P = \{l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \mid l, m, n \in \mathbb{Z}\}$ form a proper sublattice of $\mathbf{L}$ such that $\mathbf{L}$ is the union of $\mathbf{L}_P$ with the translates of $\mathbf{L}_P$ by centring vectors $\mathbf{v}_1, \ldots, \mathbf{v}_s$, *i.e.* $\mathbf{L} = \mathbf{L}_P \cup (\mathbf{v}_1 + \mathbf{L}_P) \cup \ldots \cup (\mathbf{v}_s + \mathbf{L}_P)$.

Typically, the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is a conventional basis and in this case one often briefly says that a lattice $\mathbf{L}$ is a *primitive lattice* or a *centred lattice* without explicitly mentioning the conventional basis.

Example

A rectangular lattice has as conventional basis a vector $\mathbf{a}$ of minimal length and a vector $\mathbf{b}$ of minimal length amongst the vectors perpendicular to $\mathbf{a}$. The resulting primitive lattice $\mathbf{L}_P$ is indicated by the filled nodes in Fig. 1.3.2.3. Now consider the lattice $\mathbf{L}$ having both the filled and the open nodes in Fig. 1.3.2.3 as its lattice nodes. One sees that $\mathbf{a}' = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, $\mathbf{b}' = -\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$ is a primitive basis for $\mathbf{L}$, but it is more convenient to regard $\mathbf{L}$ as a centred lattice with respect to the basis $\mathbf{a}, \mathbf{b}$ with centring vector $\mathbf{v} = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$. The filled nodes then show the sublattice $\mathbf{L}_P$ of $\mathbf{L}$, the open nodes are the translate $\mathbf{v} + \mathbf{L}_P$ and $\mathbf{L}$ is the union $\mathbf{L}_P \cup (\mathbf{v} + \mathbf{L}_P)$.

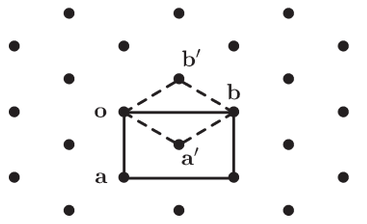

Figure 1.3.2.4
Primitive cell (dashed line) and centred cell (solid lines) for the centred rectangular lattice.

Recalling that a lattice is in particular a group (with addition of vectors as operation), the sublattice $\mathbf{L}_P$ spanned by the basis of a centred lattice is a subgroup of the centred lattice $\mathbf{L}$. Together with the zero vector $\mathbf{v}_0 = \mathbf{0}$, the centring vectors form a set $\mathbf{v}_0, \mathbf{v}_1, \ldots, \mathbf{v}_s$ of coset representatives of $\mathbf{L}$ relative to $\mathbf{L}_P$ and the index $[i]$ of $\mathbf{L}_P$ in $\mathbf{L}$ is $s + 1$. In particular, the sum of two centring vectors is, up to a vector in $\mathbf{L}_P$, again a centring vector, *i.e.* for centring vectors $\mathbf{v}_i$, $\mathbf{v}_j$ there is a unique centring vector $\mathbf{v}_k$ (possibly $\mathbf{0}$) such that $\mathbf{v}_i + \mathbf{v}_j = \mathbf{v}_k + \mathbf{w}$ for a vector $\mathbf{w} \in \mathbf{L}_P$.

The concepts of primitive and centred lattices suggest corresponding notions of primitive and centred unit cells. If $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is a primitive basis for the lattice $\mathbf{L}$, then the parallelepiped spanned by $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called a *primitive unit cell* (or primitive cell); if $\mathbf{a}, \mathbf{b}, \mathbf{c}$ spans a proper sublattice $\mathbf{L}_P$ of index $[i]$ in $\mathbf{L}$, then the parallelepiped spanned by $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called a *centred unit cell* (or centred cell). Since translating a centred cell by translations from the sublattice $\mathbf{L}_P$ covers the full space, the centred cell contains one representative from each coset of the centred lattice $\mathbf{L}$ relative to $\mathbf{L}_P$. This means that the centred cell contains $[i]$ lattice vectors of the centred lattice and due to this a centred cell is also called a *multiple cell*. As a consequence, the volume of the centred cell is $[i]$ times as large as that of a primitive cell for $\mathbf{L}$.

For a conventional basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of the lattice $\mathbf{L}$, the parallelepiped spanned by $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called a *conventional unit cell* (or conventional cell) of $\mathbf{L}$. Depending on whether the conventional basis is a primitive basis or not, *i.e.* whether the lattice is primitive or centred, the conventional cell is a primitive or a centred cell.

Remark: It is important to note that the cell parameters given in the description of a crystallographic structure almost always refer to a conventional cell. When in the crystallographic literature the term 'unit cell' is used without further attributes, in most cases a conventional unit cell (as specified by the cell parameters) is meant, which is a primitive or centred (multiple) cell depending on whether the lattice is primitive or centred.

Example (continued)

In the example of a centred rectangular lattice, the conventional basis $\mathbf{a}, \mathbf{b}$ spans the centred unit cell indicated by solid lines in Fig. 1.3.2.4, whereas the primitive basis $\mathbf{a}' = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, $\mathbf{b}' = -\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$ spans the primitive unit cell indicated by dashed lines. One observes that the centred cell contains two lattice vectors, $\mathbf{o}$ and $\mathbf{a}'$, whereas the primitive cell only contains the zero vector $\mathbf{o}$ (note that due to the condition $0 \leq x, y < 1$ for the points in the unit cell the other vertices

$\mathbf{a}', \mathbf{b}', \mathbf{b}$ of the cell are excluded). The volume of the centred cell is clearly twice as large as that of the primitive cell.

Figures displaying the different primitive and centred unit cells as well as tables describing the metric properties of the different primitive and centred lattices are given in Section 3.1.2.

Examples

(i) The conventional basis for a *primitive cubic lattice* (*cP*) is a basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of vectors of equal length which are pairwise perpendicular, *i.e.* with $|\mathbf{a}| = |\mathbf{b}| = |\mathbf{c}|$ and $\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{c} = \mathbf{c} \cdot \mathbf{a} = 0$. As the name indicates, this basis is a primitive basis.

(ii) A *body-centred cubic lattice* (*cI*) has as its conventional basis the conventional basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of a primitive cubic lattice, but the lattice also contains the centring vector $\mathbf{v} = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b} + \frac{1}{2}\mathbf{c}$ which points to the centre of the conventional cell. If we denote the primitive cubic lattice by $\mathbf{L}_P$, then the body-centred cubic lattice $\mathbf{L}_I$ is the union of $\mathbf{L}_P$ and the translate $\mathbf{v} + \mathbf{L}_P = \{\mathbf{v} + \mathbf{w} \mid \mathbf{w} \in \mathbf{L}_P\}$. Since $\mathbf{L}_P$ is a sublattice of index 2 in $\mathbf{L}_I$, the ratio of the volumes of the centred and the primitive cell of the body-centred cubic lattice is 2.
A possible primitive basis for $\mathbf{L}_I$ is $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$. With respect to this basis, the metric tensor of $\mathbf{L}_I$ is

$$a^2 \cdot \begin{pmatrix} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{3}{4} \end{pmatrix}$$

(where $a = \mathbf{a} \cdot \mathbf{a}$). However, it is more common to use a primitive basis with vectors of the same length and equal interaxial angles. Such a basis is $\mathbf{a}'' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{b}'' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c})$, $\mathbf{c}'' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$ (*cf.* Fig. 1.5.1.3), and with respect to this basis the metric tensor of $\mathbf{L}_I$ is

$$\frac{a^2}{4} \cdot \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}.$$

(iii) The conventional basis for a *face-centred cubic lattice* (*cF*) is again the conventional basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of a primitive cubic lattice, but the lattice also contains the three centring vectors $\mathbf{v}_1 = \frac{1}{2}\mathbf{b} + \frac{1}{2}\mathbf{c}$, $\mathbf{v}_2 = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{c}$, $\mathbf{v}_3 = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$ which point to the centres of faces of the conventional cell.
The face-centred cubic lattice $\mathbf{L}_F$ is the union of the primitive cubic lattice $\mathbf{L}_P$ with its translates $\mathbf{v}_i + \mathbf{L}_P$ by the three centring vectors. The ratio of the volumes of the centred and the primitive cell of the face-centred cubic lattice is 4. In this case, the centring vectors actually form a primitive basis of $\mathbf{L}_F$. With respect to the basis $\mathbf{a}' = \frac{1}{2}(\mathbf{b} + \mathbf{c})$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{c})$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$ (*cf.* Fig. 1.5.1.4) the metric tensor of $\mathbf{L}_F$ is

$$\frac{a^2}{4} \cdot \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}.$$

(iv) In the conventional basis of a primitive hexagonal lattice, the basis vector $\mathbf{c}$ is chosen as a shortest vector along a sixfold axis. The vectors $\mathbf{a}$ and $\mathbf{b}$ then are shortest vectors along twofold axes in a plane perpendicular to $\mathbf{c}$ and such that they enclose an angle of 120°. The corresponding metric tensor has the form

$$\begin{pmatrix} a^2 & -\frac{a^2}{2} & 0 \\ -\frac{a^2}{2} & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}.$$

(v) In the unit cell of the primitive hexagonal lattice $\mathbf{L}_P$, a point with coordinates $\frac{2}{3}, \frac{1}{3}, z$ is mapped to the points $-\frac{1}{3}, \frac{1}{3}, z$ and $-\frac{1}{3}, -\frac{2}{3}, z$ under the threefold rotation around the c axis. Both of these points are translates of $\frac{2}{3}, \frac{1}{3}, z$ by lattice vectors of $\mathbf{L}_P$. This means that a centring vector of the form $\frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b} + z\mathbf{c}$ will result in a lattice which is invariant under the threefold rotation. Choosing $\mathbf{v}_1 = \frac{1}{3}(2\mathbf{a} + \mathbf{b} + \mathbf{c})$ as centring vector, the lattice generated by $\mathbf{L}_P$ and $\mathbf{v}_1$ contains $\mathbf{L}_P$ as a sublattice of index 3 with coset representatives $\mathbf{0}$, $\mathbf{v}_1$ and $2\mathbf{v}_1 = \frac{1}{3}(4\mathbf{a} + 2\mathbf{b} + 2\mathbf{c})$. The coset representative $2\mathbf{v}_1$ is commonly replaced by $\mathbf{v}_2 = \frac{1}{3}(\mathbf{a} + 2\mathbf{b} + 2\mathbf{c})$ and the centred lattice $\mathbf{L}_R$ with centring vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ so obtained is called the *rhombohedrally centred lattice* (*hR*). The ratio of the volumes of the centred and the primitive cell of the rhombohedrally centred lattice is 3.
For this lattice, the primitive basis of $\mathbf{L}_R$ consisting of three shortest non-coplanar vectors which are permuted by the threefold rotation is also regarded as a conventional basis. With respect to the above lattice basis of the primitive hexagonal lattice, this basis can be chosen as $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{c}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$. The metric tensor with respect to this basis is

$$\frac{1}{9} \cdot \begin{pmatrix} 3a^2 + c^2 & -\frac{3}{2}a^2 + c^2 & -\frac{3}{2}a^2 + c^2 \\ -\frac{3}{2}a^2 + c^2 & 3a^2 + c^2 & -\frac{3}{2}a^2 + c^2 \\ -\frac{3}{2}a^2 + c^2 & -\frac{3}{2}a^2 + c^2 & 3a^2 + c^2 \end{pmatrix}.$$

Details about the transformations between hexagonal and rhombohedral lattices are given in Section 1.5.3.1 and Table 1.5.1.1 (see also Fig. 1.5.1.6).

Remark: In three-dimensional space $\mathbb{V}^3$, the conventional bases have been chosen in such a way that any isometry of a centred lattice maps the sublattice generated by the conventional basis to itself. This means that the matrices of the isometries of the lattice are not only integral with respect to a primitive basis, but also when written with respect to the conventional basis. The advantage of the conventional basis is that the matrices are much simpler.

In dimensions $n \geq 4$, such a choice of a conventional basis is in general no longer possible. For example, one will certainly regard the standard orthonormal basis

$$\mathbf{a} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{c} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad \mathbf{d} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

of the four-dimensional hypercubic lattice as a conventional basis. The body-centred lattice with centring vector $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c} + \mathbf{d})$ is invariant under all the isometries of the hypercubic lattice, but

the body-centred lattice itself allows isometries that do not leave the hypercubic lattice invariant. Thus, not all isometries of the body-centred lattice are integral with respect to the conventional basis of the hypercubic lattice.

1.3.2.5. Reciprocal lattice

For crystallographic applications, a lattice $\mathbf{L}^*$ related to $\mathbf{L}$ is of utmost importance. If the atoms are placed at the nodes of a lattice $\mathbf{L}$, then the diffraction pattern will have sharp Bragg peaks at the nodes of the *reciprocal lattice* $\mathbf{L}^*$. More generally, if the crystal pattern is invariant under translations from $\mathbf{L}$, then the locations of the Bragg peaks in the diffraction pattern will be invariant under translations from $\mathbf{L}^*$.

Definition

Let $\mathbf{L} \subset \mathbb{V}^3$ be a lattice with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$. Then the *reciprocal basis* $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ is defined by the properties

$$\mathbf{a} \cdot \mathbf{a}^* = \mathbf{b} \cdot \mathbf{b}^* = \mathbf{c} \cdot \mathbf{c}^* = 1$$

and

$$\mathbf{b} \cdot \mathbf{a}^* = \mathbf{c} \cdot \mathbf{a}^* = \mathbf{c} \cdot \mathbf{b}^* = \mathbf{a} \cdot \mathbf{b}^* = \mathbf{a} \cdot \mathbf{c}^* = \mathbf{b} \cdot \mathbf{c}^* = 0,$$

which can conveniently be written as the matrix equation

$$\begin{pmatrix} \mathbf{a} \cdot \mathbf{a}^* & \mathbf{a} \cdot \mathbf{b}^* & \mathbf{a} \cdot \mathbf{c}^* \\ \mathbf{b} \cdot \mathbf{a}^* & \mathbf{b} \cdot \mathbf{b}^* & \mathbf{b} \cdot \mathbf{c}^* \\ \mathbf{c} \cdot \mathbf{a}^* & \mathbf{c} \cdot \mathbf{b}^* & \mathbf{c} \cdot \mathbf{c}^* \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \boldsymbol{I}_3.$$

This means that $\mathbf{a}^*$ is perpendicular to the plane spanned by $\mathbf{b}$ and $\mathbf{c}$ and its projection to the line along $\mathbf{a}$ has length $1/|\mathbf{a}|$. Analogous properties hold for $\mathbf{b}^*$ and $\mathbf{c}^*$.

The *reciprocal lattice* $\mathbf{L}^*$ of $\mathbf{L}$ is defined to be the lattice with lattice basis $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$.

In three-dimensional space $\mathbb{V}^3$, the reciprocal basis can be determined *via* the vector product. Assuming that $\mathbf{a}, \mathbf{b}, \mathbf{c}$ form a right-handed system that spans a unit cell of volume V, the relation $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = V$ and the defining conditions $\mathbf{a} \cdot \mathbf{a}^* = 1$, $\mathbf{b} \cdot \mathbf{a}^* = \mathbf{c} \cdot \mathbf{a}^* = 0$ imply that $\mathbf{a}^* = \frac{1}{V}(\mathbf{b} \times \mathbf{c})$. Analogously, one has $\mathbf{b}^* = \frac{1}{V}(\mathbf{c} \times \mathbf{a})$ and $\mathbf{c}^* = \frac{1}{V}(\mathbf{a} \times \mathbf{b})$.

The reciprocal lattice can also be defined independently of a lattice basis by stating that the vectors of the reciprocal lattice have integral scalar products with all vectors of the lattice:

$$\mathbf{L}^* = \{\mathbf{w}^* \in \mathbb{V}^3 \mid \mathbf{v} \cdot \mathbf{w}^* \in \mathbb{Z} \text{ for all } \mathbf{v} \in \mathbf{L}\}.$$

Owing to the symmetry $\mathbf{v} \cdot \mathbf{w} = \mathbf{w} \cdot \mathbf{v}$ of the scalar product, the roles of the basis and its reciprocal basis can be interchanged. This means that $(\mathbf{L}^*)^* = \mathbf{L}$, *i.e.* taking the reciprocal lattice $(\mathbf{L}^*)^*$ of the reciprocal lattice $\mathbf{L}^*$ results in the original lattice $\mathbf{L}$ again.

Remark: In parts of the literature, especially in physics, the reciprocal lattice is defined slightly differently. The condition there is that $\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi$ if $i = j$ and 0 otherwise and thus the reciprocal lattice is scaled by the factor 2π as compared to the above definition. By this variation the exponential function $\exp(-2\pi i\, \mathbf{v} \cdot \mathbf{w})$ is changed to $\exp(-i\, \mathbf{v} \cdot \mathbf{w})$, which simplifies the formulas for the Fourier transform.

Example

Let $\mathbf{a}, \mathbf{b}, \mathbf{c}$ be the lattice basis of a primitive cubic lattice. Then the body-centred cubic lattice $\mathbf{L}_I$ with centring vector $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ is the reciprocal lattice of the rescaled face-centred cubic lattice $2\mathbf{L}_F$, *i.e.* the lattice spanned by $2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ and the centring vectors $\mathbf{b} + \mathbf{c}$, $\mathbf{a} + \mathbf{c}$, $\mathbf{a} + \mathbf{b}$.

This example illustrates that a lattice and its reciprocal lattice need not have the same type. The reciprocal lattice of a body-centred cubic lattice is a face-centred cubic lattice and *vice versa*. However, the conventional bases are chosen such that for a primitive lattice with a conventional basis as lattice basis, the reciprocal lattice is a primitive lattice of the same type. Therefore the reciprocal lattice of a centred lattice is always a centred lattice for the same type of primitive lattice.

The reciprocal basis can be read off the inverse matrix of the metric tensor $\boldsymbol{G}$: We denote by $\boldsymbol{P}^*$ the matrix containing the coordinate columns of $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$, so that $\mathbf{a}^* = P_{11}^*\mathbf{a} + P_{21}^*\mathbf{b} + P_{31}^*\mathbf{c}$ *etc*. Recalling that scalar products can be computed by multiplying the metric tensor $\boldsymbol{G}$ from the left and right with coordinate columns with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$, the conditions

$$\begin{pmatrix} \mathbf{a} \cdot \mathbf{a}^* & \mathbf{a} \cdot \mathbf{b}^* & \mathbf{a} \cdot \mathbf{c}^* \\ \mathbf{b} \cdot \mathbf{a}^* & \mathbf{b} \cdot \mathbf{b}^* & \mathbf{b} \cdot \mathbf{c}^* \\ \mathbf{c} \cdot \mathbf{a}^* & \mathbf{c} \cdot \mathbf{b}^* & \mathbf{c} \cdot \mathbf{c}^* \end{pmatrix} = \boldsymbol{I}_3$$

defining the reciprocal basis result in the matrix equation $\boldsymbol{I}_3 \cdot \boldsymbol{G} \cdot \boldsymbol{P}^* = \boldsymbol{I}_3$, since the coordinate columns of the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ with respect to itself are the rows of the identity matrix $\boldsymbol{I}_3$, and $\boldsymbol{P}^*$ was just defined to contain the coordinate columns of $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$. But $\boldsymbol{G} \cdot \boldsymbol{P}^* = \boldsymbol{I}_3$ means that $\boldsymbol{P}^* = \boldsymbol{G}^{-1}$ and thus the coordinate columns of $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are precisely the columns of the inverse matrix $\boldsymbol{G}^{-1}$ of the metric tensor $\boldsymbol{G}$.

From $\boldsymbol{P}^* = \boldsymbol{G}^{-1}$ one also derives that the metric tensor $\boldsymbol{G}^*$ of the reciprocal basis is

$$\boldsymbol{G}^* = \boldsymbol{P}^{*\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{P}^* = \boldsymbol{G}^{-1} \cdot \boldsymbol{G} \cdot \boldsymbol{G}^{-1} = \boldsymbol{G}^{-1}.$$

This means that the metric tensors of a basis and its reciprocal basis are inverse matrices of each other. As a further consequence, the volume V^* of the unit cell spanned by the reciprocal basis is $V^* = V^{-1}$, *i.e.* the inverse of the volume of the unit cell spanned by $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

Of course, the reciprocal basis can also be computed from the vectors $\mathbf{a}_i$ directly. If $\boldsymbol{B}$ and $\boldsymbol{B}^*$ are the matrices containing as ith column the vectors $\mathbf{a}_i$ and $\mathbf{a}_i^*$, respectively, then the relation defining the reciprocal basis reads as $\boldsymbol{B}^{\mathrm{T}} \cdot \boldsymbol{B}^* = \boldsymbol{I}_3$, *i.e.* $\boldsymbol{B}^* = (\boldsymbol{B}^{-1})^{\mathrm{T}}$. Thus, the reciprocal basis vector $\mathbf{a}_i^*$ is the ith column of the transposed matrix of $\boldsymbol{B}^{-1}$ and thus the ith *row* of the inverse of the matrix $\boldsymbol{B}$ containing the $\mathbf{a}_i$ as columns.

The relations between the parameters of the unit cell spanned by the reciprocal basis vectors and those of the unit cell spanned by the original basis can either be obtained from the vector product expressions for $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ or by explicitly inverting the metric tensor $\boldsymbol{G}$ (*e.g.* using Cramer's rule). The latter approach would also be applicable in n-dimensional space. Either way, one finds

$$a^* = \frac{bc \sin\alpha}{V}, \quad b^* = \frac{ca \sin\beta}{V}, \quad c^* = \frac{ab \sin\gamma}{V},$$
$$\sin\alpha^* = \frac{V}{abc \sin\beta \sin\gamma}, \quad \cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma},$$
$$\sin\beta^* = \frac{V}{abc \sin\gamma \sin\alpha}, \quad \cos\beta^* = \frac{\cos\gamma\cos\alpha - \cos\beta}{\sin\gamma\sin\alpha},$$
$$\sin\gamma^* = \frac{V}{abc \sin\alpha \sin\beta}, \quad \cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}.$$