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

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.

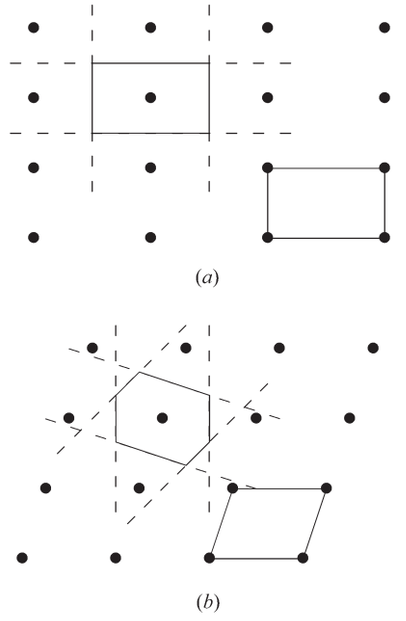

Figure 1.3.2.2
Voronoï domains and primitive unit cells for a rectangular lattice (*a*) and an oblique lattice (*b*).

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