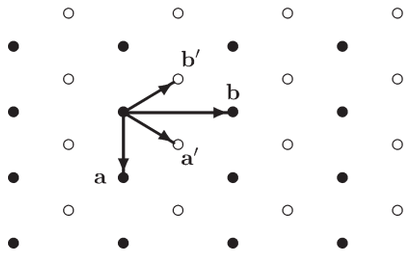

Figure 1.3.2.3
Primitive rectangular lattice (only the filled nodes) and centred rectangular lattice (filled and open nodes).

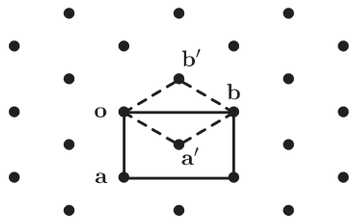

Figure 1.3.2.4
Primitive cell (dashed line) and centred cell (solid lines) for the centred rectangular lattice.

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 $\mathbf{L}_P \cup (\mathbf{v} + \mathbf{L}_P)$.

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