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Duality of spaces and the origin of integral reflection conditions

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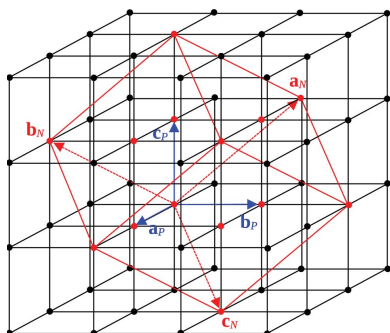
Keywords: reflection conditions; unit cells; direct lattices; reciprocal lattices.

The dualism between direct and reciprocal space is at the origin of well known relations between basis vectors in the two spaces. It is shown that when a coordinate system corresponding to a non-primitive unit cell is adopted, this dualism has to be handled with care. In particular, the reciprocal of a non-primitive unit cell is not a unit cell but a region in reciprocal space that does not represent a unit of repetition by translation. The basis vectors do not correspond to reciprocal-space cell lengths, contrary to what is stated even in the core CIF dictionary. The corresponding unit cell is a multiple of this region. The broken correspondence between basis vectors and unit cell is at the origin of the integral reflection conditions.

1. Introduction

Physical objects, including atoms that build up a crystal structure, are described in a Euclidean space \mathbb{E} known as the physical space, where the position of each object is given through its coordinates $|xyz\rangle^1$ with respect to a chosen coordinate system $O\mathbf{abc}$. The fundamental objects in a Euclidean space are called points and for this reason this space is also known as the point space. When we provide the fractional atomic coordinates of an atom within a unit cell² we implicitly treat it as a zero-dimensional point; this approximation is corrected by the tensor of the atomic displacement parameters, which provide a measure of the volume spanned by the atoms undergoing displacements about their equilibrium positions.

The set of vectors relating pairs of points in a Euclidean space \mathbb{E} build up a vector space \mathbb{V} ; it has no origin, and two parallel vectors with the same length are considered the same vector. The two spaces have the same metric; in crystallography, we commonly use the ångström, although this is not a unit recognized by the International System of Units (SI). For any two points of a Euclidean space \mathbb{E} , $|x_1y_1z_1\rangle$ and $|x_2y_2z_2\rangle$, a pair of vectors \mathbf{v} and $-\mathbf{v}$ are defined by the difference between the coordinates, $x_2 - x_1$, $y_2 - y_1$, $z_2 - z_1$ and $x_1 - x_2$, $y_1 - y_2$, $z_1 - z_2$. When $|x_1y_1z_1\rangle = |x_2y_2z_2\rangle$ one gets the zero vector. For any pair of points in the Euclidean space \mathbb{E} , the vectors \mathbf{v} and $-\mathbf{v}$ connecting them are uniquely defined, while there are infinitely many possible pairs of points in \mathbb{E} for any vector \mathbf{v} . This $\infty \rightarrow 1$ correspondence represents one of the challenges in solving crystal structures from diffraction data; from the experimental intensities one gets direct



¹ In the following, for brevity of notation we use the symbols (| and \rangle) for row and column matrices, respectively.

² For the sake of readers landing here from different fields, we clarify that in crystallography we use the term *unit cell* to indicate *any* unit of repetition by translation, whereas in mathematics it is common to reserve this term for the smallest units, *i.e.* primitive cells.

information on interatomic vectors, not on atomic coordinates. This information is the basis of the well known Patterson function (Patterson, 1934) and explains the phenomenon of diffraction enhancement of symmetry which is observed in some modular structures (Umayahara *et al.*, 2022).

The experimental diffraction pattern consists of a regular distribution of intensities that can be calculated as the Fourier transform of the electron density of the crystal structure. It is commonly interpreted as a periodic distribution of points, building the ‘index space’ (Bienenstock & Ewald, 1962), each of which is associated with an intensity; the position of these points in space is periodic, whereas the intensity distribution is not, although for some modular structures a periodic component of the intensity distribution can be extracted (Nespolo *et al.*, 1999). The characteristic features of the Fourier transform result in the metric of the space where diffraction is measured, also known as Fourier space (Bienenstock & Ewald, 1962), being the reciprocal of the metric of the physical space. In crystallography it is known as reciprocal space, precisely because its metric is Å^{-1} . The geometric distribution of points in reciprocal space that correspond to the measured reflections builds up a lattice, known as the reciprocal lattice; its non-periodic counterpart obtained by associating to each point the corresponding structure factor, or intensity, is known as the weighted reciprocal lattice (Shmueli, 2008).

The reciprocal lattice can be introduced in two equivalent but slightly different ways:

(i) As a reciprocal system of vectors, for which $\mathbf{v}_i \cdot \mathbf{v}_j^* = \delta_{ij}$ (Gibbs, 1881; Gibbs & Wilson, 1947).

(ii) By drawing a set of normals to each lattice plane (hkl) and adding lattice nodes onto these normals, having a periodicity $1/d(hkl)$.

The result is a set of vectors \mathbf{r}_{hkl}^* that are perpendicular to the families of planes (hkl); these vectors define a vector space with the metric Å^{-1} . Exactly like in direct space, vectors in reciprocal space satisfy the axioms of vector space, in particular the associativity and commutativity of vector addition, the compatibility of scalar multiplication with field multiplication $-p(q\mathbf{r}^*) = (pq)\mathbf{r}^*$, where p and q are scalars – and the distributivity of scalar multiplication with respect to vector addition and field addition. This means that any combination $m(p\mathbf{r}_1^* + q\mathbf{r}_2^*)$, with $m, p, q \in \mathbb{Z}$, is still a vector in reciprocal space (the symbol \mathbb{Z} indicates the ring of integer numbers). By choosing the three shortest non-coplanar vectors \mathbf{a}^* , \mathbf{b}^* and \mathbf{c}^* as basis vectors of reciprocal space, any reciprocal-lattice vector can be expressed as $m(p\mathbf{a}^* + q\mathbf{b}^* + r\mathbf{c}^*)$, with $m, p, q, r \in \mathbb{Z}$. Because \mathbf{a}^* , \mathbf{b}^* and \mathbf{c}^* are the three shortest vectors, they define a primitive unit cell.

For each vector \mathbf{r}^* there exist an infinite number of pairs of points in reciprocal space that can be connected by this vector; once an origin O^* has been chosen on one of these points, the coordinates of any pair of points connected by the vector \mathbf{r}^* with respect to the basis $O^*\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*$ are (nh, nk, nl) and $((n+1)h, (n+1)k, (n+1)l)$ for any integer value of n . The result is a Euclidean space with metric Å^{-1} and with a periodic three-dimensional distribution of points nh, nk, nl which are

known as the reciprocal-lattice nodes. To each node nh, nk, nl is associated an intensity which corresponds to the n th diffraction order from the direct-lattice planes (hkl); accordingly, nh, nk, nl are also known as the Laue indices of that reflection.

Direct and reciprocal spaces are dual because the same transformation leads from one to the other. If the transformation from direct to reciprocal space is denoted as $\mathbb{V} \rightarrow \mathbb{V}^*$, then the same transformation applied to \mathbb{V}^* is $\mathbb{V}^* \rightarrow \mathbb{V}^{**}$, which, as is well known, gives back \mathbb{V} : $\mathbb{V}^{**} = \mathbb{V}$.

Lattice directions in reciprocal space are defined by the vectors \mathbf{r}_{hkl}^* perpendicular to the families of lattice planes (hkl) in direct space. A vector \mathbf{r}_{hkl}^* connects the origin of reciprocal space to the node hkl . A direction parallel to this vector passes through all the lattice nodes with coordinates nh, nk, nl , where $n \in \mathbb{Z} \cup]-\infty, +\infty[$ ³. The direction indices are $[hkl]^*$ and they correspond to the coordinates of the first reciprocal-lattice node along the direction after the origin. The investigator chooses whether hkl or \overline{hkl} have to be selected; if hkl are all positive, then $[hkl]^*$ is normally used instead of $[\overline{hkl}]^*$.

Lattice planes in reciprocal space are defined exactly like in direct space, as geometric planes that pass through reciprocal-lattice nodes. The indexing is performed in a similar way; however, because of the duality between the two spaces, a plane in reciprocal space is by construction perpendicular to a lattice direction in direct space. If the direction indices of the latter are $[uvw]$, then the indices of the reciprocal-lattice plane normal to it are $(uvw)^*$ (Hammond, 2015). Because they are defined in exactly the same way as the Miller indices in direct space, in the following we call them Miller indices of reciprocal space.

We define here some symbols that we use in the following.

L: the direct lattice.

L^{*}: the reciprocal lattice.

U : a unit cell of **L**, subdivided into U_P and U_N for primitive and non-primitive, respectively. It is congruent to the cell spanned by the basis vectors $O\mathbf{a}_P\mathbf{b}_P\mathbf{c}_P$ of a primitive or $O\mathbf{a}_N\mathbf{b}_N\mathbf{c}_N$ of a non-primitive coordinate system, respectively.

U_P^* : a primitive unit cell of reciprocal space. It is congruent to the region spanned by the basis vectors of a primitive coordinate system $O^*\mathbf{a}_P^*\mathbf{b}_P^*\mathbf{c}_P^*$.

$(U_N)^*$: the reciprocal of a non-primitive unit cell U_N of **L**. It is congruent to the region spanned by the basis vectors $\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$ obtained by the inverse transformation that gives a non-primitive unit cell in direct space. As we are going to see, this is not a unit cell of **L**^{*}.

U_N^* : a non-primitive unit cell of reciprocal space. Some of its edges are multiples of the basis vectors $\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$ obtained by the inverse transformation that gives a non-primitive unit cell in direct space. It is not congruent to the region spanned by the basis vectors $\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$. As we are going to see, this is a unit cell of **L**^{*}.

³ The reader should not confuse the open and close intervals, written as $]$ and $[$, respectively, with the notation of lattice directions, $[uvw]$ and $[hkl]^*$. The interval $]-\infty, +\infty[$ is open because the points $-\infty, +\infty$ can never be reached.

Table 1

Transformation matrices between U_P and U_N for all the unit cells to which a letter has been assigned in the literature, and the corresponding relation with the unit cells in reciprocal space.

Unit cells of types *A*, *B* and *C* are collectively indicated as *S*.

Type of unit cell in direct space and their centring vectors	\mathbf{M}	$\det(\mathbf{M})$	\mathbf{M}^{-1}	$\det(\mathbf{M}^{-1})$	$z_1 z_2 z_3$	Multiplicity of $U_N^* = V(U_N^*)/V(U_P^*)$	$V(U_N^*)/V(U_N)^*$	Type of unit cell in reciprocal space	Integral reflection conditions
<i>P</i>	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	1	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	1	111	1	1	<i>P</i>	–
<i>A</i> $0, \frac{1}{2}, \frac{1}{2}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \bar{1} \\ 0 & 1 & 1 \end{pmatrix}$	2	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	$\frac{1}{2}$	122	2	4	<i>A</i>	$k + l = 2n$
<i>B</i> $\frac{1}{2}, 0, \frac{1}{2}$	$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 1 \end{pmatrix}$	2	$\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$	$\frac{1}{2}$	212	2	4	<i>B</i>	$h + l = 2n$
<i>C</i> $\frac{1}{2}, \frac{1}{2}, 0$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\frac{1}{2}$	221	2	4	<i>C</i>	$h + k = 2n$
<i>I</i> $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	2	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	$\frac{1}{2}$	222	4	8	<i>F</i>	$h + k + l = 2n$
<i>F</i> $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$	4	$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	$\frac{1}{4}$	222	2	8	<i>I</i>	$h + k = 2n,$ $h + l = 2n,$ $k + l = 2n$
<i>R</i> $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$ $\frac{1}{3}, \frac{1}{3}, \frac{2}{3}$	$\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}$	3	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{2}{3} \end{pmatrix}$	$\frac{1}{3}$	333	9	27	<i>X</i>	$-h + k + l = 3n$
<i>H</i> $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	3	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{2}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\frac{1}{3}$	331	3	9	<i>X</i>	$-h + k = 3n$
<i>D</i> $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ $\frac{2}{3}, \frac{2}{3}, \frac{2}{3}$ $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$	$\begin{pmatrix} 1 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{pmatrix}$	3	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{2}{3} \end{pmatrix}$	$\frac{1}{3}$	333	9	27	<i>X</i>	$h + k + l = 3n$

2. Transformation between primitive and non-primitive unit cells

Let us call \mathbf{M} the matrix transforming the basis vectors in direct space that define a primitive unit cell (U_P) to those defining a centred (U_N) unit cell. We use *N* for ‘non-primitive’ instead of *C* for ‘centred’ in order to avoid confusion with *C*-centred cells. In symbols,

$$(\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P | \mathbf{M} = (\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N |; (\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N | \mathbf{M}^{-1} = (\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P |. \quad (1)$$

Equation (1) implicitly assumes that the origin of U_N coincides with the origin of U_P . If that is not the case, a translation has to be added, which has no influence on what follows.

Covariant quantities transform like the basis vectors and are written as row vectors (|; the Miller indices (*hkl*) of \mathbf{L} planes, the Laue indices *hkl* of the reflections, the coordinates *hkl* of \mathbf{L}^* and the direction indices [*hkl*] * of \mathbf{L}^* are covariant quantities. Contravariant quantities transform opposite to the basis vectors, *i.e.* through the matrix \mathbf{M}^{-1} , and are written as column vectors |); the basis vectors of \mathbf{L}^* , $\mathbf{a}^* \mathbf{b}^* \mathbf{c}^*$, the coordinates in direct space *xyz*, the direction indices [*uvw*] of \mathbf{L} and

the Miller indices (*uvw*) * of \mathbf{L}^* planes are contravariant quantities. Lattice rows in direct and reciprocal space are expressed, respectively, as

$$u\mathbf{a} + v\mathbf{b} + w\mathbf{c} = (\mathbf{abc} | uvw); h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* = (hkl | \mathbf{a}^* \mathbf{b}^* \mathbf{c}^*).$$

The effect of a change of coordinate system is straightforward (\mathbf{I} is the 3×3 identity matrix),

$$\begin{aligned} (\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P | \mathbf{I} | u_P v_P w_P) &= (\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P | \mathbf{M} \mathbf{M}^{-1} | u_P v_P w_P) \\ &= (\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N | \mathbf{M}^{-1} | u_P v_P w_P) \\ &= (\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N | u_N v_N w_N), \\ (\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P | \mathbf{I} | x_P y_P z_P) &= (\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P | \mathbf{M} \mathbf{M}^{-1} | x_P y_P z_P) \\ &= (\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N | \mathbf{M}^{-1} | x_P y_P z_P) \\ &= (\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N | x_N y_N z_N), \\ (h_P k_P l_P | \mathbf{I} | \mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*) &= (h_P k_P l_P | \mathbf{M} \mathbf{M}^{-1} | \mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*) \\ &= (h_N k_N l_N | \mathbf{M}^{-1} | \mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*) \\ &= (h_N k_N l_N | \mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*), \end{aligned} \quad (2)$$

confirming that *hkl* are transformed by the \mathbf{M} matrix, whereas *uvw*, *xyz* and $\mathbf{a}^* \mathbf{b}^* \mathbf{c}^*$ are transformed by the \mathbf{M}^{-1} matrix. Table 1 lists the \mathbf{M} and \mathbf{M}^{-1} matrices for all the unit cells to

which a conventional symbol has been assigned in the literature: P, S (A, B or C), I, F, R, H and D ; any other unit cell is indicated as X . Because hkl represent both the Miller indices of \mathbf{L} planes and the Laue indices of reflections, the restrictions on the parities of the Miller indices (hkl) in non-primitive unit cells translate directly in the integral reflection conditions on Laue indices hkl . However, hkl are also the coordinates of points in reciprocal space and the restriction on their parities arises from the fact that, contrary to what is universally stated in the literature, $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$ do not define a unit cell of \mathbf{L}^* .

3. Direction indices, Miller indices and unit cells in direct and reciprocal space

Direction indices $[uvw]$ and Miller indices (hkl) are relatively prime integers only if the coordinate system $O\mathbf{abc}$ corresponds to a primitive basis, *i.e.* if the basis vectors \mathbf{a}, \mathbf{b} and \mathbf{c} are non-coplanar shortest vectors: in other words, if all vectors $\mathbf{v} \in \mathbb{V}$ can be expressed as a linear combination $m\mathbf{a} + p\mathbf{b} + q\mathbf{c}$ with $m, p, q \in \mathbb{Z}$. If the coordinate system $O\mathbf{abc}$ does not correspond to a primitive basis, *i.e.* if the whole set of vectors $m\mathbf{a} + p\mathbf{b} + q\mathbf{c}$ with $m, p, q \in \mathbb{Z}$ forms a proper sublattice, then the direction indices for at least some directions are rational (as opposed to integer) numbers and the Miller indices for at least some families of lattice planes are not relatively prime integers, *i.e.* they contain a common integer factor (Nespolo, 2015, 2017a). This is a direct result of the transformations in equation (2). For example, when the coordinate system $O\mathbf{abc}$ defines a C -centred unit cell, the Miller indices of the family of planes parallel to \mathbf{b} and \mathbf{c} are (200), because the first plane of this family, after the one that passes through the origin, has an intercept $\frac{1}{2}$ on \mathbf{a} . Analogously, the direction characterized by $u = v$ and $w = 0$ has indices $[\frac{11}{22}0]$, because the first lattice node after the origin along this direction has coordinates $xyz = \frac{11}{22}0$.

Because of the duality between direct and reciprocal space, the choice of a non-primitive basis leads to the same result in reciprocal space: $[hkl]^*$ are no longer restricted to relatively prime integers, while $(uvw)^*$ take rational (as opposed to integer) values.

The transformation of the direct and reciprocal metric tensors, \mathbf{G}_P and \mathbf{G}_P^* , is performed by the \mathbf{M} and \mathbf{M}^{-1} matrices respectively:

$$\mathbf{G}_N = \mathbf{M}^T \mathbf{G}_P \mathbf{M}; \quad \mathbf{G}_N^* = \mathbf{M}^{-1} \mathbf{G}_P^* \mathbf{M}^{-1,T}, \quad (3)$$

where \mathbf{M}^T is the transpose matrix of \mathbf{M} . Remembering that the volume V of the unit cell is the square root of the determinant of the metric tensor, and that $\det(\mathbf{M}^T) = \det(\mathbf{M})$ and $\det(\mathbf{M}^{-1}) = \det(\mathbf{M})^{-1}$, the following relations hold:

$$\begin{aligned} V(U_N) &= [\det(\mathbf{M}^T) \det(\mathbf{G}_P) \det(\mathbf{M})]^{1/2} = \det(\mathbf{M}) V(U_P); \\ V(U_N)^* &= [\det(\mathbf{M}^{-1}) \det(\mathbf{G}_P^*) \det(\mathbf{M}^{-1,T})]^{1/2} \\ &= \det(\mathbf{M}^{-1}) V(U_P^*) = V(U_P^*) / \det(\mathbf{M}). \end{aligned} \quad (4)$$

The region of reciprocal space $(U_N)^*$ spanned by the $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$ vectors is not a unit of repetition by translation: it has lattice nodes on $8 \times \det(\mathbf{M}^{-1}) = 8/\det(\mathbf{M}) < 8$ corners.

Therefore, $(U_N)^*$ cannot correspond to a unit cell, its volume being smaller than that of the smallest possible unit cell (primitive). A unit cell in reciprocal space U_N^* is congruent to the region spanned by the reciprocal-space vectors $z_1 \mathbf{a}^* z_2 \mathbf{b}^* z_3 \mathbf{c}^*$, where z_i depend on the type of unit cell in direct space, U_N . If we indicate the basis vectors as $\mathbf{v}_i, i = 1, 3$ ($\mathbf{v}_1 = \mathbf{a}, \mathbf{v}_2 = \mathbf{b}, \mathbf{v}_3 = \mathbf{c}$), the transformation from $|\mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*|$ to $|\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*|$ is simply

$$\mathbf{v}_{i,N}^* = \sum_j \mathbf{M}_{ij}^{-1} \mathbf{v}_{j,P}^*, \quad (5)$$

where $\mathbf{M}_{ij}^{-1} = \mathbf{A}_{ij} / \det(\mathbf{M})$, \mathbf{A} being the adjugate matrix of \mathbf{M} (the transpose of the cofactor matrix of \mathbf{M}). Because $\mathbf{v}_{j,P}^*$ define a primitive basis of \mathbf{L}^* , if $0 < |\mathbf{M}_{ij}^{-1}| < 1$ for at least one of the three values of j , then the vector $\mathbf{v}_{i,N}^*$ does not connect two \mathbf{L}^* nodes; the edge of $(U_N)^*$, congruent with $\mathbf{v}_{i,N}^*$, is not the edge of a unit cell. To obtain the edge of a unit cell, one has to choose a vector $z_i \mathbf{v}_{i,N}^*$ that connects two \mathbf{L}^* nodes, *i.e.* a multiple of $\mathbf{v}_{i,N}^*$. The coefficient to apply is the largest absolute value between $1/\mathbf{M}_{i1}^{-1}, 1/\mathbf{M}_{i2}^{-1}$ and $1/\mathbf{M}_{i3}^{-1}$ computed for non-zero values of \mathbf{M}_{ij}^{-1} . In symbols,

$$z_i = \max[\text{abs}(1/\mathbf{M}_{ij}^{-1}) | \mathbf{M}_{ij}^{-1} \neq 0, j = 1, 3]. \quad (6)$$

The volume of U_N^* is obtained from that of $(U_N)^*$ by acting on $(\mathbf{G}_N)^*$ with a diagonal matrix \mathbf{Z} having $z_1 z_2 z_3$ as non-zero elements, whose determinant is $\det(\mathbf{Z}) = \prod_i z_i$. Therefore,

$$\begin{aligned} \mathbf{G}_N^* &= \mathbf{Z}^T (\mathbf{G}_N)^* \mathbf{Z} = \mathbf{Z}^T \mathbf{M}^{-1,T} \mathbf{G}_P^* \mathbf{M}^{-1} \mathbf{Z}, \\ \det(\mathbf{G}_N^*) &= \det(\mathbf{Z})^2 \det(\mathbf{M}^{-1})^2 \det(\mathbf{G}_P^*) \\ &= \left(\prod_i z_i \right)^2 \det(\mathbf{M})^{-2} \det(\mathbf{G}_P^*), \quad (7) \\ V(U_N^*) &= V(U_P^*) \prod_i z_i / \det(\mathbf{M}) = \prod_i z_i V(U_N)^*. \end{aligned}$$

Table 1 summarizes the results. For example, the reciprocal of an A -centred cell, $(U_A)^*$, is a region in reciprocal space that has nodes on four of the eight corners, so that it contains only $4/8 = 0.5$ lattice nodes. This is also evident from the determinant of the matrix \mathbf{M}^{-1} , which is $\frac{1}{2}$, whereas the volume of U_A is twice the volume of U_P , the volume of $(U_A)^*$ is half the volume of U_P^* . Therefore, $(U_A)^*$ – the region of reciprocal space defined by the basis vectors $\mathbf{a}_A^* \mathbf{b}_A^* \mathbf{c}_A^*$ – cannot correspond to a unit cell. The corresponding non-primitive unit cell in reciprocal space, U_A^* , is obtained by taking $\mathbf{a}_A^* 2\mathbf{b}_A^* 2\mathbf{c}_A^*$, the denominator of the non-zero elements of the second and third rows of the \mathbf{M}^{-1} matrix being 2, and is an A -centred unit cell, exactly like the conventional cell in direct space. The correspondence between basis vectors and unit cells is therefore no longer valid for the reciprocal of non-primitive unit cells.

The integral reflection conditions observed when the diffraction pattern is indexed with respect to basis vectors $\mathbf{a}_A^* \mathbf{b}_A^* \mathbf{c}_A^*$, which are the reciprocals of basis vectors $\mathbf{a}_A \mathbf{b}_A \mathbf{c}_A$ defining a non-primitive unit cell in direct space, are the result of this broken correspondence between basis vectors and unit cell. The restrictions on the possible values of hkl that we interpret as reflection conditions find their origin in the fact

that $\mathbf{v}_{i,N}^*$ (here $N = A$) do not connect \mathbf{L}^* nodes, contrary to $z_i \mathbf{v}_{i,N}^*$.

3.1. S-centred unit cell

An *S*-centred unit cell ($N = A, B$ or C) has additional translation vectors on one plane; for the *A*-centring, these vectors are $(2m + 1)\mathbf{b}/2$, $(2p + 1)\mathbf{c}/2$, with $m, p \in \mathbb{Z}$; for the *B*- and *C*-centrings, the difference consists just in a permutation of the axes.

The transformation from $(\mathbf{a}_p \mathbf{b}_p \mathbf{c}_p)$ to $(\mathbf{a}_A \mathbf{b}_A \mathbf{c}_A)$ can be obtained in four ways: $(\mathbf{a}_A \mathbf{b}_A \mathbf{c}_A) = (\mathbf{a}_p, \mathbf{b}_p + \mathbf{c}_p, -\mathbf{b}_p + \mathbf{c}_p)$ and $(\mathbf{a}_A \mathbf{b}_A \mathbf{c}_A) = (\mathbf{a}_p, \mathbf{b}_p - \mathbf{c}_p, \mathbf{b}_p + \mathbf{c}_p)$, plus two transformations obtained from these two by taking the negative senses of \mathbf{b}_A and \mathbf{c}_A . We choose the first transformation, the conclusions being independent of the choice. The transformation matrices are in Table 1. The determinant of \mathbf{M} is 2 and that of \mathbf{M}^{-1} is $\frac{1}{2}$; accordingly, $V(U_A) = 2V(U_p)$, whereas $V(U_A)^* = V(U_p^*)/2$ and $V(U_A^*) = 2V(U_p^*) = 4V(U_A)^*$ [equations (3) and (7)].

Miller indices (hkl) , Laue indices hkl , \mathbf{L}^* nodes hkl and direction indices $[hkl]^*$, covariant with respect to the basis vectors, are transformed by the matrix \mathbf{M} ,

$$(h_p k_p l_p) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \bar{1} \\ 0 & 1 & 1 \end{pmatrix} = (h_p, k_p + l_p, -k_p + l_p) = (h_A k_A l_A). \quad (8)$$

Accordingly, $h_A = h_p$, $k_A = k_p + l_p$ and $l_A = -k_p + l_p$, which implies the restriction $k_A + l_A = 2l_p$, an even number. We obtain immediately the integral condition typical of an *A*-centred cell: $hkl: k + l = 2n$, which depends only on the choice of unit cell and is not influenced by the atomic structure.

Direction indices $[uvw]$ and Miller indices in reciprocal space $(uvw)^*$, contravariant with respect to the basis vectors, are transformed by the matrix \mathbf{M}^{-1} ,

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} u_p \\ v_p \\ w_p \end{pmatrix} = \begin{pmatrix} u_p \\ \frac{v_p + w_p}{2} \\ \frac{-v_p + w_p}{2} \end{pmatrix} = \begin{pmatrix} u_A \\ v_A \\ w_A \end{pmatrix}. \quad (9)$$

Because $[uvw]_p$ are integers, u_A is always integer, whereas v_A and w_A are integers or half-integers depending on whether v_p and w_p have the same (*ee* or *oo*) or opposite (*eo* or *oe*) parity, where *e* = even and *o* = odd. For example, $[011]_p$ transforms to $[010]_A$, whereas $[010]_p$ transforms to $[0\frac{1}{2}\frac{1}{2}]_A$ and $[001]_p$ transforms to $[0\frac{1}{2}\frac{1}{2}]_A$. The direction indices v and w of an *A*-centred cell are therefore no longer restricted to integer values, as should be evident from the definition itself of direction indices (the coordinates of the first lattice node after the origin along that direction). The same holds for the Miller indices of \mathbf{L}^* planes, $(uvw)^*$. We therefore find a perfect duality between direct and reciprocal space. In direct space, the direction indices $[uvw]$ are half-integers, whereas the Miller indices (hkl) are not restricted to relatively prime integers. In reciprocal space, the direction indices $[hkl]^*$ are not restricted to relatively prime integers, whereas the Miller indices $(uvw)^*$ are half-integers. It is worth analysing the geometric meaning of this duality.

Fig. 1 shows the (100) projection of a Bravais lattice \mathbf{L} , indexed with respect to a coordinate system defining (a) a primitive (blue) unit cell and (b) the conventional *A*-centred (red) unit cell. In this example, $\|\mathbf{b}_p\| = \|\mathbf{c}_p\|$, so that $\alpha_N = 90^\circ$. For a general value of α_N , U_N would not be a conventional unit cell but the conclusions would be the same, because they

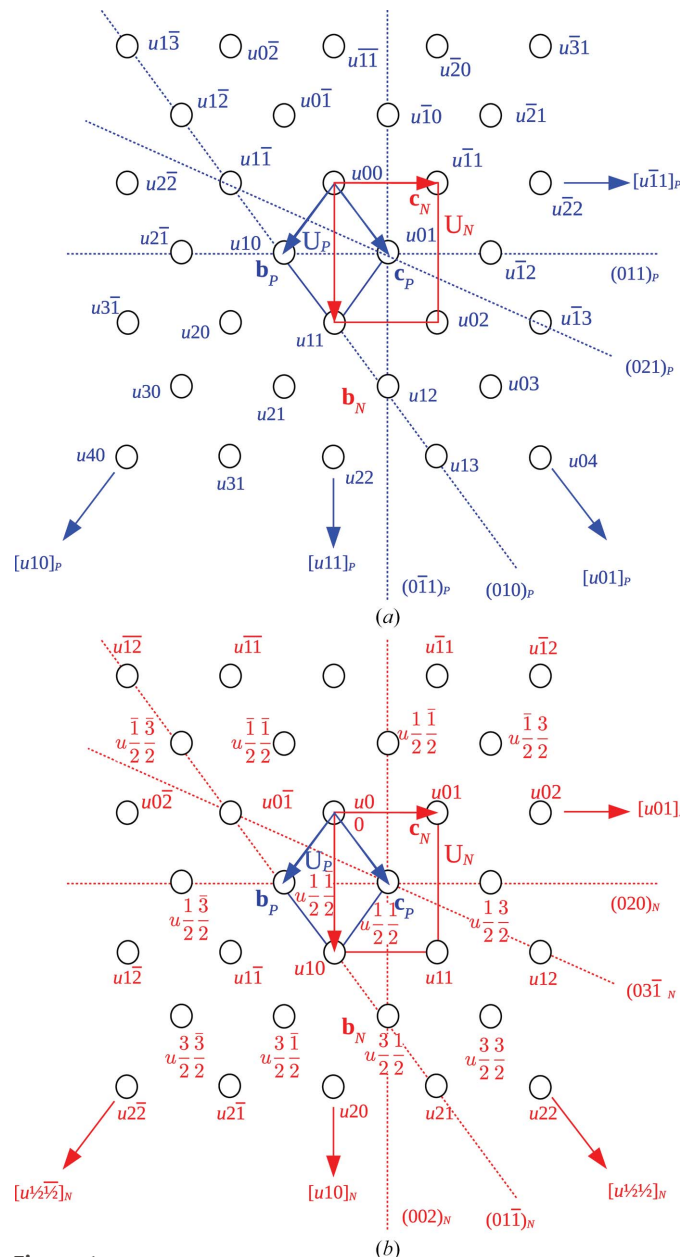


Figure 1 (a) The projection on the (100) plane of a portion of a direct Bravais lattice \mathbf{L} indexed with respect to a primitive coordinate system $O\mathbf{a}_p\mathbf{b}_p\mathbf{c}_p$. Because this is a projection on (100), \mathbf{a}_p is not shown; the basis vectors $\mathbf{b}_p\mathbf{c}_p$ and the corresponding unit cell U_p are shown in blue. The traces of three lattice planes $(0kl)$ are shown by dotted lines. A non-primitive coordinate system $O\mathbf{a}_N\mathbf{b}_N\mathbf{c}_N$ ($N = A$ in this example) and the corresponding unit cell U_N are shown in red. The direction indices $[uvw]$ and Miller indices (hkl) are all integer numbers without common factors. (b) The same lattice indexed with respect to the $O\mathbf{a}_N\mathbf{b}_N\mathbf{c}_N$ coordinate system. The direction indices $[uvw]$ are rational (as opposite to integer) numbers, whereas the Miller indices (hkl) are integer numbers which may contain a common factor and obey the restriction $k + l = 2n$.

depend only on the choice of the coordinate system used to index the lattice, not on the symmetry of the lattice. With respect to U_P in Fig. 1(a), the coordinates of \mathbf{L} nodes uvw are

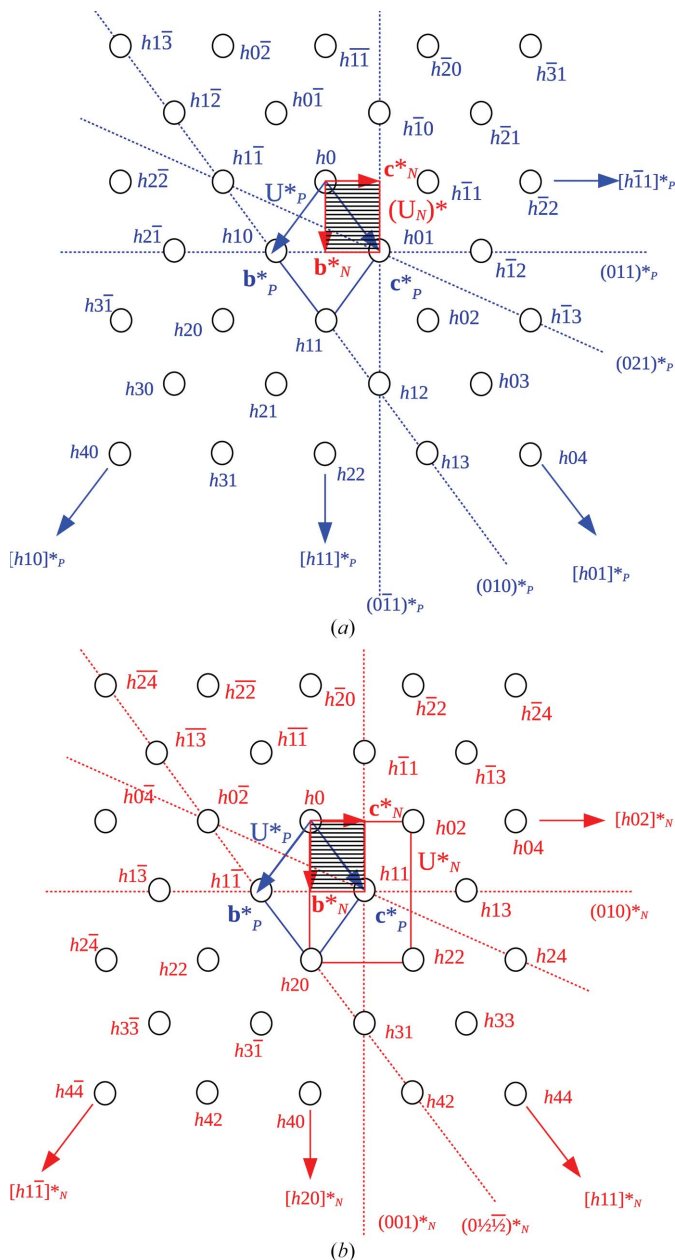


Figure 2 The projection on the $(100)^*$ plane of a portion of the reciprocal \mathbf{L}^* of the Bravais lattice \mathbf{L} in Fig. 1, indexed with respect to (a) $O^*\mathbf{a}_P^*\mathbf{b}_P^*\mathbf{c}_P^*$ and (b) $O^*\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$. The region spanned by the vectors $\mathbf{a}_P^*, \mathbf{b}_P^*, \mathbf{c}_P^*$ defines a primitive unit cell U_P^* which is the reciprocal of U_P in panel (a); with respect to these vectors, the direction indices $[hkl]^*$ and Miller indices $(uvw)^*$ are all integer numbers without common factors. The region $(U_N^*)^*$ spanned by the vectors $\mathbf{a}_N^*, \mathbf{b}_N^*, \mathbf{c}_N^*$ (hatched) is the reciprocal of U_N but it does not correspond to a unit cell; the latter, U_N^* , is obtained by taking $z_1\mathbf{a}_N^*z_2\mathbf{b}_N^*z_3\mathbf{c}_N^*$ (here $z_1 = 1, z_2 = z_3 = 2$) [panel (b)]. When indexed with respect to $O^*\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$, the direction indices $[hkl]^*$ are integer numbers which may contain a common factor, whereas the Miller indices $(uvw)^*$ are rational (as opposed to integer) numbers. The coordinates of the nodes of \mathbf{L}^* , which are also the Laue indices of the reflections, obey the same restriction $k + l = 2n$ as the Miller indices of planes of \mathbf{L} and correspond to the reflection conditions observed when the diffraction pattern is indexed with respect to $O^*\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$.

all integers and the direction indices $[uvw]$ and Miller indices (hkl) are relatively prime integers. With respect to U_N , the conventional A -centred unit cell in Fig. 1(b), the coordinates of \mathbf{L} nodes uvw and direction indices $[uvw]$ are half-integers, whereas the Miller indices (hkl) are integers that obey the condition $k + l = 2n$.

Fig. 2 shows the projection of \mathbf{L}^* on the $(100)^*$ plane, indexed with respect to a coordinate system defining (a) the reciprocal of the primitive (blue) unit cell U_P^* and (b) the reciprocal of the conventional A -centred (red) unit cell $(U_N^*)^*$. The basis vectors $\mathbf{a}_P^*, \mathbf{b}_P^*, \mathbf{c}_P^*$ define a unit cell in reciprocal space [Fig. 2(a)] which is primitive; the coordinates of \mathbf{L}^* nodes hkl are all integers and the direction indices $[hkl]$ and Miller indices $(uvw)^*$ are relatively prime integer. Instead, the basis vectors $\mathbf{a}_N^*, \mathbf{b}_N^*, \mathbf{c}_N^*$ define $(U_N^*)^*$ – here $N = A$ – which is not a unit cell in reciprocal space [Fig. 2(b)]: it contains 0.5 lattice nodes, at 000, 011, 100 and 111, each counting for $\frac{1}{8}$. The corresponding unit cell U_N^* is congruent with the region of reciprocal space spanned by vectors $z_1\mathbf{a}_N^*z_2\mathbf{b}_N^*z_3\mathbf{c}_N^*$, where $z_1 = 1$ and $z_2 = z_3 = 2$ [equation (6) and Table 1]. U_N^* is an A -centred unit cell, exactly like for the conventional cell in direct space. As expected from the duality of direct and reciprocal space, the possible values of the coordinates of \mathbf{L}^* nodes hkl obey the same restrictions as the Miller indices (hkl) of \mathbf{L} planes, i.e. $hkl: k + l = 2n$, with respect to the basis $O^*\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$ which does not define a unit cell in reciprocal space.

3.2. I-centred unit cell

An I -centred unit cell has additional translation vectors $(2m + 1)\mathbf{a}/2, (2p + 1)\mathbf{b}/2, (2q + 1)\mathbf{c}/2$, with $m, p, q \in \mathbb{Z}$. The transformation from $(\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P)$ to $(\mathbf{a}_I, \mathbf{b}_I, \mathbf{c}_I)$ is $(\mathbf{a}_I, \mathbf{b}_I, \mathbf{c}_I) = (\mathbf{b}_P + \mathbf{c}_P, \mathbf{a}_P + \mathbf{c}_P, \mathbf{a}_P + \mathbf{b}_P)$ (Table 1 and Fig. 3). The determinant of \mathbf{M} is 2 and that of \mathbf{M}^{-1} is $\frac{1}{2}$; accordingly [equation (7)], $V(U_I) = 2V(U_P)$ and $V(U_I)^* = V(U_P^*)/2$.

The transformation of hkl leads to

$$(h_p k_p l_p) \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} = (k_p + l_p, h_p + l_p, h_p + k_p) = (h_I k_I l_I). \quad (10)$$

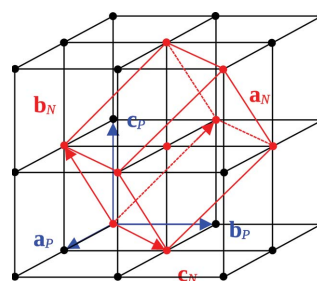


Figure 3 A portion of a Bravais lattice \mathbf{L} indexed with respect to a primitive coordinate system $O\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P$ (blue) and a non-primitive coordinate system $O\mathbf{a}_N, \mathbf{b}_N, \mathbf{c}_N$ (red) which corresponds to an I -centred unit cell U_N (here, $N = I$). To improve readability, the lattice nodes at the corners of and centring U_N are shown in red.

Accordingly, $h_I = k_P + l_P$, $k_I = h_P + l_P$, $l_I = h_P + k_P$, which implies the restriction $h_I + k_I + l_I = 2h_P + 2k_P + 2l_P$, an even number. We obtain immediately the integral condition typical of an I -centred cell: hkl : $h + k + l = 2n$.

The transformation of uvw leads to

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} u_P \\ v_P \\ w_P \end{pmatrix} = \begin{pmatrix} \frac{-u_P + v_P + w_P}{2} \\ \frac{u_P - v_P + w_P}{2} \\ \frac{u_P + v_P - w_P}{2} \end{pmatrix} = \begin{pmatrix} u_I \\ v_I \\ w_I \end{pmatrix}. \quad (11)$$

Because $|u_P v_P w_P|$ are integers, u_I , v_I and w_I are integers if either u_P , v_P and w_P are all even or one of the three is even, and half-integers otherwise. For example, $|011\rangle_P$ transforms to $|100\rangle_I$, whereas $|010\rangle_P$ transforms to $|\frac{1}{2}\frac{1}{2}1\rangle_I$ and $|001\rangle_P$ transforms to $|\frac{1}{2}\frac{1}{2}\frac{1}{2}\rangle_I$. The direction indices u , v and w of an I -centred cell are therefore no longer restricted to integer values. The same holds for the Miller indices of \mathbf{L}^* planes, $(uvw)^*$.

Fig. 3 shows a portion of \mathbf{L} , indexed with respect to a coordinate system defining a primitive (blue) and conventional (red) coordinate system. The basis vectors of the conventional coordinate system define the conventional cell, I -centred, whose edges are congruent to the basis vectors $\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N$. With respect to the primitive unit cell, the coordinates of \mathbf{L} nodes uvw , the direction indices $[uvw]$ and the Miller indices (hkl) are all relatively prime integers. With respect to the conventional I -centred unit cell, the coordinates of \mathbf{L}

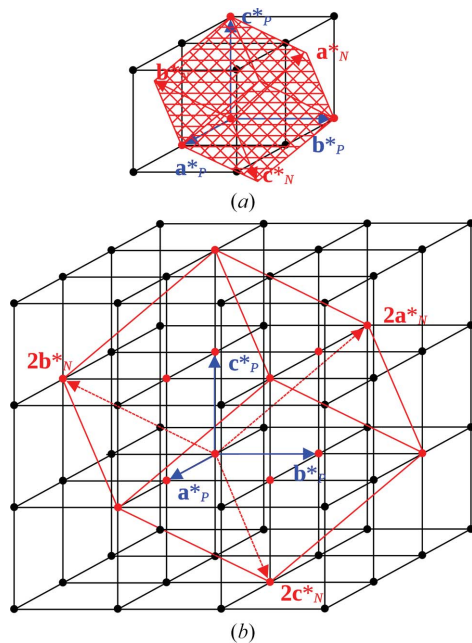


Figure 4
A portion of the reciprocal \mathbf{L}^* of the Bravais lattice \mathbf{L} in Fig. 3. (a) Two primitive (black) unit cells U_P^* , defined by the coordinate system $O^* \mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$ (blue), are shown, together with the $(U_N)^*$ (hatched in red) defined by the vectors $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$ (red). $(U_N)^*$ is the reciprocal of U_N in Fig. 3 but is not a unit cell; the latter, U_N^* , is obtained by taking $z_1 \mathbf{a}_N^* z_2 \mathbf{b}_N^* z_3 \mathbf{c}_N^*$ (here $z_1 = z_2 = z_3 = 2$) [panel (b)]. When indexed with respect to $O^* \mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$, the nodes of \mathbf{L}^* obey the restriction $h + k + l = 2n$ corresponding to the reflection condition of an I -centred unit cell in \mathbf{L} , which corresponds also to the F -centred unit cell of \mathbf{L}^* defined by the vectors $2\mathbf{a}_N^* 2\mathbf{b}_N^* 2\mathbf{c}_N^*$ [panel (b)]. To improve readability, the lattice nodes at the corners of and centring the faces of U_N^* are shown in red.

nodes uvw and the direction indices $[uvw]$ are half-integers, whereas the Miller indices (hkl) are integers that obey the condition $h + k + l = 2n$ [equation (10)].

Fig. 4(a) shows two primitive unit cells (black) of \mathbf{L}^* , indexed with respect to $\mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$ (blue) and $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$ (red). The latter do not define a unit cell but a region of reciprocal space, $(U_N)^*$, that is not a unit cell: it contains 0.5 lattice nodes, at 000, 011, 110 and 101, each counting for $\frac{1}{8}$. A unit cell in reciprocal space is congruent with a region spanned by vectors $2\mathbf{a}_N^* 2\mathbf{b}_N^* 2\mathbf{c}_N^*$, which define an F -centred unit cell [Fig. 4(b)]: U_N^* : $V(U_N^*) = 4V(U_P^*) = 8V(U_N)$. With respect to the primitive unit cell of Fig. 4(a), the coordinates of \mathbf{L}^* nodes hkl , the direction indices $[hkl]^*$ and Miller indices $(uvw)^*$ are relatively prime integers. With respect to the conventional F -centred unit cell [Fig. 4(b)], the coordinates of \mathbf{L}^* nodes hkl and the direction indices $[hkl]^*$ are integers that obey the condition $h + k + l = 2n$, whereas the Miller indices $(uvw)^*$ are half-integers.

3.3. F -centred unit cell

An F -centred unit cell has additional translation vectors $(2m + 1)\mathbf{a}/2$, $(2p + 1)\mathbf{b}/2$, $q\mathbf{c}$, $(2m + 1)\mathbf{a}/2$, $p\mathbf{b}$, $m(2q + 1)\mathbf{c}/2$ and $m\mathbf{a}$, $(2p + 1)\mathbf{b}/2$, $(2q + 1)\mathbf{c}/2$, with $m, p, q \in \mathbb{Z}$. The transformation from $(\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P)$ to $(\mathbf{a}_F \mathbf{b}_F \mathbf{c}_F)$ is $(\mathbf{a}_F \mathbf{b}_F \mathbf{c}_F) = (-\mathbf{a}_P + \mathbf{b}_P + \mathbf{c}_P, \mathbf{a}_P - \mathbf{b}_P + \mathbf{c}_P, \mathbf{a}_P + \mathbf{b}_P - \mathbf{c}_P)$ (Table 1 and Fig. 5). The determinant of \mathbf{M} is 4 and that of \mathbf{M}^{-1} is $\frac{1}{4}$; accordingly [equation (7)], $V(U_F) = 4V(U_P)$ and $V(U_F)^* = V(U_P^*)/4$.

The transformation of hkl leads to

$$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix} \begin{pmatrix} h_P k_P l_P \end{pmatrix} = \begin{pmatrix} -h_P + k_P + l_P, h_P - k_P + l_P, h_P + k_P - l_P \end{pmatrix} = \begin{pmatrix} h_F k_F l_F \end{pmatrix}. \quad (12)$$

Accordingly, $h_F = -h_P + k_P + l_P$, $k_F = h_P - k_P + l_P$ and $l_F = h_P + k_P - l_P$, which implies the restrictions $h_F + k_F = 2l_P$, $h_F + l_F = 2k_P$, $k_F + l_F = 2h_P$, which are all even numbers. We obtain

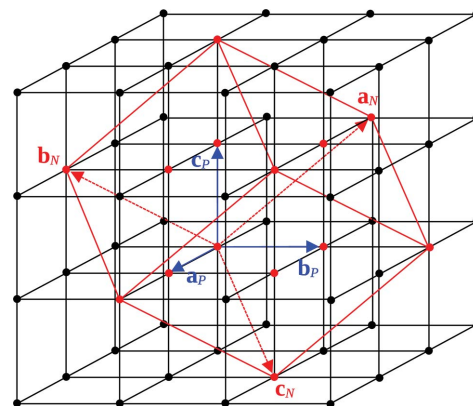


Figure 5
A portion of a Bravais lattice \mathbf{L} indexed with respect to a primitive coordinate system $O \mathbf{a}_P \mathbf{b}_P \mathbf{c}_P$ (blue) and a non-primitive coordinate system $O \mathbf{a}_N \mathbf{b}_N \mathbf{c}_N$ (red) which corresponds to an F -centred unit cell U_N (here, $N = F$). To improve readability, the lattice nodes at the corners of and centring the faces of U_N are shown in red.

immediately the integral conditions typical of an F -centred cell: hkl : $h + k = 2n$, $h + l = 2n$, $k + l = 2n$.

The transformation of uvw leads to

$$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} u_P \\ v_P \\ w_P \end{pmatrix} = \begin{pmatrix} \frac{v_P + w_P}{2} \\ \frac{u_P + w_P}{2} \\ \frac{u_P + v_P}{2} \end{pmatrix} = \begin{pmatrix} u_F \\ v_F \\ w_F \end{pmatrix}. \quad (13)$$

Because $|u_P v_P w_P|$ are integers, u_F , v_F and w_F are all integers if u_P , v_P and w_P are either all even or all odd; otherwise, two of them are half-integers. For example, $[111]_P$ transforms to $[111]_F$, whereas $[011]_P$ transforms to $[1\frac{1}{2}0]_F$ and $[001]_P$ transforms to $[\frac{1}{2}\frac{1}{2}0]_F$. The direction indices u , v and w of an F -centred cell are therefore no longer restricted to integer values. The same holds for the Miller indices of \mathbf{L}^* planes, $(uvw)^*$. In direct space, the direction indices $[uvw]$ are half-integers, whereas the Miller indices (hkl) are not restricted to relatively prime integers. In reciprocal space, the direction indices $[hkl]^*$ are not restricted to relatively prime integers, whereas the Miller indices $(uvw)^*$ are half-integers.

Fig. 5 shows a portion of \mathbf{L} , indexed with respect to a coordinate system defining a primitive (blue) and conventional (red) coordinate system. The basis vectors of the conventional coordinate system define the conventional cell, F -centred, whose edges are congruent to the basis vectors $\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N$. With respect to the primitive unit cell, the coordinates of \mathbf{L} nodes uvw are all integers and the direction indices $[uvw]$ and Miller indices (hkl) are relatively prime integers. With respect to the conventional F -centred unit cell, the coordinates of \mathbf{L} nodes uvw and the direction indices $[uvw]$ are half-

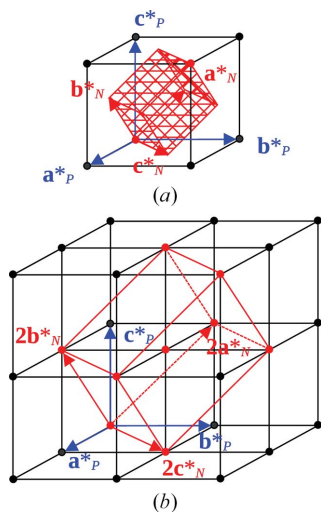


Figure 6 The reciprocal \mathbf{L}^* of the Bravais lattice \mathbf{L} in Fig. 5. (a) A primitive (black) unit cell U_P^* , defined by the coordinate system $O^* \mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$ (blue) is shown, together with the $(U_N)^*$ (hatched in red) defined by the vectors $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$ (red). $(U_N)^*$ is the reciprocal of U_N in Fig. 5 but is not a unit cell; the latter, U_N^* , is obtained by taking $z_1 \mathbf{a}_N^* z_2 \mathbf{b}_N^* z_3 \mathbf{c}_N^*$ (here $z_1 = z_2 = z_3 = 2$) [panel (b)]. When indexed with respect to $O^* \mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$, the nodes of \mathbf{L}^* obey the restrictions $h + k = 2n$, $h + l = 2n$, $k + l = 2n$, corresponding to the reflection condition of an F -centred unit cell in \mathbf{L} , which corresponds also to the I -centred unit cell of \mathbf{L}^* defined by the vectors $2\mathbf{a}_N^* 2\mathbf{b}_N^* 2\mathbf{c}_N^*$. To improve readability, the lattice nodes at the corners of and centring U_N^* are shown in red.

integers, whereas the Miller indices (hkl) are integers that obey the condition $h + k = 2n$, $h + l = 2n$, $k + l = 2n$ [equation (12)].

Fig. 6 shows a primitive unit cell (black) of \mathbf{L}^* , indexed with respect to $\mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$ (blue) and $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$ (red) [Fig. 6(a)]. The latter do not define a unit cell but a region of reciprocal space, $(U_N)^*$, that is not a unit cell: it contains 0.25 lattice nodes, at 000 and 111, each counting for $\frac{1}{8}$. A unit cell in reciprocal space has its edges coherent with $2\mathbf{a}_N^* 2\mathbf{b}_N^* 2\mathbf{c}_N^*$, which define an I -centred unit cell [Fig. 6(b)] U_N^* : $V(U_N^*) = 2V(U_P^*) = 8V(U_N)$. With respect to the primitive unit cell [Fig. 6(a)], the coordinates of \mathbf{L}^* nodes hkl are all integers and the direction indices $[hkl]^*$ and Miller indices $(uvw)^*$ are relatively prime integers. With respect to the I -centred unit cell [Fig. 6(b)], the coordinates of \mathbf{L}^* nodes hkl and the direction indices $[hkl]^*$ are integers that obey the condition $h + k = 2n$, $h + l = 2n$, $k + l = 2n$, whereas the Miller indices $(uvw)^*$ are half-integers.

3.4. R-centred unit cell

An R -centred unit cell has additional translation vectors $(3m + 2)\mathbf{a}/3$, $(3p + 1)\mathbf{b}/3$, $(3q + 1)\mathbf{c}/3$ and $(3m + 1)\mathbf{a}/3$, $(3p + 2)\mathbf{b}/3$, $(3q + 2)\mathbf{c}/3$, with $m, p, q \in \mathbb{Z}$. The transformation from $(\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P)$ to $(\mathbf{a}_R \mathbf{b}_R \mathbf{c}_R)$ is $(\mathbf{a}_R \mathbf{b}_R \mathbf{c}_R) = (\mathbf{a}_P + \mathbf{b}_P, \mathbf{b}_P - \mathbf{c}_P, \mathbf{a}_P + \mathbf{b}_P - \mathbf{c}_P)$ (Table 1 and Fig. 7). The determinant of \mathbf{M} is 3 and that of \mathbf{M}^{-1} is $\frac{1}{3}$; accordingly [equation (7)], $V(U_R) = 3V(U_P)$ and $V(U_R)^* = V(U_P^*)/3$.

The transformation of hkl leads to

$$(h_P k_P l_P) \begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix} = (h_P - k_P, k_P - l_P, h_P + k_P + l_P) = (h_R k_R l_R). \quad (14)$$

Accordingly, $h_R = h_P - k_P$, $k_R = k_P - l_P$, $l_R = h_P + k_P + l_P$, which implies the restriction $-h_R + k_R + l_R = 3k_P$. We obtain immediately the integral condition typical of an R -centred cell: hkl : $-h + k + l = 3n$.

The transformation of uvw leads to

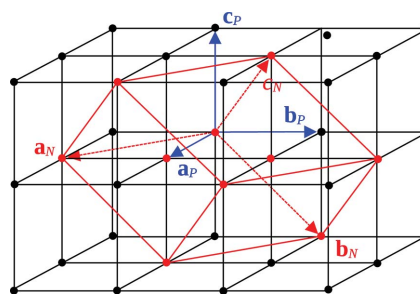


Figure 7 A portion of a Bravais lattice \mathbf{L} indexed with respect to a primitive coordinate system $O\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P$ (blue) and a non-primitive coordinate system $O\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N$ (red) which corresponds to an R -centred unit cell U_N (here, $N = R$). For U_N to be an R -centred unit cell, $O\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P$ should obey the restrictions $a_P = b_P = c_P$ and $\alpha_P = \beta_P = \gamma_P$. The figure is drawn for the special case $\alpha_P = 90^\circ$, which corresponds to a cubic metric, but this does not affect the results. To improve readability, the lattice nodes at the corners of and centring U_N are shown in red.

Table 2

Lattice nodes contained in $(U_R)^*$ depending on its position in \mathbf{L}^* .

Computation performed in the interval $[0, 2]$ of h, k and l , i.e. for eight locations. Each $(U_R)^*$ contains either $\frac{3}{8}$ or $\frac{1}{4}$ of a lattice node, leading to an average of $(5 \times \frac{3}{8} + 3 \times \frac{1}{4})/8 = 21/64$, approaching $\frac{1}{3}$, the determinant of the matrix \mathbf{M}^{-1} for the R -centred unit cell.

	Location of $(U_R)^*$							
	$h_N, k_N, l_N \in [0, 1]$	$h_N \in [1, 2], k_N, l_N \in [0, 1]$	$k_N \in [1, 2], h_N, l_N \in [0, 1]$	$l_N \in [1, 2], h_N, k_N \in [0, 1]$	$h_N, k_N \in [1, 2], l_N \in [0, 1]$	$h_N, l_N \in [1, 2], k_N \in [0, 1]$	$k_N, l_N \in [1, 2], h_N \in [0, 1]$	$h_N, k_N, l_N \in [1, 2]$
Coordinates of nodes with respect to $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$	000 ($\frac{1}{8}$)	110 ($\frac{1}{8}$)	110 ($\frac{1}{8}$)	101 ($\frac{1}{8}$)	110 ($\frac{1}{8}$)	101 ($\frac{1}{8}$)	021 ($\frac{1}{8}$)	211 ($\frac{1}{8}$)
	110 ($\frac{1}{8}$)	101 ($\frac{1}{8}$)	021 ($\frac{1}{8}$)	012 ($\frac{1}{8}$)	220 ($\frac{1}{8}$)	211 ($\frac{1}{8}$)	012 ($\frac{1}{8}$)	122 ($\frac{1}{8}$)
	101 ($\frac{1}{8}$)	211 ($\frac{1}{8}$)			211 ($\frac{1}{8}$)	202 ($\frac{1}{8}$)	122 ($\frac{1}{8}$)	
Coordinates of nodes with respect to $\mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$	000	10 $\bar{1}$	10 $\bar{1}$	100	10 $\bar{1}$	100	11 $\bar{1}$	20 $\bar{1}$
	10 $\bar{1}$	100	11 $\bar{1}$	110	20 $\bar{2}$	20 $\bar{1}$	110	21 $\bar{1}$
	100	20 $\bar{1}$			20 $\bar{1}$	200	21 $\bar{1}$	
Multiplicity	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{4}$

$$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} u_P \\ v_P \\ w_P \end{pmatrix} = \begin{pmatrix} \frac{2u_P - v_P - w_P}{3} \\ \frac{u_P + v_P - 2w_P}{3} \\ \frac{u_P + v_P + w_P}{3} \end{pmatrix} = \begin{pmatrix} u_R \\ v_R \\ w_R \end{pmatrix}. \quad (15)$$

Whereas $|u_P v_P w_P|$ are integers, u_R, v_R and w_R are rational numbers. For example, $|111|_P$ transforms to $|001|_{R_2}$, whereas $|011|_P$ transforms to $|\frac{2}{3}\frac{1}{3}\frac{2}{3}|_R$ and $|001|_P$ transforms to $|\frac{1}{3}\frac{2}{3}\frac{1}{3}|_R$. The direction indices u, v and w of an R -centred cell are therefore no longer restricted to integer values. The same holds for the Miller indices of \mathbf{L}^* planes, $(uvw)^*$. In direct space, the direction indices $[uvw]$ are rational numbers, whereas the Miller indices (hkl) are not restricted to relatively prime integers. In reciprocal space, the direction indices $[hkl]^*$ are not restricted to relatively prime integers, whereas the Miller indices $(uvw)^*$ are rational numbers.

Fig. 7 shows a portion of \mathbf{L} , indexed with respect to a coordinate system defining a primitive (blue) and conventional (red) coordinate system. The basis vectors of the conventional coordinate system define an R -centred unit cell, whose edges are congruent to the basis vectors $\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N$ and whose cell parameters obey the restrictions $a_N = b_N, c_N, \alpha_N = \beta_N = 90^\circ$ and $\gamma_N = 120^\circ$, leaving two degrees of freedom (a_N and c_N). The corresponding restrictions on U_P are $a_P = b_P = c_P$ and $\alpha_P = \beta_P = \gamma_P$, again with two degrees of freedom (a_P and α_P). Three special cases, $\alpha = 90^\circ, \alpha = 60^\circ$ and $\alpha = \cos^{-1}(-\frac{1}{3})$ ($\sim 109.47^\circ$), correspond to the primitive cells of a cubic lattice, whose conventional cells are, respectively, primitive (cP), F -centred (cF) and I -centred (cI). For these special cases, the metric of the R -centred cell corresponds to $a_N = b_N = a_P 2^{1/2}, c_N = c_P 3^{1/2}$ (cP), $a_N = b_N = a_P, c_N = c_P 6^{1/2}$ (cF) and $a_N = b_N = a_P (8/3)^{1/2}, c_N = c_P$ (cI). These cases are sometimes called the ‘hexagonal cubes’. With respect to the primitive unit cell, the coordinates of \mathbf{L} nodes uvw are all integers, and the direction indices $[uvw]$ and Miller indices (hkl) are relatively prime integers. With respect to the conventional R -centred unit cell, the coordinates of \mathbf{L} nodes uvw and the direction indices $[uvw]$ are rational numbers, whereas the Miller indices (hkl) are integers that obey the condition $-h + k + l = 3n$ [equation (14)].

Fig. 8(a) shows four primitive unit cells (black) of \mathbf{L}^* , indexed with respect to $\mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$ (blue) and $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$ (red). The latter do not define a unit cell but a region of reciprocal space, $(U_N)^*$, that is not a unit cell: it contains on average $\frac{1}{3}$ of a lattice

node (the determinant of the transformation matrix being $\frac{1}{3}$) but the fraction of lattice nodes is not constant and depends on

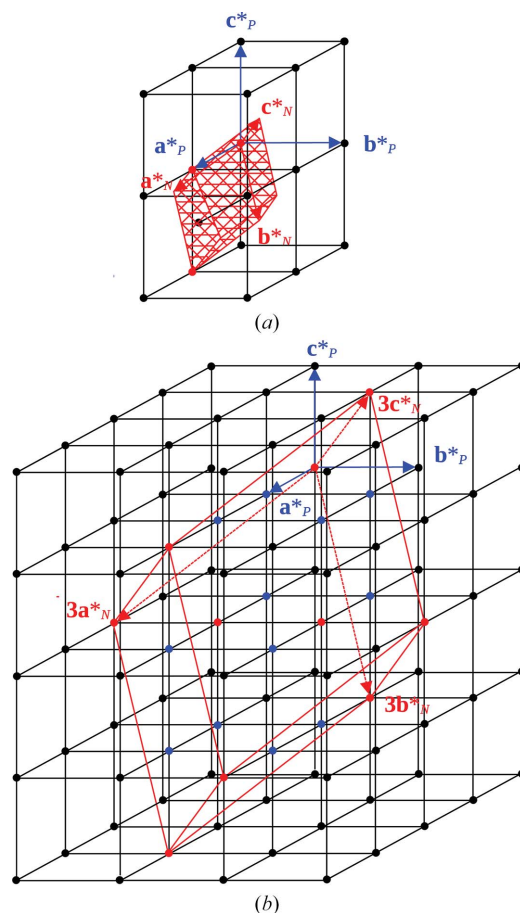


Figure 8

The reciprocal \mathbf{L}^* of the Bravais lattice \mathbf{L} in Fig. 7. (a) Four primitive (black) unit cells U_P^* , defined by the coordinate system $O^* \mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$ (blue) are shown, together with the $(U_N)^*$ (hatched in red) defined by the vectors $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$ (red). $(U_N)^*$ is the reciprocal of U_N in Fig. 7 but is not a unit cell; the latter, U_N^* , is obtained by taking $z_1 \mathbf{a}_N^* z_2 \mathbf{b}_N^* z_3 \mathbf{c}_N^*$ (here $z_1 = z_2 = z_3 = 3$) [panel (b)]. When indexed with respect to $O^* \mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$, the nodes of \mathbf{L}^* obey the restriction $-h + k + l = 3n$, corresponding to the reflection condition of an R -centred unit cell in \mathbf{L} . The unit cell U_N^* defined by $3\mathbf{a}_N^* 3\mathbf{b}_N^* 3\mathbf{c}_N^*$ has multiplicity 9 and is therefore indicated with the generic symbol X . To improve readability, the lattice nodes at the corners of U_N^* and rhombohedrally centring it are shown in red and those centring the faces of U_N^* in blue.

Table 3

Coordinates hkl of lattice nodes in the unit cell U_R^* with respect to three coordinate systems.

When expressed with respect to $\mathbf{a}_N^*, \mathbf{b}_N^*, \mathbf{c}_N^*$, they obey the restriction $-h + k + l = 3n$ typical of an R -centred unit cell in direct space, U_R . The unit cell in reciprocal space contains nine lattice nodes and does not correspond to any of the nine types to which a letter has been assigned in the literature. It is therefore indicated with the generic symbol X .

Position	Coordinates of nodes with respect to $\mathbf{a}_P^*, \mathbf{b}_P^*, \mathbf{c}_P^*$	Coordinates of nodes with respect to $3\mathbf{a}_N^*, 3\mathbf{b}_N^*, 3\mathbf{c}_N^*$	Coordinates of nodes with respect to $\mathbf{a}_N^*, \mathbf{b}_N^*, \mathbf{c}_N^*$
Corners ($\times \frac{1}{8}$)	000, $11\bar{2}$, 111 , $2\bar{1}\bar{1}$, $2\bar{2}\bar{1}$, $30\bar{3}$, 300 , $41\bar{2}$;	000, 010, 001, 100, 011, 110, 101, 111	000, 030, 003, 300, 033, 330, 303, 333
Faces ($\times \frac{1}{2}$)	$10\bar{1}$, $20\bar{2}$, 210 , $31\bar{1}$, 100 , 200 , $21\bar{2}$, $31\bar{2}$, $11\bar{1}$, 110 , $30\bar{2}$, $30\bar{1}$	$\frac{11}{3}0$, $\frac{22}{3}0$, $\frac{11}{33}1$, $\frac{22}{33}1$, $\frac{1}{3}0\frac{1}{3}$, $\frac{2}{3}0\frac{2}{3}$, $\frac{1}{3}1\frac{1}{3}$, $\frac{2}{3}1\frac{2}{3}$, $0\frac{1}{33}$, $0\frac{2}{33}$, $\frac{1}{33}1$, $\frac{2}{33}1$	110, 220, 113, 223, 101, 202, 131, 232, 021, 012, 321, 312
Body ($\times 1$)	$20\bar{1}$, $21\bar{1}$	$\frac{211}{333}$, $\frac{122}{333}$	211, 122

the location of $(U_N)^*$. Table 2 shows the lattice nodes partially contained in $(U_N)^*$ depending on its location. The computation has been performed through equation (14) in the interval $[0, 2]$ of h_N , k_N and l_N , i.e. for eight locations.⁴ Each $(U_N)^*$ contains either $\frac{3}{8}$ or $\frac{1}{4}$ of a lattice node, leading to an average of $(5 \times \frac{3}{8} + 3 \times \frac{1}{4})/8 = 21/64$, approaching $\frac{1}{3}$, the determinant of the matrix \mathbf{M}^{-1} for the R -centred unit cell. The value $\frac{1}{3}$ is obtained by enlarging the interval (omitted for brevity). A unit cell in reciprocal space has its edges coherent with $3\mathbf{a}_N^*, 3\mathbf{b}_N^*, 3\mathbf{c}_N^*$, which define a centred unit cell [Fig. 8(b)], U_N^* , containing nine lattice nodes (Table 3), and is therefore of type X . With respect to $\mathbf{a}_P^*, \mathbf{b}_P^*, \mathbf{c}_P^*$ [Fig. 8(a)], the coordinates of \mathbf{L}^* nodes hkl are all integers and the direction indices $[hkl]^*$ and Miller indices $(uvw)^*$ are relatively prime integers. With respect to $\mathbf{a}_N^*, \mathbf{b}_N^*, \mathbf{c}_N^*$ [Fig. 8(b)], the coordinates of \mathbf{L}^* nodes hkl and the direction indices $[hkl]^*$ are integers that obey the condition $-h + k + l = 3n$, whereas the Miller indices $(uvw)^*$ are rational numbers.

3.5. H -centred unit cell

An H -centred unit cell has additional translation vectors $(3m + 2)\mathbf{a}/3$, $(3p + 1)\mathbf{b}/3$ and $(3m + 1)\mathbf{a}$, $(3p + 2)\mathbf{b}/3$, with $m, p \in \mathbb{Z}$. It is used e.g. to describe the aristotype of hexagonal crystal structures or the family structure of order–disorder polytypes (Nespolo & Āuroviĉ, 2002).

Three transformations can be chosen from $(\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P |$ to $(\mathbf{a}_H \mathbf{b}_H \mathbf{c}_H |$: H_1 , $(\mathbf{a}_H \mathbf{b}_H \mathbf{c}_H | = (\mathbf{a}_P - \mathbf{b}_P, \mathbf{a}_P + 2\mathbf{b}_P, \mathbf{c}_P |$, H_2 , $(\mathbf{a}_H \mathbf{b}_H \mathbf{c}_H | = (2\mathbf{a}_P + \mathbf{b}_P, -\mathbf{a}_P + \mathbf{b}_P, \mathbf{c}_P |$ and H_3 , $(\mathbf{a}_H \mathbf{b}_H \mathbf{c}_H | = (\mathbf{a}_P + 2\mathbf{b}_P, -2\mathbf{a}_P - \mathbf{b}_P, \mathbf{c}_P |$. We choose the first one (Table 1 and Fig. 9), the result of our analysis being independent of the choice among the three unit cells. The determinant of \mathbf{M} is 3 and that of \mathbf{M}^{-1} is $\frac{1}{3}$; accordingly [equation (7)], $V(U_H) = 3V(U_P)$ and $V(U_H)^* = V(U_P^*)/3$.

The transformation of hkl leads to

$$(h_P k_P l_P) \begin{pmatrix} 1 & 1 & 1 \\ \bar{1} & 2 & 1 \\ 0 & 0 & 1 \end{pmatrix} = (h_P - k_P, h_P + 2k_P, h_P + k_P + l_P) = (h_H k_H l_H). \quad (16)$$

Accordingly, $h_H = h_P - k_P$, $k_H = h_P + 2k_P$, $l_H = l_P$, which implies the restriction $-h_H + k_H = 3k_P$. We obtain immedi-

ately the integral condition typical of an H -centred cell: hkl : $-h + k = 3n$.

The transformation of uvw leads to

$$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_P \\ v_P \\ w_P \end{pmatrix} = \begin{pmatrix} \frac{2u_P - v_P}{3} \\ \frac{u_P + v_P}{3} \\ w_P \end{pmatrix} = \begin{pmatrix} u_H \\ v_H \\ w_H \end{pmatrix}. \quad (17)$$

Whereas $|u_P v_P w_P|$ are integers, u_H , v_H and w_H are rational numbers. For example, $|101|_P$ transforms to $|\frac{21}{33}1|_H$, $|011|_P$ transforms to $|\frac{1}{3}11|_H$ and $|1\bar{1}1|_P$ transforms to $|101|_H$. The direction indices u, v and w of an H -centred cell are therefore no longer restricted to integer values. The same holds for the Miller indices of \mathbf{L}^* planes, $(uvw)^*$. In direct space, the direction indices $[uvw]$ are rational numbers, whereas the Miller indices (hkl) are not restricted to relatively prime integers. In reciprocal space, the direction indices $[hkl]^*$ are not restricted to relatively prime integers, whereas the Miller indices $(uvw)^*$ are rational numbers.

Fig. 9 shows a portion of \mathbf{L} , indexed with respect to a coordinate system defining a primitive and conventional (blue) and a centred (red) coordinate system. The latter defines the H -centred cell with multiplicity three. With respect to the primitive unit cell, the coordinates of \mathbf{L} nodes uvw are all integers and the direction indices $[uvw]$ and Miller indices (hkl) are relatively prime integers. With respect to the H -centred unit cell, the coordinates of \mathbf{L} nodes uvw and the direction indices $[uvw]$ are rational numbers, whereas the Miller indices (hkl) are integers that obey the condition $-h + k = 3n$ [equation (16)].

Fig. 10(a) shows two unit cells U_P^* of \mathbf{L}^* , indexed with respect to $\mathbf{a}_P^*, \mathbf{b}_P^*, \mathbf{c}_P^*$ (blue) and $\mathbf{a}_N^*, \mathbf{b}_N^*, \mathbf{c}_N^*$ (red). The latter do not define a unit cell but a region of reciprocal space, $(U_N)^*$,

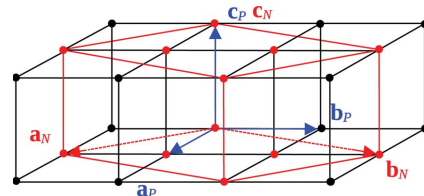


Figure 9

A portion of a Bravais lattice \mathbf{L} indexed with respect to a primitive coordinate system $O\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P$ (blue) and a non-primitive coordinate system $O\mathbf{a}_N \mathbf{b}_N \mathbf{c}_N$ (red) which corresponds to an H -centred unit cell U_N (here, $N = H$). To improve readability, the lattice nodes at the corners of and centring U_N are shown in red.

⁴ Concretely, a larger interval of $h_P k_P l_P$ is used to compute $h_N k_N l_N$ through equation (14) and the results in the intervals $[0, 1]$ or $[1, 2]$ are retained.

Table 4
Lattice nodes contained in $(U_H)^*$ depending on its position in \mathbf{L}^* .

Computation performed in the interval $[0, 2]$ of h, k and l , i.e. for eight locations. Each $(U_H)^*$ contains either $\frac{1}{2}$ or $\frac{1}{4}$ of a lattice node, leading to an average of $(4 \times \frac{1}{2} + 4 \times \frac{1}{4})/8 = 3/8$, approaching $\frac{1}{3}$, the determinant of the matrix \mathbf{M}^{-1} for the H -centred unit cell.

	Location of $(U_H)^*$							
	$h_N, k_N, l_N \in [0, 1]$	$h_N \in [1, 2], k_N, l_N \in [0, 1]$	$k_N \in [1, 2], h_N, l_N \in [0, 1]$	$l_N \in [1, 2], h_N, k_N \in [0, 1]$	$h_N, k_N \in [1, 2], l_N \in [0, 1]$	$h_N, l_N \in [1, 2], k_N \in [0, 1]$	$k_N, l_N \in [1, 2], h_N \in [0, 1]$	$h_N, k_N, l_N \in [1, 2]$
Coordinates of nodes with respect to $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$	000 ($\frac{1}{8}$) 001 ($\frac{1}{8}$) 110 ($\frac{1}{8}$) 111 ($\frac{1}{8}$)	110 ($\frac{1}{8}$) 111 ($\frac{1}{8}$)	110 ($\frac{1}{8}$) 111 ($\frac{1}{8}$)	001 ($\frac{1}{8}$) 002 ($\frac{1}{8}$) 111 ($\frac{1}{8}$) 112 ($\frac{1}{8}$)	110 ($\frac{1}{8}$) 111 ($\frac{1}{8}$) 220 ($\frac{1}{8}$) 221 ($\frac{1}{8}$)	111 ($\frac{1}{8}$) 112 ($\frac{1}{8}$)	111 ($\frac{1}{8}$) 112 ($\frac{1}{8}$)	111 ($\frac{1}{8}$) 222 ($\frac{1}{8}$) 112 ($\frac{1}{8}$) 221 ($\frac{1}{8}$)
Coordinates of nodes with respect to $\mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$	000 001 100 101	100 101	100 101	001 002 101 102	100 101 200 201	101 102	101 102	101 202 102 201
Multiplicity	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$

Table 5
Coordinates hkl of lattice nodes in the unit cell U_H^* with respect to three coordinate systems.

When expressed with respect to $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$, they obey the restriction $h + k = 3n$ typical of an H -centred unit cell in direct space, U_H . The unit cell in reciprocal space contains three lattice nodes and is of type X .

Position	Coordinates of nodes with respect to $\mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$	Coordinates of nodes with respect to $3\mathbf{a}_N^* 3\mathbf{b}_N^* \mathbf{c}_N^*$	Coordinates of nodes with respect to $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$
Corners ($\times \frac{1}{8}$)	000, 110, 111, 001, 300, 301, $2\bar{1}0, 2\bar{1}\bar{1}$	000, 010, 011, 001, 110, 111, 100, 101	000, 030, 031, 001, 330, 331, 300, 301
Faces ($\times \frac{1}{2}$)	100, 101, 200, 201	$\frac{11}{33}, \frac{11}{33}, \frac{22}{33}, \frac{22}{33}$	110, 111, 220, 221

that is not a unit cell: it contains *on average* $\frac{1}{3}$ of a lattice node (the determinant of the transformation matrix being $\frac{1}{3}$) but the fraction of lattice nodes is not constant and depends on the location of $(U_N)^*$. Table 4 shows the lattice nodes partially contained in $(U_N)^*$ depending on the location of $(U_N)^*$. The computation has been performed in the interval $[0, 2]$ of h, k and l , i.e. for eight locations. Each $(U_H)^*$ contains either $\frac{1}{2}$ or $\frac{1}{4}$ of a lattice node, leading to an average of $(4 \times \frac{1}{2} + 4 \times \frac{1}{4})/8 =$

$\frac{1}{3}$, approaching $\frac{1}{3}$, the determinant of the matrix \mathbf{M}^{-1} for the H -centred unit cell. A unit cell in reciprocal space has its edges coherent with $3\mathbf{a}_N^* 3\mathbf{b}_N^* \mathbf{c}_N^*$, which define a centred unit cell [Fig. 10(b)], U_H^* , containing three lattice nodes (Table 5), and is again of type X . With respect to $\mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$ [Fig. 10(a)], the coordinates of \mathbf{L}^* nodes hkl are all integers and the direction indices $[hkl]^*$ and Miller indices $(uvw)^*$ are relatively prime integers. With respect to $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$ [Fig. 10(b)], the coordinates of \mathbf{L}^* nodes hkl and the direction indices $[hkl]^*$ are integers that obey the condition $-h + k = 3n$, whereas the Miller indices $(uvw)^*$ are rational numbers.

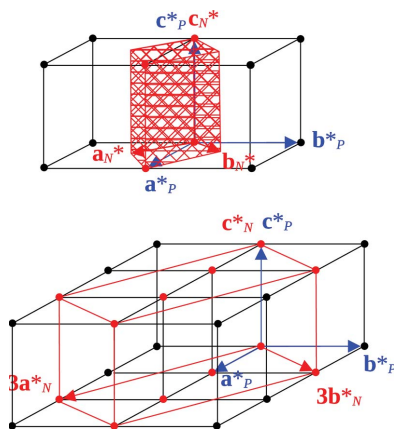


Figure 10
The reciprocal \mathbf{L}^* of the Bravais lattice \mathbf{L} in Fig. 9. (a) Two primitive (black) unit cells U_P^* , defined by the coordinate system $O^* \mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$ (blue) are shown, together with the $(U_N)^*$ (hatched in red) defined by the vectors $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$ (red). $(U_N)^*$ is the reciprocal of U_N in Fig. 9 but is not a unit cell; the latter, U_N^* , is obtained by taking $z_1 \mathbf{a}_N^* z_2 \mathbf{b}_N^* z_3 \mathbf{c}_N^*$ (here $z_1 = z_2 = 3, z_3 = 1$) [panel (b)]. When indexed with respect to $O^* \mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$, the nodes of \mathbf{L}^* obey the restriction $-h + k = 3n$, corresponding to the reflection condition of an H -centred unit cell in \mathbf{L} . The unit cell U_N^* defined by $3\mathbf{a}_N^* 3\mathbf{b}_N^* \mathbf{c}_N^*$ is also an H -centred cell. To improve readability, the lattice nodes at the corners of and centring U_N^* are shown in red.

3.6. D -centred unit cell

A D -centred unit cell has additional translation vectors $(3m + 1)\mathbf{a}/3, (3p + 1)\mathbf{b}/3, (3q + 1)\mathbf{c}/3$ and $(3m + 2)\mathbf{a}/3, (3p + 2)\mathbf{b}/3, (3q + 2)\mathbf{c}/3$, with $m, p, q \in \mathbb{Z}$. It was introduced by Buerger (1942) as the ‘hexagonal centering’, i.e. the rhombohedral description of a hexagonal lattice; today it has mainly a historical interest and is seldom used. Nevertheless, for the sake of completeness, we consider it interesting to show the consequences of choosing this unit cell on the diffraction pattern.

The transformation from $(\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P)$ to $(\mathbf{a}_D \mathbf{b}_D \mathbf{c}_D)$ is $(\mathbf{a}_D \mathbf{b}_D \mathbf{c}_D) = (\mathbf{a}_P + \mathbf{c}_P, \mathbf{b}_P + \mathbf{c}_P, -\mathbf{a}_P - \mathbf{b}_P + \mathbf{c}_P)$ (Table 1 and Fig. 11). The determinant of \mathbf{M} is 3 and that of \mathbf{M}^{-1} is $\frac{1}{3}$, accordingly [equation (7)], $V(U_D) = 3V(U_P)$ and $V(U_D)^* = V(U_P^*)/3$.

The transformation of hkl leads to

$$\begin{aligned}
 (h_P k_P l_P) \begin{pmatrix} 1 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{pmatrix} &= (h_P + l_P, k_P + l_P, -h_P - k_P + l_P) \\
 &= (h_D k_D l_D). \tag{18}
 \end{aligned}$$

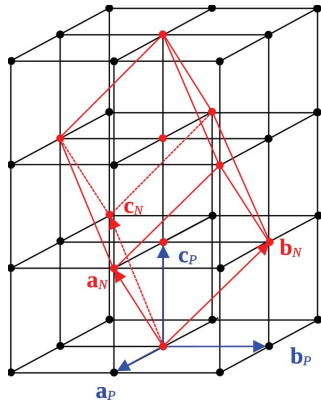


Figure 11
A portion of a Bravais lattice \mathbf{L} indexed with respect to a primitive coordinate system $O\mathbf{a}_p\mathbf{b}_p\mathbf{c}_p$ (blue) and a non-primitive coordinate system $O\mathbf{a}_N\mathbf{b}_N\mathbf{c}_N$ (red) which corresponds to a D -centred unit cell U_N (here, $N = D$). To improve readability, the lattice nodes at the corners of and centring U_N are shown in red.

Accordingly, $h_D = h_P + l_P$, $k_D = k_P + l_P$, $l_D = -h_P - k_P + l_P$, which implies the restriction $h_D + k_D + l_D = 3l_P$. We obtain immediately the integral condition typical of a D -centred cell (Buerger, 1942): hkl : $h + k + l = 3n$.

The transformation of uvw leads to

$$\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 3 \end{pmatrix} \begin{pmatrix} u_P \\ v_P \\ w_P \end{pmatrix} = \begin{pmatrix} 2u_P - v_P + w_P \\ -u_P + 2v_P + w_P \\ -u_P - v_P + w_P \end{pmatrix} = \begin{pmatrix} u_D \\ v_D \\ w_D \end{pmatrix}. \quad (19)$$

Whereas $|u_P v_P w_P|$ are integers, u_D , v_D and w_D are rational numbers. For example, $|111|_P$ transforms to $|\frac{2}{3}\frac{2}{3}\frac{1}{3}|_D$, $|110|_P$ transforms to $|\frac{1}{3}\frac{1}{3}\frac{2}{3}|_D$ and $|101|_P$ transforms to $|100|_D$. The direction indices u , v and w of a D -centred cell are therefore no longer restricted to integer values. The same holds for the Miller indices of \mathbf{L}^* planes, $(uvw)^*$. In direct space, the direction indices $[uvw]$ are rational numbers, whereas the Miller indices (hkl) are not restricted to relatively prime integers. In reciprocal space, the direction indices $[hkl]^*$ are not restricted to relatively prime integers, whereas the Miller indices $(uvw)^*$ are rational numbers.

Fig. 11 shows a portion of \mathbf{L} , indexed with respect to a coordinate system defining a primitive and conventional (blue) and a centred (red) coordinate system. Because the D -centred unit cell is defined for a hexagonal lattice, the angle γ_P is assumed to be 120° . The basis vectors $\mathbf{a}_N\mathbf{b}_N\mathbf{c}_N$ define the D -centred cell. With respect to the primitive unit cell (black), the coordinates of \mathbf{L} nodes uvw are all integers and the direction indices $[uvw]$ and Miller indices (hkl) are relatively prime integers. With respect to the D -centred unit cell (red), the coordinates of \mathbf{L} nodes uvw and the direction indices $[uvw]$ are rational numbers, whereas the Miller indices (hkl) are integers that obey the condition $h + k + l = 3n$ [equation (18)].

Fig. 12(a) shows four primitive unit cells (black) of \mathbf{L}^* , indexed with respect to $\mathbf{a}_p^*\mathbf{b}_p^*\mathbf{c}_p^*$ (blue) and $\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$ (red). The latter do not define a unit cell but a region of reciprocal space, $(U_N)^*$, that is not a unit cell: it contains on average $\frac{1}{3}$ of a lattice node (the determinant of the transformation matrix being $\frac{1}{3}$)

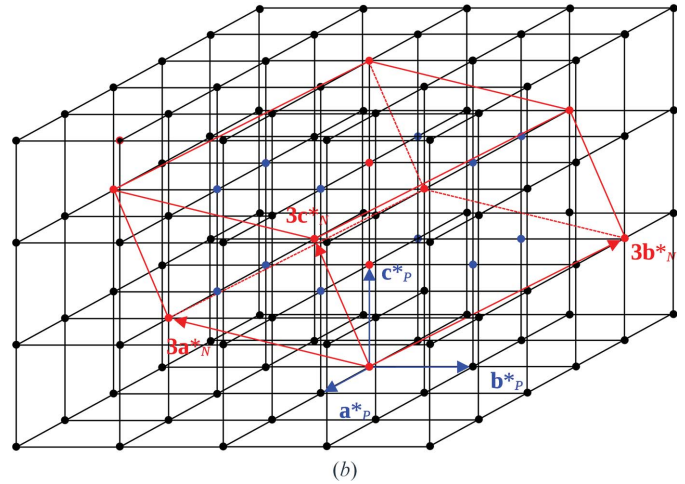
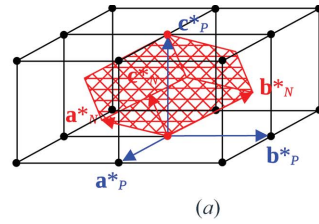


Figure 12

The reciprocal \mathbf{L}^* of the Bravais lattice \mathbf{L} in Fig. 11. (a) Four primitive (black) unit cells U_p^* , defined by the coordinate system $O^*\mathbf{a}_p^*\mathbf{b}_p^*\mathbf{c}_p^*$ (blue) are shown, together with the $(U_N)^*$ (hatched in red) defined by the vectors $\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$ (red). $(U_N)^*$ is the reciprocal of U_N in Fig. 11 but is not a unit cell; the latter, U_N^* , is obtained by taking $z_1\mathbf{a}_N^*z_2\mathbf{b}_N^*z_3\mathbf{c}_N^*$ (here $z_1 = z_2 = z_3 = 3$) [panel (b)]. When indexed with respect to $O^*\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$, the nodes of \mathbf{L}^* obey the restriction $h + k + l = 3n$, corresponding to the reflection condition of a D -centred unit cell in \mathbf{L} . The unit cell U_N^* defined by $3\mathbf{a}_N^*3\mathbf{b}_N^*3\mathbf{c}_N^*$ has multiplicity 9 and is therefore indicated with the generic symbol X . To improve readability, the lattice nodes at the corners of U_N^* and centring it are shown in red and those centring the faces of U_N^* in blue.

but the fraction of lattice nodes is not constant and depends on the location of $(U_N)^*$. Table 6 shows the lattice nodes partially contained in $(U_N)^*$ depending on the location of $(U_N)^*$. The computation has been performed in the interval $[0, 2]$ of h , k and l , i.e. for eight locations. Each $(U_N)^*$ contains either $\frac{3}{8}$ or $\frac{1}{4}$ of a lattice node, leading to an average of $(6 \times \frac{3}{8} + 2 \times \frac{1}{4})/8 = 22/64$, approaching $\frac{1}{3}$, the determinant of the matrix \mathbf{M}^{-1} for the D -centred unit cell. A unit cell in reciprocal space has its edges coherent with $3\mathbf{a}_N^*3\mathbf{b}_N^*3\mathbf{c}_N^*$, which define a centred unit cell [Fig. 12(b)], U_N^* , containing nine lattice nodes (Table 7), and is therefore of type X . With respect to $\mathbf{a}_p^*\mathbf{b}_p^*\mathbf{c}_p^*$ [Fig. 12(a)], the coordinates of \mathbf{L}^* nodes hkl are all integers and the direction indices $[hkl]^*$ and Miller indices $(uvw)^*$ are relatively prime integers. With respect to $\mathbf{a}_N^*\mathbf{b}_N^*\mathbf{c}_N^*$ [Fig. 12(b)], the coordinates of \mathbf{L}^* nodes hkl and the direction indices $[hkl]^*$ are integers that obey the condition $h + k + l = 3n$, whereas the Miller indices $(uvw)^*$ are rational numbers.

4. Discussion

In direct space, the edges of the unit cell are congruent with the basis vectors. This is no longer true in reciprocal space,

Table 6

Lattice nodes contained in $(U_D)^*$ depending on its position in \mathbf{L}^* .

Computation performed in the interval $[0, 2]$ of h, k and l , i.e. for eight locations. Each $(U_D)^*$ contains either $\frac{3}{8}$ or $\frac{1}{4}$ of a lattice node, leading to an average of $(6 \times \frac{3}{8} + 2 \times \frac{1}{4})/8 = 22/64$, approaching $\frac{1}{3}$, the determinant of the matrix \mathbf{M}^{-1} for the D -centred unit cell.

	Location of $(U_D)^*$							
	$h_N, k_N, l_N \in [0, 1]$	$h_N \in [1, 2], k_N, l_N \in [0, 1]$	$k_N \in [1, 2], h_N, l_N \in [0, 1]$	$l_N \in [1, 2], h_N, k_N \in [0, 1]$	$h_N, k_N \in [1, 2], l_N \in [0, 1]$	$h_N, l_N \in [1, 2], k_N \in [0, 1]$	$k_N, l_N \in [1, 2], h_N \in [0, 1]$	$h_N, k_N, l_N \in [1, 2]$
Coordinates of nodes with respect to $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$	000 ($\frac{1}{8}$) 111 ($\frac{1}{8}$)	111 ($\frac{1}{8}$) 201 ($\frac{1}{8}$) 210 ($\frac{1}{8}$)	021 ($\frac{1}{8}$) 111 ($\frac{1}{8}$) 120 ($\frac{1}{8}$)	012 ($\frac{1}{8}$) 102 ($\frac{1}{8}$) 111 ($\frac{1}{8}$)	111 ($\frac{1}{8}$) 120 ($\frac{1}{8}$) 210 ($\frac{1}{8}$)	102 ($\frac{1}{8}$) 111 ($\frac{1}{8}$) 201 ($\frac{1}{8}$)	012 ($\frac{1}{8}$) 021 ($\frac{1}{8}$) 111 ($\frac{1}{8}$)	111 ($\frac{1}{8}$) 222 ($\frac{1}{8}$)
Coordinates of nodes with respect to $\mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$	000 001	001 111 101	111 001 011	101 011 001	001 011 101	011 001 111	101 111 001	001 002
Multiplicity	$\frac{1}{4}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{4}$

Table 7

Coordinates hkl of lattice nodes in the unit cell U_D^* with respect to three coordinate systems.

When expressed with respect to $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$, they obey the restriction $h + k + l = 3n$ typical of a D -centred unit cell in direct space, U_D . The unit cell in reciprocal space contains nine lattice nodes and does not correspond to any of the nine types to which a letter has been assigned in the literature. It is therefore indicated with the generic symbol X .

Position	Coordinates of nodes with respect to $\mathbf{a}_P^* \mathbf{b}_P^* \mathbf{c}_P^*$	Coordinates of nodes with respect to $3\mathbf{a}_N^* 3\mathbf{b}_N^* 3\mathbf{c}_N^*$	Coordinates of nodes with respect to $\mathbf{a}_N^* \mathbf{b}_N^* \mathbf{c}_N^*$
Corners ($\times \frac{1}{8}$)	000, 212, 111, 121, 003, 122, 112, 211	000, 011, 001, 010, 111, 101, 110, 100	000, 033, 003, 030, 333, 303, 330, 300
Faces ($\times \frac{1}{2}$)	101, 102, 111, 112, 011, 012, 111, 112, 101, 102	$0\frac{12}{33}, \frac{12}{33}1, 0\frac{21}{33}, \frac{12}{33}2, \frac{10}{33}, \frac{21}{33}1, \frac{12}{33}0, \frac{1}{3}1\frac{1}{3}, \frac{2}{3}0\frac{1}{3}, 1\frac{12}{33}$ $\frac{21}{33}0, 1\frac{12}{33}$	012, 123, 021, 132, 102, 213, 120, 231, 201, 312, 210, 321
Body ($\times 1$)	001, 002	$\frac{111}{333}, \frac{222}{333}$	111, 222

unless a primitive unit cell is adopted. In the daily crystallographic routine of structure solution from diffraction data, it is customary to call $V^* = \det(\mathbf{G}^*)^{1/2}$ the ‘volume of the unit cell of the reciprocal lattice’. The core CIF dictionary calls a^*, b^*, c^* (collectively indicated as a_i^*) the ‘reciprocal-space cell lengths’ (Hall *et al.*, 2005). These are incorrect statements unless the unit cell is primitive. V^* is the volume, and a^*, b^*, c^* are the edges, of a region which is smaller than the unit cell; the latter is a multiple of this region. The integral reflection conditions that appear when the diffraction pattern is indexed with respect to a coordinate system that is the reciprocal of a non-primitive coordinate system in direct space come precisely from this broken correspondence between basis vectors and unit cell and, contrary to the zonal and serial reflection conditions, are not related to the crystal structure. Accordingly, the integral reflection conditions are the same for every crystal structure in any type of space group if the same type of unit cell is adopted; a change in the coordinate system from centred to primitive makes the integral reflection conditions disappear. This is not true for zonal and serial reflection conditions, which do depend on the crystal structure, and therefore on the type of space group, and do not disappear when changing the coordinate system, although their expression does depend on that choice. For example, by describing in a primitive coordinate system two crystal structures whose space groups are, respectively, of type $Fmm2$ (symmorphic) and $Fdd2$ (non-symmorphic), the integral reflection conditions disappear for both of them. The structure crystallizing in the symmorphic space group does not show zonal or serial reflection conditions because the e -glides $\frac{1}{4}yz$

and $x\frac{1}{4}z$ and the n -glides $0yz$ and $x0z$ are parallel to the mirror planes, and the screw axes are parallel to the rotation axes. Accordingly, the zonal reflection conditions $0kl: k, l = 2n$ (e -glide), $0kl: k + l = 2n$ (n -glide), $h0l: h, l = 2n$ (e -glide) and $h0l: h + l = 2n$ (n -glide) are also a specialization of the integral reflection conditions $hkl: h + l = 2n, h + k = 2n, k + l = 2n$; the same holds for the serial reflection conditions $00l: l = 2n$. When the structure is described in the unconventional primitive coordinate system, $\mathbf{a}_P = \mathbf{b}_F + \mathbf{c}_F/2, \mathbf{b}_P = \mathbf{a}_F + \mathbf{c}_F/2, \mathbf{c}_P = \mathbf{a}_F + \mathbf{b}_F/2$, the consequences of the change of basis are:

- (i) The integral reflection conditions disappear, the unit cell being primitive.
- (ii) The directions $[100], [010]$ and $[001]$ become $[\bar{1}11], [1\bar{1}1]$ and $[11\bar{1}]$, respectively.
- (iii) The $e_{[100]}$ -glide and $n_{[100]}$ -glide become $e_{[\bar{1}11]}$ and $n_{[1\bar{1}1]}$, respectively; their zonal reflection conditions are always satisfied because $k_F = 2l_P$ and $l_F = 2k_P$.
- (iv) The $e_{[010]}$ -glide and $n_{[010]}$ -glide become $e_{[1\bar{1}1]}$ and $n_{[1\bar{1}1]}$, respectively; their zonal reflection conditions are always satisfied because $h_F = 2l_P$ and $l_F = 2h_P$.
- (v) The $2_{[001]}$ becomes $2_{[1\bar{1}1]}$ and its serial reflection condition $00l: l = 2n$ becomes $hh0: h \in \mathbb{Z}$, which is always true in a primitive coordinate system.

The conclusion is the well known fact that a symmorphic space group does not show any reflection condition when described in a primitive coordinate system (Nespolo, 2017b). However, a structure crystallizing in a non-symmorphic space group shows zonal reflection conditions also when it is described in the unconventional primitive coordinate system. In the example $Fdd2$, the d -glide planes perpendicular to $[100]$

and [010] become, respectively, an a -glide plane perpendicular to $[1\bar{1}1]$ and a b -glide plane perpendicular to $[\bar{1}11]$. Following the change in coordinate system, the zonal reflection conditions are modified from $0kl: k + l = 4n$ and $h0l: h + l = 4n$ to, respectively, the unconventional expressions $hkl: h = k + l = 2n$ and $hkl: k = h + l = 2n$. The presence of glide planes in non-symmorphic space groups is still visible in the diffraction pattern whatever coordinate system is adopted, contrary to the integral reflection conditions.

This fundamental difference between integral reflection conditions on one side, and zonal and serial reflection conditions on the other side, should be taken into account to avoid propagating widespread misunderstandings, but also to facilitate the comprehension of a phenomenon – the occurrence of integral reflection conditions – which too often remains a relatively obscure point in the education of crystallographers.

The polar lattice, the ancestor of the reciprocal lattice (Nespolo & Souvignier, 2010), does not suffer from the same breaking of correspondence between basis vectors and unit cell because it is a dual lattice defined by having the same volume of the unit cell. It was, however, introduced for the morphological study of crystals and is not suitable to index a diffraction pattern.

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