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

1.3.2.5. Reciprocal lattice

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

Definition

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

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

and

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

which can conveniently be written as the matrix equation

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

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

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

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

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

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

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

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

Example

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

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

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

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

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

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

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

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

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

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

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

Examples

(i) The lattice **L** spanned by the vectors

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

has metric tensor

$$\boldsymbol{G} = \begin{pmatrix} 3 & 2 & 0 \\ 2 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

The inverse of the metric tensor is

$$\boldsymbol{G}^* = \boldsymbol{G}^{-1} = \frac{1}{2}\begin{pmatrix} 2 & -2 & 0 \\ -2 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Interpreting the columns of $\boldsymbol{G}^{-1}$ as coordinate vectors with respect to the original basis, one concludes that the reciprocal basis is given by

$$\mathbf{a}^* = \mathbf{a} - \mathbf{b}, \quad \mathbf{b}^* = \tfrac{1}{2}(-2\mathbf{a} + 3\mathbf{b}), \quad \mathbf{c}^* = \tfrac{1}{2}\mathbf{c}.$$

Inserting the columns for **a**, **b**, **c**, one obtains

$$\mathbf{a}^* = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{b}^* = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}, \quad \mathbf{c}^* = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}.$$

For the direct computation, the matrix $\boldsymbol{B}$ with the basis vectors **a**, **b**, **c** as columns is

$$\boldsymbol{B} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 0 & 0 \end{pmatrix}$$

and has as its inverse the matrix

$$\boldsymbol{B}^{-1} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 2 \\ 1 & 1 & -2 \\ 1 & -1 & 0 \end{pmatrix}.$$

The rows of this matrix are indeed the vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ as computed above.

(ii) The body-centred cubic lattice **L** has the vectors

$$\mathbf{a} = \frac{1}{2}\begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \quad \mathbf{c} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}$$

as primitive basis.
The matrix

$$\boldsymbol{B} = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

with the basis vectors **a**, **b**, **c** as columns has as its inverse the matrix

$$\boldsymbol{B}^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

The rows of $\boldsymbol{B}^{-1}$ are the vectors

$$\mathbf{a}^* = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b}^* = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{c}^* = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix},$$

showing that the reciprocal lattice of a body-centred cubic lattice is a face-centred cubic lattice.

1.3.3. The structure of space groups

1.3.3.1. Point groups of space groups

The multiplication rule for symmetry operations

$$(\boldsymbol{W}_2,\ \boldsymbol{w}_2)(\boldsymbol{W}_1,\ \boldsymbol{w}_1) = (\boldsymbol{W}_2\boldsymbol{W}_1,\ \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2)$$

shows that the mapping $\Pi : (\boldsymbol{W}, \boldsymbol{w}) \mapsto \boldsymbol{W}$ which assigns a space-group operation to its linear part is actually a group homomorphism, because the first component of the combined operation is simply the product of the linear parts of the two operations. As a consequence, the linear parts of a space group form a group themselves, which is called the point group of $\mathcal{G}$. The kernel of the homomorphism Π consists precisely of the translations $(\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}$, and since kernels of homomorphisms are always normal subgroups (*cf.* Section 1.1.6), the translation subgroup $\mathcal{T}$ forms a normal subgroup of $\mathcal{G}$. According to the *homomorphism theorem* (see Section 1.1.6), the point group is isomorphic to the factor group $\mathcal{G}/\mathcal{T}$.

Definition

The *point group* $\mathcal{P}$ of a space group $\mathcal{G}$ is the group of linear parts of operations occurring in $\mathcal{G}$. It is isomorphic to the factor group $\mathcal{G}/\mathcal{T}$ of $\mathcal{G}$ by the translation subgroup $\mathcal{T}$.

When $\mathcal{G}$ is considered with respect to a coordinate system, the operations of $\mathcal{P}$ are simply 3×3 matrices.

The point group plays an important role in the analysis of the macroscopic properties of crystals: it describes the symmetry of the set of face normals and can thus be directly observed. It is usually obtained from the *diffraction record* of the crystal, where adding the information about the translation subgroup explains the sharpness of the Bragg peaks in the diffraction pattern.

Although we have already deduced that the translation subgroup $\mathcal{T}$ of a space group $\mathcal{G}$ forms a normal subgroup in $\mathcal{G}$ because it is the kernel of the homomorphism mapping each operation to its linear part, it is worth investigating this fact by an explicit computation. Let $t = (\boldsymbol{I},\ \boldsymbol{t})$ be a translation in $\mathcal{T}$ and $W = (\boldsymbol{W},\ \boldsymbol{w})$ an arbitrary operation in $\mathcal{G}$, then one has

$$\begin{aligned} WtW^{-1} &= (\boldsymbol{W},\ \boldsymbol{w})(\boldsymbol{I},\ \boldsymbol{t})(\boldsymbol{W}^{-1},\ -\boldsymbol{W}^{-1}\boldsymbol{w}) \\ &= (\boldsymbol{W},\ \boldsymbol{Wt} + \boldsymbol{w})(\boldsymbol{W}^{-1},\ -\boldsymbol{W}^{-1}\boldsymbol{w}) \\ &= (\boldsymbol{I},\ -\boldsymbol{w} + \boldsymbol{Wt} + \boldsymbol{w}) = (\boldsymbol{I},\ \boldsymbol{Wt}), \end{aligned}$$

which is again a translation in $\mathcal{G}$, namely by $\boldsymbol{Wt}$. This little computation shows an important property of the translation subgroup with respect to the point group, namely that every vector from the translation lattice is mapped again to a lattice vector by each operation of the point group of $\mathcal{G}$.

Proposition. Let $\mathcal{G}$ be a space group with point group $\mathcal{P}$ and translation subgroup $\mathcal{T}$ and let $\mathbf{L} = \{\boldsymbol{t} \mid (\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}\}$ be the lattice of translations in $\mathcal{T}$. Then $\mathcal{P}$ acts on the lattice **L**, *i.e.* for every $\boldsymbol{W} \in \mathcal{P}$ and $\boldsymbol{t} \in \mathbf{L}$ one has $\boldsymbol{Wt} \in \mathbf{L}$.

A point group that acts on a lattice is a subgroup of the full group of symmetries of the lattice, obtained as the group of orthogonal mappings that map the lattice to itself. With respect to a primitive basis, the group of symmetries of a lattice consists of all integral basis transformations that fix the metric tensor of the lattice.