1.1. Summary of general formulae

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In an ideal crystal structure, the arrangement of atoms is three-dimensionally periodic. This periodicity is usually described in terms of point lattices, vector lattices, and translation groups [*cf. IT* A (1983, Section 8.1.3)].

1.1.1. General relations between direct and reciprocal lattices

1.1.1.1. *Primitive crystallographic bases*

The vectors **a**, **b**, **c** form a primitive crystallographic basis of the vector lattice **L**, if each translation vector $\mathbf{t} \in \mathbf{L}$ may be expressed as

$$\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

with u, v, w being integers.

A primitive basis defines a primitive unit cell for a corresponding point lattice. Its volume V may be calculated as the mixed product (triple scalar product) of the three basis vectors:

$$\begin{aligned} V &= (\mathbf{abc}) = \mathbf{a} \times \mathbf{b} \cdot \mathbf{c} \\ &= \left[\begin{vmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{vmatrix} \right]^{1/2} \\ &= abc[1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma \\ &\quad + 2\cos\alpha\cos\beta\cos\gamma]^{1/2} \\ &= 2abc\left[\sin\frac{\alpha+\beta+\gamma}{2} \sin\frac{-\alpha+\beta+\gamma}{2} \right. \\ &\quad \left. \times \sin\frac{\alpha-\beta+\gamma}{2} \sin\frac{\alpha+\beta-\gamma}{2} \right]^{1/2}. \end{aligned} \tag{1.1.1.1}$$

Here a, b and c designate the lengths of the three basis vectors and $\alpha = \mathbf{b} \wedge \mathbf{c}$, $\beta = \mathbf{c} \wedge \mathbf{a}$ and $\gamma = \mathbf{a} \wedge \mathbf{b}$ the angles between them.

Each vector lattice **L** and each primitive crystallographic basis **a**, **b**, **c** is uniquely related to a reciprocal vector lattice $\mathbf{L}^*$ and a primitive reciprocal basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$:

$$\left.\begin{aligned} \mathbf{a}^* &= \frac{\mathbf{b}\times\mathbf{c}}{V} \quad \text{or} \quad \mathbf{a}^*\cdot\mathbf{b} = \mathbf{a}^*\cdot\mathbf{c} = 0, \quad \mathbf{a}^*\cdot\mathbf{a} = 1; \\ \mathbf{b}^* &= \frac{\mathbf{c}\times\mathbf{a}}{V} \quad \text{or} \quad \mathbf{b}^*\cdot\mathbf{a} = \mathbf{b}^*\cdot\mathbf{c} = 0, \quad \mathbf{b}^*\cdot\mathbf{b} = 1; \\ \mathbf{c}^* &= \frac{\mathbf{a}\times\mathbf{b}}{V} \quad \text{or} \quad \mathbf{c}^*\cdot\mathbf{a} = \mathbf{c}^*\cdot\mathbf{b} = 0, \quad \mathbf{c}^*\cdot\mathbf{c} = 1. \end{aligned}\right\} \tag{1.1.1.2}$$

$$\mathbf{L}^* = \{\mathbf{r}^* | \mathbf{r}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \text{ and } h, k, l \text{ integers}\}.$$

The lengths a^*, b^* and c^* of the reciprocal basis vectors and the angles $\alpha^* = \mathbf{b}^* \wedge \mathbf{c}^*$, $\beta^* = \mathbf{c}^* \wedge \mathbf{a}^*$ and $\gamma^* = \mathbf{a}^* \wedge \mathbf{b}^*$ are given by:

$$\left.\begin{aligned} a^* &= \frac{bc\sin\alpha}{V}, \quad b^* = \frac{ac\sin\beta}{V}, \quad c^* = \frac{ab\sin\gamma}{V}, \\ \cos\alpha^* &= \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}, \\ \cos\beta^* &= \frac{\cos\alpha\cos\gamma - \cos\beta}{\sin\alpha\sin\gamma}, \\ \cos\gamma^* &= \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}. \end{aligned}\right\} \tag{1.1.1.3}$$

$\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ define a primitive unit cell in a corresponding reciprocal point lattice. Its volume V^* may be expressed by analogy with V [equation (1.1.1.1)]:

$$\begin{aligned} V^* &= (\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*) = \mathbf{a}^* \times \mathbf{b}^* \cdot \mathbf{c}^* \\ &= \left[\begin{vmatrix} a^{*2} & a^*b^*\cos\gamma^* & a^*c^*\cos\beta^* \\ a^*b^*\cos\gamma^* & b^{*2} & b^*c^*\cos\alpha^* \\ a^*c^*\cos\beta^* & b^*c^*\cos\alpha^* & c^{*2} \end{vmatrix} \right]^{1/2} \\ &= a^*b^*c^*[1 - \cos^2\alpha^* - \cos^2\beta^* - \cos^2\gamma^* \\ &\quad + 2\cos\alpha^*\cos\beta^*\cos\gamma^*]^{1/2} \\ &= 2a^*b^*c^*\left[\sin\frac{\alpha^*+\beta^*+\gamma^*}{2} \sin\frac{-\alpha^*+\beta^*+\gamma^*}{2} \right. \\ &\quad \left. \times \sin\frac{\alpha^*-\beta^*+\gamma^*}{2} \sin\frac{\alpha^*+\beta^*-\gamma^*}{2} \right]^{1/2}. \end{aligned} \tag{1.1.1.4}$$

In addition, the following equation holds:

$$VV^* = 1. \tag{1.1.1.5}$$

As all relations between direct and reciprocal lattices are symmetrical, one can calculate **a**, **b**, **c** from $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$:

$$\mathbf{a} = \frac{\mathbf{b}^*\times\mathbf{c}^*}{V^*}, \quad \mathbf{b} = \frac{\mathbf{c}^*\times\mathbf{a}^*}{V^*}, \quad \mathbf{c} = \frac{\mathbf{a}^*\times\mathbf{b}^*}{V^*}, \tag{1.1.1.6}$$

$$\left.\begin{aligned} a &= \frac{b^*c^*\sin\alpha^*}{V^*}, \\ b &= \frac{a^*c^*\sin\beta^*}{V^*}, \\ c &= \frac{a^*b^*\sin\gamma^*}{V^*}, \\ \cos\alpha &= \frac{\cos\beta^*\cos\gamma^* - \cos\alpha^*}{\sin\beta^*\sin\gamma^*}, \\ \cos\beta &= \frac{\cos\alpha^*\cos\gamma^* - \cos\beta^*}{\sin\alpha^*\sin\gamma^*}, \\ \cos\gamma &= \frac{\cos\alpha^*\cos\beta^* - \cos\gamma^*}{\sin\alpha^*\sin\beta^*}. \end{aligned}\right\} \tag{1.1.1.7}$$

The unit-cell volumes V and V^* may also be obtained from:

$$\begin{aligned} V &= abc\sin\alpha^*\sin\beta\sin\gamma \\ &= abc\sin\alpha\sin\beta^*\sin\gamma \\ &= abc\sin\alpha\sin\beta\sin\gamma^*, \end{aligned} \tag{1.1.1.8}$$

Table 1.1.1.1. *Direct and reciprocal lattices described with respect to conventional basis systems*

Direct lattice $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$			Reciprocal lattice		
			$\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*$		
Bravais letter	Centring vectors	Unit-cell volume V_c	Conditions for reciprocal-lattice vectors $h\mathbf{a}_c^* + k\mathbf{b}_c^* + l\mathbf{c}_c^*$	Unit-cell volume V_c^*	Bravais letter
A	$\frac{1}{2}\mathbf{b}_c + \frac{1}{2}\mathbf{c}_c$	$2V$	$k + l = 2n$	$\frac{1}{2}V^*$	A
B	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{c}_c$	$2V$	$h + l = 2n$	$\frac{1}{2}V^*$	B
C	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{b}_c$	$2V$	$h + k = 2n$	$\frac{1}{2}V^*$	C
I	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{b}_c + \frac{1}{2}\mathbf{c}_c$	$2V$	$h + k + l = 2n$	$\frac{1}{2}V^*$	F
F	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{b}_c$, $\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{c}_c$, $\frac{1}{2}\mathbf{b}_c + \frac{1}{2}\mathbf{c}_c$	$4V$	$h + k = 2n$, $h + l = 2n$, $k + l = 2n$	$\frac{1}{4}V^*$	I
R	$\frac{1}{3}\mathbf{a}_c + \frac{2}{3}\mathbf{b}_c + \frac{2}{3}\mathbf{c}_c$, $\frac{2}{3}\mathbf{a}_c + \frac{1}{3}\mathbf{b}_c + \frac{1}{3}\mathbf{c}_c$	$3V$	$-h + k + l = 3n$	$\frac{1}{3}V^*$	R

$$\begin{aligned} V^* &= a^*b^*c^* \sin\alpha \sin\beta^* \sin\gamma^* \\ &= a^*b^*c^* \sin\alpha^* \sin\beta \sin\gamma^* \\ &= a^*b^*c^* \sin\alpha^* \sin\beta^* \sin\gamma. \end{aligned} \quad (1.1.1.9)$$

1.1.1.2. *Non-primitive crystallographic bases*

For certain lattice types, it is usual in crystallography to refer to a 'conventional' crystallographic basis $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ instead of a primitive basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$. In that case, $\mathbf{a}_c$, $\mathbf{b}_c$, and $\mathbf{c}_c$ with all their integral linear combinations are lattice vectors again, but there exist other lattice vectors $\mathbf{t} \in \mathbf{L}$,

$$\mathbf{t} = t_1\mathbf{a}_c + t_2\mathbf{b}_c + t_3\mathbf{c}_c,$$

with at least two of the coefficients t_1, t_2, t_3 being fractional.

Such a conventional basis defines a conventional or centred unit cell for a corresponding point lattice, the volume V_c of which may be calculated by analogy with V by substituting $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ for $\mathbf{a}, \mathbf{b}$, and $\mathbf{c}$ in (1.1.1.1).

If m designates the number of centring lattice vectors $\mathbf{t}$ with $0 \le t_1, t_2, t_3 < 1$, V_c may be expressed as a multiple of the primitive unit-cell volume V:

$$V_c = mV. \quad (1.1.1.10)$$

With the aid of equations (1.1.1.2) and (1.1.1.3), the reciprocal basis $\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*$ may be derived from $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$. Again, each reciprocal-lattice vector

$$\mathbf{r}^* = h\mathbf{a}_c^* + k\mathbf{b}_c^* + l\mathbf{c}_c^* \in \mathbf{L}^*$$

is an integral linear combination of the reciprocal basis vectors, but in contrast to the use of a primitive basis only certain triplets h, k, l refer to reciprocal-lattice vectors.

Equation (1.1.1.5) also relates V_c to V_c^*, the reciprocal cell volume referred to $\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*$. From this it follows that

$$V_c^* = \frac{1}{m}V^*. \quad (1.1.1.11)$$

Table 1.1.1.1 contains detailed information on 'centred lattices' described with respect to conventional basis systems.

As a direct lattice and its corresponding reciprocal lattice do not necessarily belong to the same type of Bravais lattices [*IT* A (1987, Section 8.2.4)], the Bravais letter of $\mathbf{L}^*$ is given in the last column of Table 1.1.1.1. Except for P lattices, a conventionally chosen basis for $\mathbf{L}^*$ coincides neither with $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ nor with $\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*$. This third basis, however, is not used in crystallography. The designation of scattering vectors and the indexing of Bragg reflections usually refers to $\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*$.

If the differences with respect to the coefficients of direct- and reciprocal-lattice vectors are disregarded, all other relations discussed in Part 1 are equally true for primitive bases and for conventional bases.

1.1.2. Lattice vectors, point rows, and net planes

The length t of a vector $\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$ is given by

$$\begin{aligned} t^2 = {} & u^2\mathbf{a}^2 + v^2\mathbf{b}^2 + w^2\mathbf{c}^2 + 2uvab\cos\gamma \\ & + 2uwac\cos\beta + 2vwbc\cos\alpha. \end{aligned} \quad (1.1.2.1)$$

Accordingly, the length r^* of a reciprocal-lattice vector $\mathbf{r}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$ may be calculated from

$$\begin{aligned} r^{*2} = {} & h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2hka^*b^*\cos\gamma^* \\ & + 2hla^*c^*\cos\beta^* + 2klb^*c^*\cos\alpha^*. \end{aligned} \quad (1.1.2.2)$$

If the coefficients u, v, w of a vector $\mathbf{t} \in \mathbf{L}$ are coprime, $[uvw]$ symbolizes the direction parallel to $\mathbf{t}$. In particular, $[uvw]$ is used to designate a crystal edge, a zone axis, or a point row with that direction.

The integer coefficients h, k, l of a vector $\mathbf{r}^* \in \mathbf{L}^*$ are also the coordinates of a point of the corresponding reciprocal lattice and designate the Bragg reflection with scattering vector $\mathbf{r}^*$. If h, k, l are coprime, the direction parallel to $\mathbf{r}^*$ is symbolized by $[hkl]^*$.

Each vector $\mathbf{r}^*$ is perpendicular to a family of equidistant parallel nets within a corresponding direct point lattice. If the coefficients h, k, l of $\mathbf{r}^*$ are coprime, the symbol (hkl) describes that family of nets. The distance $d(hkl)$ between two neighbouring nets is given by

references