1.1. SUMMARY OF GENERAL FORMULAE

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

$$d(hkl) = r^{*-1}. \tag{1.1.2.3}$$

Parallel to such a family of nets, there may be a face or a cleavage plane of a crystal.

The net planes (hkl) obey the equation

$$hx + ky + lz = n \quad (n = \text{integer}). \tag{1.1.2.4}$$

Different values of n distinguish between the individual nets of the family; x, y, z are the coordinates of points on the net planes (not necessarily of lattice points). They are expressed in units a, b, and c, respectively.

Similarly, each vector $\mathbf{t} \in \mathbf{L}$ with coprime coefficients u, v, w is perpendicular to a family of equidistant parallel nets within a corresponding reciprocal point lattice. This family of nets may be symbolized $(uvw)^*$. The distance $d^*(uvw)$ between two neighbouring nets can be calculated from

$$d^*(uvw) = t^{-1}. \tag{1.1.2.5}$$

A layer line on a rotation pattern or a Weissenberg photograph with rotation axis $[uvw]$ corresponds to one such net of the family $(uvw)^*$ of the reciprocal lattice.

The nets $(uvw)^*$ obey the equation

$$uh + vk + wl = n \quad (n = \text{integer}). \tag{1.1.2.6}$$

Equations (1.1.2.6) and (1.1.2.4) are essentially the same, but may be interpreted differently. Again, n distinguishes between the individual nets out of the family $(uvw)^*$. h, k, l are the coordinates of the reciprocal-lattice points, expressed in units a^*, b^*, c^*, respectively.

A family of nets (hkl) and a point row with direction $[uvw]$ out of the same point lattice are parallel if and only if the following equation is satisfied:

$$hu + kv + lw = 0. \tag{1.1.2.7}$$

This equation is called the 'zone equation' because it must also hold if a face (hkl) of a crystal belongs to a zone $[uvw]$.

Two (non-parallel) nets $(h_1k_1l_1)$ and $(h_2k_2l_2)$ intersect in a point row with direction $[uvw]$ if the indices satisfy the condition

$$u : v : w = \begin{vmatrix} k_1 l_1 \\ k_2 l_2 \end{vmatrix} : \begin{vmatrix} l_1 h_1 \\ l_2 h_2 \end{vmatrix} : \begin{vmatrix} h_1 k_1 \\ h_2 k_2 \end{vmatrix}. \tag{1.1.2.8}$$

The same condition must be satisfied for a zone axis $[uvw]$ defined by the crystal faces $(h_1k_1l_1)$ and $(h_2k_2l_2)$.

Three nets $(h_1k_1l_1)$, $(h_2k_2l_2)$, and $(h_3k_3l_3)$ intersect in parallel rows, or three faces with these indices belong to one zone if

$$\begin{vmatrix} h_1 k_1 l_1 \\ h_2 k_2 l_2 \\ h_3 k_3 l_3 \end{vmatrix} = 0. \tag{1.1.2.9}$$

Two (non-parallel) point rows $[u_1v_1w_1]$ and $[u_2v_2w_2]$ in the direct lattice are parallel to a family of nets (hkl) if

$$h : k : l = \begin{vmatrix} v_1 w_1 \\ v_2 w_2 \end{vmatrix} : \begin{vmatrix} w_1 u_1 \\ w_2 u_2 \end{vmatrix} : \begin{vmatrix} u_1 v_1 \\ u_2 v_2 \end{vmatrix}. \tag{1.1.2.10}$$

The same condition holds for a face (hkl) belonging to two zones $[u_1v_1w_1]$ and $[u_2v_2w_2]$.

Three point rows $[u_1v_1w_1]$, $[u_2v_2w_2]$, and $[u_3v_3w_3]$ are parallel to a net (hkl), or three zones of a crystal with these indices have a common face (hkl) if

$$\begin{vmatrix} u_1 v_1 w_1 \\ u_2 v_2 w_2 \\ u_3 v_3 w_3 \end{vmatrix} = 0. \tag{1.1.2.11}$$

A net (hkl) is perpendicular to a point row $[uvw]$ if

$$\begin{aligned} &\frac{a}{h}(au + bv\cos\gamma + cw\cos\beta) \\ &\quad = \frac{b}{k}(au\cos\gamma + bv + cw\cos\alpha) \\ &\quad = \frac{c}{l}(au\cos\beta + bv\cos\alpha + cw). \end{aligned} \tag{1.1.2.12}$$

1.1.3. Angles in direct and reciprocal space

The angles between the normal of a crystal face and the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are called the direction angles of that face. They may be calculated as angles between the corresponding reciprocal-lattice vector $\mathbf{r}^*$ and the basis vectors $\lambda = \mathbf{r}^* \wedge \mathbf{a}$, $\mu = \mathbf{r}^* \wedge \mathbf{b}$ and $\nu = \mathbf{r}^* \wedge \mathbf{c}$:

$$\left.\begin{aligned} \cos\lambda = \frac{h}{a}d(hkl), \quad \cos\mu = \frac{k}{b}d(hkl), \\ \cos\nu = \frac{l}{c}d(hkl). \end{aligned}\right\} \tag{1.1.3.1}$$

The three equations can be combined to give

$$\left.\begin{aligned} a : b : c = \frac{h}{\cos\lambda} : \frac{k}{\cos\mu} : \frac{l}{\cos\nu} \\ \text{or} \\ h : k : l = a\cos\lambda : b\cos\mu : c\cos\nu. \end{aligned}\right\} \tag{1.1.3.2}$$

The first formula gives the ratios between a, b, and c, if for any face of the crystal the indices (hkl) and the direction angles λ, μ, and ν are known. Once the axial ratios are known, the indices of any other face can be obtained from its direction angles by using the second formula.

Similarly, the angles between a direct-lattice vector $\mathbf{t}$ and the reciprocal basis vectors $\lambda^* = \mathbf{t} \wedge \mathbf{a}^*$, $\mu^* = \mathbf{t} \wedge \mathbf{b}^*$ and $\nu^* = \mathbf{t} \wedge \mathbf{c}^*$ are given by

$$\left.\begin{aligned} \cos\lambda^* = \frac{u}{a^*}d^*(uvw), \quad \cos\mu^* = \frac{v}{b^*}d^*(uvw), \\ \cos\nu^* = \frac{w}{c^*}d^*(uvw). \end{aligned}\right\} \tag{1.1.3.3}$$

The angle ψ between two direct-lattice vectors $\mathbf{t}_1$ and $\mathbf{t}_2$ or between two corresponding point rows $[u_1v_1w_1]$ and $[u_2v_2w_2]$ may be derived from the scalar product

$$\begin{aligned} \mathbf{t}_1 \cdot \mathbf{t}_2 = {} & u_1u_2a^2 + v_1v_2b^2 + w_1w_2c^2 + (u_1v_2 + u_2v_1)ab\cos\gamma \\ & + (u_1w_2 + u_2w_1)ac\cos\beta + (v_1w_2 + v_2w_1)bc\cos\alpha \end{aligned} \tag{1.1.3.4}$$

as

$$\cos\psi = \frac{\mathbf{t}_1 \cdot \mathbf{t}_2}{t_1 t_2}. \tag{1.1.3.5}$$

Analogously, the angle φ between two reciprocal-lattice vectors $\mathbf{r}_1^*$ and $\mathbf{r}_2^*$ or between two corresponding point rows $[h_1k_1l_1]^*$ and $[h_2k_2l_2]^*$ or between the normals of two corresponding crystal faces $(h_1k_1l_1)$ and $(h_2k_2l_2)$ may be calculated as

$$\cos\varphi = \frac{\mathbf{r}_1^* \cdot \mathbf{r}_2^*}{r_1 r_2} \tag{1.1.3.6}$$

with

$$\begin{aligned} \mathbf{r}_1^* \cdot \mathbf{r}_2^* = {} & h_1h_2a^{*2} + k_1k_2b^{*2} + l_1l_2c^{*2} \\ & + (h_1k_2 + h_2k_1)a^*b^*\cos\gamma^* \\ & + (h_1l_2 + h_2l_1)a^*c^*\cos\beta^* \\ & + (k_1l_2 + k_2l_1)b^*c^*\cos\alpha^*. \end{aligned} \tag{1.1.3.7}$$

references