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

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

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

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

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

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

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

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:

$$hu + kv + lw = 0. \qquad (1.1.2.7)$$

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

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

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

$$\begin{vmatrix} h_1k_1l_1 \\ h_2k_2l_2 \\ h_3k_3l_3 \end{vmatrix} = 0. \qquad (1.1.2.9)$$

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

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

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

$$\begin{vmatrix} u_1v_1w_1 \\ u_2v_2w_2 \\ u_3v_3w_3 \end{vmatrix} = 0. \qquad (1.1.2.11)$$

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

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

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 $\nu = \mathbf{r}^* \wedge \mathbf{c}$:

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

The three equations can be combined to give

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

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

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

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

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

as

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

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

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

with

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

Finally, the angle ω between a first direction $[uvw]$ of the direct lattice and a second direction $[hkl]$ of the reciprocal lattice may also be derived from the scalar product of the corresponding vectors $\mathbf{t}$ and $\mathbf{r}^*$.

$$\cos\omega = \frac{\mathbf{t}\cdot\mathbf{r}^*}{tr^*} = \frac{uh + vk + wl}{tr^*}. \qquad (1.1.3.8)$$

1.1.4. The Miller formulae

Consider four faces of a crystal that belong to the same zone in consecutive order: $(h_1k_1l_1)$, $(h_2k_2l_2)$, $(h_3k_3l_3)$, and $(h_4k_4l_4)$. The angles between the ith and the jth face normals are designated φ_{ij}. Then the Miller formulae relate the indices of these faces to the angles φ_{ij}:

$$\frac{\sin\varphi_{12}\sin\varphi_{43}}{\sin\varphi_{13}\sin\varphi_{42}} = \frac{u_{12}u_{43}}{u_{13}u_{42}} = \frac{v_{12}v_{43}}{v_{13}v_{42}} = \frac{w_{12}w_{43}}{w_{13}w_{42}} \qquad (1.1.4.1)$$

with

$$u_{ij} = \begin{vmatrix} k_i l_i \\ k_j l_j \end{vmatrix}, \quad v_{ij} = \begin{vmatrix} l_i h_i \\ l_j h_j \end{vmatrix}, \quad w_{ij} = \begin{vmatrix} h_i k_i \\ h_j k_j \end{vmatrix}.$$

If all angles between the face normals and also the indices for three of the faces are known, the indices of the fourth face may be calculated. Equation (1.1.4.1) cannot be used if two of the faces are parallel.

From the definition of u_{ij}, v_{ij}, and w_{ij}, it follows that all fractions in (1.1.4.1) are rational:

$$\frac{\sin\varphi_{12}\sin\varphi_{43}}{\sin\varphi_{13}\sin\varphi_{42}} = \frac{p}{q} \quad \text{with } p, q \text{ integers.}$$

Therefore, (1.1.4.1) may be rearranged to

$$p\cot\varphi_{12} - q\cot\varphi_{13} = (p - q)\cot\varphi_{14}. \qquad (1.1.4.2)$$

This equation allows the determination of one angle if two of the angles and the indices of all four faces are known.

references