Appendix 3
Lattice Geometry

A3-1 PLANE SPACINGS

The value of d, the distance between adjacent planes in the set (hkl), may be found from the following equations.

Cubic:
$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Tetragonal:
$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

Hexagonal:
$$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

Rhombohedral:
$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + hl)(\cos^2\alpha - \cos\alpha)}{a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)}$$

Orthorhombic:
$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Monoclinic:
$$\frac{1}{d^2} = \frac{1}{\sin^2\beta}\left(\frac{h^2}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right)$$

Triclinic:
$$\frac{1}{d^2} = \frac{1}{V^2}(S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl)$$

In the equation for triclinic crystals,

V = volume of unit cell (see below),

$$S_{11} = b^2c^2\sin^2\alpha,$$

$$S_{22} = a^2c^2\sin^2\beta,$$

$$S_{33} = a^2b^2\sin^2\gamma,$$

$$S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma),$$

$$S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha),$$

$$S_{13} = ab^2c(\cos\gamma\cos\alpha - \cos\beta).$$

A3-2 CELL VOLUMES

The following equations give the volume V of the unit cell.

Cubic: $V = a^3$

Tetragonal: $V = a^2c$

Hexagonal: $V = \dfrac{\sqrt{3}a^2c}{2} = 0.866a^2c$

Rhombohedral: $V = a^3\sqrt{1 - 3\cos^2\alpha + 2\cos^2\alpha}$

Orthorhombic: $V = abc$

Monoclinic: $V = abc\sin\beta$

Triclinic: $V = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$

A3-3 INTERPLANAR ANGLES

The angle ϕ between the plane $(h_1k_1l_1)$, of spacing d_1, and the plane $(h_2k_2l_2)$, of spacing d_2, may be found from the following equations. (V is the volume of the unit cell.)

Cubic:
$$\cos\phi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)(h_2^2 + k_2^2 + l_2^2)}}$$

Tetragonal:
$$\cos\phi = \frac{\dfrac{h_1h_2 + k_1k_2}{a^2} + \dfrac{l_1l_2}{c^2}}{\sqrt{\left(\dfrac{h_1^2 + k_1^2}{a^2} + \dfrac{l_1^2}{c^2}\right)\left(\dfrac{h_2^2 + k_2^2}{a^2} + \dfrac{l_2^2}{c^2}\right)}}$$

Hexagonal:
$$\cos\phi = \frac{h_1h_2 + k_1k_2 + \frac{1}{2}(h_1k_2 + h_2k_1) + \dfrac{3a^2}{4c^2}l_1l_2}{\sqrt{\left(h_1^2 + k_1^2 + h_1k_1 + \dfrac{3a^2}{4c^2}l_1^2\right)\left(h_2^2 + k_2^2 + h_2k_2 + \dfrac{3a^2}{4c^2}l_2^2\right)}}$$

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