

number Z of the scattering atom. Elements with almost the same values of Z may have quite different neutron-scattering powers, and elements with widely separated values of Z may scatter neutrons equally well. Furthermore, some light elements, such as carbon, scatter neutrons more intensely than some heavy elements, such as tungsten. It follows that structure analyses can be carried out with neutron diffraction that are impossible, or possible only with great difficulty, with x-ray or electron diffraction. In a compound of hydrogen or carbon, for example, with a heavy metal, x-rays will not "see" the light hydrogen or carbon atom because of its relatively low scattering power, whereas its position in the lattice can be determined with ease by neutron diffraction. Neutrons can also distinguish in many cases between elements differing by only one atomic number, elements which scatter x-rays with almost equal intensity; neutron diffraction, for example, shows strong superlattice lines from ordered FeCo , whereas with x-rays they are practically invisible.

3. Neutrons have a small magnetic moment. If the scattering atom also has a net magnetic moment, the two interact and modify the total scattering. In substances that have an ordered arrangement of atomic moments (antiferromagnetic, ferrimagnetic, and ferromagnetic materials) neutron diffraction can disclose both the magnitude and direction of the moments. Only neutron diffraction can furnish such information, and it has had a major impact on studies of magnetic structure.

Diffuse scattering at small angles (in transmission), mentioned in regard to x-rays at the end of Sec. 9-3 and in Chap. 19, also occurs with neutrons. Neutron small-angle scattering has certain advantages over x-rays as a means of studying inhomogeneities in materials, particularly because thick specimens, rather than thin foils, can be examined.

Neutron diffraction would doubtless have wider application if all potential investigators had easy access to high-intensity neutron sources, but the number of such sources is very limited.

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:

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

(Trigonal) **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),

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

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

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

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

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

CELL VOLUMES

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

Cubic: $V = a^3$

Tetragonal: $V = a^2c$

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

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

Orthorhombic: $V = abc$

Monoclinic: $V = abc\sin\beta$

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

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

Hexagonal:

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

Rhombohedral:

$$\cos\phi = \frac{a^4d_1d_2}{V^2} \left[\sin^2\alpha(h_1h_2 + k_1k_2 + l_1l_2) + (\cos^2\alpha - \cos\alpha)(k_1l_2 + k_2l_1 + l_1h_2 + l_2h_1 + h_1k_2 + h_2k_1) \right]$$

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

Monoclinic:

$$\cos\phi = \frac{d_1d_2}{\sin^2\beta} \left[\frac{h_1h_2}{a^2} + \frac{k_1k_2\sin^2\beta}{b^2} + \frac{l_1l_2}{c^2} - \frac{(l_1h_2 + l_2h_1)\cos\beta}{ac} \right]$$

Triclinic:

$$\cos\phi = \frac{d_1d_2}{V^2} [S_{11}h_1h_2 + S_{22}k_1k_2 + S_{33}l_1l_2 + S_{23}(k_1l_2 + k_2l_1) + S_{13}(l_1h_2 + l_2h_1) + S_{12}(h_1k_2 + h_2k_1)]$$