3.27: Structure Factor

The **structure factor** $\mathbf{F}_{hkl}$ is a mathematical function describing the amplitude and phase of a wave diffracted from crystal lattice planes characterized by Miller indices h,k,l.

The structure factor may be expressed as

$$\mathbf{F}_{hkl} = F_{hkl}\exp(i\alpha_{hkl}) = \sum_j f_j\exp[2\pi i(hx_j + ky_j + lz_j) \tag{3.27.1}$$

$$= \sum_j f_j\cos[2\pi(hx_j + ky_j + lz_j)] + i\sum_j f_j\sin[2\pi(hx_j + ky_j + lz_j)] \tag{3.27.2}$$

$$= A_{hkl} + iB_{hkl} \tag{3.27.3}$$

where the sum is over all atoms in the unit cell, x_j,y_j,z_j are the positional coordinates of the jth atom, f_j is the scattering factor of the jth atom, and α_{hkl} is the phase of the diffracted beam.

The intensity of a diffracted beam is directly related to the amplitude of the structure factor, but the phase must normally be deduced by indirect means. In structure determination, phases are estimated and an initial description of the positions and anisotropic displacements of the scattering atoms is deduced. From this initial model, structure factors are calculated and compared with those experimentally observed. Iterative refinement procedures attempt to minimize the difference between calculation and experiment, until a satisfactory fit has been obtained.

Derivation

Consider Bragg's law for an array of atom scatterers in a primitive lattice with just one atom at each lattice point. An incident X-ray wave of wavelength λ diffracts strongly through an angle 2θ where the perpendicular distance between two lattice planes d_{hkl} satisfies the relation

$$2d_{hkl}\sin\theta = n\lambda$$

It is seen that the path difference between waves diffracted from the two planes shown differs by just one wave cycle.

Now consider a second atom added to the unit cell. Each original atom is now accompanied by a companion atom of the new type, offset by a displacement vector $\mathbf{r}_1$. The incident X-ray beam will also diffract from these new scatterers (since they occupy planes parallel to those originally drawn). But now there is a phase difference φ_1 between the waves scattered from the first and the new sets of atoms.

The amplitudes of the waves are proportional to the atomic scattering factors f_0 and f_1. The phases differ by the angle φ_1 . The resultant vector represents the two-atom structure factor with amplitude F_{hkl}. Note that there is a net phase φ arising from the phase difference due to the offset in position between the two sets of diffracting atoms.

As in the case of two atoms, the resultant diffracted wave is obtained from the linear superposition of the wave vectors scattered from each different atom.

Units

The units of the structure-factor amplitude depend on the incident radiation. For X-ray crystallography they are multiples of the unit of scattering by a single electron (2.82×10^{-15} m); for neutron scattering by atomic nuclei the unit of scattering length of 10^{-14} m is commonly used.

See also

The structure factor. P. Coppens. *International Tables for Crystallography* (2006). Vol. B, ch. 1.2, pp. 10-24

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