SPACE GROUPS 2

STRUCTURE FACTORS

- From experimental diffraction data, we are able to obtain 'observed and corrected' intensities I_{hkl}^{corr}, directly related to the square of the 'observed' structure factors$(F_{hkl}^{corr})^2$.
- The diffraction pattern produced is a result of the total scattering from all unit cells and represents the average content of a single unit cell. Structure factors are, in essence, a mathematical representation of the interaction between molecules in a crystal lattice with X-rays and are influenced by atomic scattering factors.

ATOMIC SCATTERING FACTORS

- The electrons in atoms are able to interact with and subsequently scatter X- rays. Atomic scattering factors, f_m, also known as atomic form factors, are the amplitude measure of X-ray waves scattered from an atom.

Table 5.1
Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

ATOMIC SCATTERING FACTORS

- The atomic scattering factor is a function of the Bragg angle. For example, if we refer to Fig. below, at low Bragg angles (e.g., when $\sin \theta/\lambda = 0$), the atom ic scattering factor, f_m, is directly proportional to the atomic number. In contrast, this value tails off at higher angles, as at these high angles not all of the electrons within an atom are scattering in phase.

Figure 5.3
Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

CALCULATING STRUCTURE FACTORS AND INTENSITIES

- The calculated structure factors F_{hkl}^{cal} relating to a given Miller index (h, k, l) for a crystal containing N atoms is given by the following equation:

$$F_{hkl} = \sum_{j=1}^{N} f_j e^{2\pi i(hu_j + kv_j + lw_j)}$$

$$Ae^{i\phi} = A\cos\phi + iA\sin\phi$$

$$F_{hkl}^{calc} = \sum_{1}^{N} f_n \cos 2\pi(hx_n + ky_n + lz_n) + i\sum_{1}^{N} f_n \sin 2\pi(hx_n + ky_n + lz_n),$$

- The atomic scattering factor is influenced by both the scattering from valence electrons, $f_{valence}$ and core electrons, f_{core} given by:

$$f_n = f_{valence} + f_{core}$$

- Scattering of the valence electrons occurs most efficiently at low Bragg angles, while at high Bragg angles. the scattering of the core electrons is more signifIcant. As the heavy elements contain more core electrons, the atomic scattering factor tends to diminish more slowly al higher Bragg angles.

$$F_{hkl}^{calc} = \sum_{1}^{N} f_n \cos 2\pi(hx_n + ky_n + lz_n) + \mathrm{i}\sum_{1}^{N} f_n \sin 2\pi(hx_n + ky_n + lz_n),$$

$$F_{hkl}^{calc} = \sum_{1}^{N} f_n \cos 2\pi(hx_n + ky_n + lz_n) + i\sum_{1}^{N} f_n \sin 2\pi(hx_n + ky_n + lz_n),$$

The calculation of the structure factor, F_{hkl}^{cal} can then be divided into two sections: the right-hand side of the equation splits easily into two halves. the summation with the cosine function and the summation with the sine function, which consider the atomic scattering factors of the atoms within the unit cell; with the sine function having an imaginary component.

$$F_{hkl}^{calc} = \sum_{1}^{N} f_n \cos 2\pi(hx_n + ky_n + lz_n) + i\sum_{1}^{N} f_n \sin 2\pi(hx_n + ky_n + lz_n),$$

Considering a centrosymmetric unit cell (a unit cell that possesses a centre of symmetry), the sine part of the equation disappears. So, F_{hkl}^{cal} for a centrosvmmetric unit cell becomes just

$$F_{hkl}^{calc} = \sum_{1}^{N} f_n \cos 2\pi(hx_n + ky_n + lz_n)$$

- For example, in the case of the bodycentered cell containing two atoms of the same kind, (position of 000 and 1/2 ; 1/2 ; 1/2) in unit cell, the structure factor is given as follows:

$$uvw = 000, \frac{1}{2}\frac{1}{2}\frac{1}{2}$$

$$F = f e^{2\pi i \times 0} + f e^{2\pi i \left(\frac{h}{2}+\frac{k}{2}+\frac{l}{2}\right)} = f[1 + f e^{\pi i (h+k+l)}]$$

When the number of $(h + k + l)$ is even: $F = 2f, F^2 = 4f^2$

When the number of $(h + k + l)$ is odd: $F = 0, F^2 = 0$