Atomic Scattering Factor

The diffraction conditons given by Bragg and Laue are concerned with scattering of x-rays from point scattering centers arranged on a space lattice. Since an electron is the smallest scattering centre, the diffraction conditions would ideally be applicable to a lattice in which every lattice point is occupied by an electron. This is, however, not a realistic situation. Lattice points are always occupied by atoms which may contain a number of electrons. Also, since the wavelength of x-rays used for diffraction purposes is of the order of atomic dimensions, the x-rays scattered from different portions of an atom are, in general, on it phase. Thus the amplitude of radiation scattered by a single atom is not necessarily equal to the product of the amplitude of radiation scattered by a single electron and the number of electrons (atomic number, Z) present in the atom. It is generally less than this value. The *atomic scattering factor* or *form factro*, f, describes the scattering power of a single atom in relation to the scattering power of a single electron and is given by

$$f = \frac{\text{amplitude of radiation scattered from an atom}}{\text{amplitude of radiation scattered from an electron}}$$

In general, $f < Z$. It approaches Z in the limiting case.

Another type of scattering centres in the atoms may be nuclei, but due to their weak interaction with x-rays, the scattering due to nuclei is neglected campared with that due to electrons. General expression for atomic scattering factor is given by:

$$f = \int \rho(r)\, e^{-i\vec{G}\cdot\vec{r}}\, dv$$

At zero scattering angle, all the scattered waves are in phase and the scattered amplitude is the simple sum of the contribution from all Z electrons, i.e. $f = Z$. As the scattering angle increases, f falls below Z because of the increasingly destructive interference effects between the Z scattered waves. Atomic scattering factors f are plotted as a function of angle (usually expressed as $\sin\theta/\lambda$). Figure 9.1 shows such a plot for the oxygen anion O^2, the neon atom Ne, and the silicon cation Si^{4+} - all of which contain 10 electrons. When $\sin\theta/\lambda = 0$, $f = 10$ but with increasing angle f falls below 10. The extent to which it does depends upon the relative sizes of the atoms or ions; the silicon cation is small, hence the phase differences are small and the destructive interference between the scattered waves is leastand conversely for the large oxygen anion.

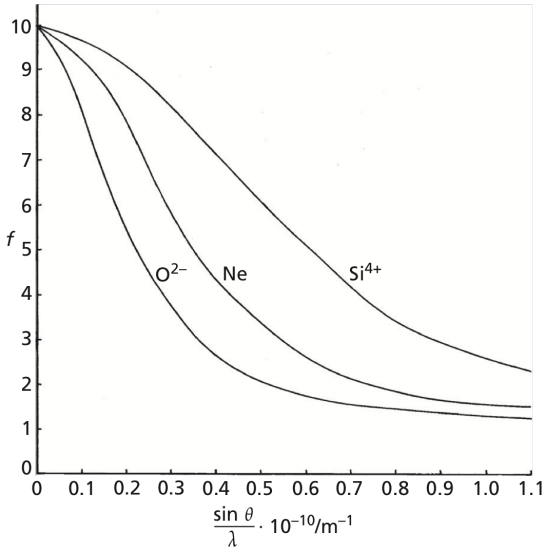

Figure 1: The variation in atomic form factor f with scattering angle (expressed as $\sin\theta/\lambda$ for atoms and ions with ten electrons. Note that the decrease in f is greatest for the (large) O^{2-} anion and least for the (small) Si^{4+} cation.

Geometrical Structure Factor

The intensity of an x-ray beam diffracted from a crystal not only depends upon the atomic scattering factors of the various atoms involved but also on the contents of the unit cell, i.e., on the number, type and distribution of atoms within the cell. The x-rays scattered from different atoms of the unit cell may or may not be in phase with each other. It is, therefore, important to know the effect of various atoms present in the unit cell on the total scattering amplitude in a given direction. The total scattering amplitude $F(h'k'l')$ for the reflection $(h'k'l')$ is defined as the ratio of the amplitude of radiation scattered by the entire unit cell to the amplitude of radiation scattered by a single point electron placed at origin for the same wavelength. It is given by

$$F(h'k'l') = \sum_j f_j e^{i\phi_j} = \sum_j f_j e^{i(2\pi/\lambda)(r_j \cdot N)}$$

where f_j is the atomic scattering factor for the j^{th} atom, ϕ_j is the phase difference between the radiation scattered from the j^{th} atom of the unit cell and that scattered from the electron placed at the origin. This gives the structure factor of given basis.