X-ray Crystallography II
Scattering by X-rays

- Two types of scattering
  - Elastic - incident and scattered radiation is the same wavelength
  - Inelastic - incident and scattered radiation is not the same wavelength
- Fluorescence occurs
- Intensity of scattered radiation is

\[ I_{\text{sca}} = \frac{(C I_o)}{r^2} \]

Where \( I_{\text{sca}} \) is scattered Intensity
\( I_o \) is incident intensity
\( r \) distance from scattering point to detector
C proportionality factor
Scattering by Two Electrons

**FIGURE 12.1**

(a) The scattering from a single electron for light polarized perpendicular to the scattering plane is independent of angle in the scattering plane. The scattering intensity decreases inversely proportional to the square of the distance from the scattering electron. (b) For scattering from two electrons, the angle dependence of the scattering amplitude depends on the interference between the two scattered waves.
Summing of Waves

FIGURE 12.3
Summing of two waves: (a) waves completely in phase; (b) waves out of phase by one-quarter wavelength (partial reinforcement occurs); (c) waves out of phase by one-half wavelength (total destructive interference occurs). [From J. P. Glusker and K. N. Trueblood, 1972, Crystal Structure Analysis: A Primer (New York: Oxford University Press), p. 19, fig. 5.]
Path Differences

Path difference \( \Delta = R \cos \Theta - R \)

FIGURE 12.2
Path difference for two beams scattered from two electrons separated by distance \( R \). The angle between the incident beam and the scattered beam is \( \Theta \). At the top, the two scatterers are on a line with the incident beam; at the bottom, the scatterers are perpendicular to the incident beam direction. Trigonometry shows that the path difference \( \Delta \) is related to the scattering angle \( \Theta \) and the distance between scattering points \( R \).
Bragg's Law

\[ n\lambda = 2d_{hkl} \sin \theta \]

**FIGURE 12.12**

Diffraction of radiation from a crystal. The parallel lines represent planes of atoms with Miller indices \( h, k, \) and \( l \). The Bragg condition for diffraction is for the incident beam and the diffracted beam to make an angle \( \theta = \sin^{-1} \left( n\lambda / 2d_{hkl} \right) \) with the planes. Note that the scattering angle \( (\theta) \) between incident and scattered beams (defined before in figure 12.2) is \( 2\theta \). Simple geometric construction shows that the extra path length traveled by the ray scattered by the top layer relative to the next layer down is \( 2d_{hkl} \sin \theta \).
Experimental arrangement for measuring the X-ray scattering from a crystal. A beam of X rays is incident on a crystal that is mounted so that it can be rotated around perpendicular axes. The intensities of the diffracted X-ray beams are measured with a photographic film or an equivalent imaging plate. A beam stop is used to attenuate the incident X-ray beam.
“Home” Source - Rotating Anode
National Synchrotron Light Source
Experimental Floor at NSLS
X29 Beamline NSLS
• The scattering intensity is a function of angle from the incident beam. Brighter reflections have a lower angle of scatter.
• The position of the reflection is dependent on orientation of the lattice to the incident beam.
Diffraction One-Dimensional Lattice

- Only get constructive reinforcement if \( a(\cos \alpha - \cos \alpha_0) = h \lambda \)
Diffraction Three-Dimensional Lattice

- Only get constructive reinforcement if
  \[ a(\cos \alpha - \cos \alpha_0) = h\lambda \]
  \[ b(\cos \alpha - \cos \alpha_0) = k\lambda \]
  \[ c(\cos \alpha - \cos \alpha_0) = l\lambda \]
  von Laue’s equations
  hkl are called Miller indices
  Each reflection is given a unique set of Miller indices
  Reciprocal Lattice
Monochromatic vs Polychromatic X-rays

Monochromatic

Polychromatic
Scattering Factors

Scattering factor ($f_0$) ratio of the amplitude scattered by an atom to the amplitude scattered by a point electron.