Theory of Diffraction: Bragg Law

- Single plane of infinite lattice points separated by $d$.
- Incident beam “reflects” off of array (why?)
- Condition for constructive interference:
  \[ n\lambda = 2d \sin \theta \]
Theory of Diffraction: Von Laue Conditions

**Key difference:** waves are not reflecting off of a plane of atoms; instead, atoms are point sources for scattered waves (see blue circles on previous slide)

**Conditions for Constructive Interference:**

\[ l\lambda = c(\cos \gamma - \cos \gamma_0) \]

From van Holde, p. 295.
1-Dimensional Diffraction

Figure 6.12  An incident beam of X-rays causes a set of scattering cones from a one-dimensional crystal aligned along the vertical axis. Each cone makes an angle $2\theta$ relative to the incident beam to conform to the von Laue conditions for diffraction. The intersection of each cone with a piece of flat photographic film is an arc. Each arc is a layer line representing the order of the reflection, the integer index $l$ in Eq. 6.6. In a three-dimensional crystal, each axis of the unit cell generates a set of concentric cones, with the conical axes aligned parallel with the crystallographic axes.

From Principles of Physical Biochemistry
van Holde, et al., Chapt. 6, p. 295
2-Dimensional Diffraction

Von Laue Conditions must be met for both cones: result is a line
Diffraction in 2D and 3D

• Multiple scattering planes are possible; each has functional form:
  \[ h\lambda = a(\cos \alpha - \cos \alpha_0) \]
  \[ k\lambda = b(\cos \beta - \cos \beta_0) \]
  \[ l\lambda = c(\cos \gamma - \cos \gamma_0) \]

• For indices \( h, k, \) and \( l \) (Miller indices) plane spacing of \( a, b, \) and \( c \) are observed

• Miller indices define the plane of scattering (reciprocal of intercept on a axes; \( \bar{1} = -1 \))

“Miller Index,” Wikipedia.
Diffraction in 2D and 3D

• Define a *scattering vector* \((\mathbf{S})\) with direction normal to the Bragg plane

• Then, condition for diffraction is given by the *von Laue* equation:

\[
|\mathbf{S}| = \left( \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right)^{1/2} = \frac{2 \sin \theta}{\lambda}
\]

• It can be shown that this is equivalent to Bragg’s law in 1D
Measuring Reflections

http://www.stolaf.edu/people/hansonr/mo/xray.gif
Measuring Reflections

Source

θ (Bragg Plane)

S

Reflection (intensity only; no phase)

R (precisely known)

Detector (CCD, Image Plate, or Film)
Measuring Reflections

From *Principles of Physical Biochemistry*
van Holde, et al., Chapt. 6, p. 298
Ewald Sphere and Reflections

Figure 6.15  Conditions for diffraction in reciprocal space. (a) A point of origin $O$ for the scattered X-ray beam is defined at the origin of a unit cell of the reciprocal lattice. A point $A$ is the crystal placed along the incident beam at a distance $1/\lambda$ from $O$. A circle with a radius of $1/\lambda$ is drawn with $A$ at the center. The point where the circle intersects the incident beam is labeled point $B$. Any other lattice point $L$ of the reciprocal lattice that intersects the circle represents a reflection in reciprocal space. (b) Bragg's law is derived by defining the diffraction angle $\theta$ as the angle $OBL$, and the trigonometric relationship between the scattering vector $S$ and the diameter of the circle. The vector $AL$ is the direction of scattered beam from the crystal in real space. This is shown as the bold arrow extending from the origin $O$ and at an angle $2\theta$ relative to the incident beam.

From *Principles of Physical Biochemistry*
van Holde, *et al.*, Chapt. 6, p. 303
Data Collection

Crystal morphology (unit cell dimensions & symmetry) can be determined by assigning indices and observing patterns in reflections – typically done by computer.

From *Diffraction*
Summary

• Bragg Planes and Von Laue Conditions are two ways of determining diffraction angle
• Each reflection corresponds to a miller index, and a set of planes responsible for diffraction
• Reciprocal space and Ewald sphere are a graphical representation von Laue conditions
• Detectors only measure intensity, not phase of scattered light
• Looking at reflections allows measurement of unit cell shape/symmetry