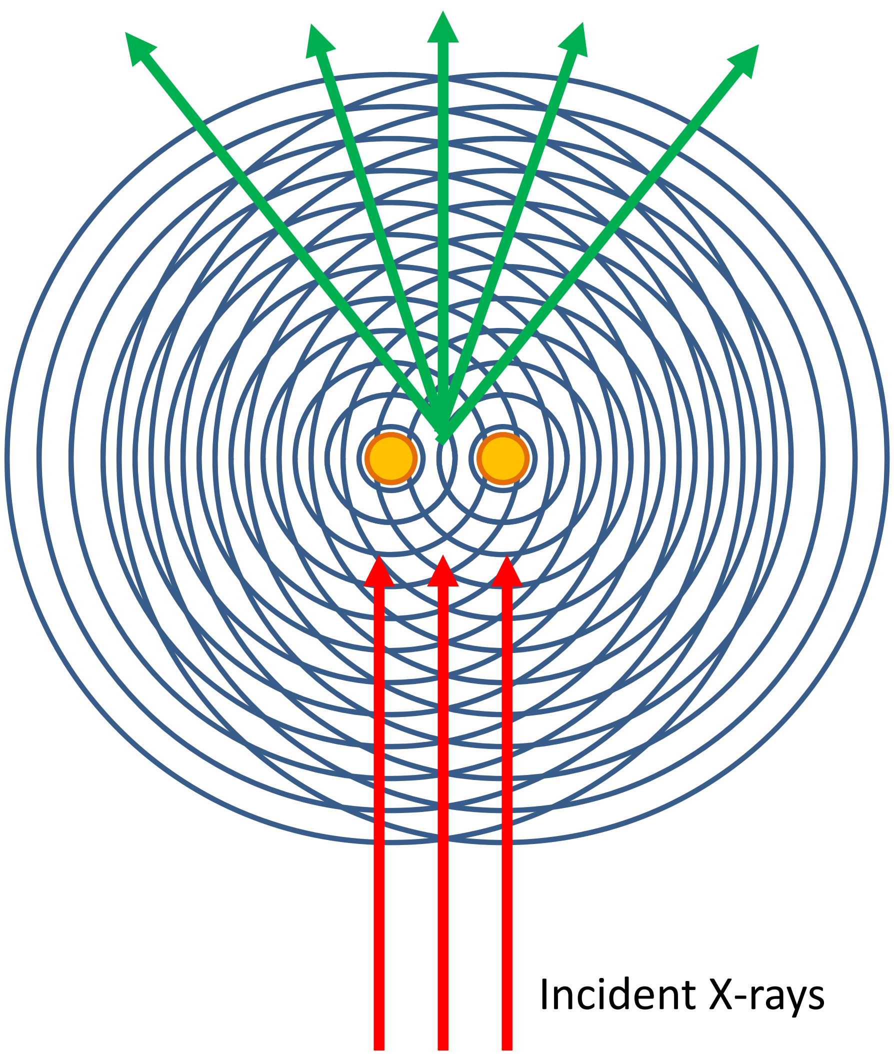
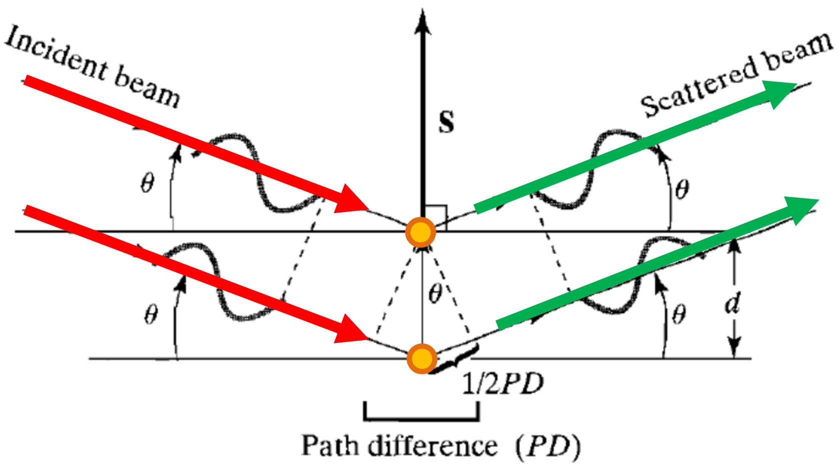
Theory of Diffraction: Bragg Law





- Single plane of infinite lattice points separated by d.
- Incident beam "reflects" off of array (why?)
- Condition for constructive interference:

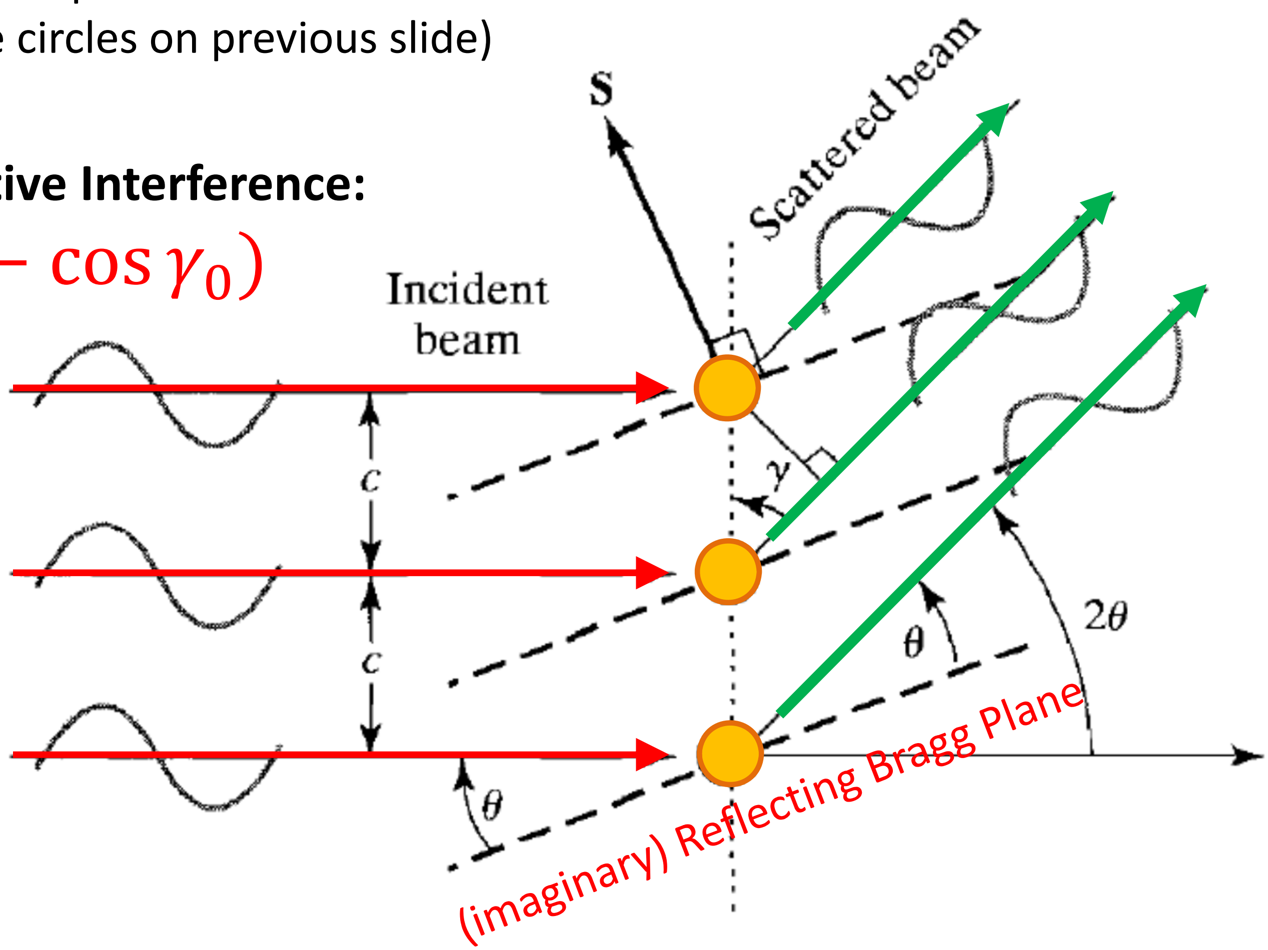
$$n\lambda = 2d\sin\theta$$

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

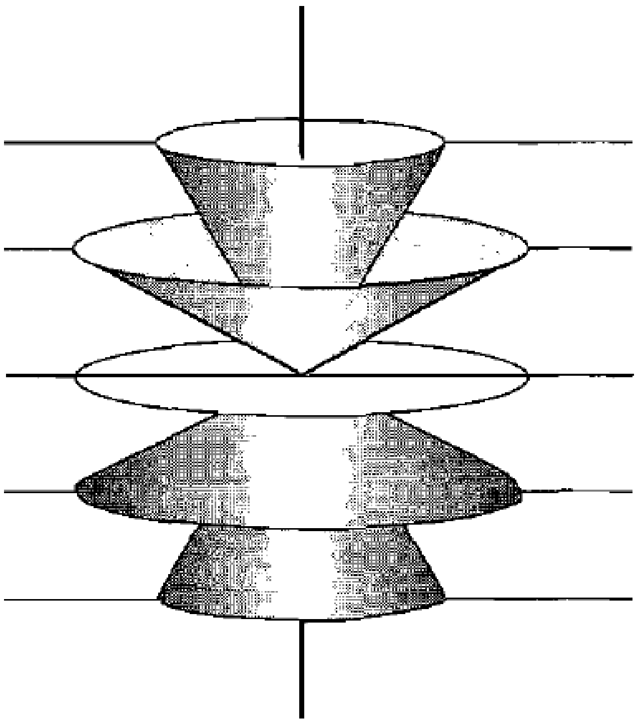
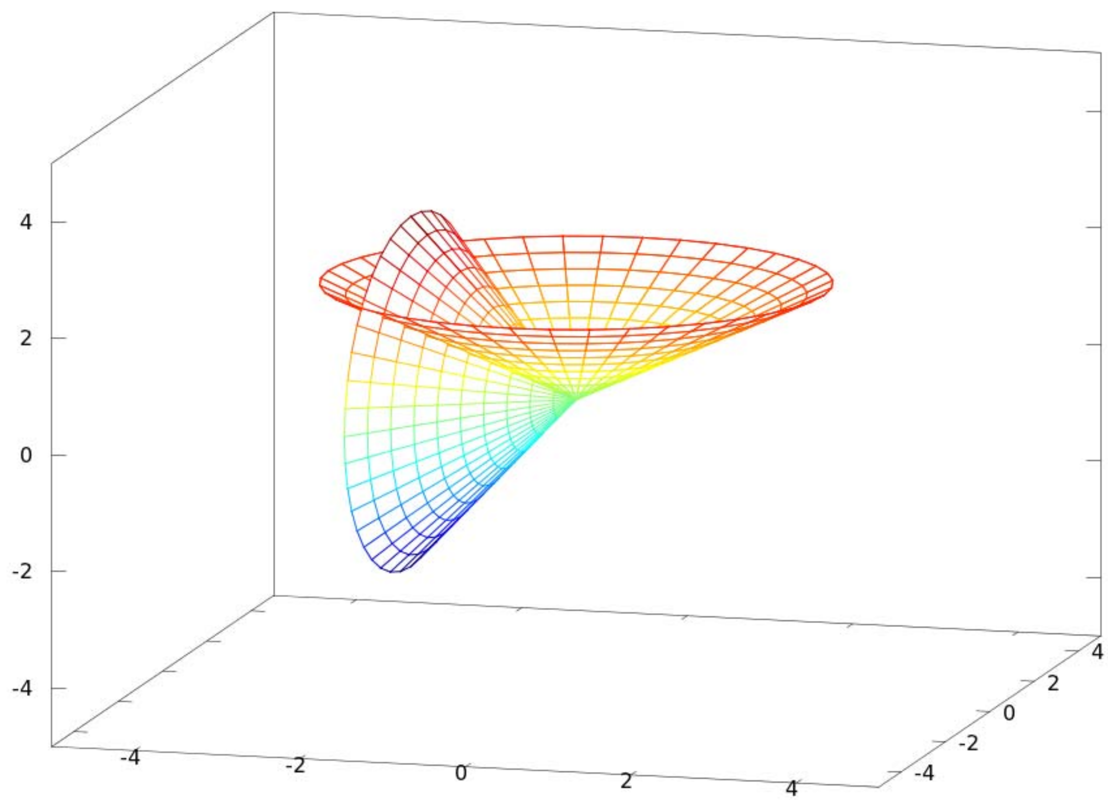


Figure 6.12 An incident beam of X-rays causes a set of scattering cones from a one-dimensional crystal aligned along the vertical axis. Each cone makes an angle 2θ relative to the incident beam to conform to the von Laue conditions for diffraction. The intersection of each cone with a piece of flat photographic 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



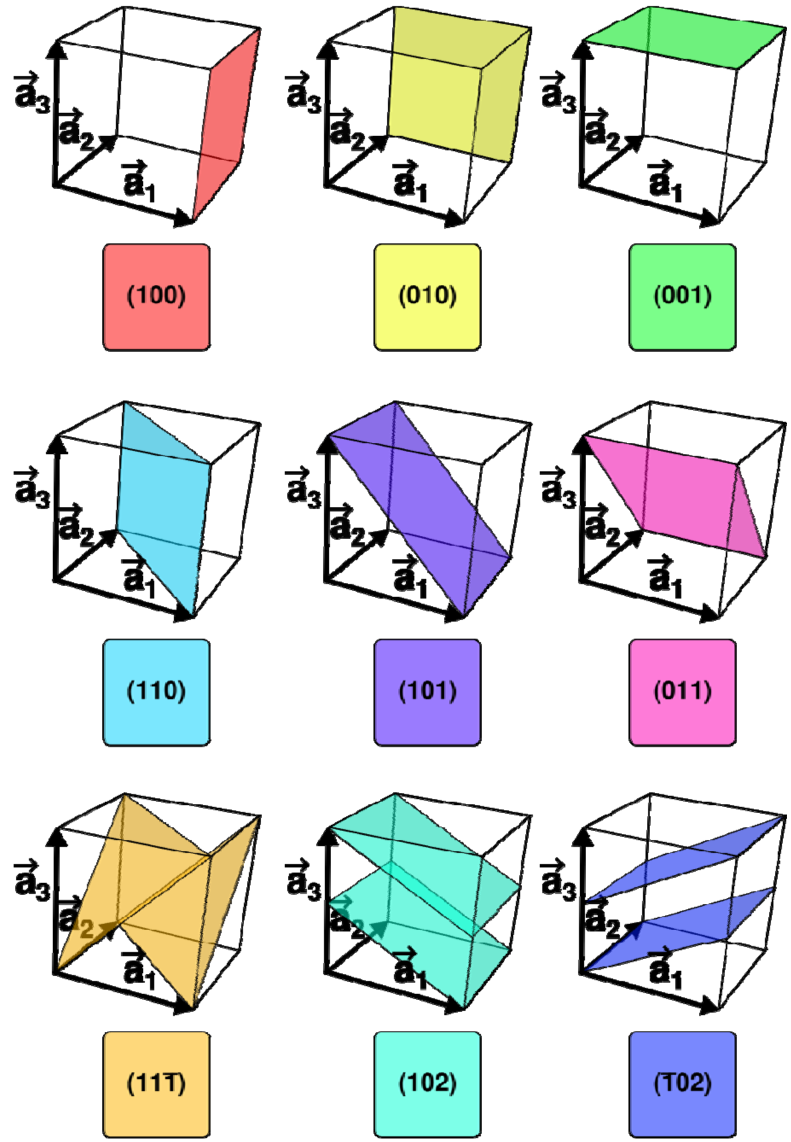
Von Laue Conditions must be met for both cones: result is a line

Diffraction in 2D and 3D

- Multiple scattering planes are possible; each has functional form:

$$h\lambda = a(\cos\alpha - \cos\alpha_0)$$
$$k\lambda = b(\cos\beta - \cos\beta_0)$$
$$\mathrm{l}\lambda = c(\cos\gamma - \cos\gamma_0)$$

- 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

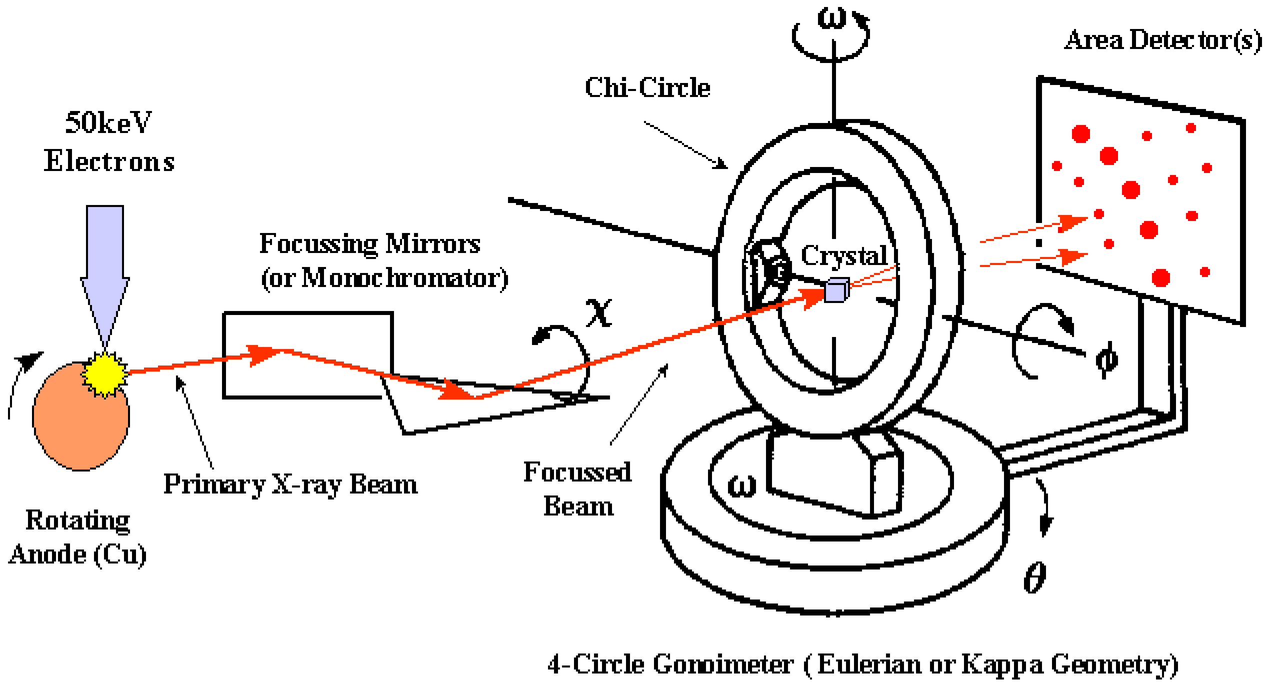
- Define a *scattering vector (**S**)* with direction normal to the Bragg plane

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

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

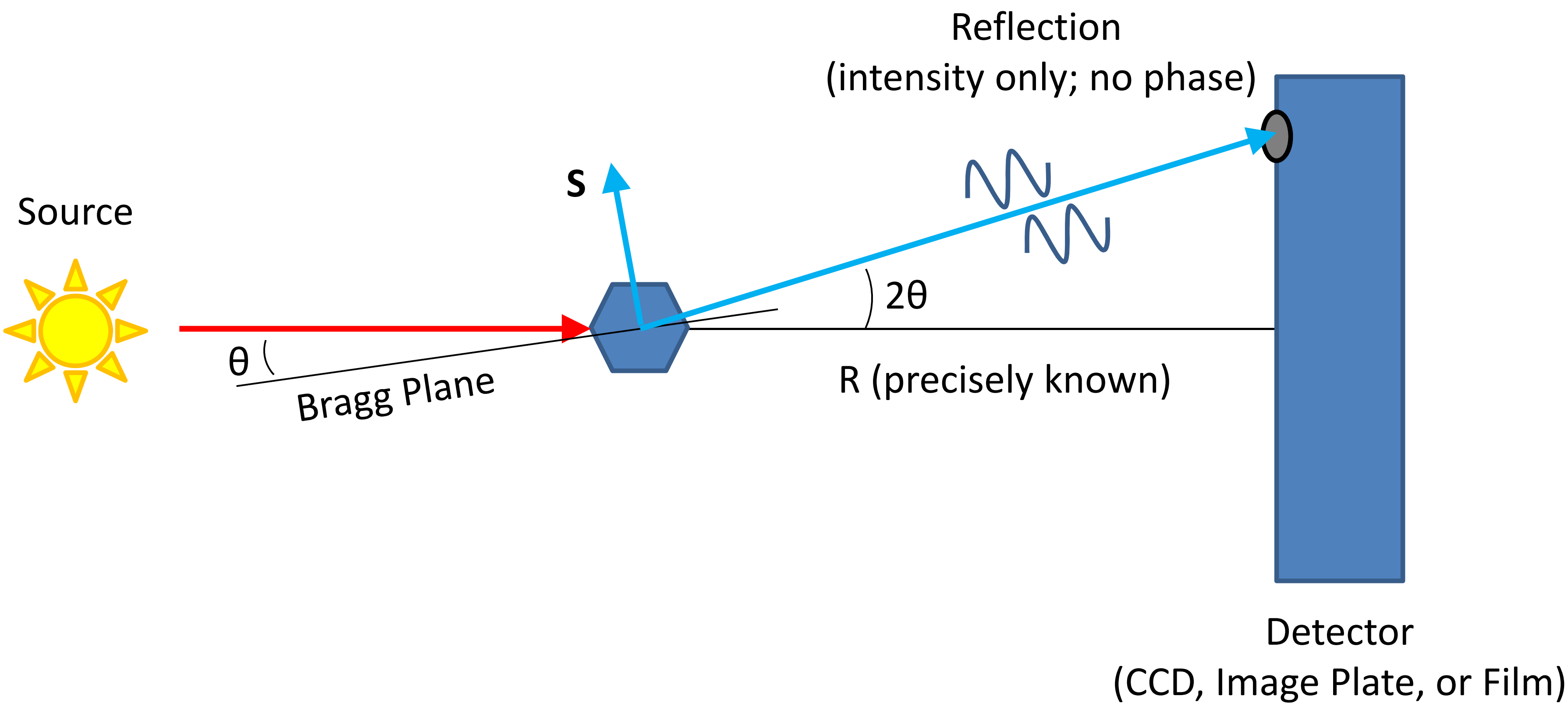
- It can be shown that this is equivalent to Bragg's law in 1D

Measuring Reflections

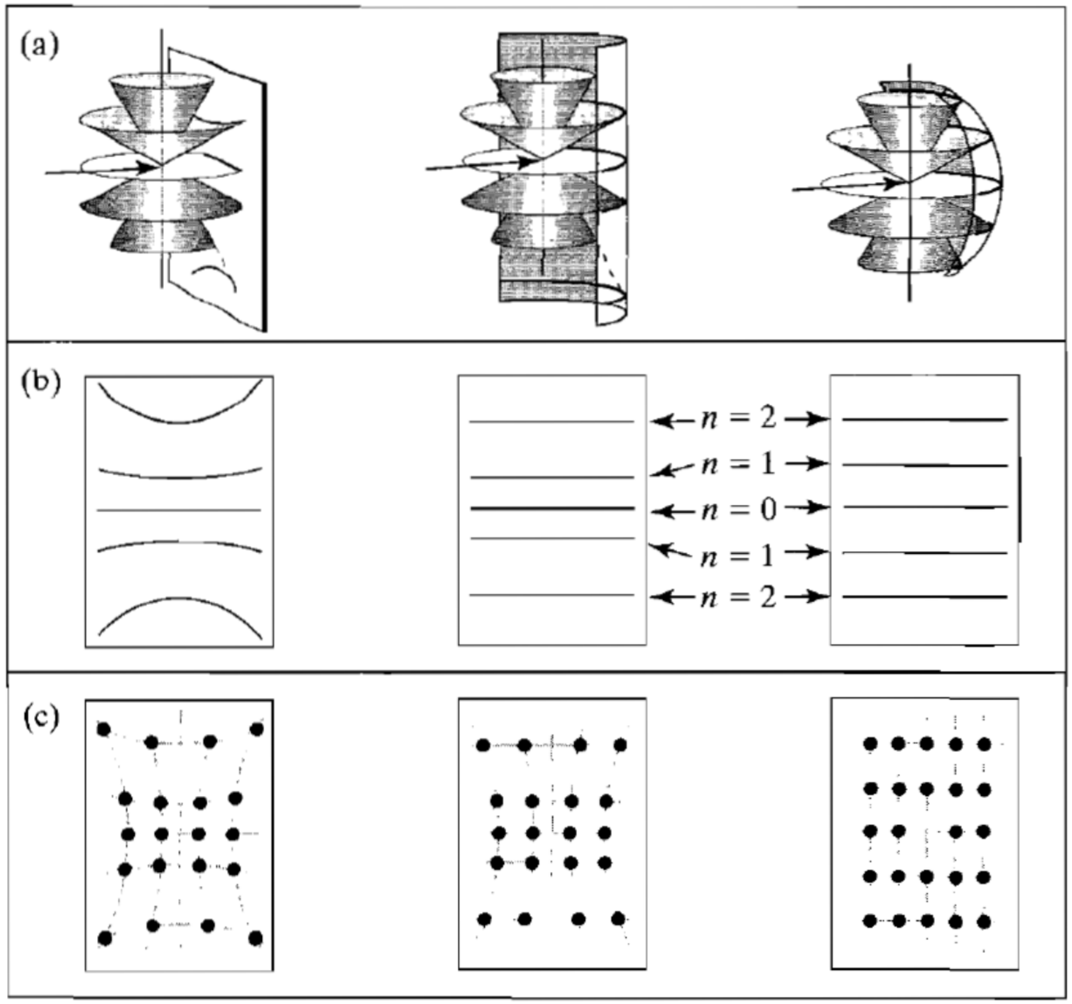


http://www.stolaf.edu/people/hansonr/mo/xray.gif

Measuring Reflections



Measuring Reflections



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

Ewald Sphere and Reflections

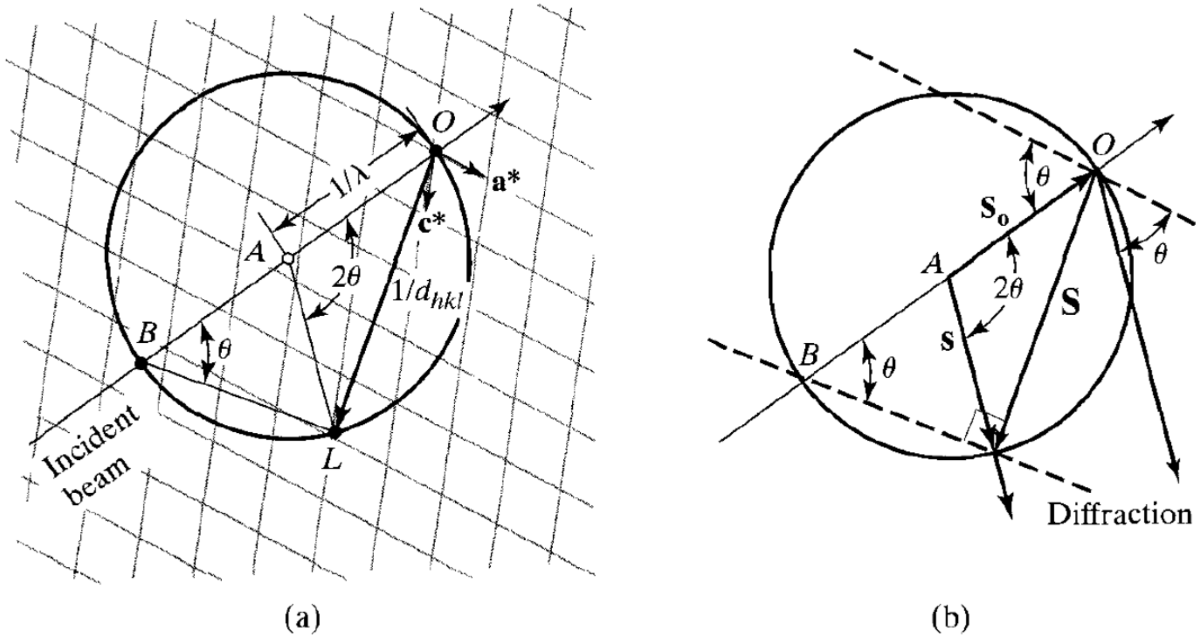
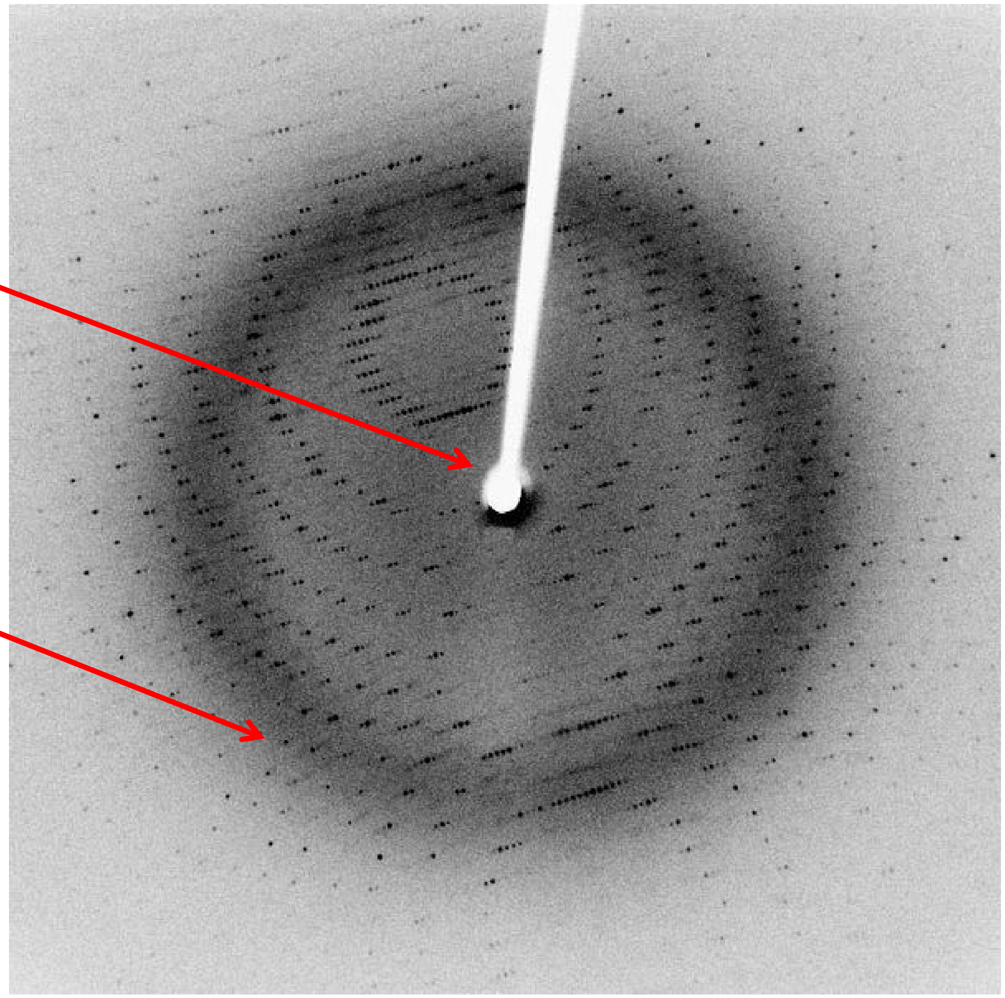


Figure 6.15 Conditions for diffraction in reciprocal space. (a) A point of origin O for the scattered X-ray beam is defined at the origin of a unit cell of the reciprocal lattice. A point A is the crystal placed along the incident beam at a distance $1/\lambda$ from O. A circle with a radius of $1/\lambda$ 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 θ 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 2θ relative to the incident beam.

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

Data Collection



Beam Stop

hkl reflections in reciprocal space (each one has an index!)

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

From *Diffraction*
http://en.wikipedia.org/wiki/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