de Broglie Waves

- de Broglie argued
  - Light exhibits both wave and particle properties
    - Wave – interference, diffraction
    - Particle – photoelectric effect, Compton effect
  - Then matter (particles) should exhibit both particle and wave properties
  - He predicted the wavelength to be

$$\text{de Broglie wavelength } \lambda = \frac{h}{p}$$

de Broglie Waves

- Consider the E, p relations for a photon

$$E = hf \text{ and } E = pc$$

then

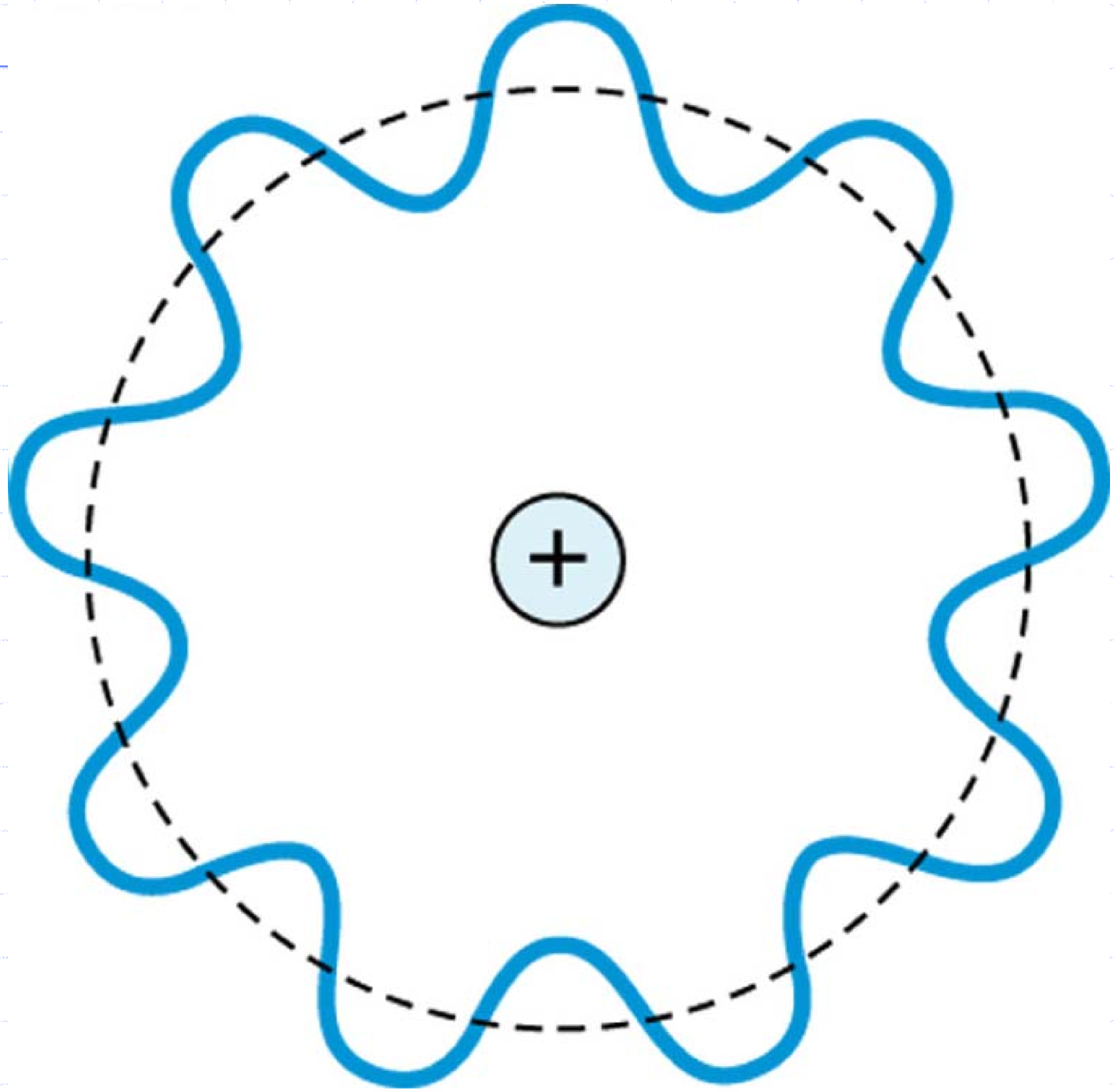
$$hf = pc$$

$$\frac{c}{f} = \frac{h}{p}$$

$$\lambda = \frac{h}{p}$$

- Guided by this, de Broglie proposed the same relation for matter

de Broglie Waves



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de Broglie Waves

- Let's apply de Broglie waves to the Bohr model
- If the electron is represented as a standing wave in an orbit about the proton

$$2\pi r = n\lambda = n\frac{h}{p}$$

$$L = rp = \frac{nh}{2\pi} = n\hbar$$

- This apparently justifies Bohr's assumption

de Broglie Waves

- de Broglie wavelength of a person running

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34} Js}{(65kg)(5m/s)}$$

$$\lambda = 2 \times 10^{-36} m$$

- de Broglie wavelength of a 50 eV electron

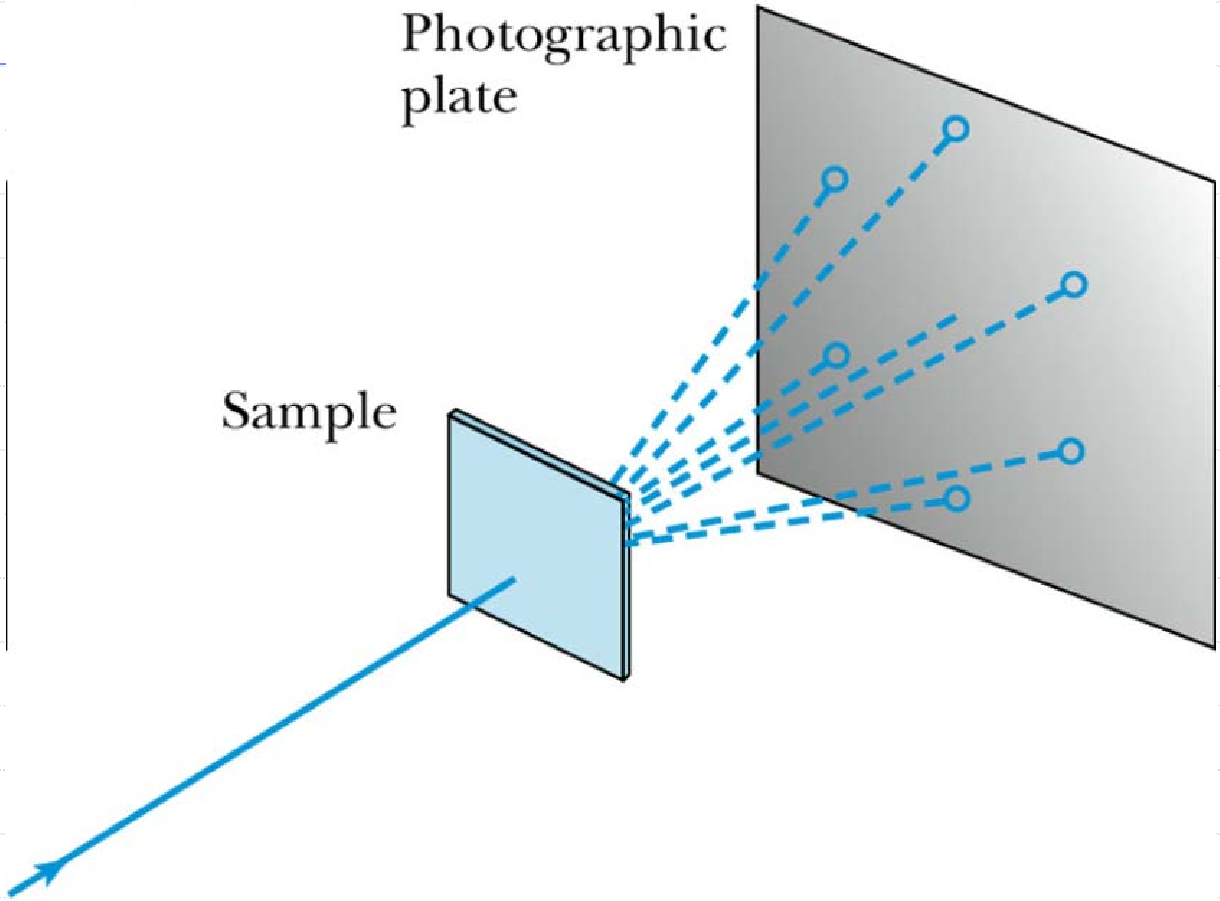
$$\lambda = \frac{h}{p} = \frac{hc}{pc} = \frac{hc}{\sqrt{2mc^2T}} = \frac{1240eVnm}{\sqrt{(2)(.511 \times 10^6)(50)}}$$

$$\lambda = 0.17nm$$

X-ray Scattering

- Before examining electron scattering from a (large) crystal, let's first look at x-ray scattering from a crystal
  - Spacing of atoms in a crystal ~ 1A
  - Wavelength of "hard" x-rays ~ 0.1-1A
  - Laue therefore expected that interference patterns should be observed
    - And they were!
  - Today, the Laue technique can be used to determine crystal orientation and assess crystal perfection from the size and shape of the spots

X-ray Scattering



(a)

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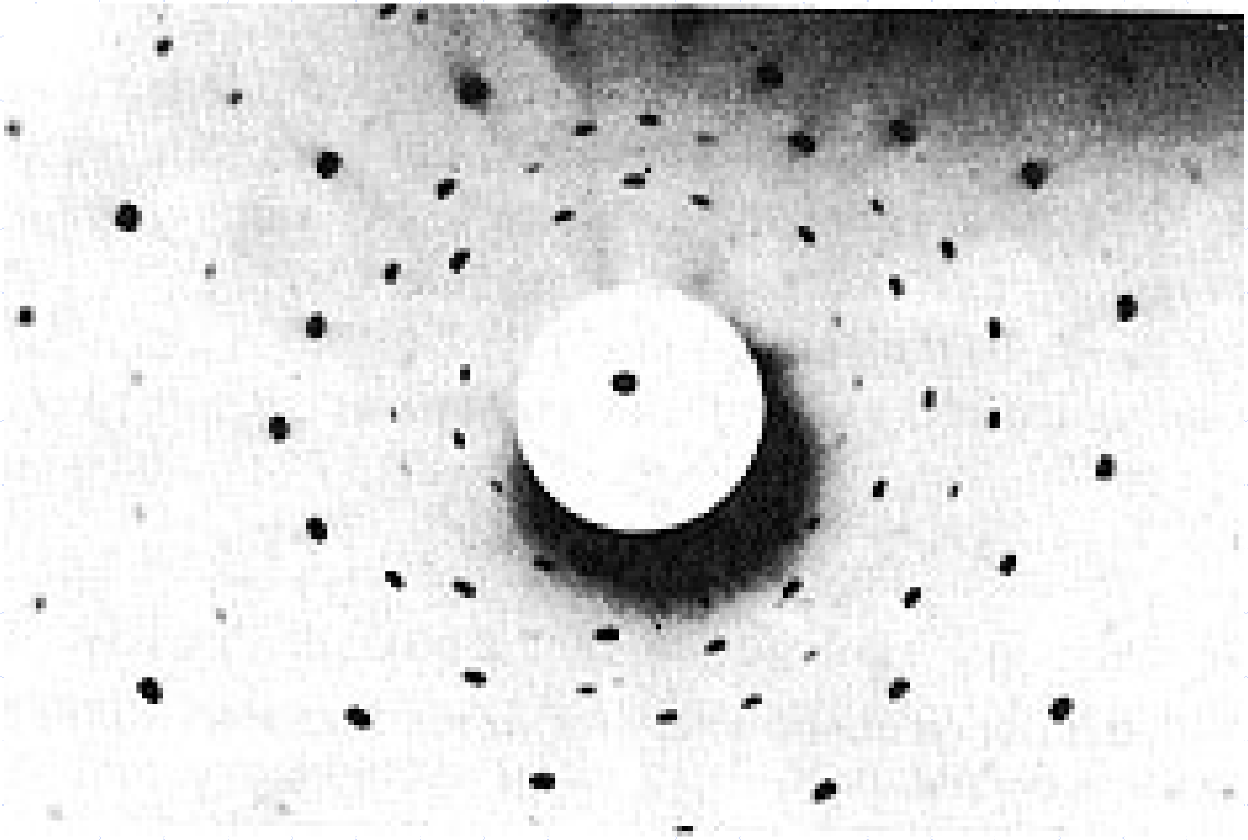
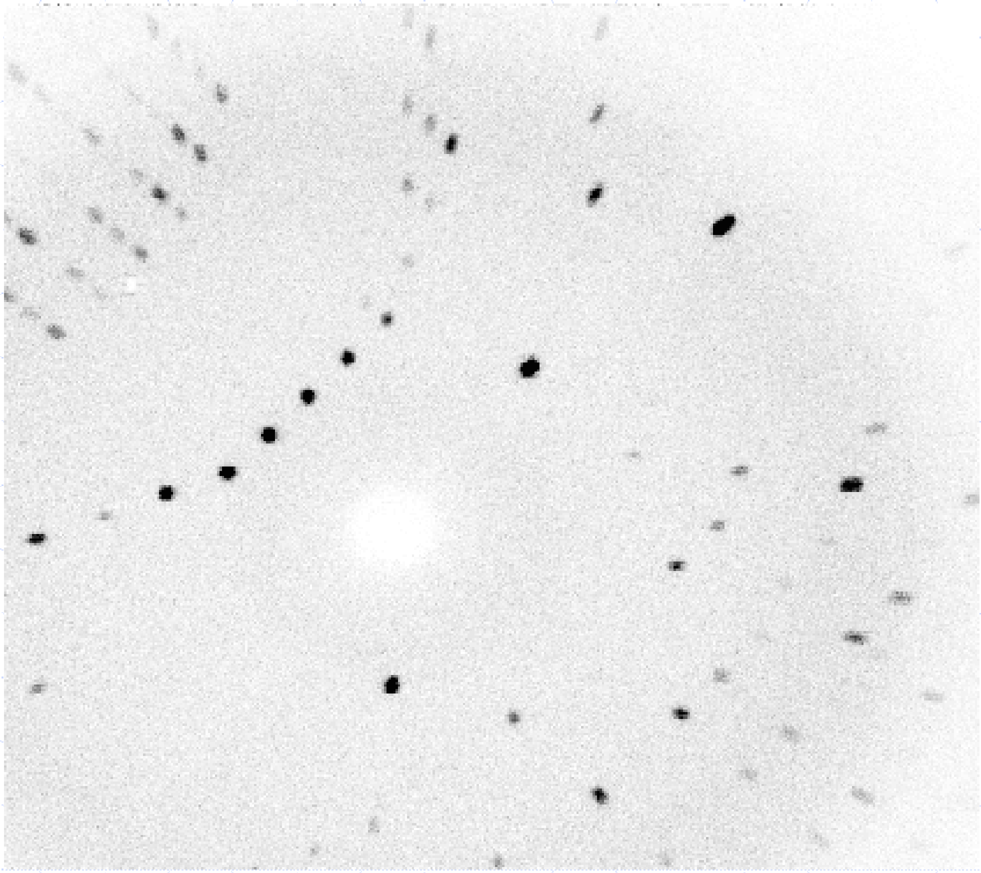
X-ray Scattering

- Laue diffraction of salt



X-ray Scattering

- Whale myoglobin
  - Of ~35,000 known protein structures, ~29,000 have been identified using x-ray diffraction



X-ray Scattering

Gregory K. Farber[†‡], Pella Machin[§¶], Steven C.

[†]Department of Chemistry, Massachusetts Institute of Technology, Cambridge
Daresbury, Warrington, Cheshire, WA4 4AD, United Kingdom; [‖]Department
**Laboratory of Molecular Biophysics, Oxford OX1 3QU, United Kingdom

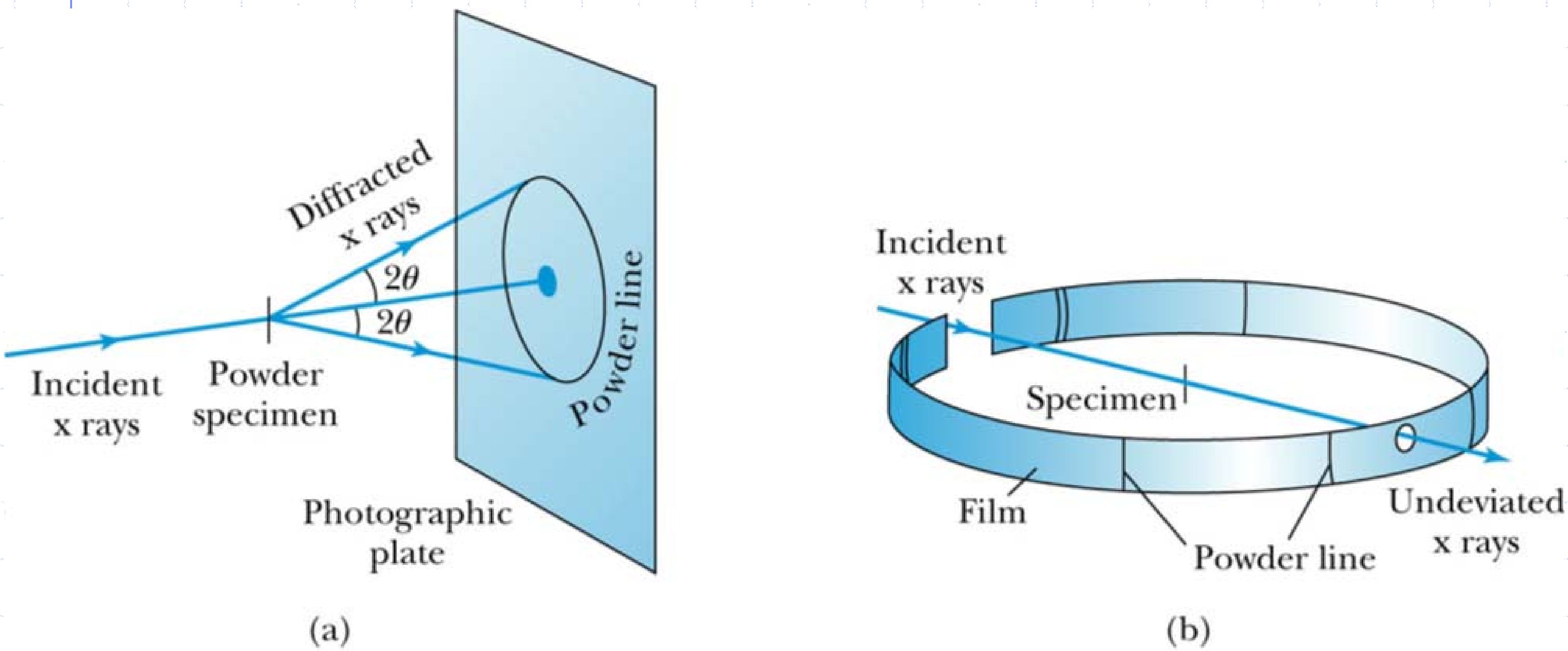
Communicated by Robert A. Alberty, September 10, 1987 (received

ABSTRACT The Laue method (stationary crystal, polychromatic x-rays) was used to collect native and heavy-atom-derivative data on crystals of xylose isomerase (EC 5.3.1.5). These data were used to find the heavy-atom positions. The positions found by use of Laue data are the same as those found by use of monochromatic data collected on a diffractometer. These results confirm that Laue diffraction data sets, which can be obtained on a millisecond time scale, can be used to locate small molecules bound to protein active sites. The successful determination of heavy-atom positions also indicates that x-ray crystallographic data collected by the Laue method can be used to solve protein structures.

X-ray Scattering

- Powder diffraction
  - Sometimes single crystals are not available
  - Sometimes materials naturally occur in a polycrystalline state
- Using many small crystals
  - Their orientation will be random
  - At least a few of the small crystals in the sample will be in the correct orientation to diffract for each of the possible planes
  - The resulting rings are called the Debye-Scherrer pattern
- The powder diffraction method is frequently used to fingerprint crystals via a large database

X-ray Scattering



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X-ray Scattering

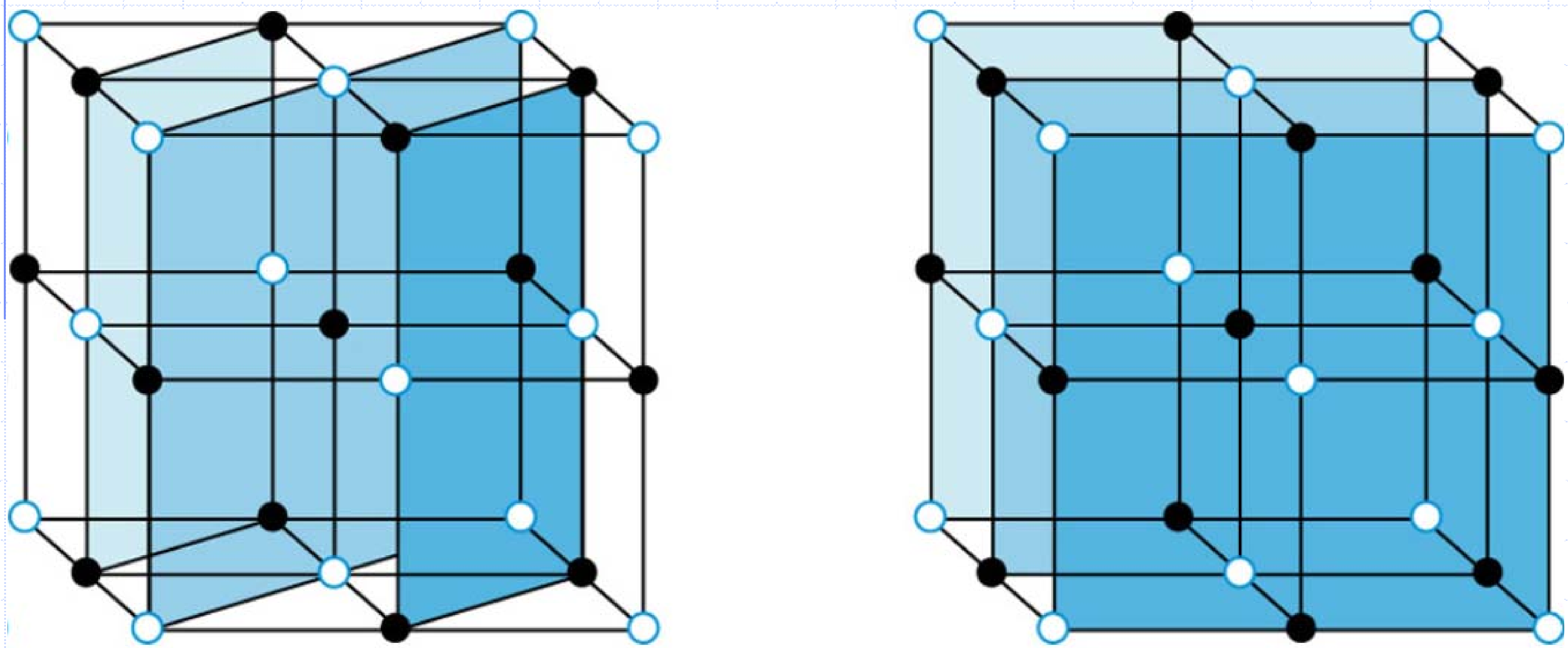
- Debye-Scherrer pattern from powder diffraction for NaCl and KCL

X-ray Scattering

- Bragg simplified Laue's three dimensional analysis by considering x-ray scattering as the reflection of the incident beam from successive lattice planes in the crystal
- If the scattered angle = incident angle (reflection), there is no phase change between the incident and reflected waves
- Waves scattered at equal angles from atoms in two different planes will constructively interfere if the path length difference is an integral number of wavelengths

X-ray Scattering

- Crystal structure of NaCl



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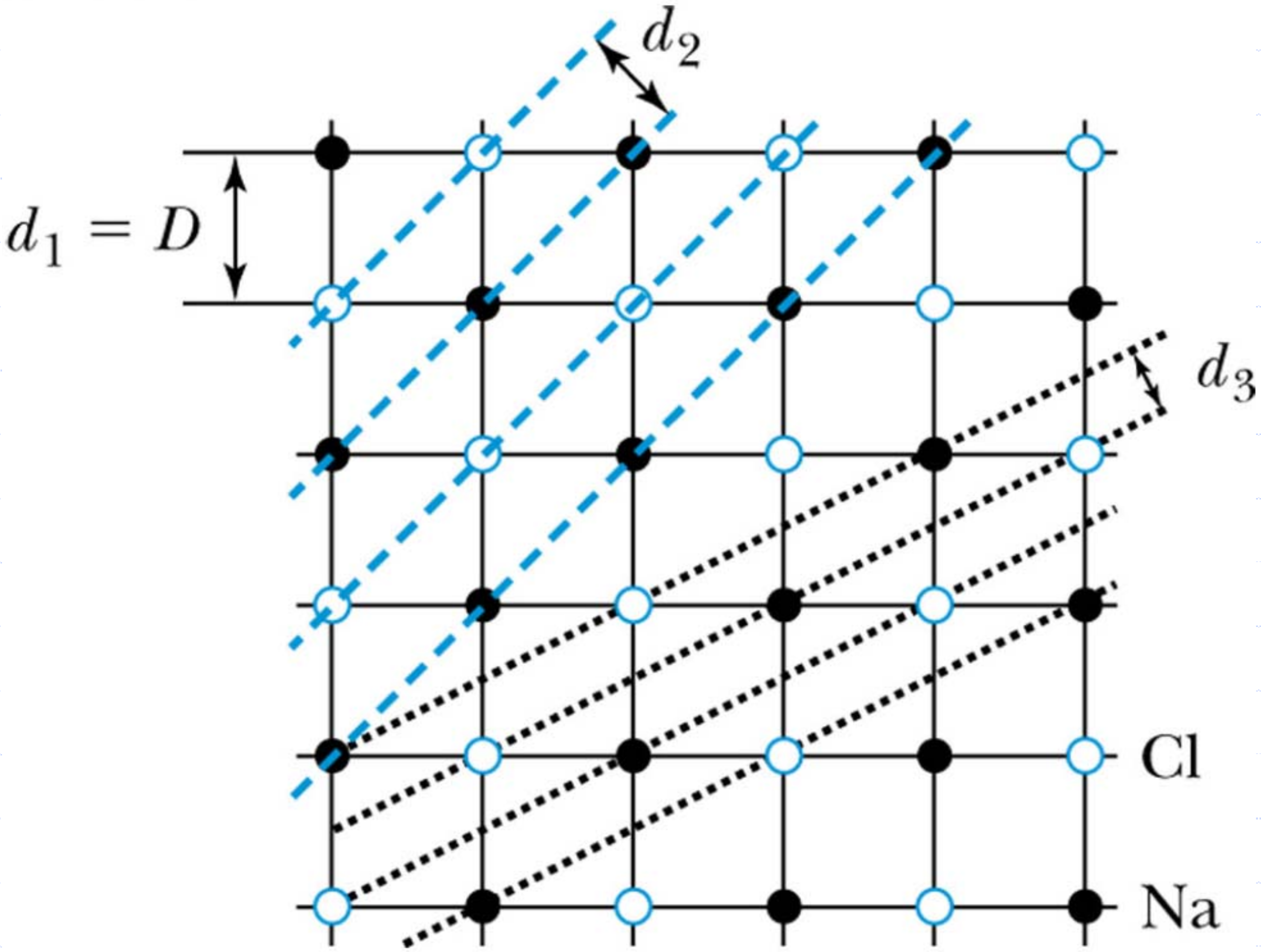
X-ray Scattering

- Crystal structure of NaCl



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X-ray Scattering

- Bragg condition

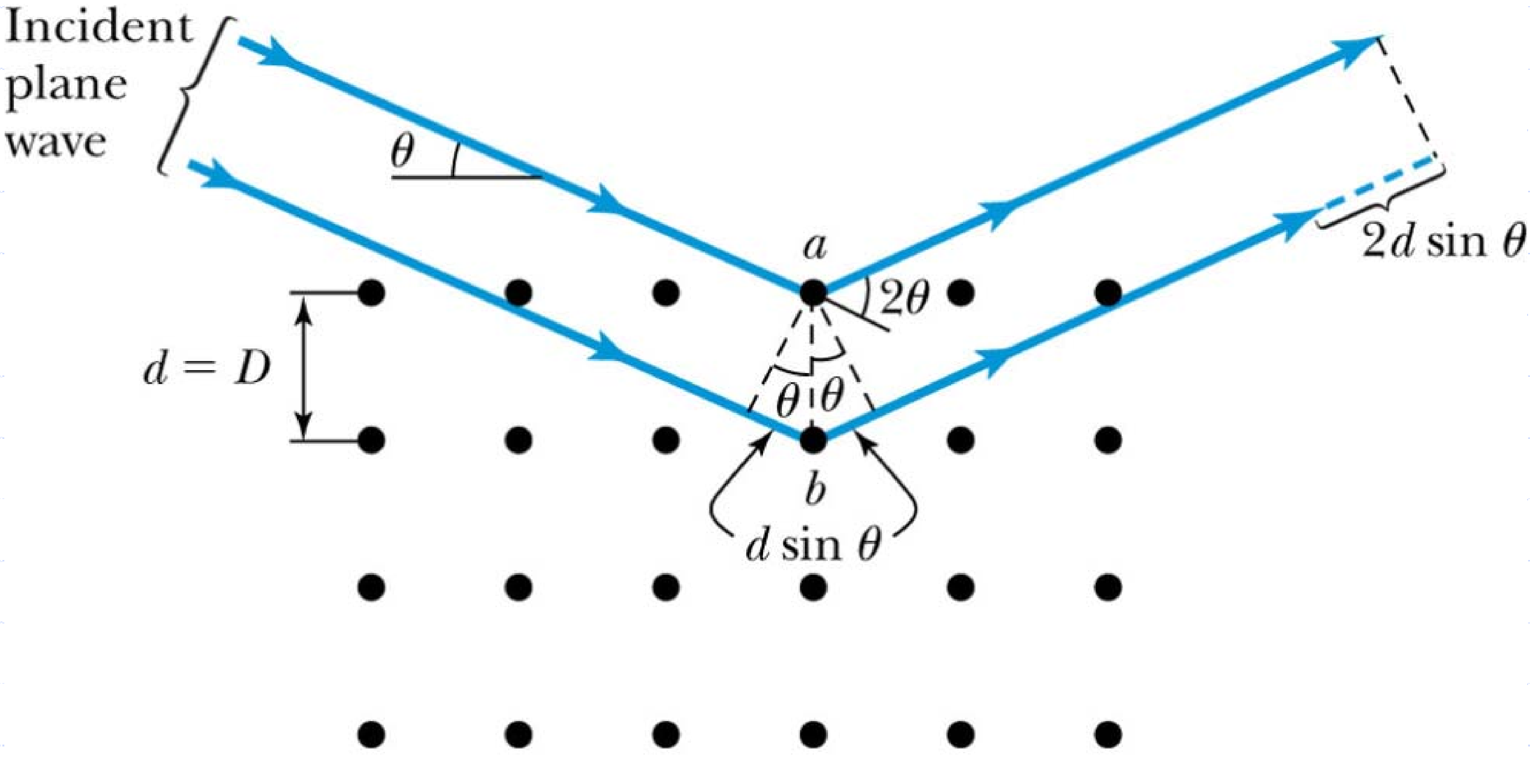
$$2d \sin\theta = m\lambda$$

  - The intensity pattern of the scattered waves of a known wavelength gives information about the structure of the crystal
  - The intensity pattern of the scattered waves from a known crystal spacing gives information about the incoming wavelengths

- Laue and Bragg scattering effectively started the field of solid state physics

X-ray Scattering

- Crystal structure of NaCl



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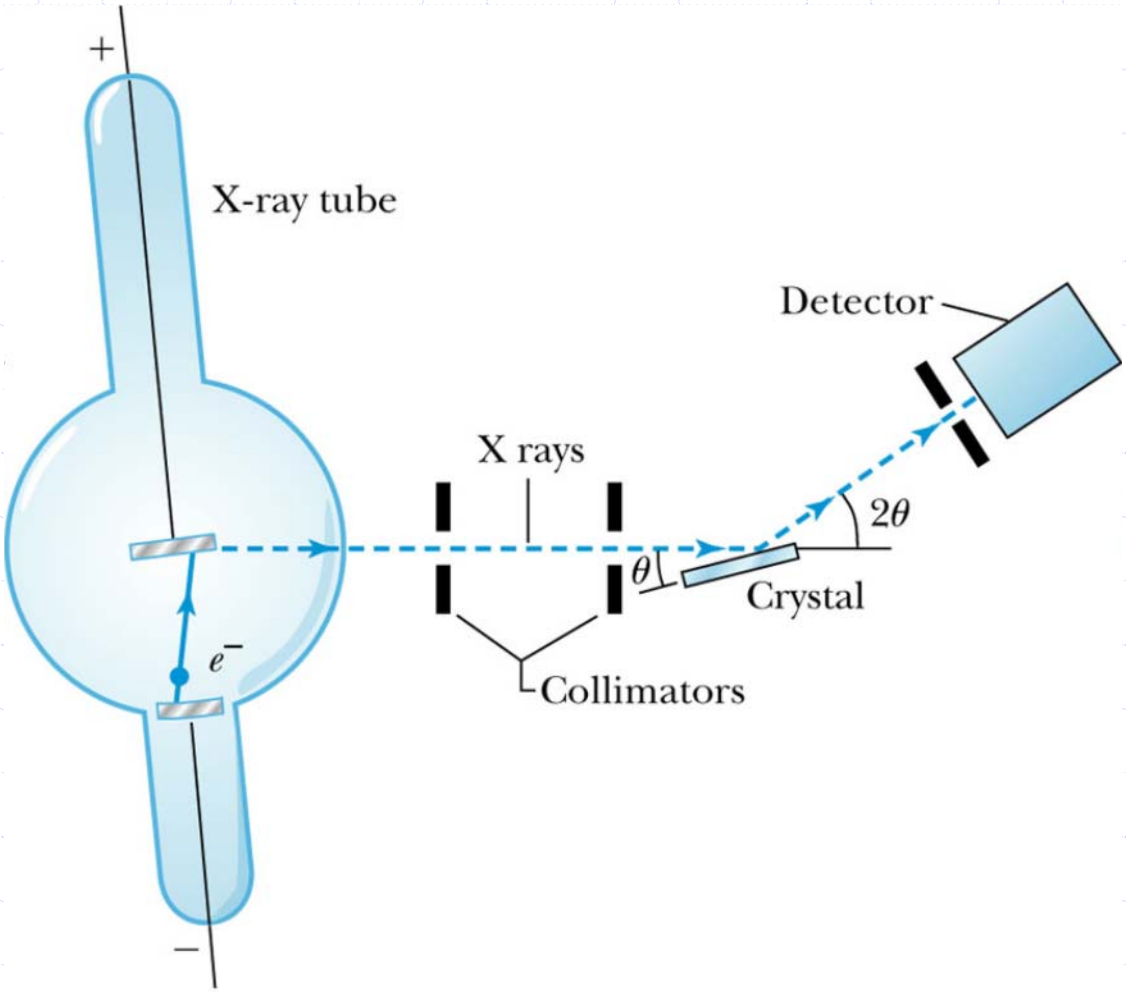
X-ray Scattering

- Crystal structure of NaCl



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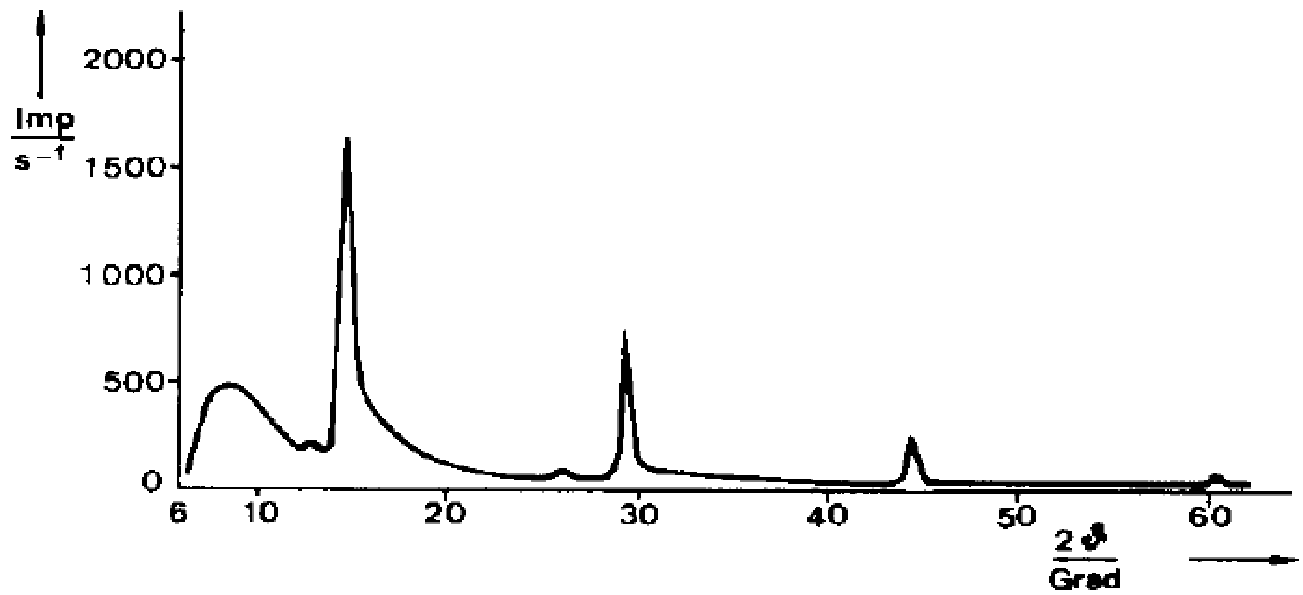
X-ray Scattering

- Bragg spectrum of NaCl

Intensity



2θ

X-ray Scattering

- To determine d

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

$$d = \frac{\lambda}{2\sin\theta} = \frac{0.073nm}{2\sin\frac{15}{2}} = 0.28nm$$

- To determine n

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

$$n = \frac{2d\sin\theta}{\lambda} = \frac{(2)(0.28)\left(\sin\frac{29.5}{2}\right)}{0.073} \approx 2$$

X-ray Scattering

- To check d
  - The volume of one atom is d^3 for a face-centered cubic crystal

$$\frac{molecules}{volume} = \frac{N_{Av}\rho}{At} = \frac{(6.02\times10^{23})(2.16g/cm^3)}{58.5g/mol} = 2.22\times10^{22}\,\frac{molecules}{cm^3}$$

$$\frac{atoms}{volume} = (2.22\times10^{22})(2)\left(\frac{10^6 cm^3}{m^3}\right) = 4.45\times10^{28}\,\frac{atoms}{m^3}$$

$$d^3 = \frac{1}{4.45\times10^{28}}\,\frac{volume}{atom}$$

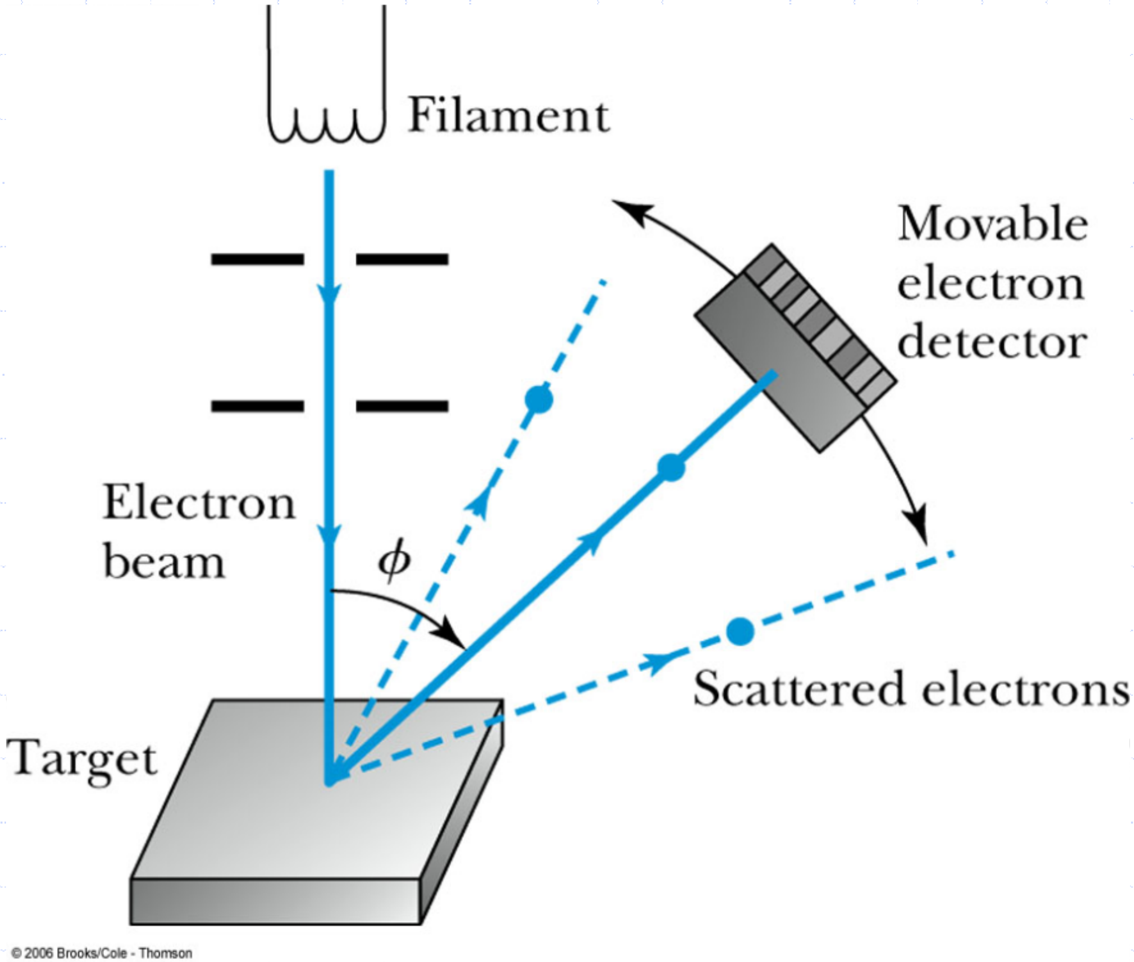
$$d = 0.282nm$$

Electron Scattering

- If x-rays of wavelength ~ 1A produce an diffraction pattern when scattered off a crystal so should matter waves of comparable wavelength
  - For example, 50 eV electrons
- Davisson and Germer verified this (accidentally)

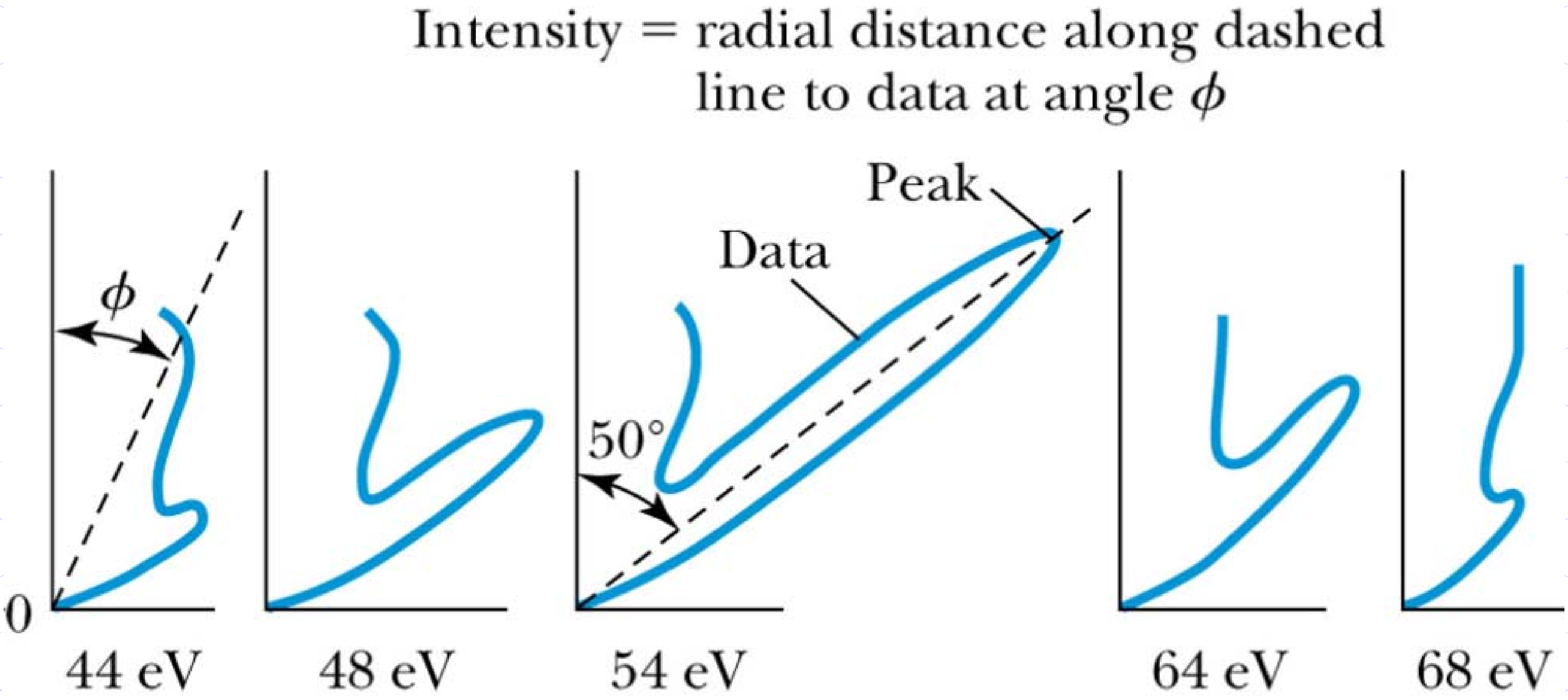
Electron Scattering

- Davisson-Germer experiment



Electron Scattering

- Davisson-Germer data



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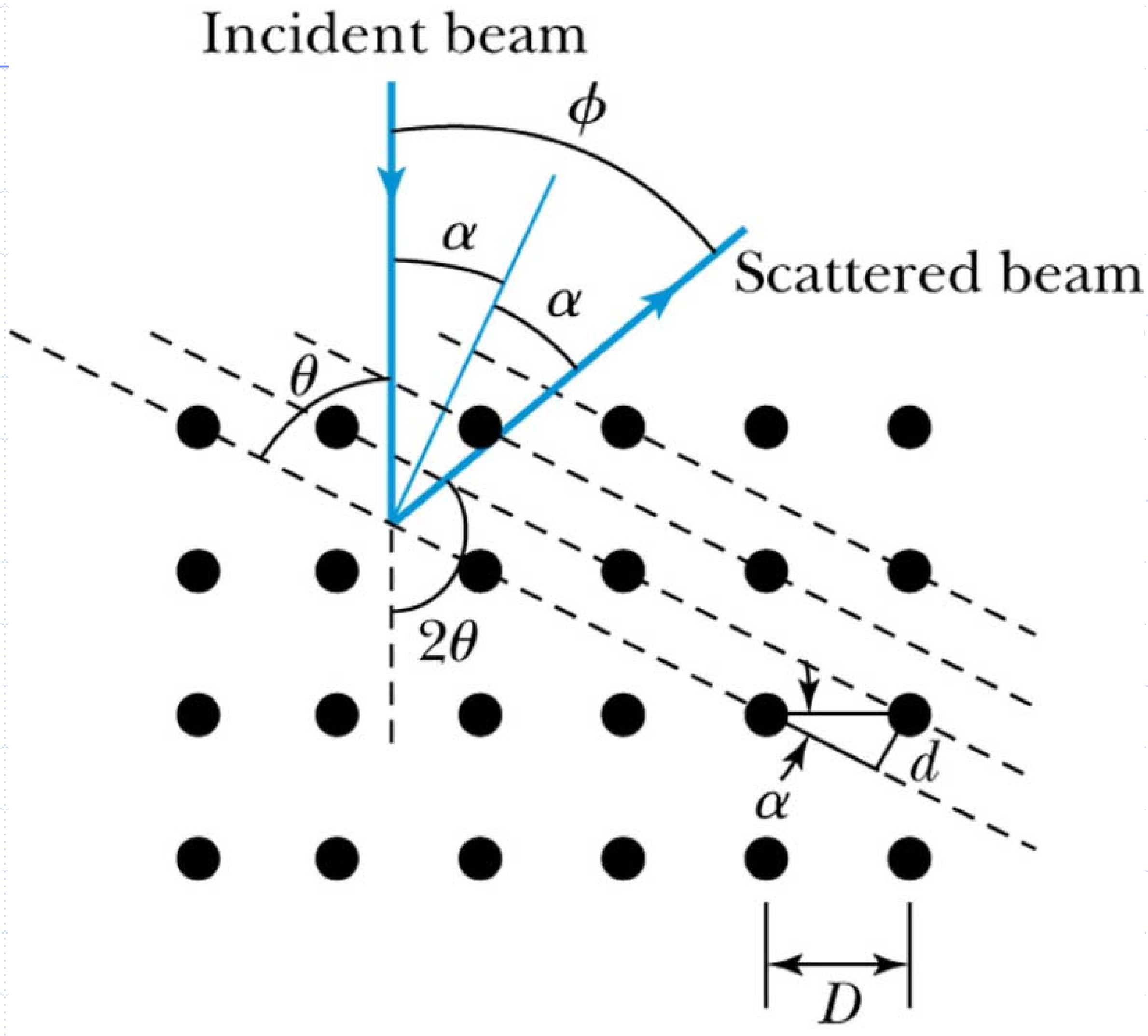
Electron Scattering



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Electron Scattering

- Bragg's law applies for electrons too

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

$$\text{D-G measured } \phi = 2\alpha, \text{ not } \theta$$

$$2\theta = \pi - 2\alpha$$

$$n\lambda = 2d\cos\alpha \text{ and } d = D\sin\alpha$$

$$n\lambda = 2D\cos\alpha\sin\alpha = D\sin 2\alpha = D\sin\phi$$

$$n\lambda = D\sin\phi$$

Electron Scattering

- Analyzing the Davisson-Germer data

$$\lambda = D\sin\phi = (0.215nm)(\sin 50^\circ)$$

$$\lambda = 0.165nm$$

The de Broglie wavelength for 54.4eV electron is

$$\lambda = \frac{h}{p} = \frac{hc}{\sqrt{2mc^2T}} = \frac{1240eV-nm}{\sqrt{(2)(0.511\times10^6eV)(54.4eV)}} = 0.167nm$$

- Experimental evidence that electrons behave as waves with the de Broglie wavelength

Electron Scattering

- Aside, these results hold true for even a low intensity electron beam
  - This means that the interference pattern does not result from interference between waves from two electrons, but from waves associated with a single electron
- Aside, diffraction patterns are also observed using neutrons, H, and He atoms

Electron Scattering

- Thomson observes diffraction patterns in electron transmission experiments similar to Laue's in x-ray transmission experiments

(a)

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