Transmission Electron Microscopy
2. Scattering and Diffraction

EMA 6518

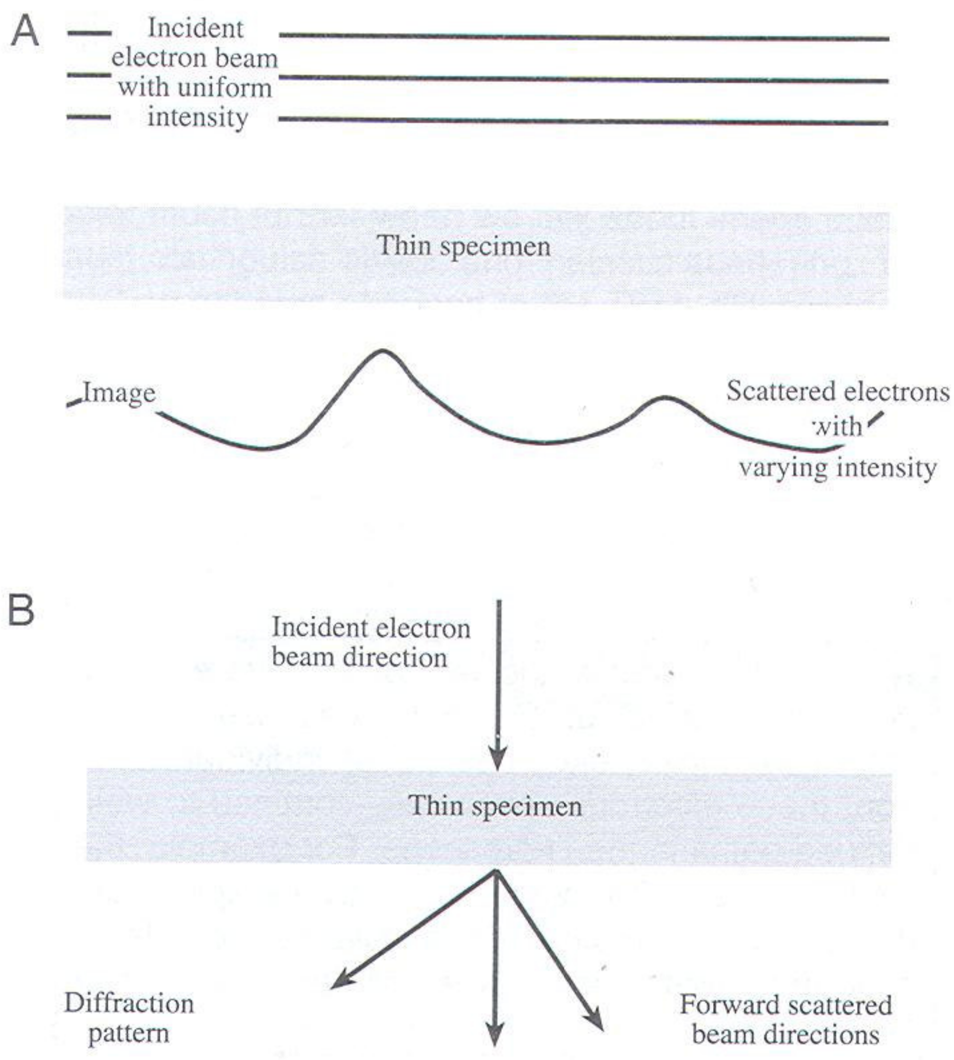
Outline

- Why are we interested in electron scattering?
- Terminology of scattering
- The characteristics of electron scattering
- The interaction cross section
- The mean free path
- Other factors affecting scattering
- Comparison to X-ray diffraction
- Fraunhofer and Fresnel diffraction
- Coherent interference
- A word about angles
- Electron diffraction patterns

Terminology of Diffraction and Scattering

- Diffraction (by Talyor)---an interaction between a wave of any kind and an object of any kind
- Diffraction (by Collins dictionary)---a deviation in the direction of a wave at the edge of an obstacle in its path
- Scattering (by Collins dictionary)---the process in which particles, atoms, etc., are deflected as a result of collisions
- Electron scattering---Nonuniform distribution of electrons---all the structural and chemical information

Nonuniform Distribution



Angular distribution

Reflection and Refraction

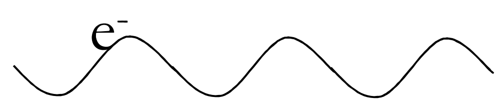
- Reflection is the change in direction of a wavefront at an interface between two different media so that the wavefront returns into the medium from which it originated.

- Refraction is the change in direction of a wave due to a change in its speed. This is most commonly seen when a wave passes from one medium to another.

$$n_1 \sin \theta_1 = n_2 \sin \theta_2$$

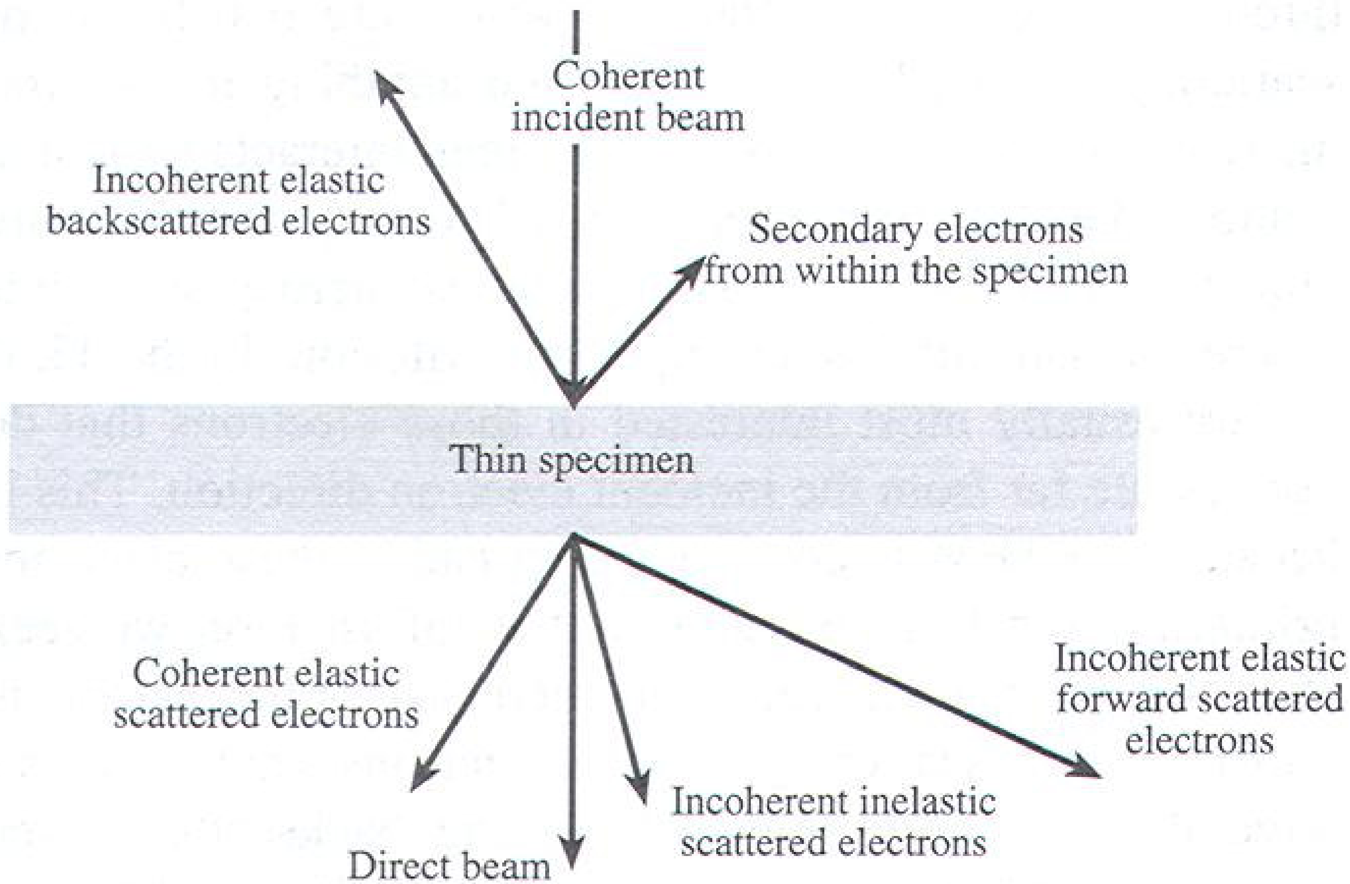
Why are we interested in electron scattering

- "Visible", "invisible", "transparent"
- Invisibility is the state of an object which cannot be "seen".
  - Black Body Radiation?
- Any nonscattering object is invisible.
- Electron scattering
  - Elastic scattering: no loss of energy
  - Inelastic scattering: measurable loss of energy
    - Billiard balls colliding
    - Coherent and incoherent



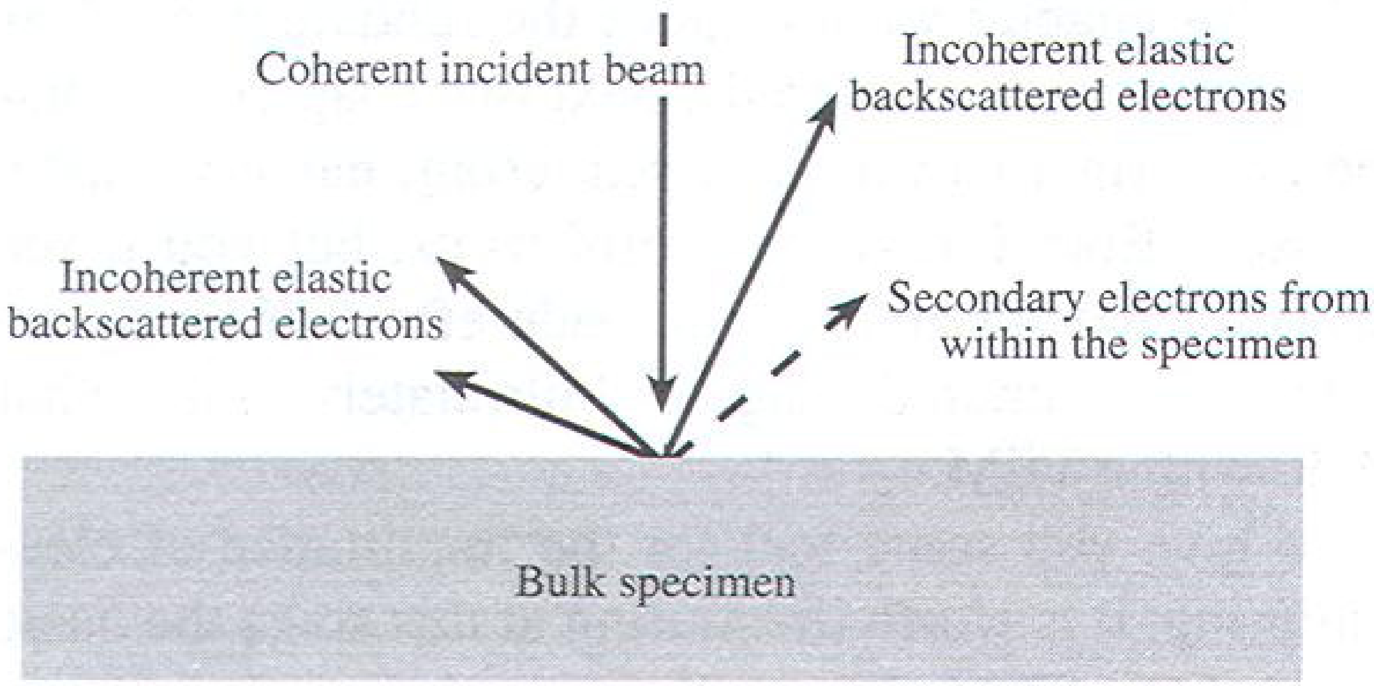
  - Forward scattering: <90º
  - Back scattering: >90º

Terminology of Scattering



Forward scattering causes most of the signals used in the TEM

Terminology of Scattering



Terminology of Scattering

- Elastic scattering is usually coherent, if the specimen is thin and crystalline
- Elastic scattering usually occurs at relatively low angles (1-10º), i.e., in the forward direction
- At higher angles (>~10º) elastic scattering becomes more incoherent
- Inelastic scattering is almost always incoherent and relatively low angle (<1º) forward scattering
- As the specimen gets thicker, less electrons are forward scattered and more are backscattered until primarily incoherent backscattering is detectable in bulk, nontransparent specimens

Terminology of Scattering

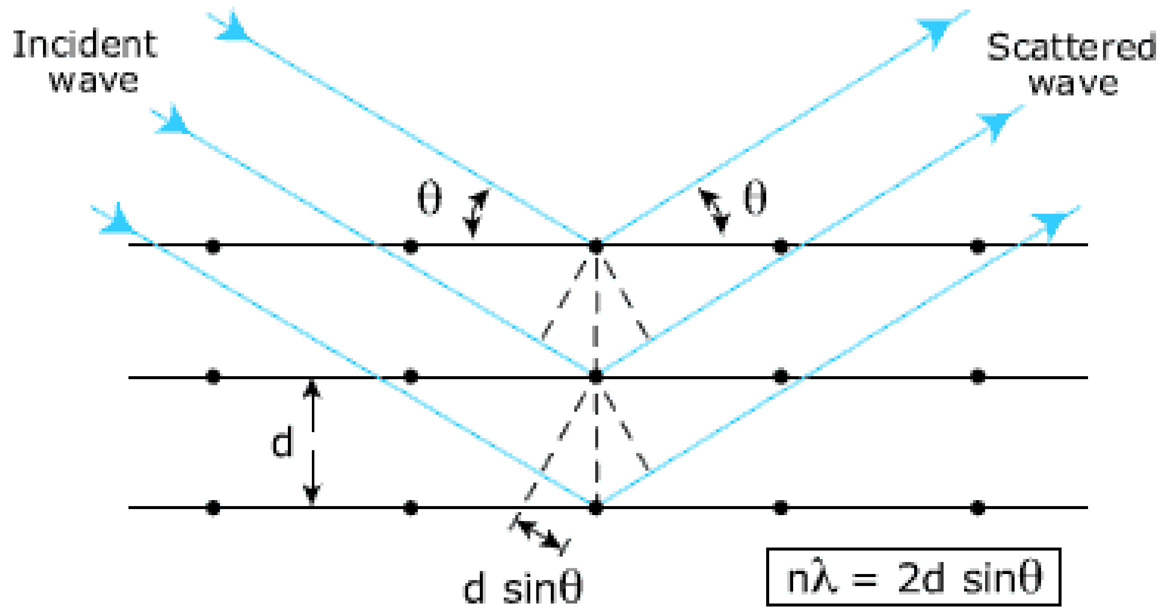
- Single scattering: thin specimen
- Plural scattering: more than once
- Multiple scattering: >20 times

- The greater the number of scattering events, the more difficult it is to predict what will happen to the electron and the more difficult it is to interpret the images, diffraction patterns and spectra

- In the TEM, electrons are not simply transmitted, but are scattered mainly in the forward direction
- Forward scattering includes elastic scattering, Bragg scattering, diffraction, refraction, and inelastic scattering

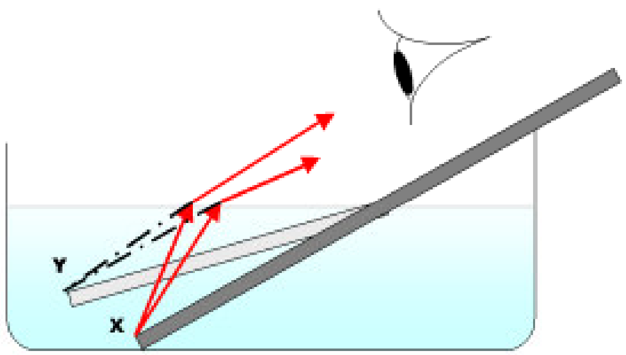
Terminology of Scattering

- Bragg scattering: the diffraction phenomenon exhibited by a crystal bombarded with x-rays in such a way that each plane of the crystal lattice acts as a reflector



Terminology of Scattering

- refraction

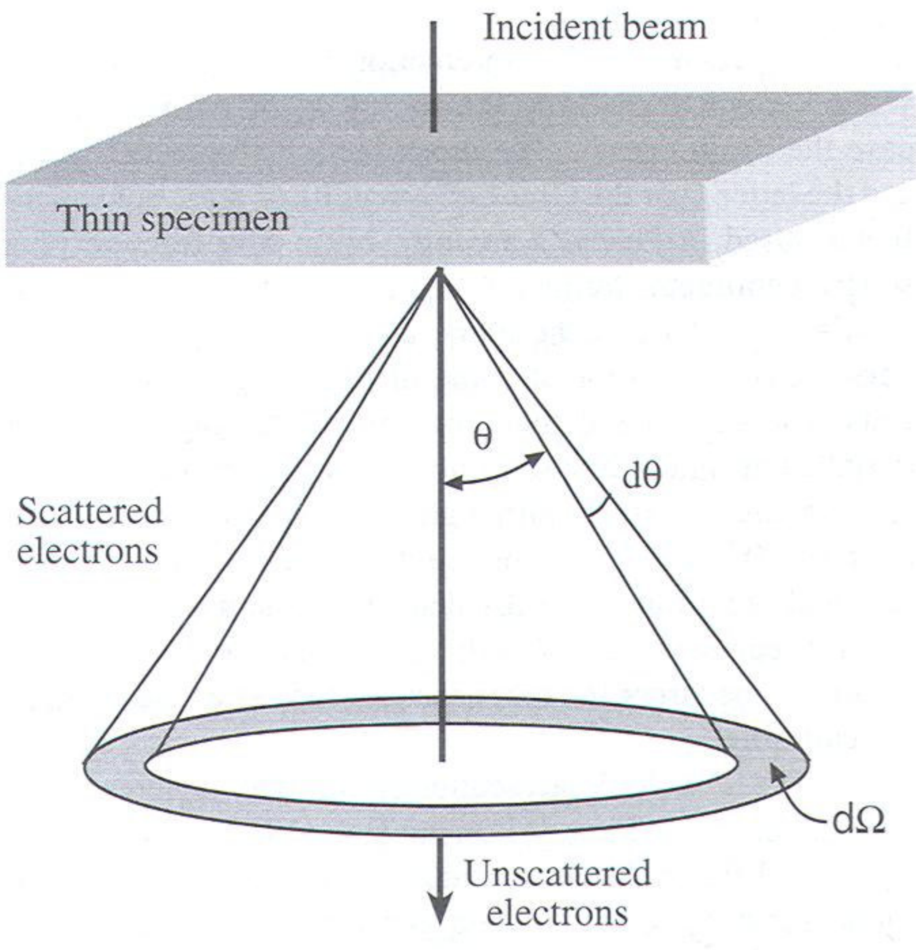


Refraction of light waves in water. The dark rectangle represents the actual position of a pencil sitting in a bowl of water.

Some representative refractive index

Material	n at λ=589.3nm
Vacuum	1
Water ice	1.31
Liquid water (20ºC)	1.333
Teflon	1.35-1.38
Acrylic Glass	1.490-1.492
Si	4.01
Diamond	2.419

Characteristics of Electron Scattering



θ is small enough

$$\sin\theta \approx \tan\theta \approx \theta$$

The Interaction Cross Section

- The chance of a particular electron undergoing any kind of interaction with an atom is determined by an interaction cross section (б)
- Cross section has units of area (isolated atom)

$$\sigma_T = \sigma_{elastic} + \sigma_{inelastic}$$

σ_T : total scattering cross section for the isolated atom

Hall 1953:

$$\sigma = \pi r^2$$

$$r_{elastic} = \frac{Ze}{V\theta}$$

r: effective radius of the scattering center
V: potential of the incoming electron
e: charge
Z: atomic number

The Interaction Cross Section

- Consider the specimen contains N atoms/unit volume

$$Q_T = N\sigma_T = \frac{N_0\sigma_T\rho}{A}$$

(Heidenreich 1964)

N_o: Avogadro's number (atoms/mole)
A: atomic weight (e/mole) of the atoms in the specimen
ρ: density

Q can be regarded as the number of scattering events per unit distance that the electron travels through the specimen.

The probability of scattering from the specimen is given by:

"Mass-thickness" of the specimen

$$Q_T t = \frac{N_0\sigma_T(\rho t)}{A}$$

t: specimen thickness

Mean Free Path

The total cross section for scattering can be expressed as the inverse of the mean free path, λ. This parameter is the average distance that the electron travels between scattering events. typical values of λ at TEM voltages are of the order of tens of nm

p: a probability of scattering as the electron travels through a specimen thickness t

$$\lambda = \frac{1}{Q_T} = \frac{A}{N_0 \sigma_T \rho}$$

$$p = \frac{t}{\lambda} = \frac{N_0 \sigma_T (\rho t)}{A}$$

Differential Cross Section

• electrons are scattered through an angle θ into a solid angle Ω. The differential scattering can be written as

$$\frac{d\theta}{d\Omega} = \frac{1}{2\pi \sin\theta} \frac{d\sigma}{d\theta}$$

$$\sigma_\theta = \int_0^\pi d\sigma = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin\theta d\theta$$

Other Factors Affecting Scattering

- Less scattering at higher angles, most of the scattered electrons are within 5º of the unscattered beam
- Higher voltage (electron energy) will result in less electron scattering
- Atomic number , Z, is more important in elastic than inelastic scattering. As Z increases elastic scattering dominates.

Electron Beam-Specimen Interactions

- What happens when the beam reaches the specimen?
- How the signals produced by the EB-specimen interactions are converted into images and/or spectra that convey useful information?
  - Size, shape, composition, certain properties, etc.

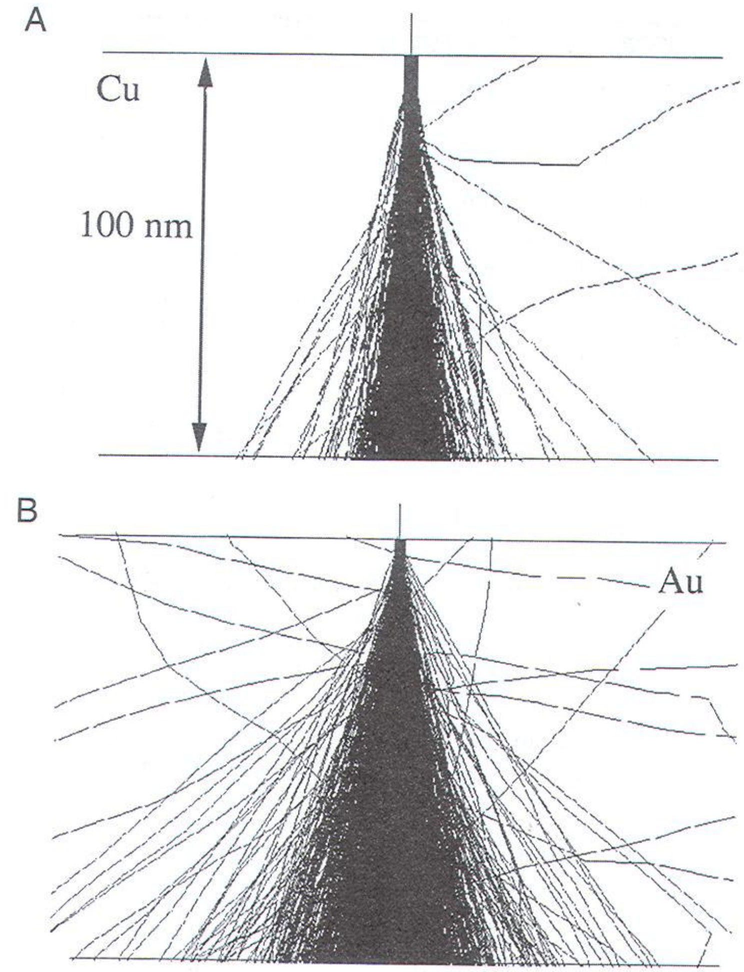
Monte Carlo Simulation of Electron Beam-Specimen Interactions

by David Joy and are based on the algorithms described in the book "Monte Carlo Modeling for Electron Microscopy and Microanalysis" published by Oxford University Press (1995).

Electron Beam-Specimen Interactions

- The process is called Monte Carlo Simulation because of the use of random numbers in the computer programs, the outcome is always predicted by statistics

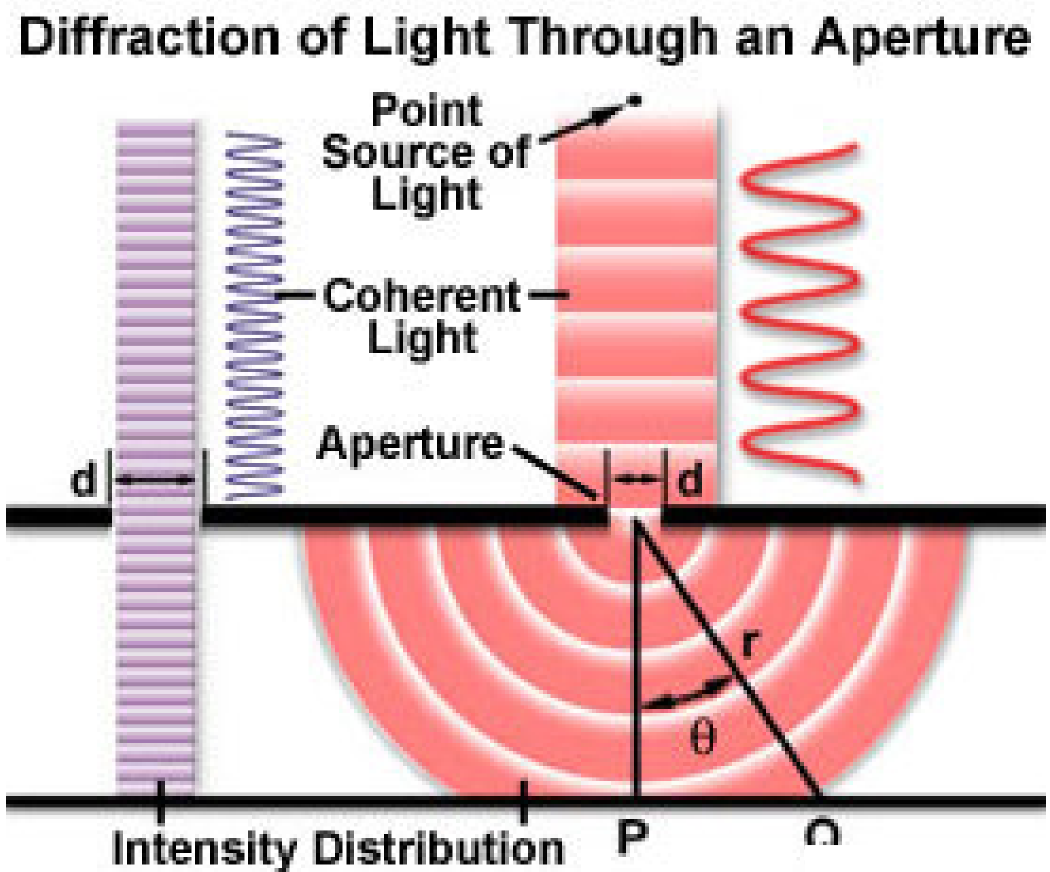
- Late 1940s devloped by J.Von Neumann and S. Ulam at Los Alamos



What will happen?

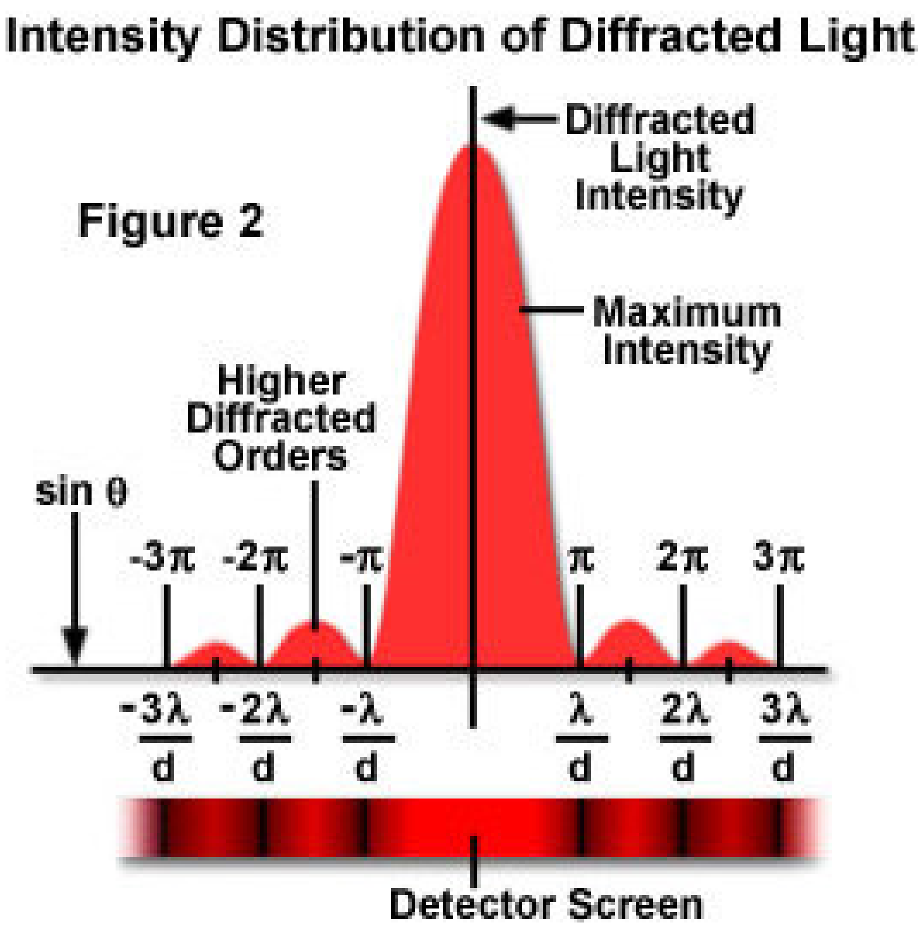
- When a beam of monochromatic red (having a wavelength of 662 nanometers) light incident on a slit aperture that is 1260 nanometers wide, ….
- When the wavelength exceeds the size of the slit, …..

Diffraction



sin(θ) = mλ/d

Diffraction

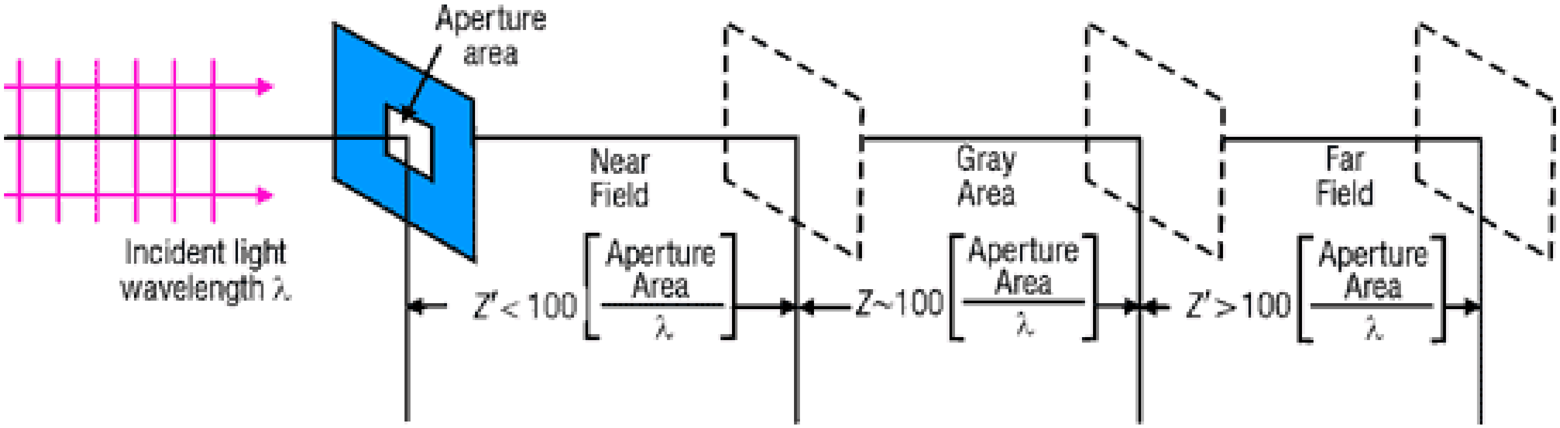


$$\sin(\theta) = m\lambda/d$$

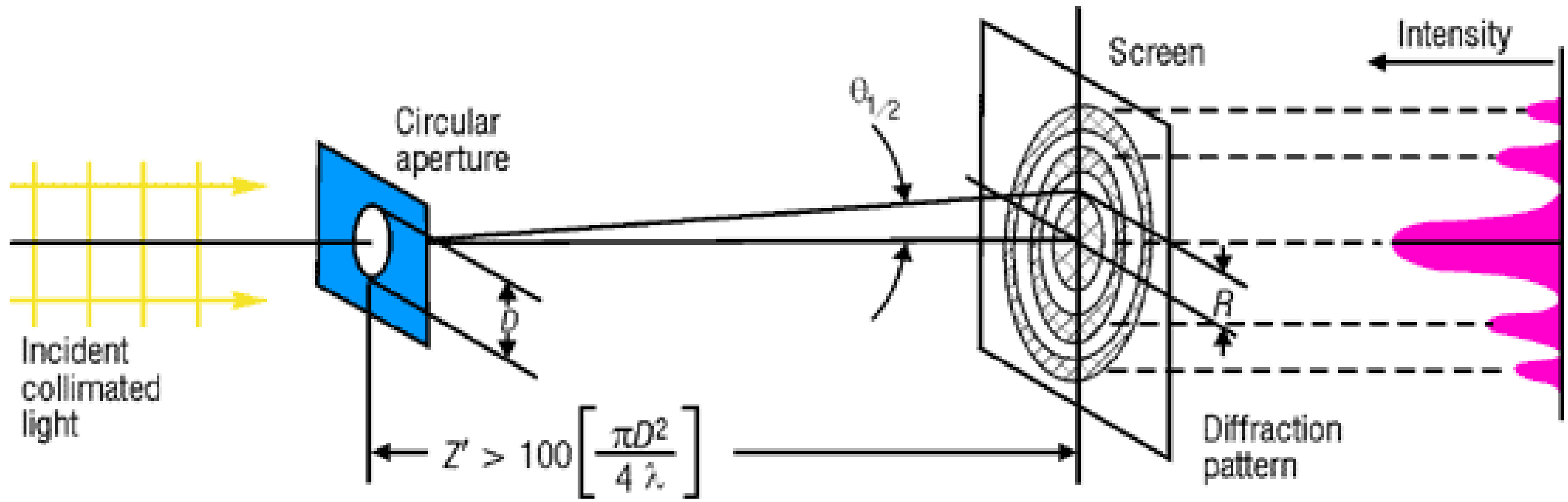
where **Θ** is the angle between the central incident propagation direction and the first minimum of the diffraction pattern, and **m** indicates the sequential number of the higher-order maxima.

Fraunhofer and Fresnel Diffraction

- Fraunhofer diffraction occurs when a flat wave-front interacts with an object. Since a wave emitted by a point becomes planar at large distances, this is known as far-field diffraction.
- Fresnel diffraction occurs when it's not Fraunhofer. This case is also known as near-field diffraction.



Fraunhofer and Fresnel Diffraction

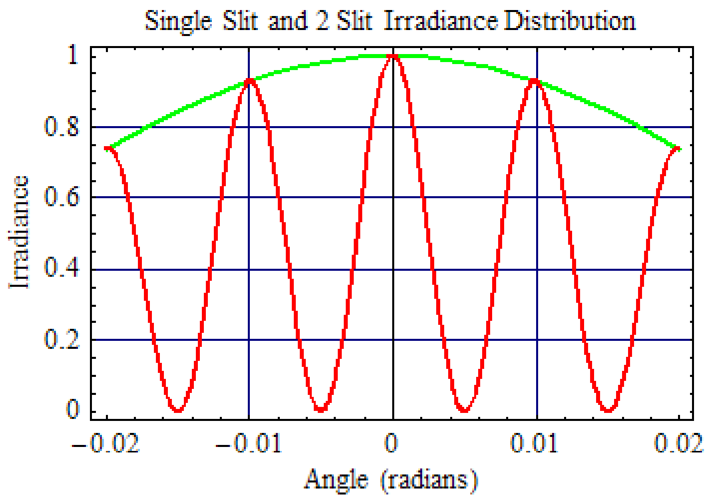


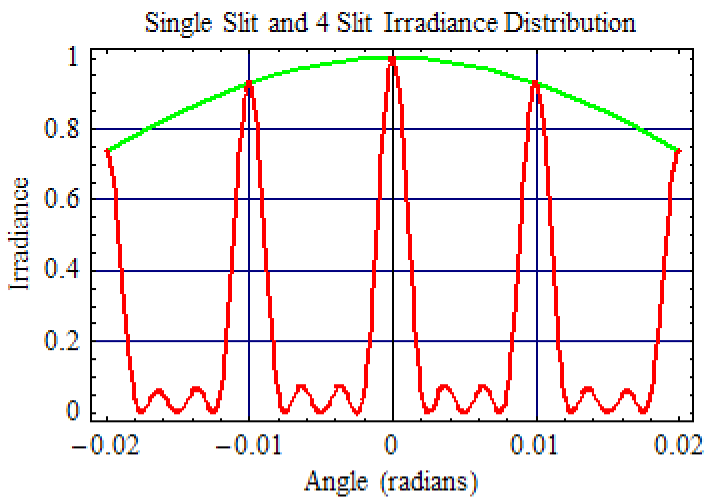
$$R = \frac{1.22\lambda Z'}{D}$$

•Electron Diffraction patterns correspond closely to the Fraunhofer case.

•The coherent interference is purely a matter of physical optics.

Fraunhofer and Fresnel Diffraction





FRAUNHOFER DIFFRACTION

- Multiple Slits
- Circular Aperture
- Rectangular Aperture

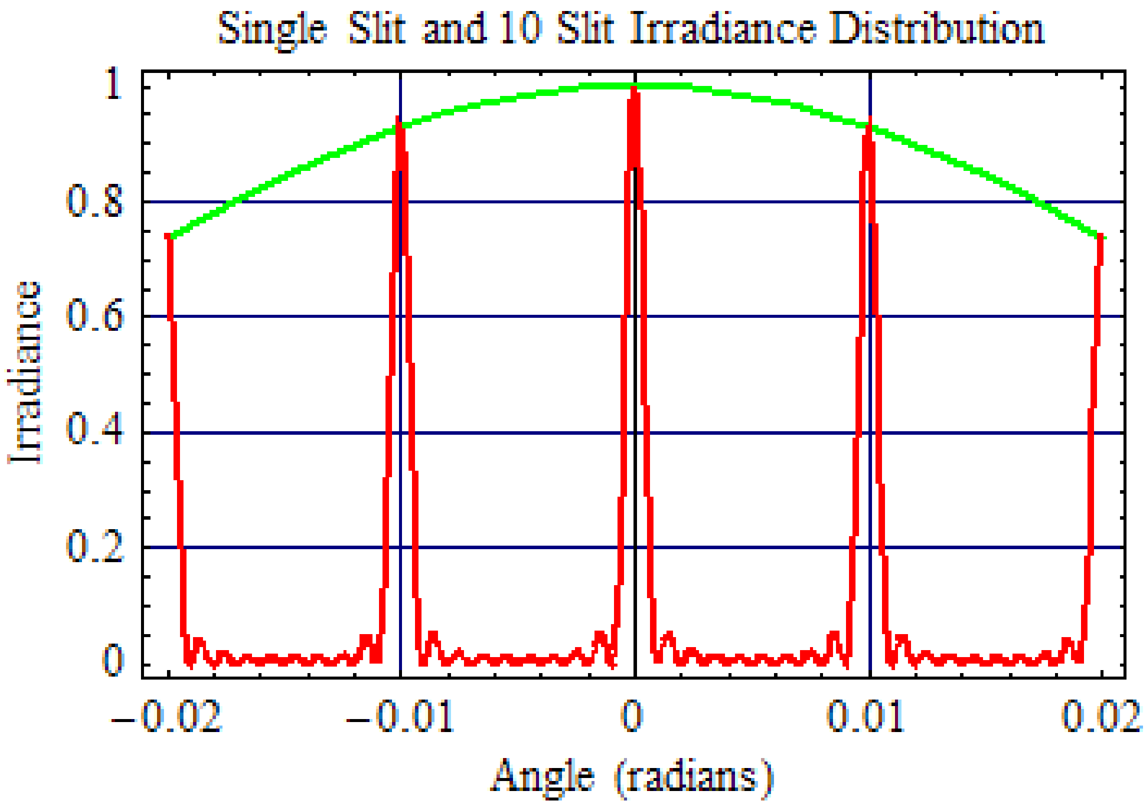
FRESNEL DIFFRACTION

- Circular Aperture
- Rectangular Aperture

http://wyant.optics.arizona.edu/math.htm

Multiple Slit Fraunhofer Diffraction Pattern

Multiple Slit Fraunhofer Diffraction Pattern



Input:

10 slits

15 wavelength slit width

100 wavelength slit spacing

0.02 radians plot range

Fraunhofer and Fresnel Diffraction

- Path difference $L = d\sin\theta$
- The two wavelets propagating in direction r are out of phase by $2\pi L/\lambda$

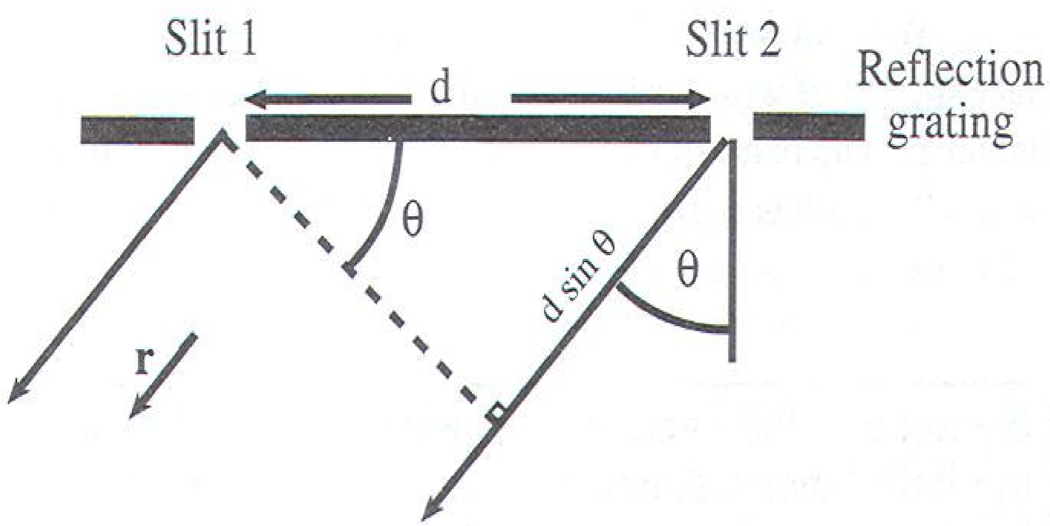
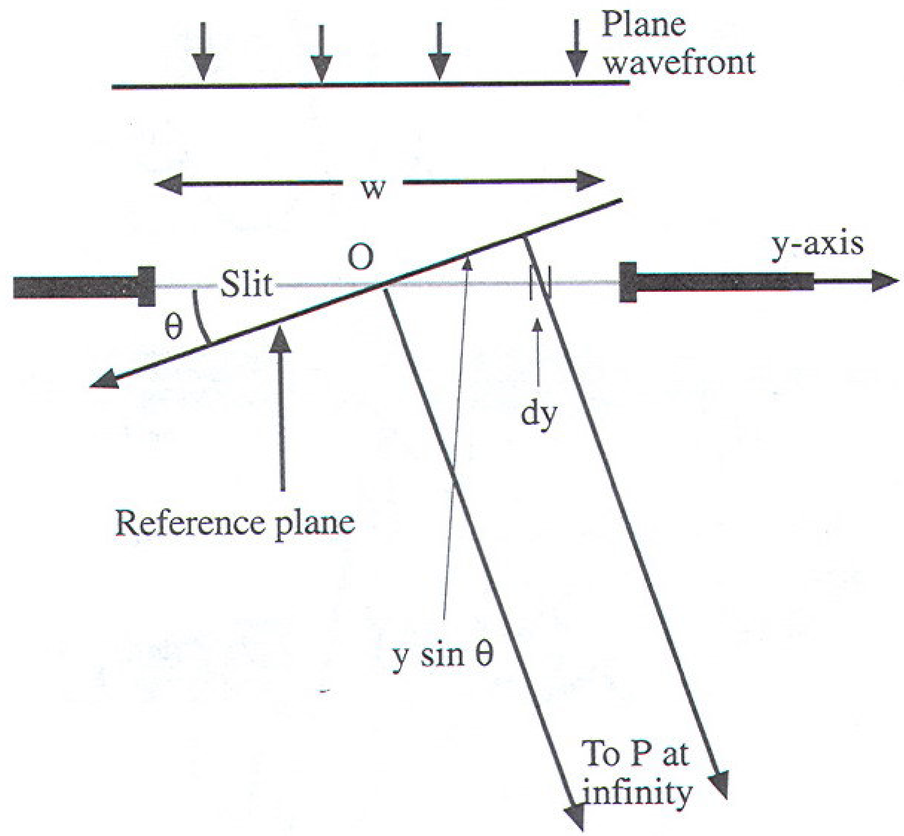


Figure 2.5. An incident plane wave is scattered by two slits, distance d apart. The scattered waves are in phase when the path difference $d\sin\theta$ is $n\lambda$.

There is an inverse relationship between d and Θ:

As d ↓, sin Θ ↑

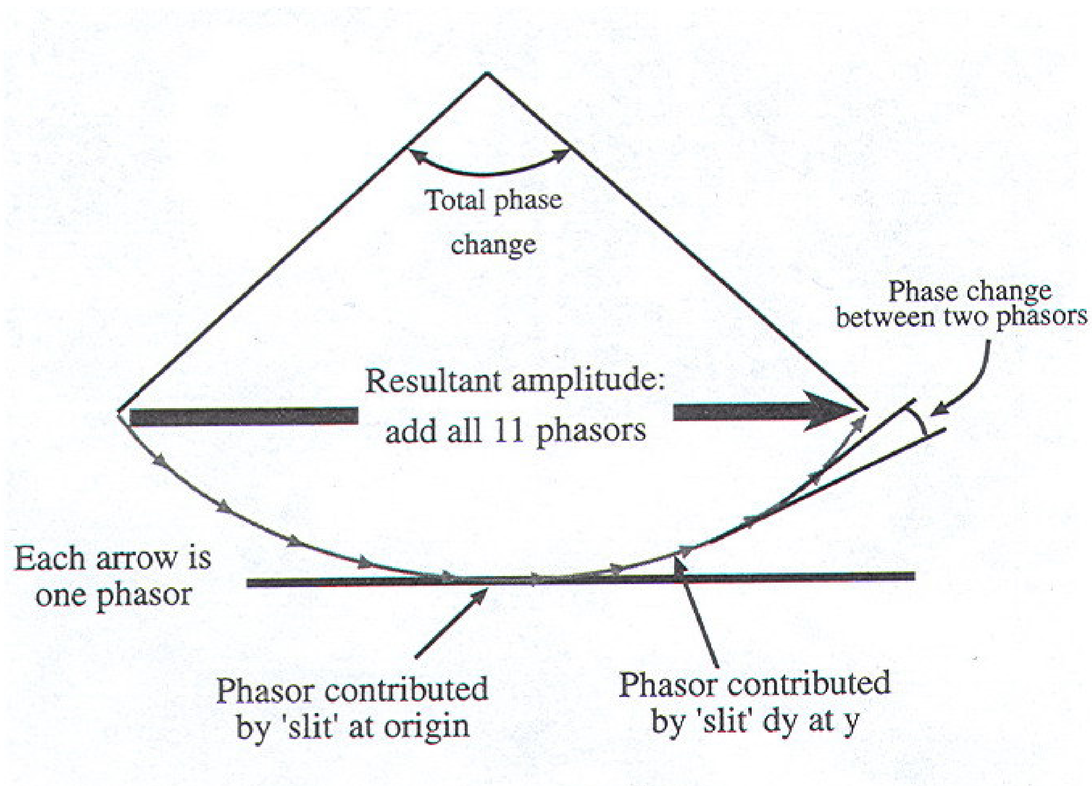
Coherent Interference

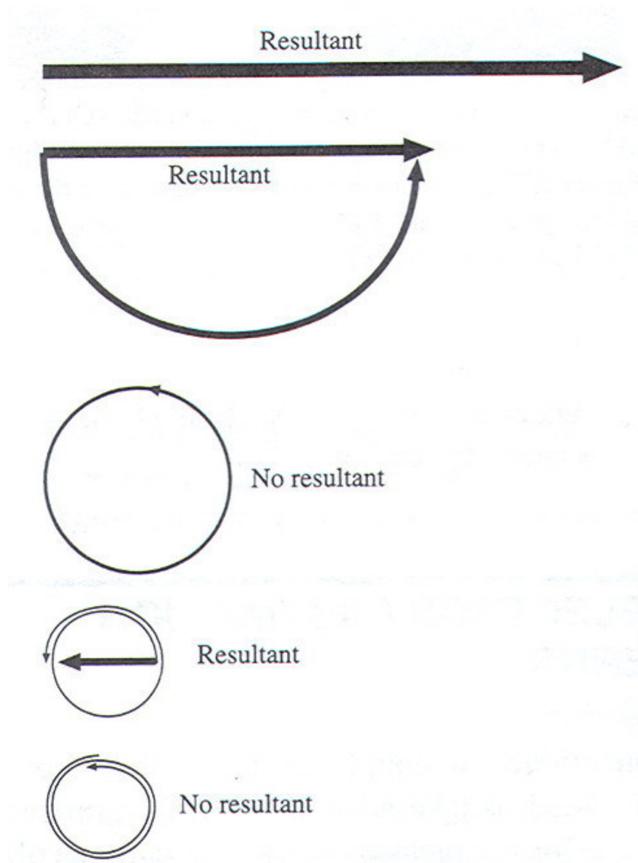


$$\psi = \psi_0 e^{i\phi}$$

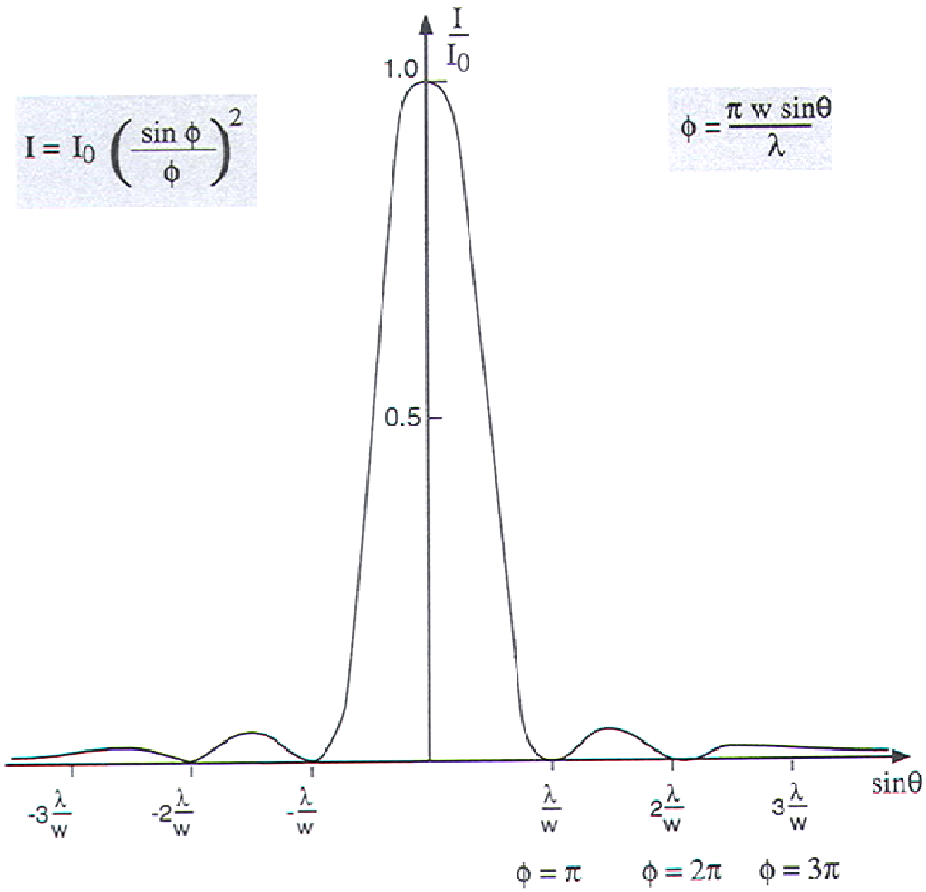
$$\Delta\phi = \frac{2\pi}{\lambda}\Delta x$$

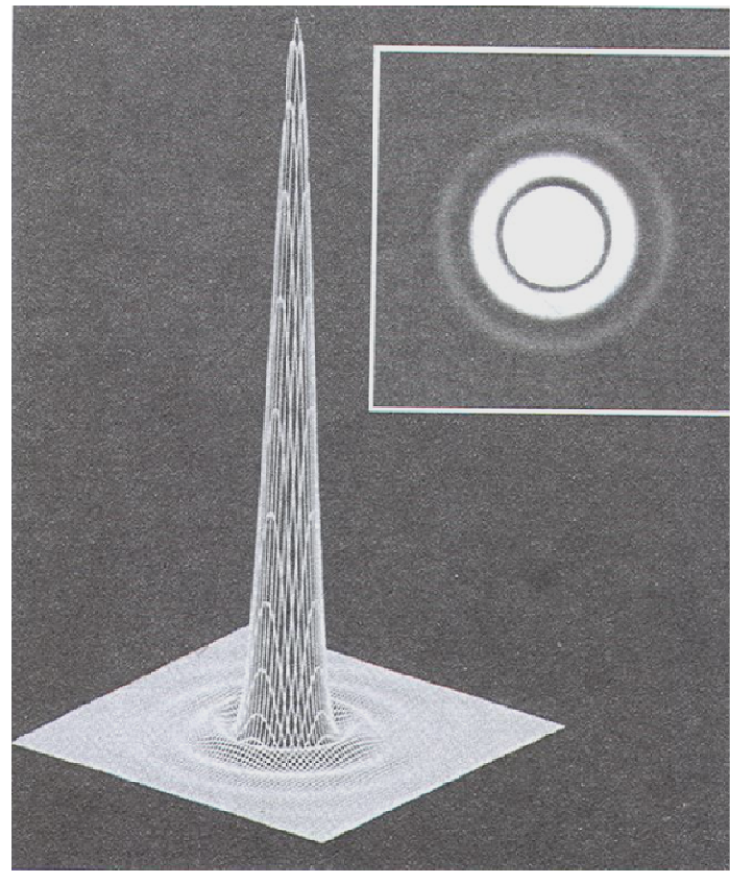
Coherent Interference





Coherent Interference





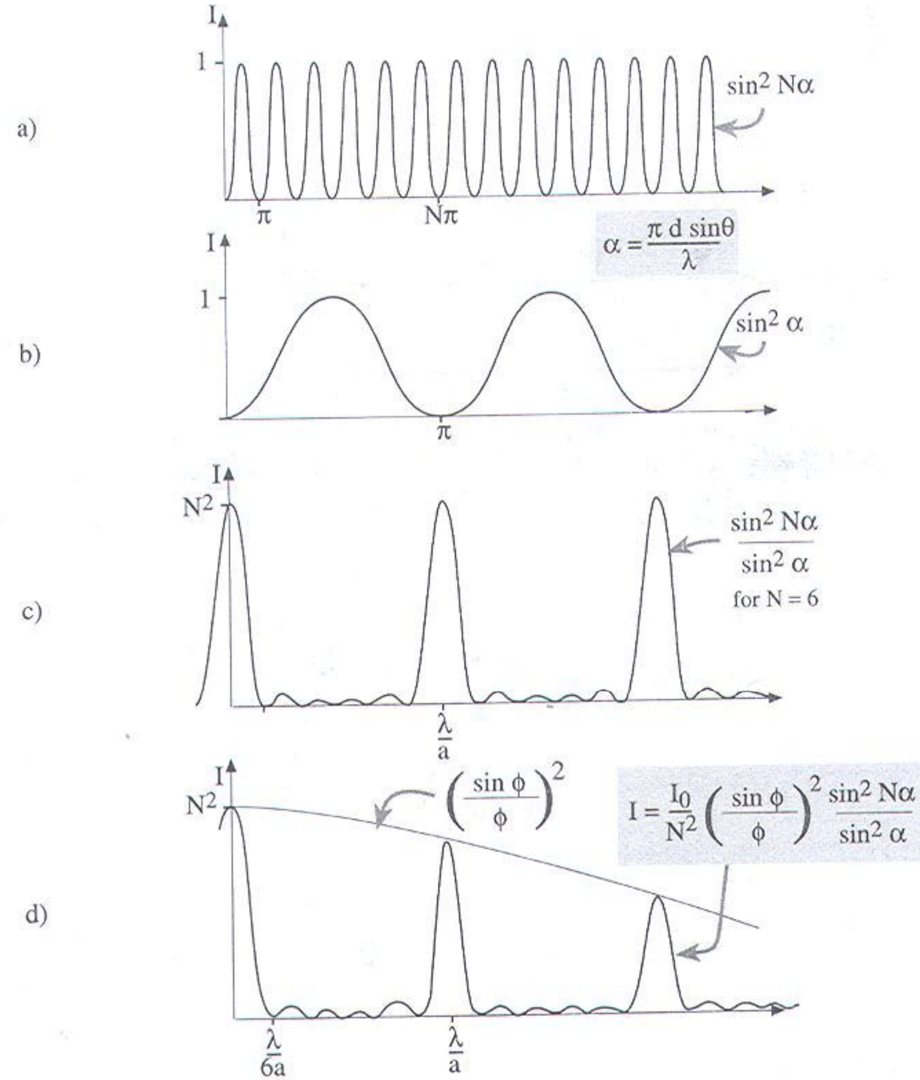
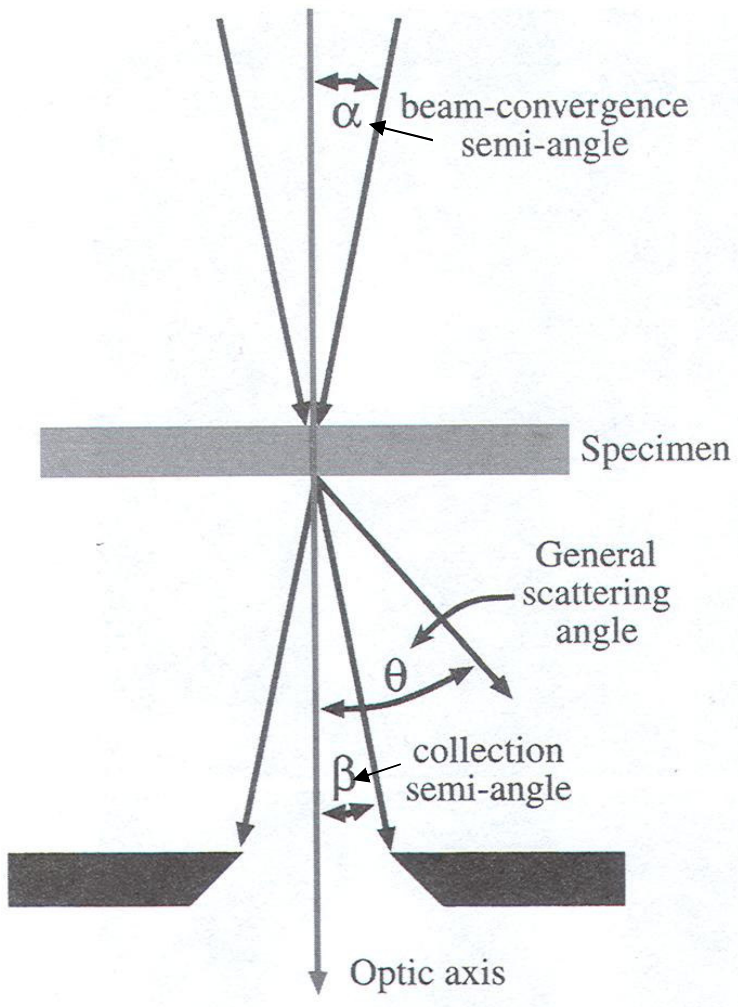
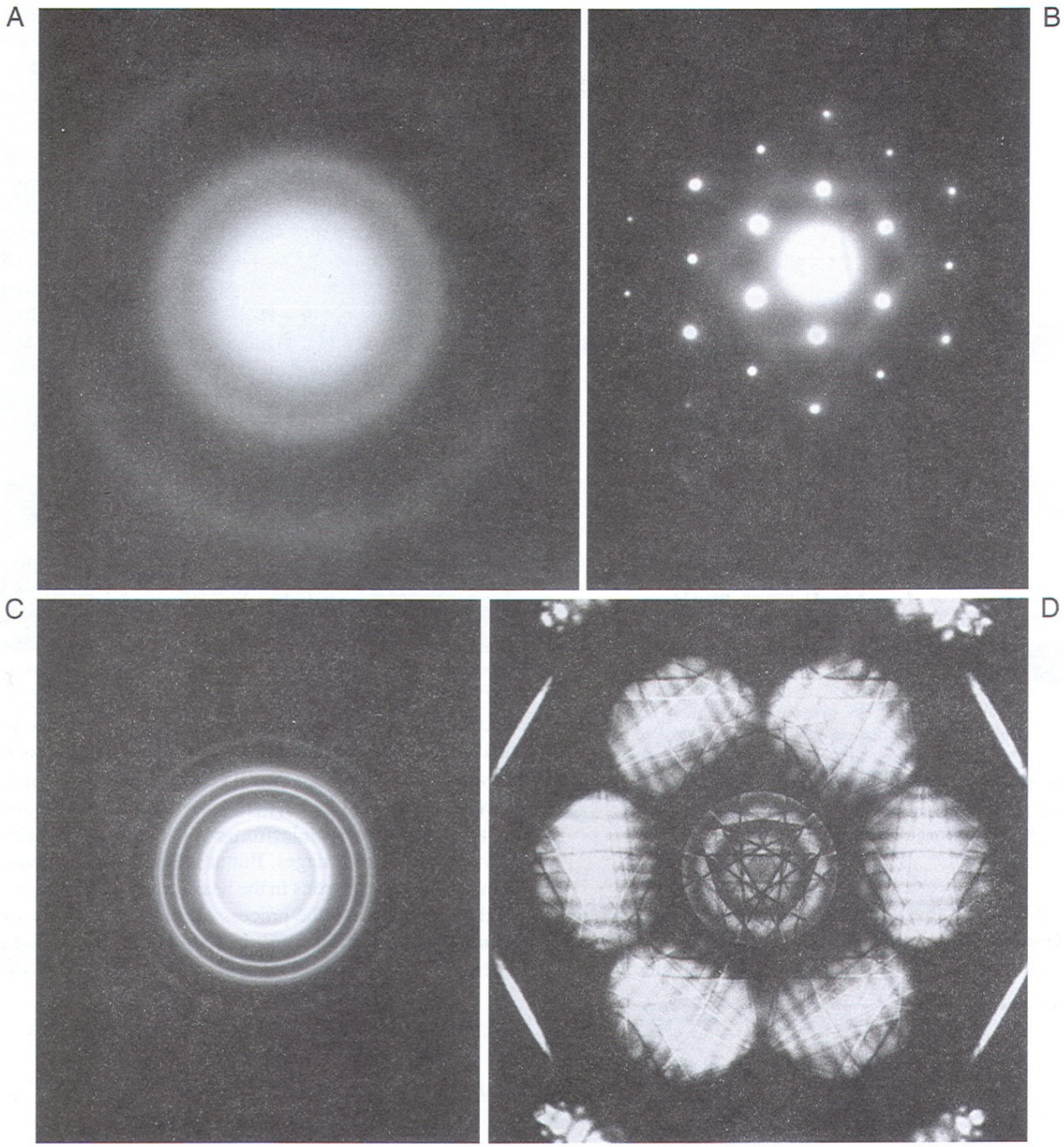


Figure 2.9. The scattered intensity from N slits (shown here for $N = 6$) where each slit would give the intensity shown in (B). (C) is the curve in (A) divided by curve in (B) and (D) is the curve in (C) multiplied by the curve in (Figure 2.7D). The distance d, the separation of the slits, and ϕ are defined in Figures 2.5 and 2.7. (λ/w has been increased compared to Figures 2.7 and 2.8 for simplicity.)

Definition of the Major Semiangles in TEM

A,β,θ





A: Amorphous carbon
B: Al single crystal
C: polycrystalline Au
D: Si illuminated with a convergent beam of electrons

Electron Diffraction Patterns

- Most of the intensity is in the direct beam, in the center of the pattern, which means that most electrons are not scattered but travel straight through the specimen.

- The scattering intensity falls with increasing θ (increasing distance from the direct beam), which reflects the decrease in the scattering cross section with θ

- The scattering intensity varies strongly with the structure of the specimen