UNIT-5

QUANTUM PHYSICS

Quantum or Wave Mechanics

L. de Broglie (1892-1987)

- Light has both wave & particle properties
- de Broglie (1924) proposed that all moving objects have wave properties.
- For light: $E = h\nu = hc / \lambda$
- For particles: $E = mc^2$ (Einstein)

Therefore, $mc = h / \lambda$

and for particles

$(\text{mass})x(\text{velocity}) = h / \lambda$

λ for particles is called the de Broglie wavelength

Property of wave

(1) Periodicity . The repeating and periodic disturbance which moves through a medium from one location to another is referred to as a wave.

(2) Waves are in general created by something oscillating. For example, sound waves are radiated by various oscillating elements as speakers, strings in guitar, etc..

(3) Waves are said to be an energy transport phenomenon. transporting energy from one location (its source) to another location without transporting matter. Or the information about the physical property are transported from one location to another location.

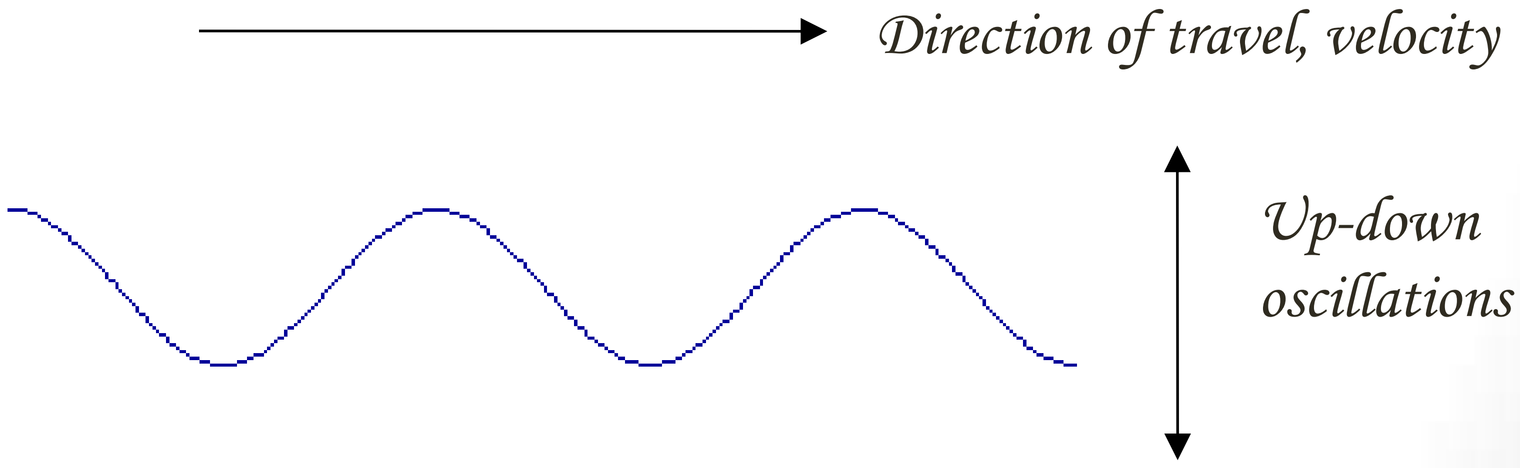
(4) Restoring forces acted on fluid particles. Each individual particle of the medium is temporarily displaced and then returns to its original equilibrium positioned by the action of restoring forces.

Waves and Particles:

Common types of waves:

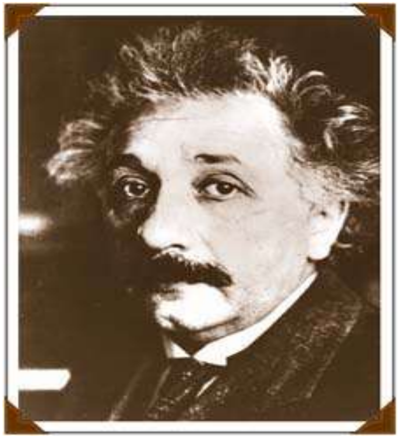
Ripples, surf, ocean waves, sound waves, radio waves.

Waves are oscillations in space and time.



Wavelength ,frequency, velocity and oscillation size defines waves

The Quantum nature of Light or the Photon



Particle nature of light was proposed by Einstein in 1905 to explain the photo-electric effect. Photo-electric effect .Particles of light are called light quanta or photons.

Energy of a Photon = h (frequency of light)
h is a fundamental constant of nature and it is very small in size.

Packet of energy in photon is so small that we are not aware of the rain of photons of light impinging on our eyes – just as you cannot feel the impact of individual air molecules, you only feel a breeze.

The Wave Nature of the Light

- Atomic structure elucidated by interaction of matter with light.
- Light properties: characterized by wavelength, λ, and frequency, ν.
- **Light** = electromagnetic radiation**,** a wave of oscillating electric and magnetic influences called fields.
- Frequency and wavelength inversely proportional to each other.

$$c = \nu\lambda$$

  where c = the speed of light = 3.00x108 m/s; units $\nu = s^{-1}$, λ = m

E.g. calculate the frequency of light with a wavelength of 500 nm.
E.g.2 calculate the frequency of light if the wavelength is 400 nm.

Quantized Energy and Photons

- Light = wave arriving as stream of particles called "photons".
- Each photon = **quantum of energy**

$$E = h\nu = \frac{hc}{\lambda}$$ where h (Planck's constant) = 6.63×10^{-34} J*s.

- An increase in the frequency = an increase in the energy
- An increase in the wavelength gives an decrease in the energy of the photon.
- Photoelectric effect: $E = h\nu - \phi$ where ϕ = constant
-
- the energy of the electron is directly related to the energy of the photon.
- the threshold of energy must be exceeded for electron emission.
- The total energy of a stream of particles (photons) of that energy will be:

$$E_{total} = n \cdot h\nu$$

where n = 1, 2, …(only discrete energies).

SUMMARY OF PHOTON PROPERTIES

Relation between particle and wave properties of light

Energy and frequency $E = h\nu$

Also have relation between momentum and wavelength

Relativistic formula relating energy and momentum

$$E^2 = p^2c^2 + m^2c^4$$

For light $E = pc$ and $c = \lambda\nu$

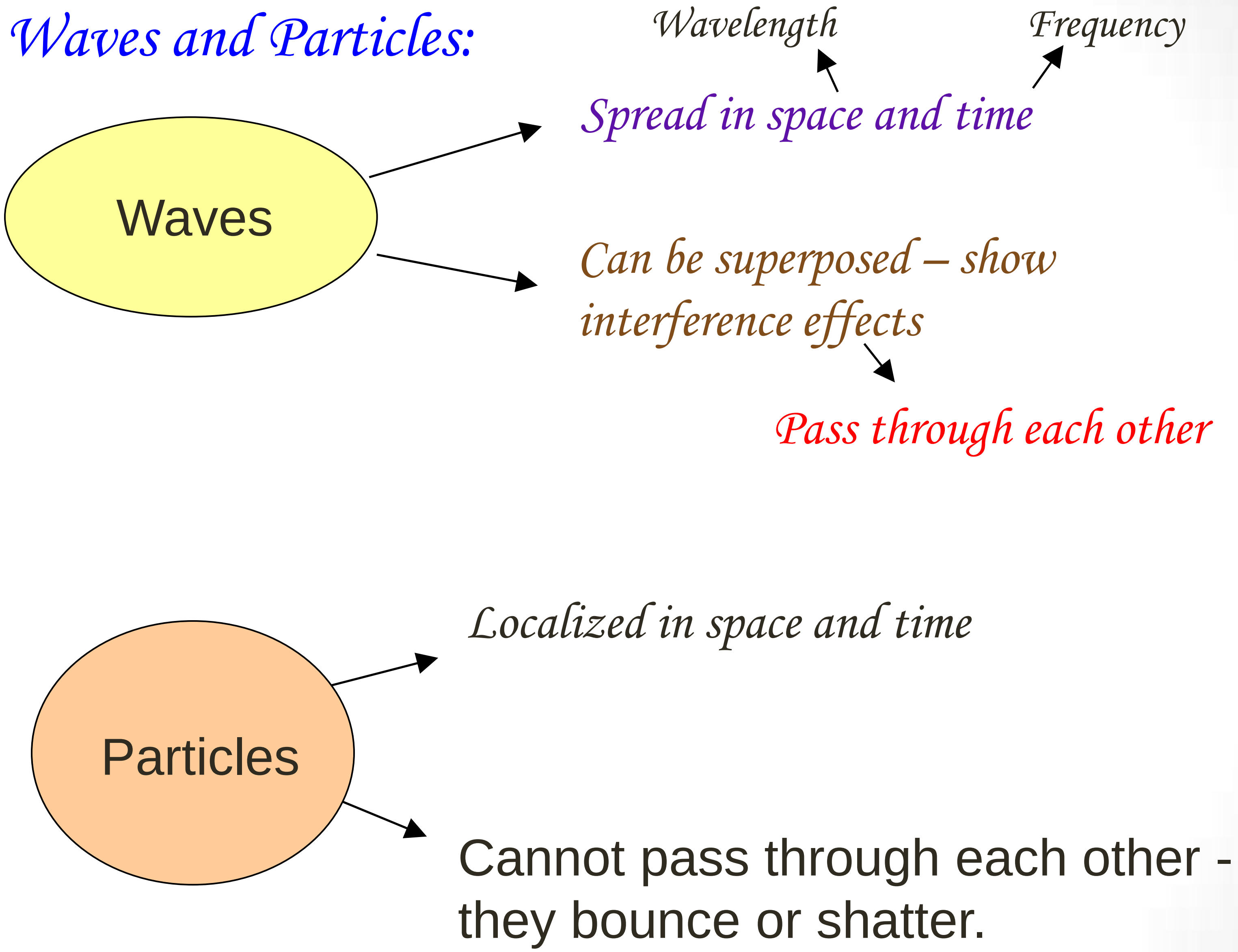
$$p = \frac{h}{\lambda} = \frac{h\nu}{c}$$

Also commonly write these as

$$E = \hbar\omega \qquad p = \hbar k \qquad \omega = 2\pi\nu \qquad k = \frac{2\pi}{\lambda} \qquad \hbar = \frac{h}{2\pi}$$

angular frequency (ω), wavevector (k), hbar ($\hbar$)

Waves and Particles:



Wave Nature of Matter

- Louis de Broglie in 1923 proposed that matter particles should exhibit wave properties just as light waves exhibited particle properties. These waves have very small wavelengths in most situations so that their presence was difficult to observe

- These waves were observed a few years later by Davisson and G.P. Thomson with high energy electrons. These electrons show the same pattern when scattered from crystals as X-rays of similar wave lengths.

De Broglie

MATTER WAVES

We have seen that light comes in discrete units (photons) with particle properties (energy and momentum) that are related to the wave-like properties of frequency and wavelength.

In 1923 Prince Louis de Broglie postulated that ordinary matter can have wave-like properties, with the wavelength λ related to momentum p in the same way as for light

de Broglie relation

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

de Broglie wavelength

Planck's constant

$$h = 6.63 \times 10^{-34}\ \text{Js}$$

NB wavelength depends on momentum, not on the physical size of the particle

Prediction: We should see diffraction and interference of matter waves

De Broglie Waves

- In his thesis in 1923, Prince Louis V. de Broglie suggested that mass particles should have wave properties similar to electromagnetic radiation.
- The energy can be written as:

$$h\nu = pc = p\lambda\nu$$

- Thus the wavelength of a matter wave is called **the de Broglie wavelength**:

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

If a light-wave could also act like a particle, why shouldn't matter-particles also act like waves?

Wave Nature of Matter

- Light behaves like matter since it can only have certain energies.
- Light had both wave- and particle-like properties $\Rightarrow$ matter did too.
- Einstein equation helps describe the duality of light:
- ➢ $E = mc^2$ --Particle behavior
- ➢ $E = h\nu$ --Wave behavior

$$h\nu = mc^2$$
$$\frac{hc}{\lambda} = mc^2$$
$$m = \frac{h}{c\lambda}$$

Wave and particle behavior

- Duality of matter expressed by replacing the speed of light with the speed of the particle to get:

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

where λ called the de Broglie wavelength of any moving particle.

The Wave-Particle Duality

- all known forms of matter (photons, electrons, muons, neutrinos,…) exhibit *both* particle-like and wave-like characteristics
- even gravity is *expected* to exhibit this duality, though no one has yet detected the “particle” of the gravitational field, dubbed the graviton.

particle-like behavior	wave-like behavior
come in discrete “pieces”, or *quanta*	amplitude can be arbitrarily small
when two particles collide, they scatter off one another	when waves “collide”, they pass through one another, producing interference effects
localized at a point in space	spread out over a region of space

The Wave-Particle Duality

- the *energy* of a particle is proportional to the *frequency* of the corresponding wave
- the *momentum* of a particle is proportional to the *wavelength* of the corresponding wave
  - these relationships require a new fundamental constant of nature: Planck's constant
  - correctly describes many effects, including
    - blackbody radiation
    - the photoelectric effect (electrons ejected off a metal surface when light shines on it)
    - the Compton effect (a photon elastically colliding with an electron)
- explains the stability of atoms
- implies the Heisenberg uncertainty principle (one aspect of this is that an experiment can never discern both the momentum and position of a particle with arbitrary accuracy).

WAVE PARTICLE DUALITY

Evidence for wave-particle duality

- Photoelectric effect
- Compton effect

- Electron diffraction
- Interference of matter-waves

Consequence: Heisenberg uncertainty principle

WAVE-PARTICLE DUALITY OF LIGHT

Evidence for wave-nature of light
- Diffraction and interference

Evidence for particle-nature of light
- Photoelectric effect
- Compton effect

- Light exhibits diffraction and interference phenomena that are *only* explicable in terms of wave properties
- Light is always detected as packets (photons); if we look, we never observe half a photon
- Number of photons proportional to energy density (i.e. to square of electromagnetic field strength)

A SUMMARY OF DUAL ITY OF NATURE
Wave particle duality of physical objects

LIGHT

Wave nature -EM wave

Optical microscope

Interference

Particle nature -photons

Convert light to electric current

Photo-electric effect

PARTICLES

Wave nature

Matter waves -electron microscope

Discrete (Quantum) states of confined systems, such as atoms.

Particle nature

Electric current photon-electron collisions

Wave properties of Particles

Particles

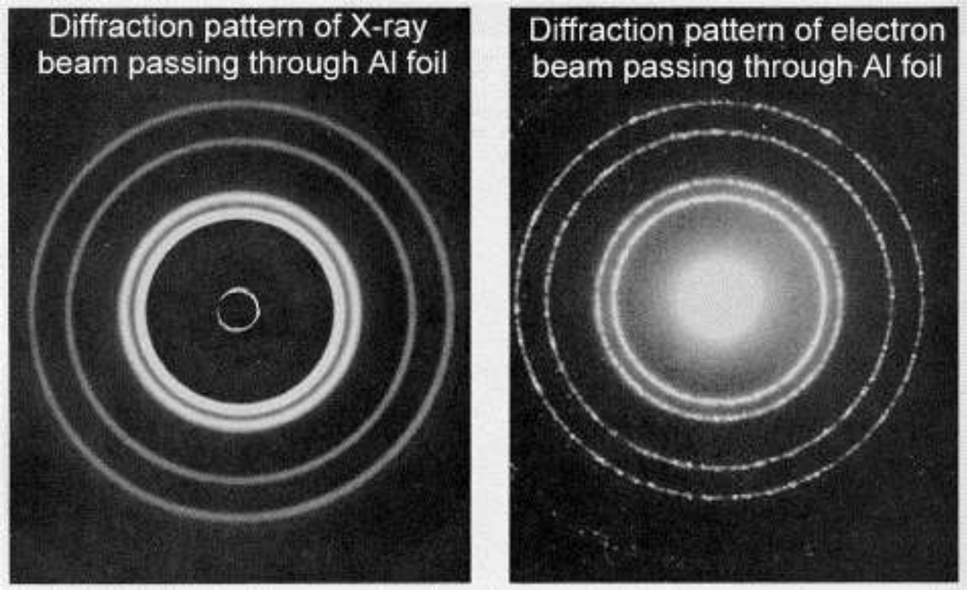
- Electrons as discrete Particles.
  - Measurement of *e* (oil-drop expt.) and *e/m* (e-beam expt.).
- Photons as discrete Particles.
  - Blackbody Radiation, Photoelectric Effect, Compton Effect

Waves

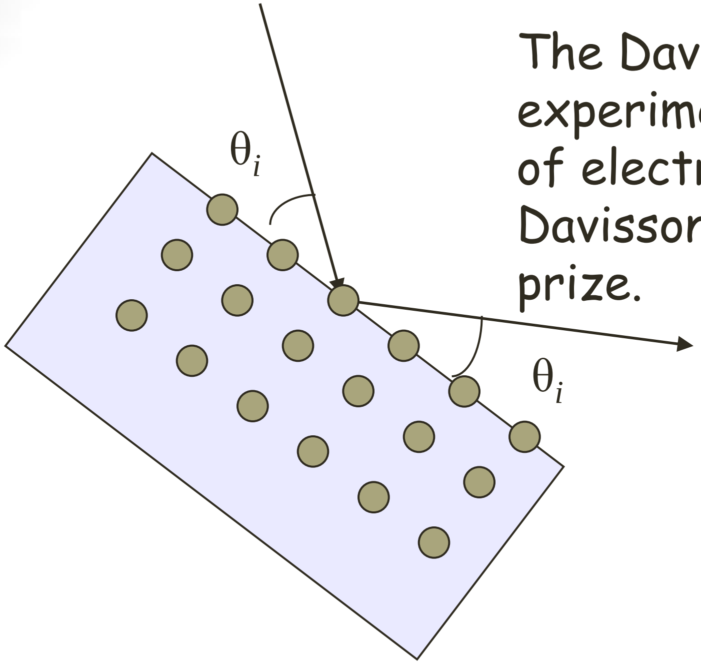
- Matter Waves
- Photons as Waves - Review: Interference and Diffraction,X-ray Diffraction (Bragg's Law)
- Electrons, neutrons as Waves

Electron Diffraction

- However, in a typical crystal lattice the interatomic spacing between atoms in the crystal is of order 10^{-10}m, and scattering a beam of electrons off a pure crystal produces an observable diffraction pattern
- this is what Davisson & Germer did in 1927 to confirm de Broglie's hypothesis

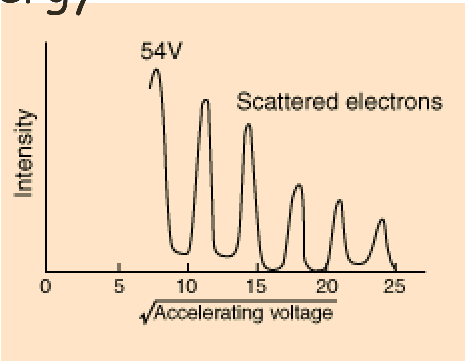


ELECTRON DIFFRACTION
The Davisson-Germer experiment (1927)



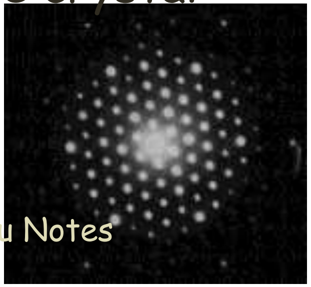
The Davisson-Germer experiment: scattering a beam of electrons from a Ni crystal. Davisson got the 1937 Nobel prize.

At fixed *angle*, find sharp peaks in intensity as a function of electron energy



Davisson, C. J., "Are Electrons Waves?," Franklin Institute Journal **205**, 597 (1928)

At fixed accelerating voltage (fixed electron energy) find a pattern of sharp reflected beams from the crystal



G.P. Thomson performed similar interference experiments with thin-film samples

Electron Diffraction

The confirmation of de Broglie's hypothesis of matter- waves and hence that of wave particle duality for matter was provided by Davisson-Germer's experiment on electron diffraction

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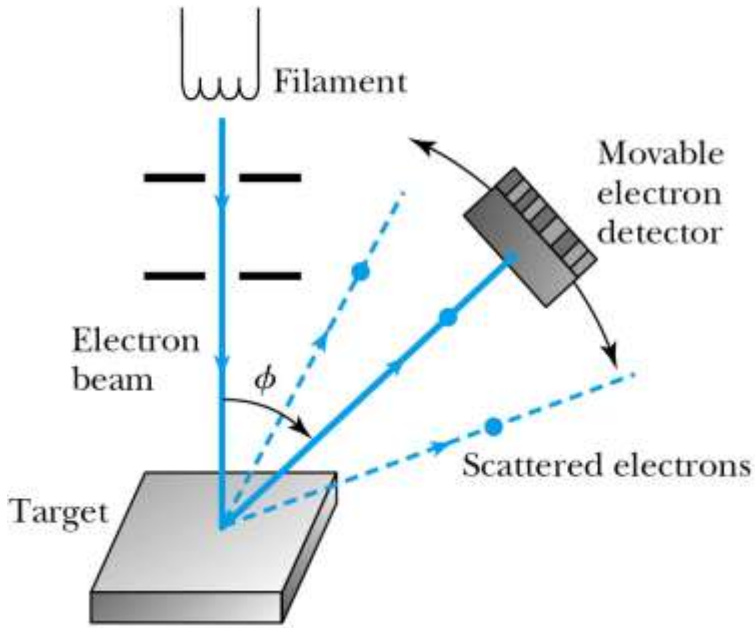
ELECTRON DIFFRACTION

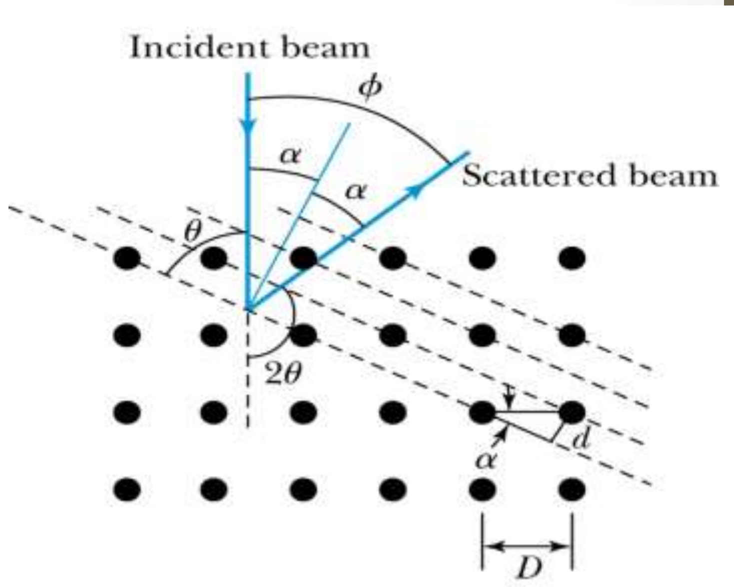
The scattered electron beam was found to have maxima and minima of intensity depending on electron energy for discrete scattering angles instead of continuous variation of intensity with an angle. This could be explained only as the consequence of diffraction of matter- waves associated with electrons. The wave length of these waves were determined from observation from calculations using l =

; both values were found to be in excellent agreement with each other.

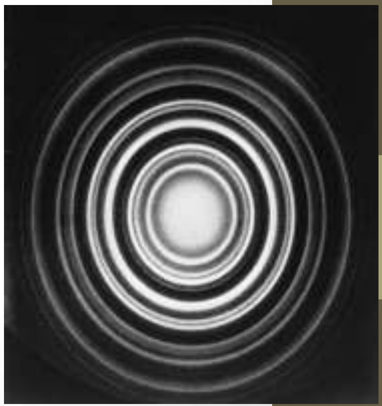
Electron Scattering

•In 1925, Davisson and Germer experimentally observed that **electrons** were diffracted (much like x-rays) in nickel crystals.



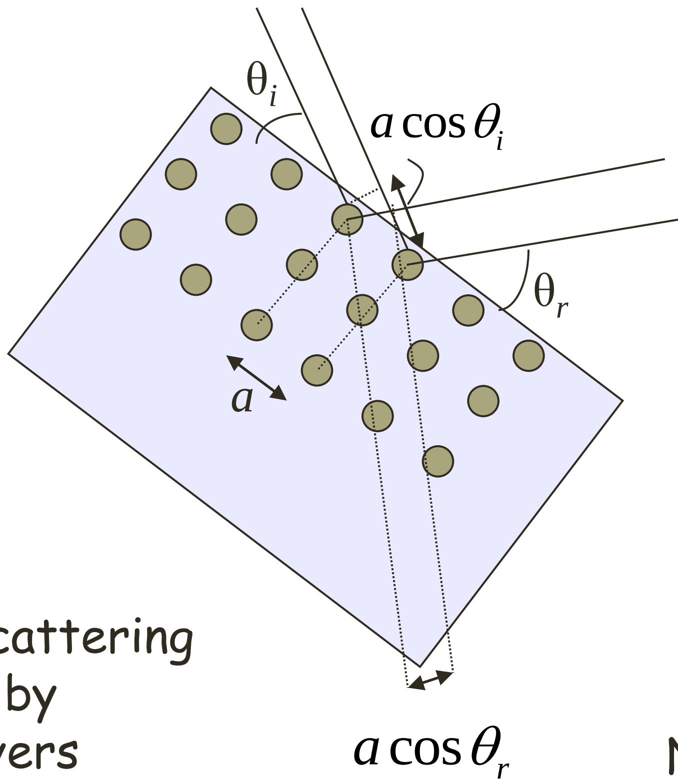


George P. Thomson (1892–1975), son of J. J. Thomson, reported seeing electron diffraction in transmission experiments on celluloid, gold, aluminum, and platinum. A randomly oriented polycrystalline sample of SnO_2 produces rings.



ELECTRON DIFFRACTION (cont)

Interpretation: similar to Bragg scattering of X-rays from crystals



Path difference:

$$a(\cos\theta_r - \cos\theta_i)$$

Constructive interference when

$$a(\cos\theta_r - \cos\theta_i) = n\lambda$$

Electron scattering dominated by *surface* layers

Note θ_i and θ_r not necessarily equal

Note difference from usual "Bragg's Law" geometry: the identical scattering planes are oriented *perpendicular* to the surface

Electron Diffraction

- an electron *is* a particle, but its dynamics (i.e. its motion) is governed by a *matter wave, or its so called wave function*

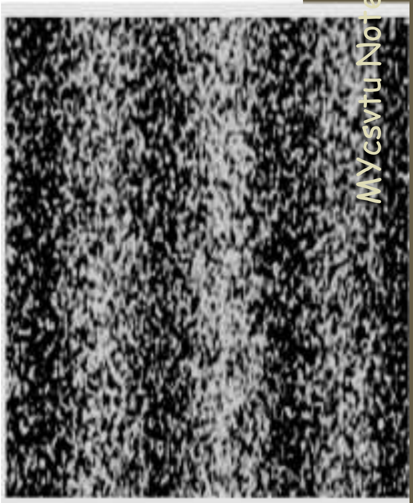
- the amplitude-squared of the electron's wave function is interpreted as the *probability* of the electron being at that location

- places where the amplitude are high (low) indicate a high (low) probability of finding the electron

- so when a single electron is sent at a double slit, its matter wave governs how it moves through the slit and strikes the screen on the other end:

- the *most probable* location on the screen for the electron to hit is where there is *constructive interference* in the matter wave (i.e., the bright fringes)

- conversely, at locations where there is destructive interference in the matter wave chances are small that the electron will strike the screen there.



(d) After 70 000 electrons

Energy quantization

- Quantum mechanical solution
  - Assume that each wave can only have an energy that is an integer multiple of a minimum energy
    - Thus short wavelength nodes have high energy, and there is not enough energy in the system (kT) to support even one node
  - In this case, the average energy per mode is not kT, but

Quantization of Energy

Energy of radiation is proportional to frequency.

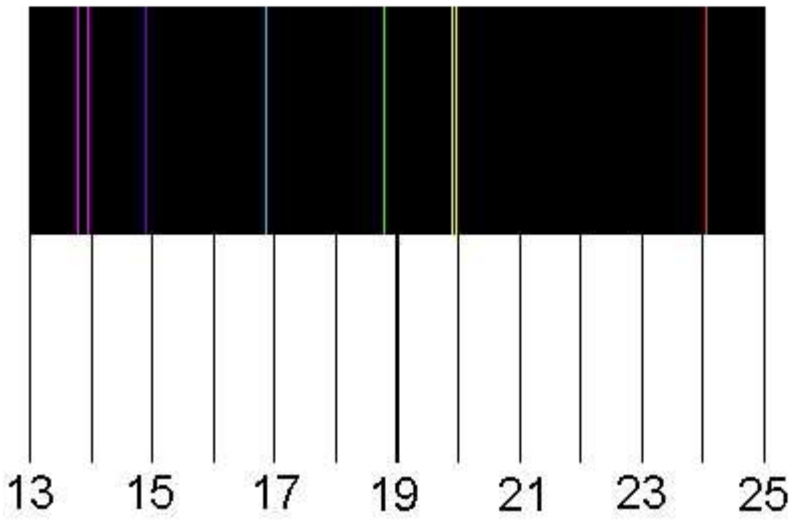
$$E = h \cdot \nu$$

where h = Planck's constant = 6.6262×10^{-34} J•s

Light with large l (small n) has a small E.

Light with a short l (large n) has a large E.

Atomic line spectra



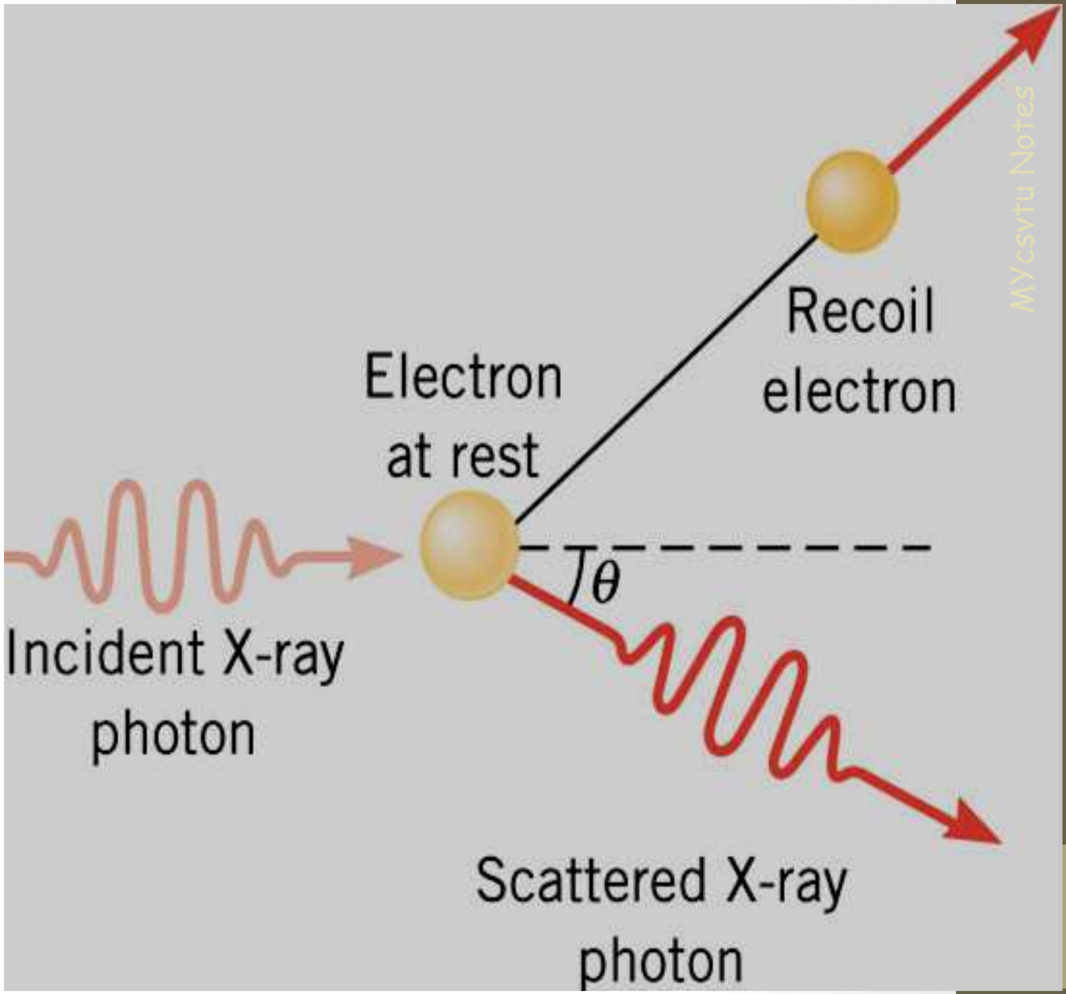
- Emission spectra from atoms show characteristic lines (unique to each atomic species)
- Spectral lines correspond to transitions between discrete atomic energy levels
- Wavelengths follow precise mathematical patterns
- Evidence for energy quantization
- Fine structure (splitting) of spectral lines is evidence of angular momentum quantization
- <<< Mercury emission spectrum

The concept of spin

- Stern-Gerlach results cannot be explained by interaction of magnetic moment from orbital angular momentum
- must be due to some additional internal source of angular momentum that does not require motion of the electron.
- internal angular momentum of electron ("spin") was suggested in 1925 by Goudsmit and Uhlenbeck building on an idea of Pauli.
- Spin is a relativistic effect and comes out directly from Dirac's theory of the electron (1928)
- spin has mathematical analogies with angular momentum, but is not to be understood as actual rotation of electron
- electrons have "half-integer" spin, i.e. $\hbar/2$
- Fermions vs Bosons

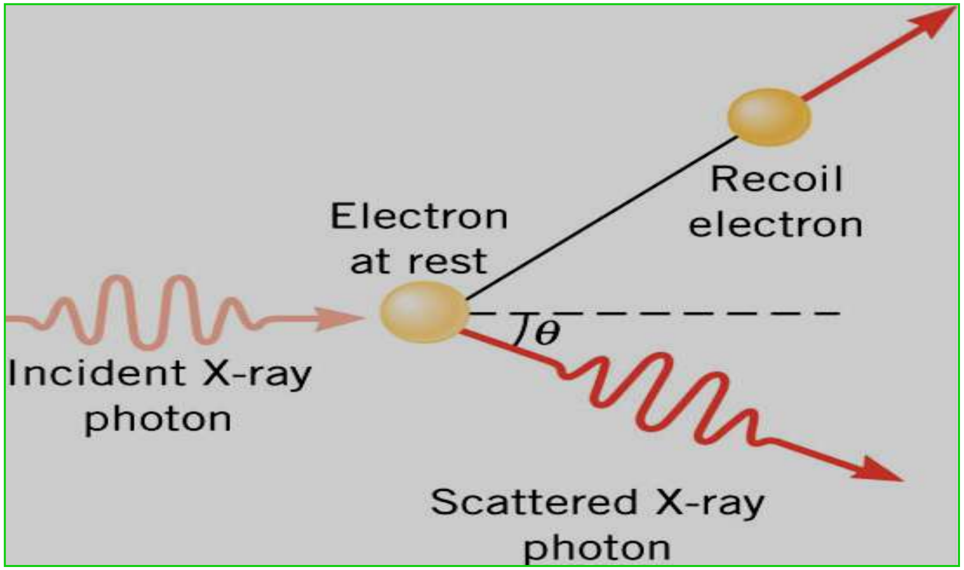
The Compton Effect

- the Compton effect is the scattering of a photon off of an electron that's initially at rest
- if the photon has enough energy (X-ray energies or higher), the scattering behaves like an *elastic collision* between particles
  - the energy and momentum of the system is conserved



The Compton Effect

- Since the photon is mass less, it *always* moves at the speed of light.
  - the photon *does* loose momentum and energy during the collision (giving it to the electron), consequently its *wavelength decreases*
  - the “reason” there is a deflection angle, is that otherwise it would be impossible for the system to conserve both energy and linear momentum



The Compton Effect

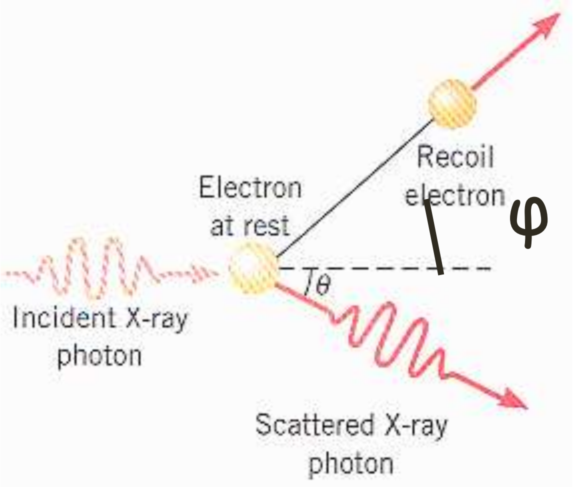
- The preceding is a rather messy set of equations to solve … here is the key result:

$$\lambda' - \lambda = \frac{h}{m_e c}\left(1 - \cos\theta\right)$$

- The quantity h/m *gth* of the electron, and has

The Compton Effect

Energy hv
Momentum hv/c



Energy hv'
Momentum hv'/c

The Compton Effect

Frequency of incident photon = v

Frequency of scattered photon = v'

Before Collision:

Energy of incident photon = hv

Momentum of incident photon = hv/c

Energy of the electron = m_0c^2

Momentum of rest electron = 0

After Collision:

Energy of scattered photon = hv'

Momentum of scattered photon = hv'/c

Energy of the electron = mc^2

Momentum of electron = mv, m is moving mass.

The Compton Effect

(1)When $\theta = 0$, $\lambda' - \lambda = 0$ or $\lambda' = \lambda$, there is no scattering along the direction of incidence.

(2) when $\theta = \pi/2$, $\lambda' - \lambda = h/m_0c = 0.02426 A^0$

(3)When $\theta = \pi$, $\lambda' - \lambda = 2h/m_0c = 0.04852 A^0$

i.e. When θ varies from 0 to π, the wavelength of scattered photon changes from λ to λ + 2h/m0c .

Matter Wave Cont

- $\psi = \psi_{real} + \psi_{imag}$, We cannot measure ψ but can measure
- $|\psi|^2 = \psi^* \psi$ = intensity of the matter wave - describes the prob of finding a particle at a particular location (& at a certain time)
- If ψ represent a single particle, $|\psi|^2$ is the probability density.
- Now (1-D case) since particle MUST be somewhere on x-axis this implies that the sum of probabilities over ALL values of x must be 1

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$$

$$\left[\begin{array}{l} \text{or generally} \\ \displaystyle\int_{\text{all space}} |\psi(r,t)|^2 \, d^3r = 1 \end{array} \right]$$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$$

That is, any wave function satifying

is said to be normalized & to fulfill the normilization condition

Wave Packets

A wave packet refers to the case where two (or more) waves exist simultaneously. A wave packet is often referred to as a wave group.

For linear system, we can apply the principle of superposition. This principle of superposition states that if any two waves are a solution to the wave equation then the sum of the waves is also a solution. Waves may therefore combine forming a wave packet .

The governing equations for fluid dynamics are nonlinear, but the perturbation method has neglected the products of the perturbation variables, the nonlinear governing equations are reduced to linear differential equations. So the principle of superposition can be applied.

WAVE FUNCTIONS, Ψ

- Ψ is a function of distance and two angles.
- For 1 electron, Ψ corresponds to an ORBITAL — the region of space within which an electron is found.
- Ψ does NOT describe the exact location of the electron.
- Ψ^2 is proportional to the probability of finding an e- at a given point.

The group velocity of a wave is the velocity with which the overall shape of the wave's amplitude (known as the envelope of the wave) propagates through space. The group velocity is defined in terms of the wave's frequency *ω* and wave number *k* by

$$\vec{c}_g = (\partial\omega/\partial k, \partial\omega/\partial l)$$

i.e. $\vec{c}_g$ is the gradient of the frequency ω in wavenumber plane.

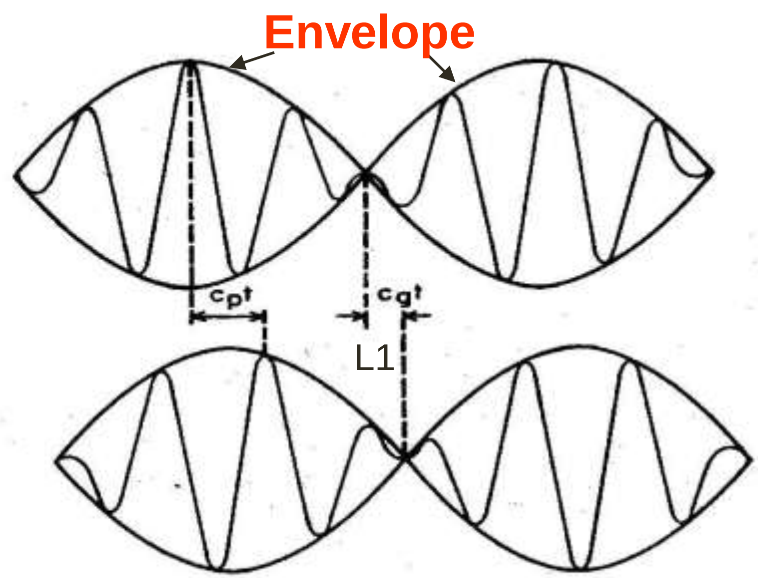


Fig. 5.7. A superposition of two sinusoidal traveling waves, illustrating the difference between the speed c_p of the wave crests and the speed c_g of the envelope of the waves, i.e., of the regions of large amplitude. The group velocity c_g equals $d\omega/dk$, which in this case is equal to $\frac{1}{2}c_p$ as for deep-water waves.

Matter Wave of a Single Electron

- described by y
- amplitude of y at any point is related to the probability of finding the particle at that point
- In analogy to $\mathbf{E^2}$, the quantity $|y|^2$ is proportional to the probability of detecting an electron in a unit volume of space
- $|y|^2$ is defined as y^*y, where y^* is the complex conjugate of y.
- In 1-D, $|y|^2dx$ is the probability of an electron being in dx. That is, P(x)dx. Where P(x) is the probability distribution function.
- Thus, $P(x)dx = |y|^2dx$
- Although amplitudes of y has no simple physical meaning, the waves behave just like classical waves exhibiting wave properties such as reflection, refraction, interference & obeying the principles of superposition.

Probability, Wave Functions, and the Copenhagen Interpretation

- The wave function determines the likelihood (or probability) of finding a particle at a particular position in space at a given time:

$$P(x) = |\Psi(x)|^2$$

- The probability of the particle being between x_1 and x_2 is given by:

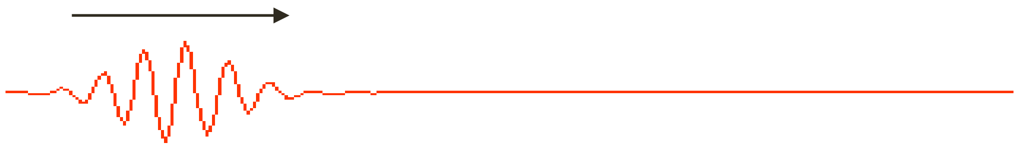
$$\int_{x_1}^{x_2} |\Psi(x)|^2 \, dx$$

- The total probability of finding the particle is 1. Forcing this condition on the wave function is called normalization.

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = 1$$

A localized wave or wave packet:

A moving particle in quantum theory



Spread in position

Spread in momentum

Superposition of waves of different wavelengths to make a packet

Narrower the packet , more the spread in momentum

Basis of Uncertainty Principle

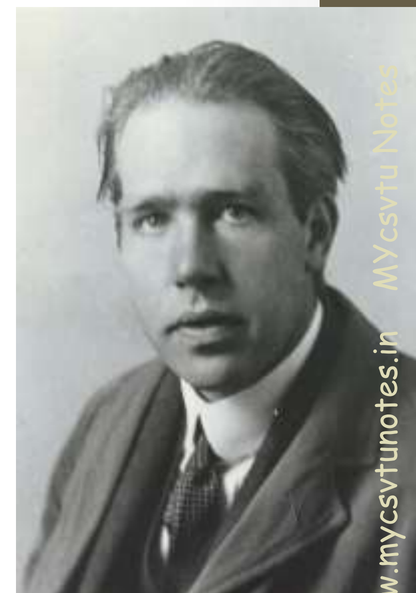
Quantum Uncertainty

The wavelike nature of particles is summarized in the famous **Heisenberg Uncertainty Principle**, which states that position and momentum cannot be known to arbitrary precision simultaneously:

$$(\Delta x) \cdot (\Delta p) > h$$

h is Planck's constant, a fundamental constant of nature.

Werner Heisenberg
(1901-1976)



Niels Bohr
(1885-1962)

Uncertainty Principle

W. Heisenberg
1901-1976

Problem of defining nature of electrons in atoms solved by W. Heisenberg.

Cannot simultaneously define the position and momentum (= m•v) of an electron.

$$\Delta x . \Delta p = h$$

At best we can describe the position and velocity of an electron by a

PROBABILITY DISTRIBUTION, which is given by Ψ^2

Uncertainty principle

- **Uncertainty principle**: (Werner Heisenberg, 1925)
  - it is impossible to simultaneously know a particle's exact position and momentum

    $\Delta p \cdot \Delta x \geq \hbar = h/(2\pi)$

    $h = 6.63 \times 10^{-34}$ J · s = 4.14×10^{-15} eV·s

    $\hbar = 1.055 \times 10^{-34}$ J · s = 6.582×10^{-16} eV·s

    (Δp means "uncertainty" in our knowledge of the momentum p)
  - also corresponding relation for energy and time:

    $\Delta E \cdot \Delta t \geq \hbar = h/(2\pi)$
- note that *there are many such uncertainty relations in quantum mechanics, for any pair of "incompatible"*

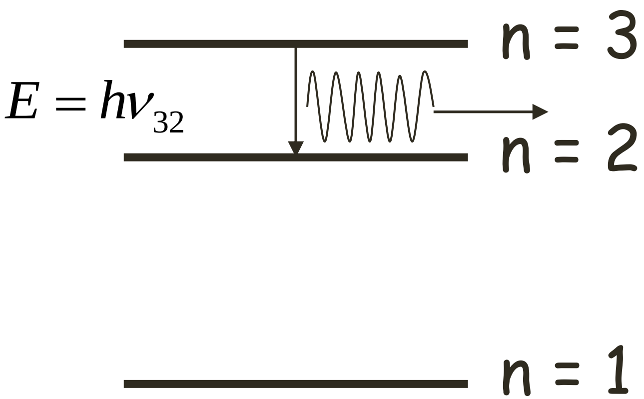
  (non-commuting) observables.
- in general, $\Delta P \cdot \Delta Q \geq \frac{1}{2} \left| \langle [P,Q] \rangle \right|$
  - [P,Q] = "commutator" of P and Q, = PQ – QP
  - $\langle A \rangle$ denotes "expectation value"

HEISENBERG UNCERTAINTY PRINCIPLE

There is also an energy-time uncertainty relation

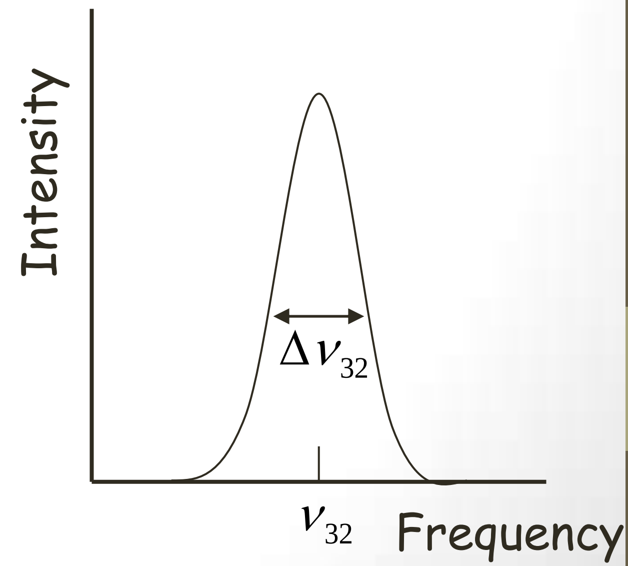
$$\Delta E \Delta t \geq \hbar / 2$$

Transitions between energy levels of atoms are not perfectly sharp in frequency.



An electron in $n = 3$ will spontaneously decay to a lower level after a lifetime of order $t \sim 10^{-8}$ s

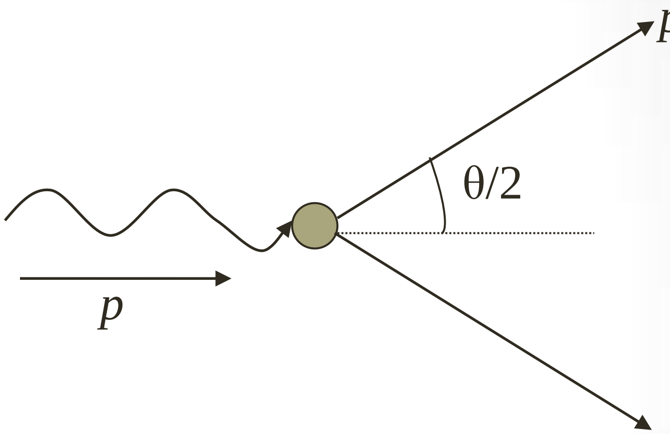
There is a corresponding 'spread' in the emitted frequency



HEISENBERG MICROSCOPE (cont)

Photons transfer momentum to the particle when they scatter.

Magnitude of p is the same before and after the collision. Why?



Uncertainty in *photon* y-momentum
= Uncertainty in *particle* y-momentum

$$-p\sin(\theta/2) \le p_y \le p\sin(\theta/2)$$

Small angle approximation

$$\Delta p_y = 2p\sin(\theta/2) \approx p\theta$$

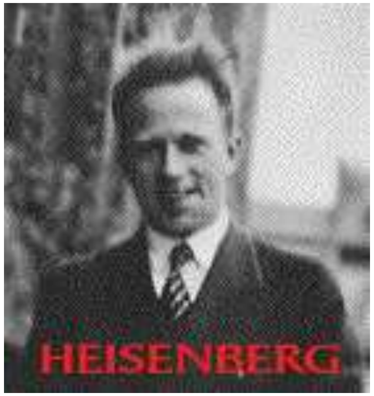
de Broglie relation gives $p = h/\lambda$ and so $\Delta p_y \approx \dfrac{h\theta}{\lambda}$

From before $\Delta y \ge \dfrac{\lambda}{\theta}$ hence

$$\Delta p_y \Delta y \approx h$$

HEISENBERG UNCERTAINTY PRINCIPLE.

ILLUSTRATION OF MEASUREMENT OF ELECTRON POSITION



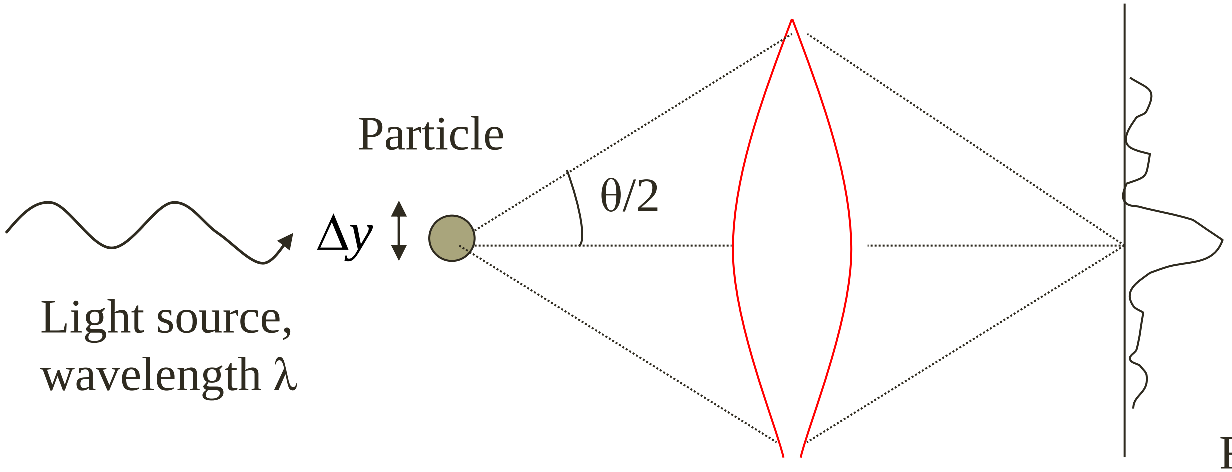
Act of measurement influences the electron -gives it a kick and it is no longer where it was ! Essence of uncertainty principle.

HEISENBERG MICROSCOPE AND THE UNCERTAINTY PRINCIPLE

(also called the Bohr microscope, but the thought experiment is mainly due to Heisenberg).

The microscope is an imaginary device to measure the position (y) and momentum (p) of a particle.

Heisenberg



Resolving power of lens:

$$\Delta y \geq \frac{\lambda}{\theta}$$

X-Rays

- Electromagnetic radiation with short wavelengths
  - Wavelengths less than for ultraviolet
  - Wavelengths are typically about 0.1 nm
  - X-rays have the ability to penetrate most materials with relative ease
- Discovered and named by Roentgen in 1895

X-rays

When a beam of fast moving electrons strikes a solid target, an invisible high penetrating radiation is produced. Because of their unknown nature, these radiations are called as X-rays.

Properties of X-rays

1. X-rays are electromagnetic waves of very short wavelength. They travel in straight lines with the velocity of light.
2. Under suitable conditions, x-rays are reflected and refracted like ordinary light.
3. They exhibit the property of interference, diffraction and polarization.
4. X-rays are not deflected by electric and magnetic fields.
5. X-rays penetrate through the substances like wood, flesh, thick paper, thin sheets of metals.
6. They cause fluorescent in many substances like Ba,Cd,W,ZnS, etc.
7. X-rays can ionize a gas through which they pass.
8. when x-rays falls on certain metals, they liberate photo electron (photo-electric effect).
9. X-rays have destructive effect on living tissues.

Production of X-rays

X-rays are produced when fast moving electrons strike a target of suitable material.

Requirement of production are:

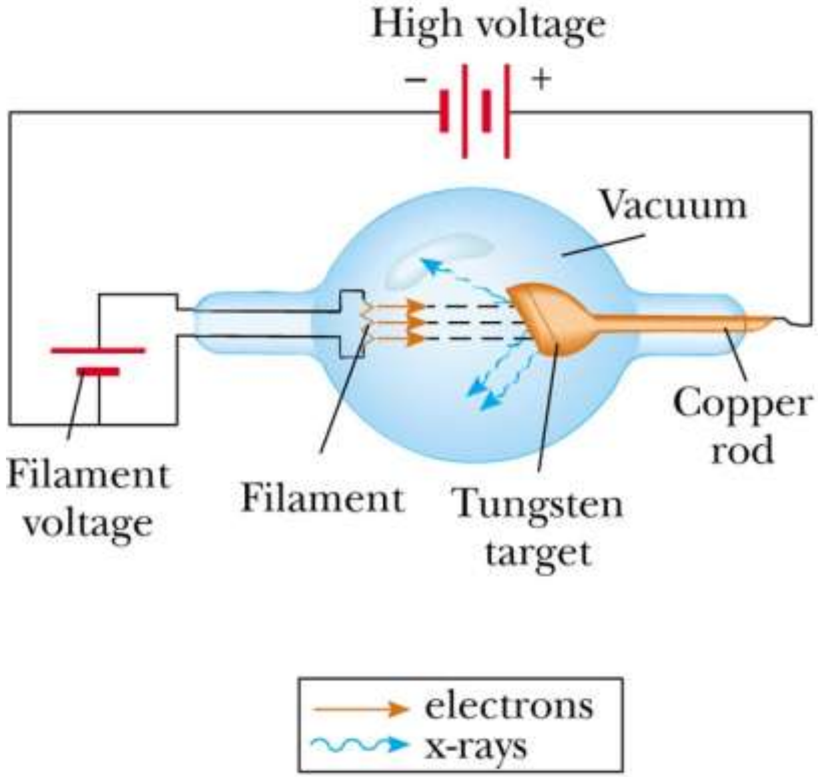
(1)A source of electrons.

(2)Effective means of accelerating the electrons.

(3)A target of suitable material of high atomic number, high melting point, high thermal conductivity.

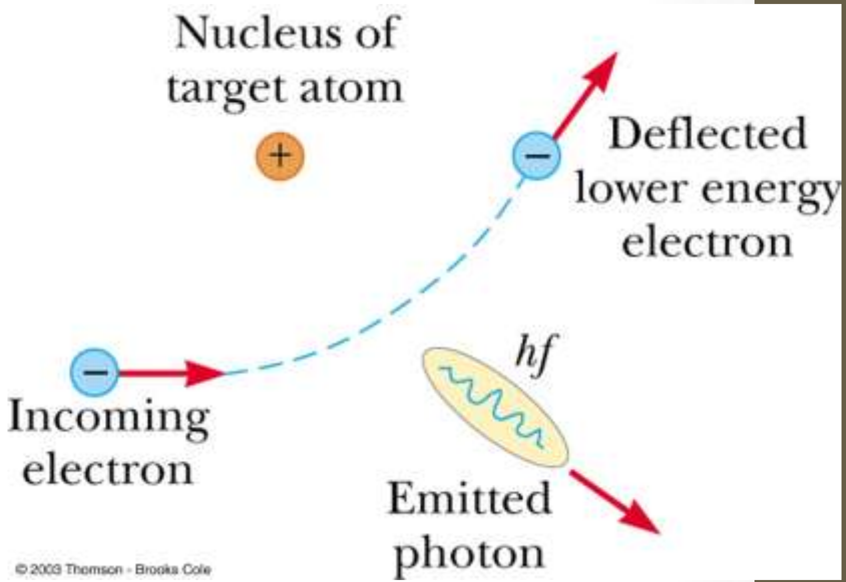
Production of X-rays, 1

- X-rays are produced when high-speed electrons are suddenly slowed down
  - Can be caused by the electron striking a metal target
- A current in the filament causes electrons to be emitted
- These freed electrons are accelerated toward a dense metal target
- The target is held at a higher potential than the filament



Production of X-rays, 2

- An electron passes near a target nucleus
- The electron is deflected from its path by its attraction to the nucleus
  - This produces an acceleration
- Due to the acceleration, the electron emits electromagnetic radiation → x-rays



In case that all the energy of the electron is transformed in emission, one gets:

$$eV = hf_{max} = hc/\lambda_{min}$$

Origin of X-rays

The loss of the kinetic energy of the electrons is responsible for the production of x-rays.

This loss is of two types:

Type-I (characteristic x-ray spectra)

- Few of fast moving electrons having velocity about $1/10^{th}$ of velocity of light may penetrate the surface atoms of the target material and knock out the tightly bound electrons from the inner most shells.
- Vacancies so created may be filled up by the electrons from higher shells.

Origin of X-rays
CHARACTERISTICS

- Electrons from higher energy levels jump to fill the created vacancies.
- The energy difference is radiated in the form of X-rays of very small but definite wavelength.
- The X-rays spectra consists of sharp lines and the characteristic of target material.
- Due to this fact it is called as characteristic spectra or line spectra.

Origin of X-rays

Type-II (continuous X-ray spectra)

- A few fast moving electrons penetrate deep into the interior of the atoms of the target material and are attracted by the attractive forces, the electron get deflected from their original paths.
- The electrons are deaccelerated.
- Their velocity is reduced by and give rise to loss of energy.
- The loss of energy during retardation is given off in the form of electromagnetic radiation i.e. X-rays of continuously varying wavelength.

Origin of X-rays

- The X-rays consists of continuous range of frequencies up to maximum frequency V_{max} or minimum wavelength λ_{min}, called as continuous X-ray spectrum.
- When the velocity of the electron changes from v to v' due to retardation, energy of radiated photon is

$$hv = mv^2/2 - mv'^2/2$$

- The liberated photon has maximum frequency, when the electron is completely brought to rest by nuclear forces.

$$mv^2/2 = hv_{max} = hc/\lambda_{min}$$

- The kinetic energy of elctron having charge e, accelerated by potential V is

$$mv^2/2 = e\,V$$

Moseley's Law

In 1913-1914, Moseley carried out an systematic study of characteristic X-rays spectra of various metallic elements, He found the following facts:

(1)The characteristic X-ray spectra of different elements are similar to each other in the sense that each consists of K, L, M series.

(2)The frequency of the lines produced from an element of higher atomic number is greater than that produced by an element of lower atomic number.

Moseley's Law

Mathematically ,the relation between frequency and atomic number is given by

$$v \alpha (Z - a)^2$$

Where v= frequency of characteristic radiation,

Z=Atomic number of element

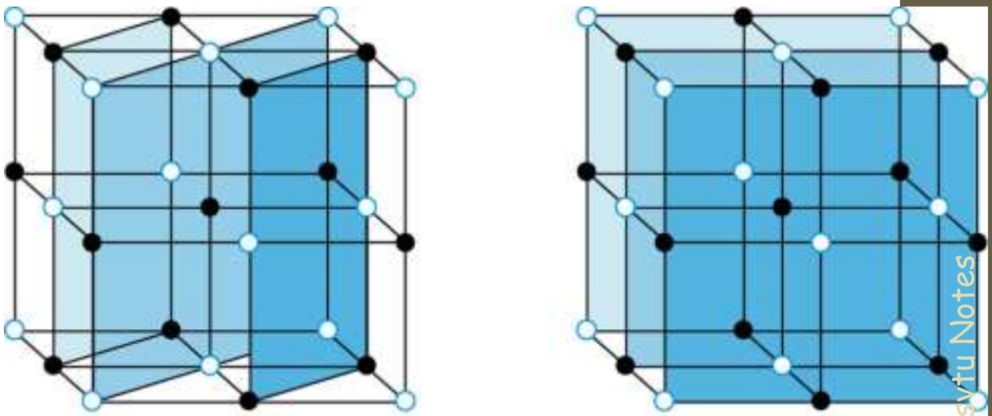
a= constant, known as screening constant and is different for different series.

b= constant, which is different for different series.

Bragg's Law

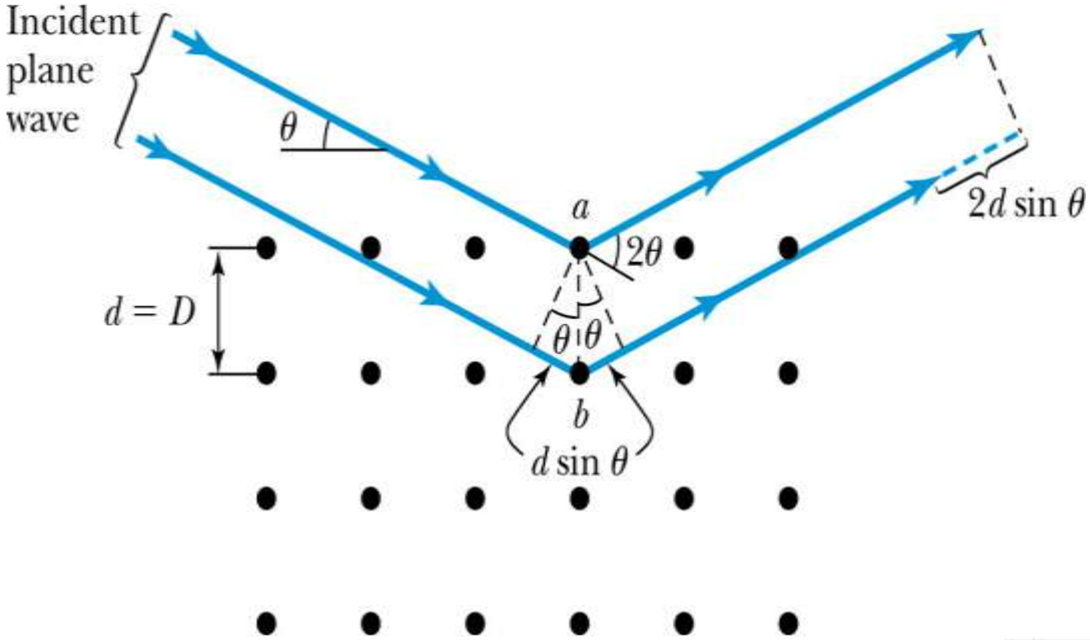
William Lawrence Bragg interpreted the x-ray scattering as the reflection of the incident x-ray beam from a unique set of planes of atoms within the crystal.

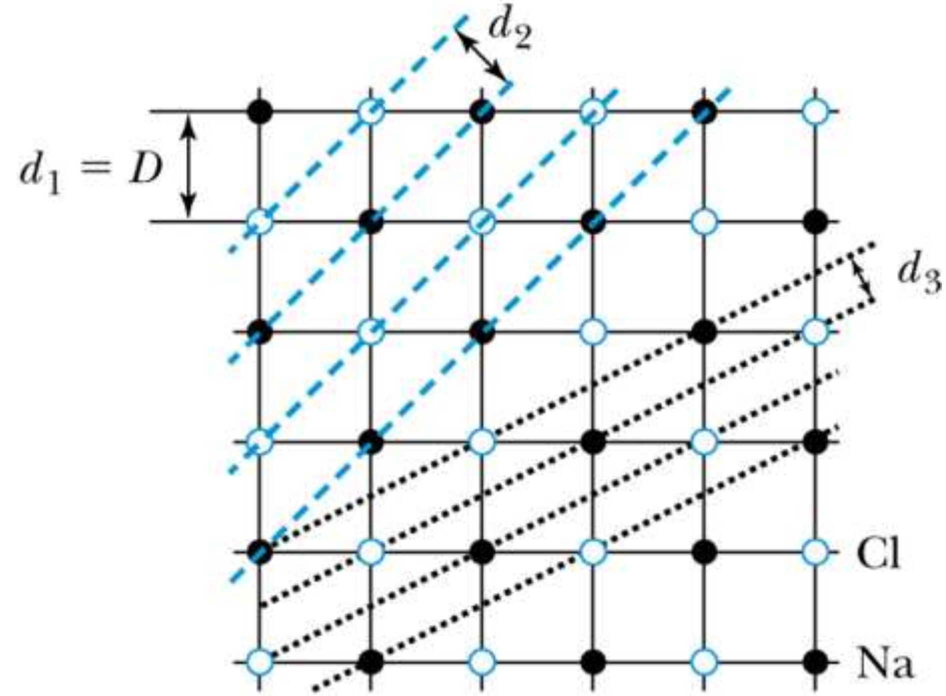
There are two conditions for constructive interference of the scattered x rays:



1) The angle of incidence must equal the angle of reflection of the outgoing wave.
2) The difference in path lengths must be an integral number of wavelengths.

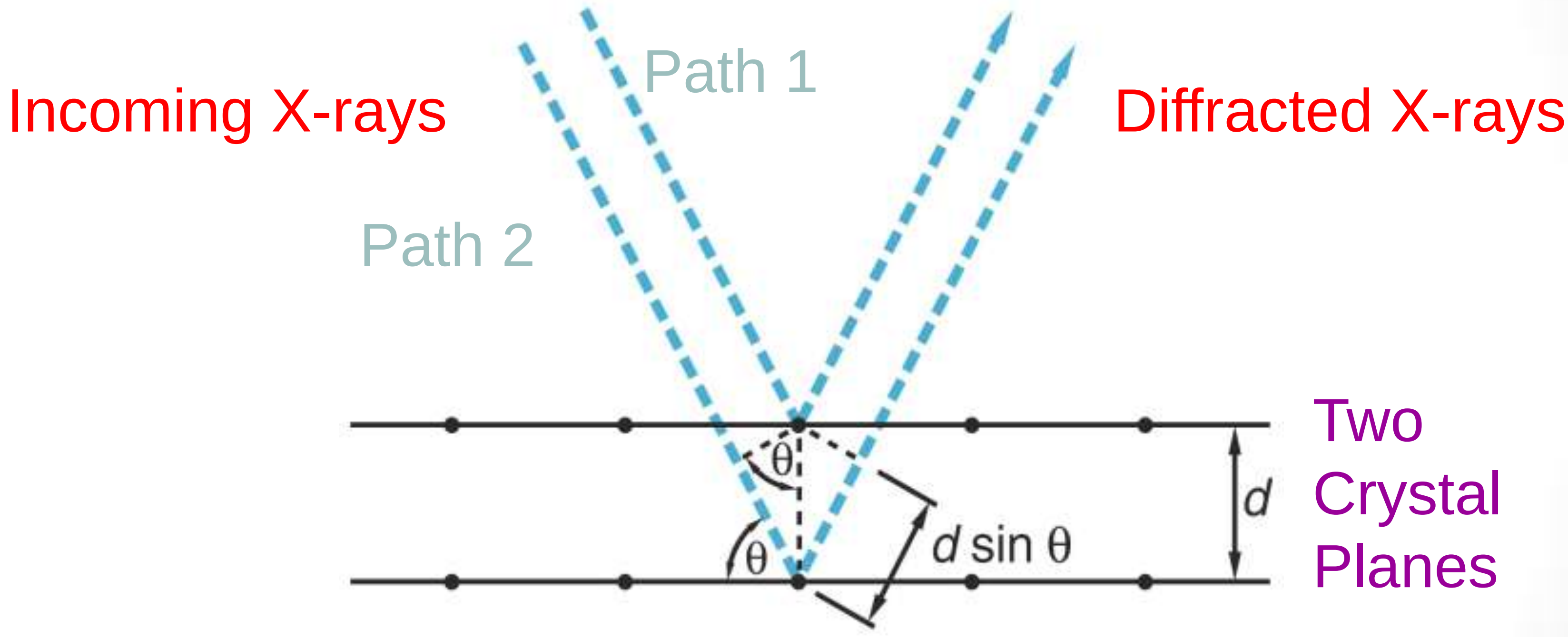
Bragg's Law: $n\lambda = 2d \sin \theta$
(n = integer)


Incident
plane
wave
θ
a
2θ
2d sin θ
d = D
θ θ
b
d sin θ


d2
d1 = D
d3
Cl
Na

X-ray Diffraction: Bragg's Law

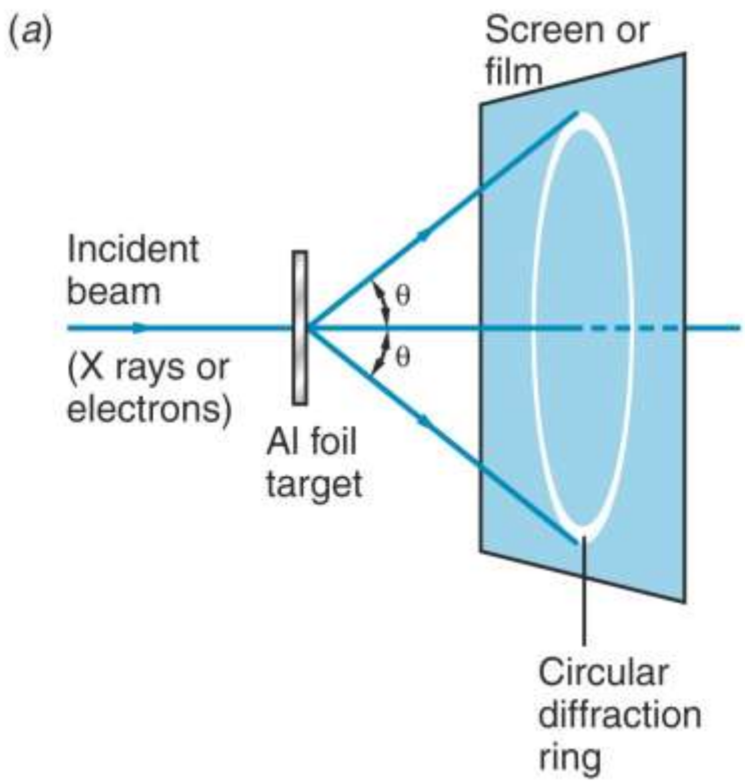
- diffraction maxima (or peaks)are observed for a path difference (2dsinθ) equal to an integer multiples of a wavelength (nλ).

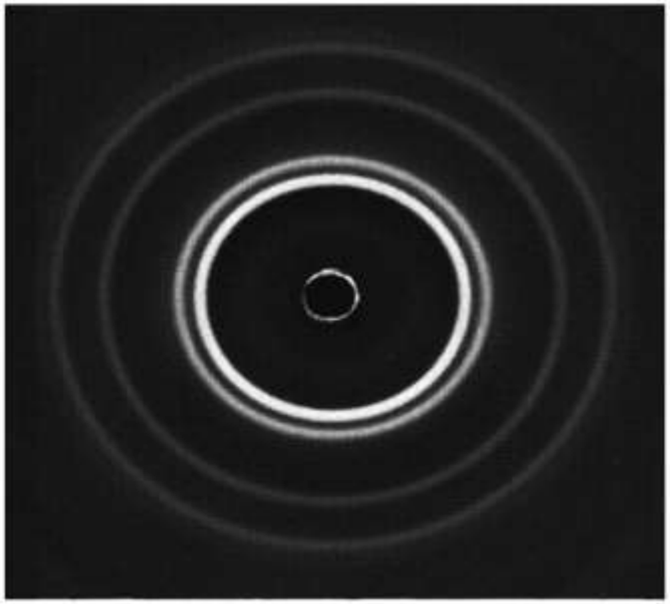


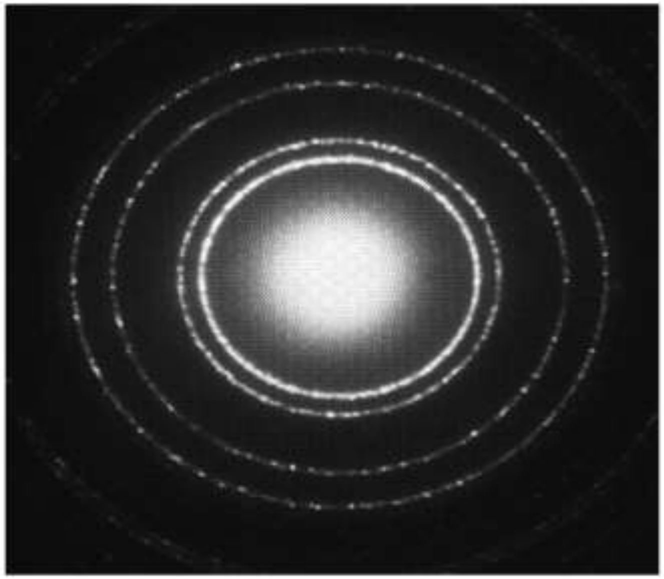
Path Difference = $$n\lambda = 2d \sin\theta$$

Diffraction Patterns

X-rays





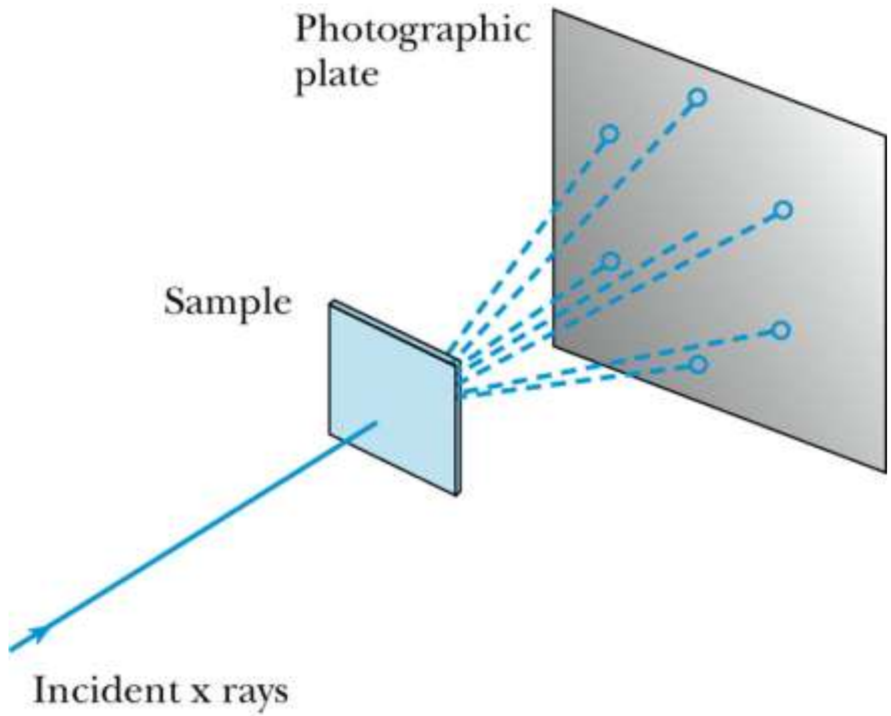


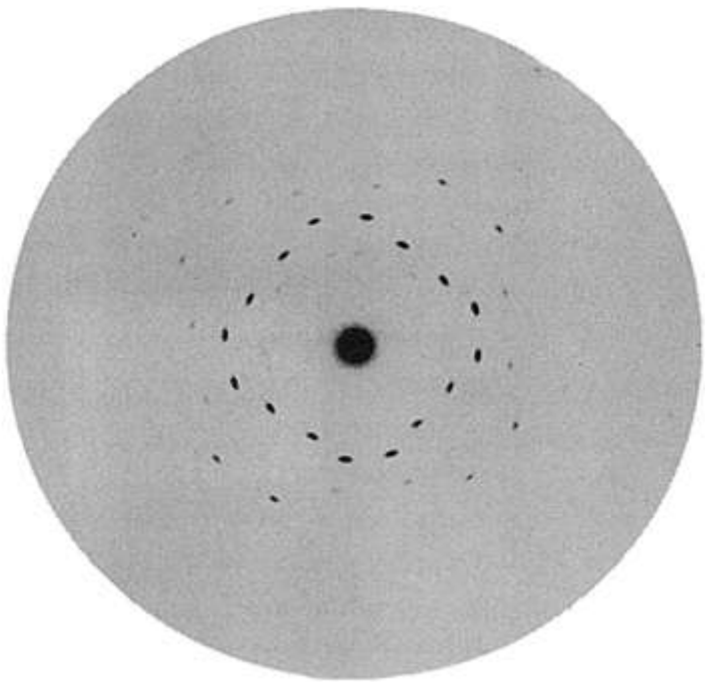
600 eV e^-

X-Ray Scattering

➢Max von Laue suggested that if x-rays were a form of electromagnetic radiation, interference effects should be observed.

➢Crystals act as three-dimensional gratings, scattering the waves and producing observable interference effects.

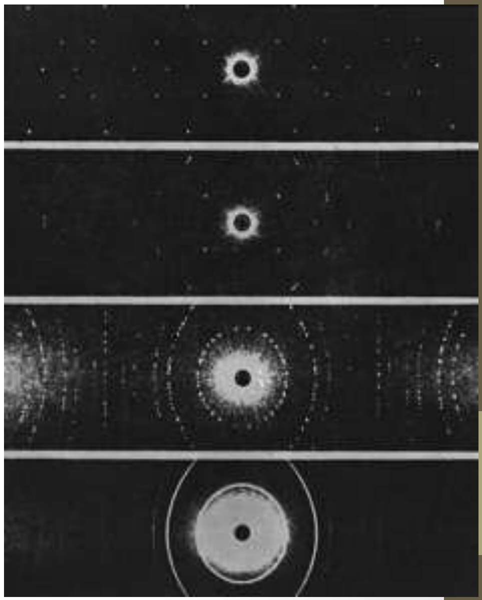




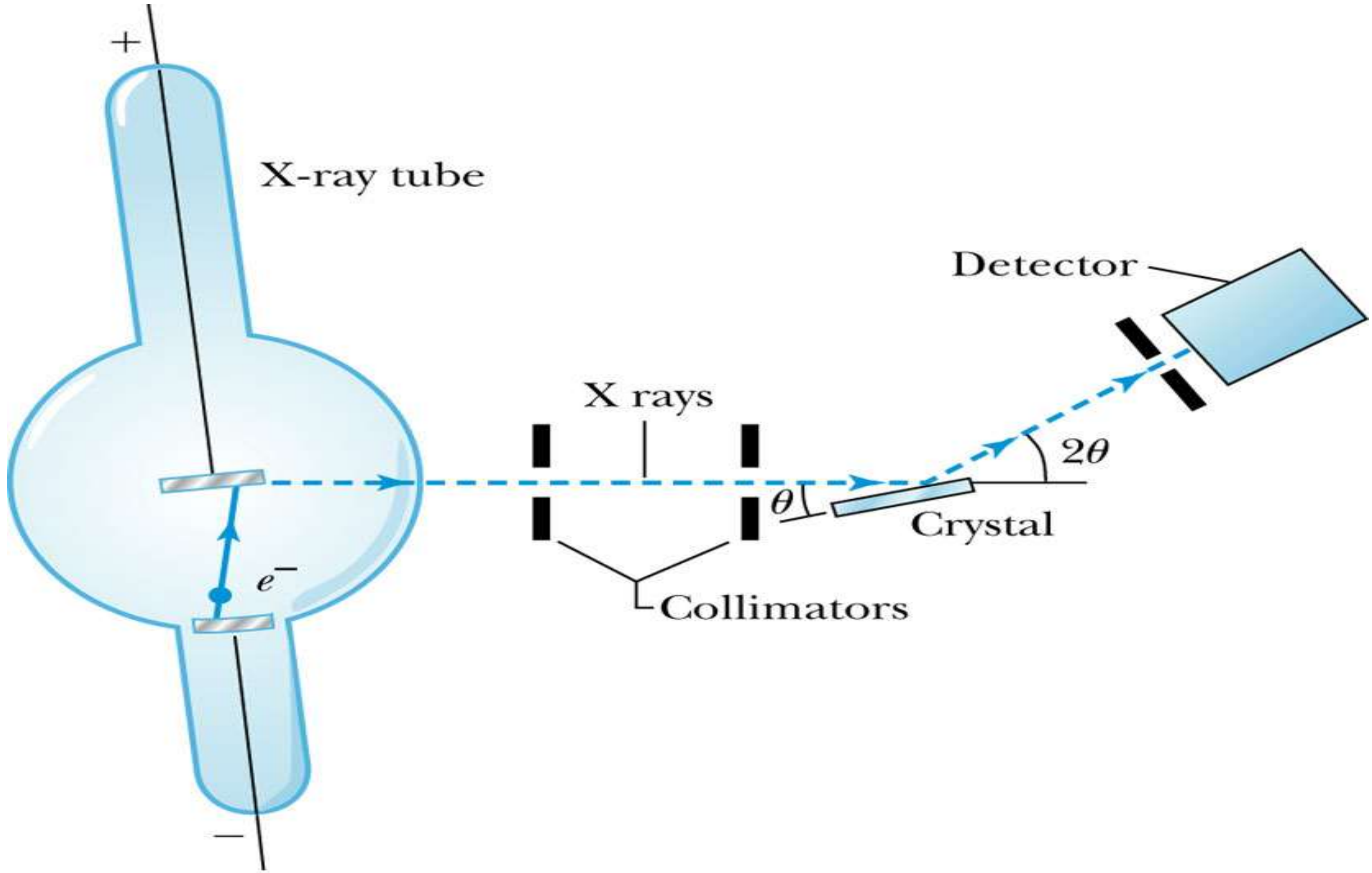
The Bragg Spectrometer

A Bragg spectrometer scatters x rays from crystals. The intensity of the diffracted beam is determined as a function of scattering angle by rotating the crystal and the detector.

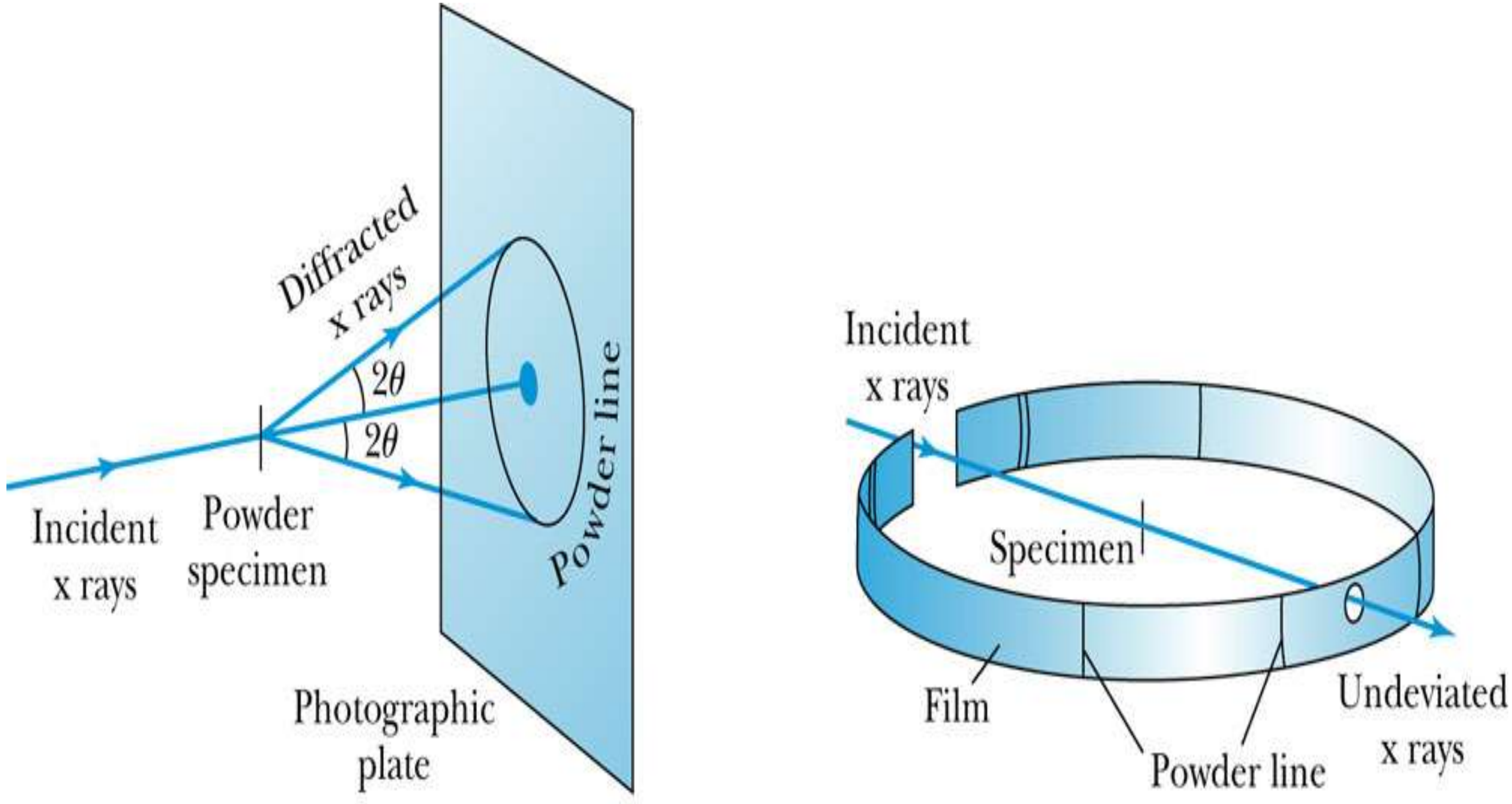
When a beam of x rays passes through a powdered crystal, the dots become a series of rings.



The Bragg Spectrometer

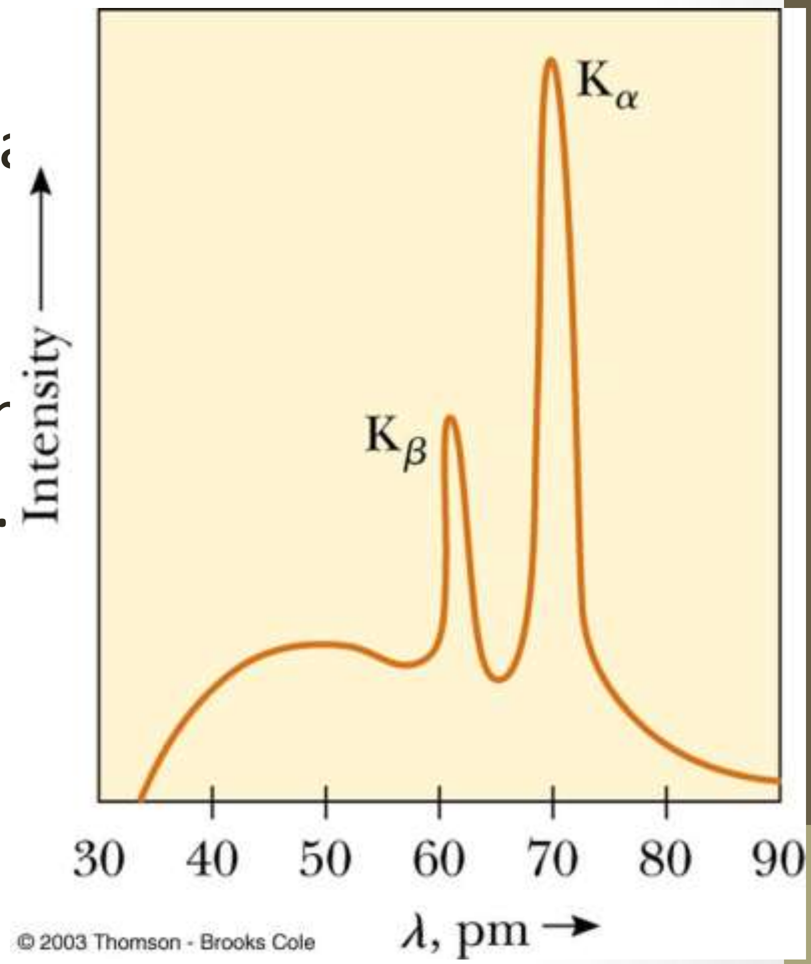


The Bragg Spectrometer



X-ray Spectrum

- The x-ray spectrum of a meta target consists of a broad continuous spectrum plus a number of sharp lines, which are due characteristic x-rays. The spectrum shown is obtained when 35 kV electrons bombarded a molybdenum target



Diffraction of X-rays by Crystals

- For diffraction to occur, the spacing between the lines must be approximately equal to the wavelength of the radiation to be measured
- For x-rays, the regular array of atoms in a crystal can act as a three-dimensional grating for diffracting x-rays

Schematic for X-ray Diffraction

- A continuous beam of x-rays is incident on the crystal
- The diffracted radiation is very intense in certain directions
    - These directions correspond to constructive interference from waves reflected from the layers of the crystal
- The diffraction pattern is detected by a photographic film

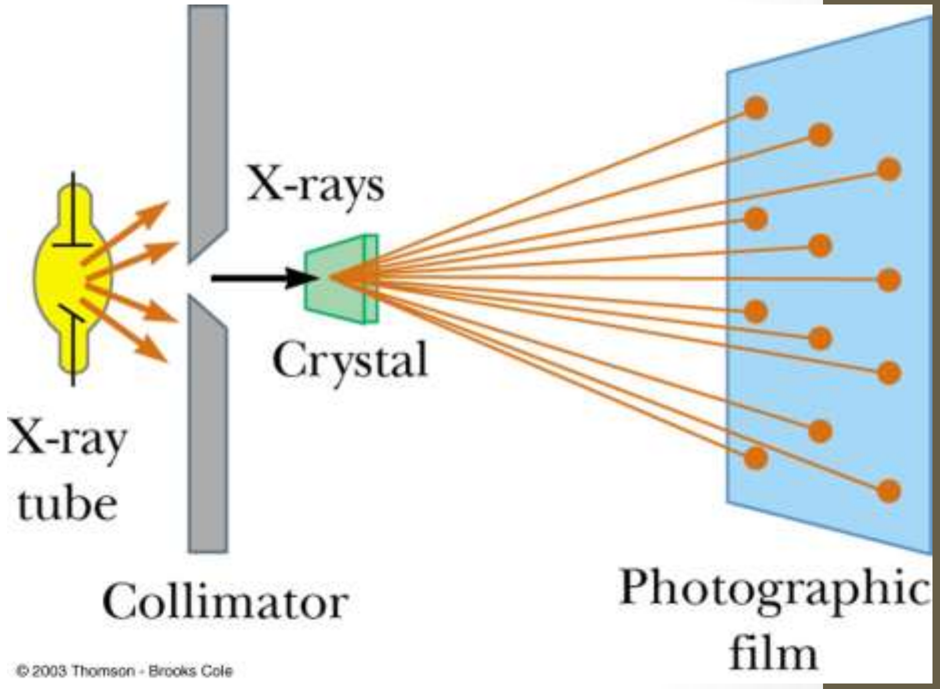
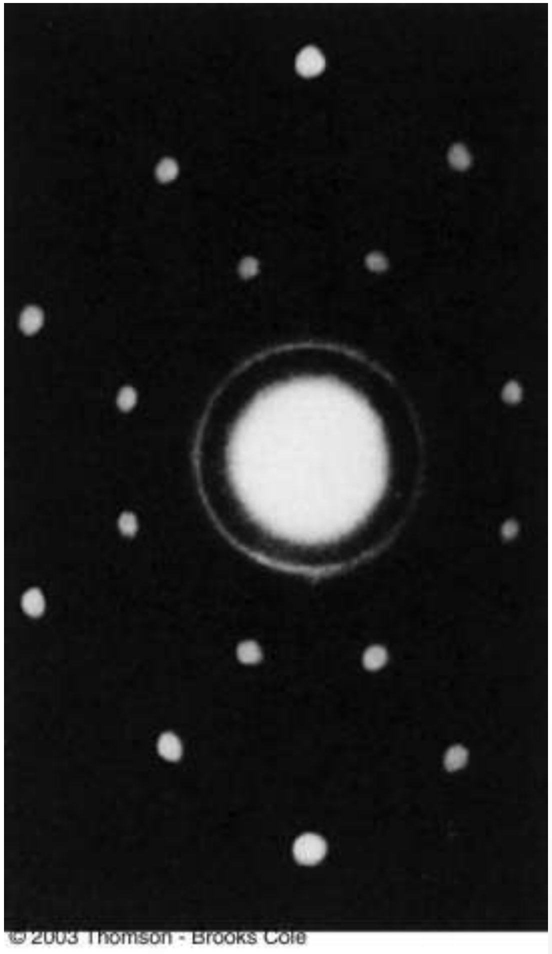


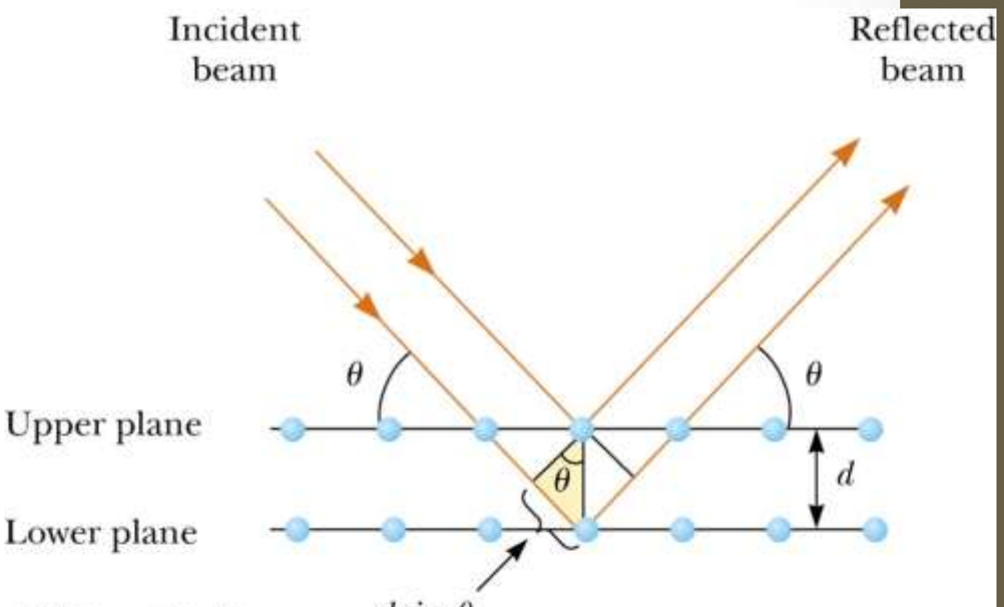
Photo of X-ray Diffraction Pattern

- The array of spots is called a *Laue* pattern
- The crystal structure is determined by analyzing the positions and intensities of the various spots
- This is for NaCl



Bragg's Law

- The beam reflected from the lower surface travels farther than the one reflected from the upper surface
- If the path difference equals some integral multiple of the wavelength, constructive interference occurs
- *Bragg's Law* gives the conditions for constructive interference

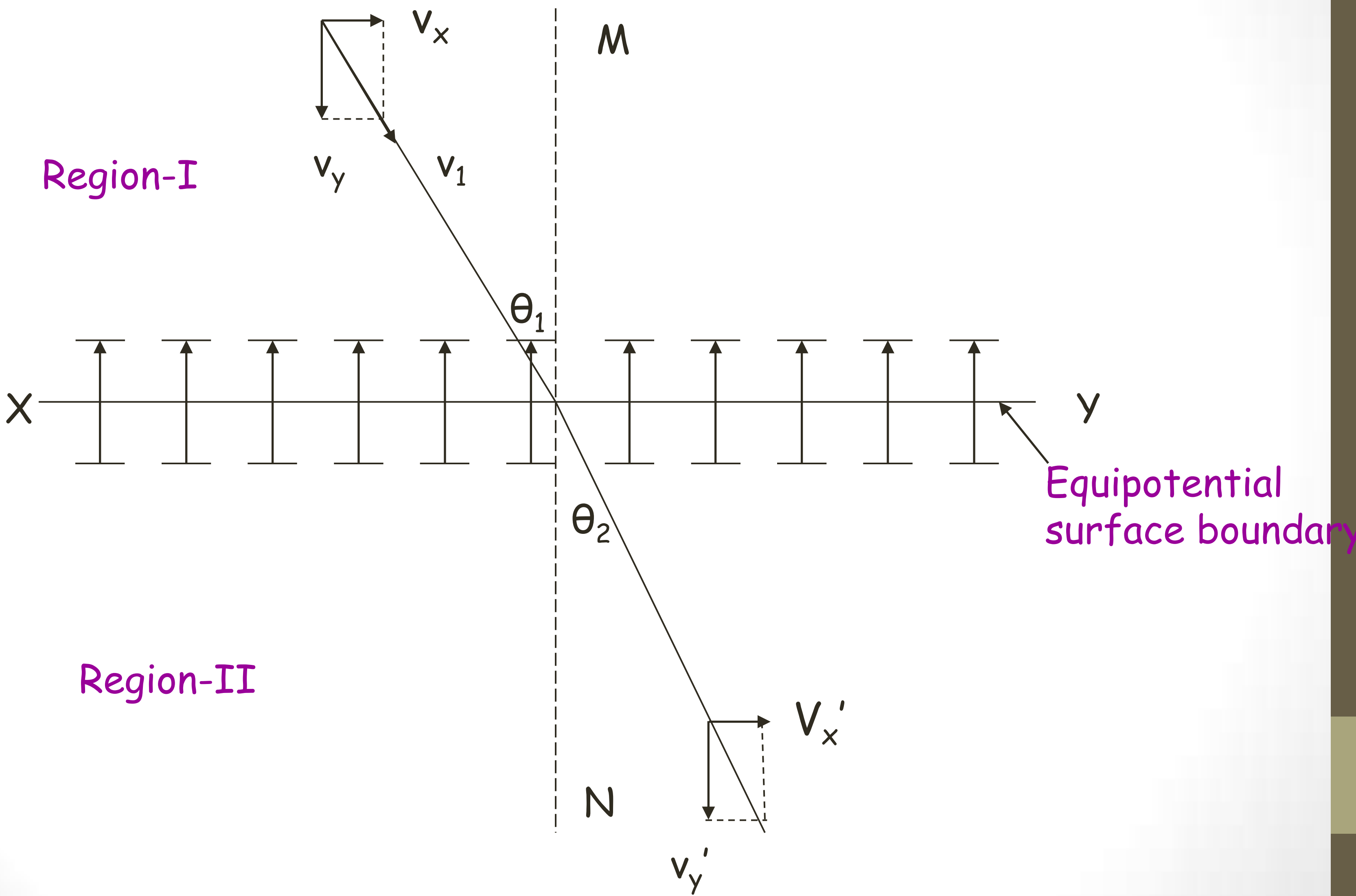


Bragg's law:
$2\, d \sin \theta = m \lambda$
$m = 1, 2, 3...$

Bethe's Law of Electron Refraction

When an electron or stream of electrons travels from a region of lower potential to a region of higher potential, its path bends at the boundary separating the two regions towards the normal in the higher potential region, known as electron refraction.

Bethe's Law of Electron Refraction



CONCLUSIONS

Light and matter exhibit wave-particle duality

Relation between wave and particle properties given by the de Broglie relations

$$E = h\nu \qquad p = \frac{h}{\lambda}$$

Evidence for particle properties of light
Photoelectric effect, Compton scattering

Evidence for wave properties of matter
Electron diffraction, interference of matter waves (electrons, neutrons, He atoms, C60 molecules)

Heisenberg uncertainty principle limits simultaneous knowledge of conjugate variables

$$\Delta x \Delta p_x \geq \hbar / 2$$
$$\Delta y \Delta p_y \geq \hbar / 2$$
$$\Delta z \Delta p_z \geq \hbar / 2$$