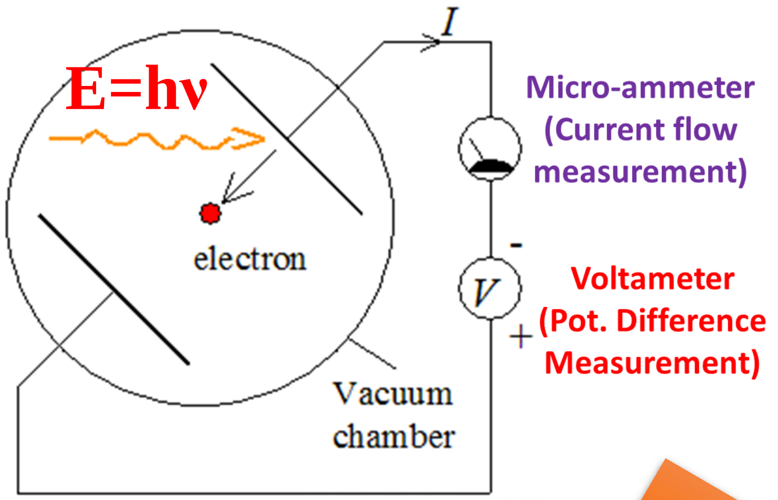
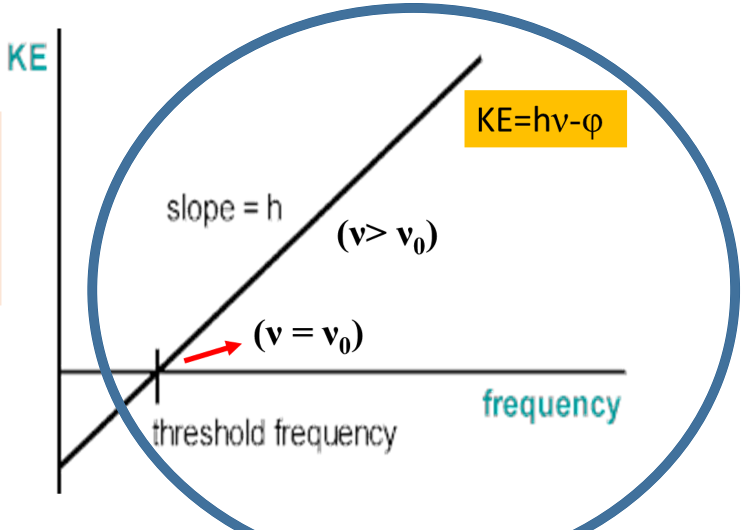
Materials Chemistry III
Day 3

Summary of Day 2

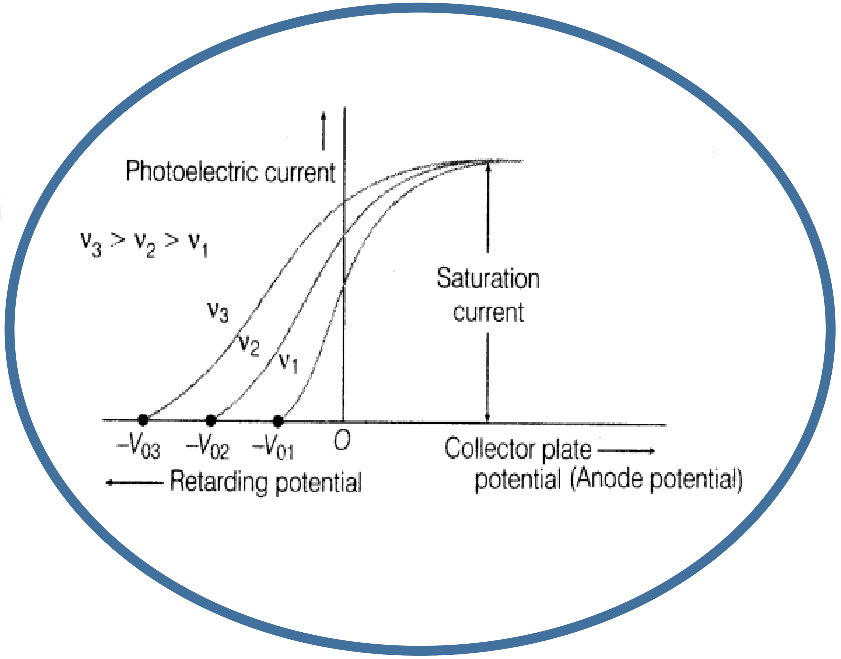


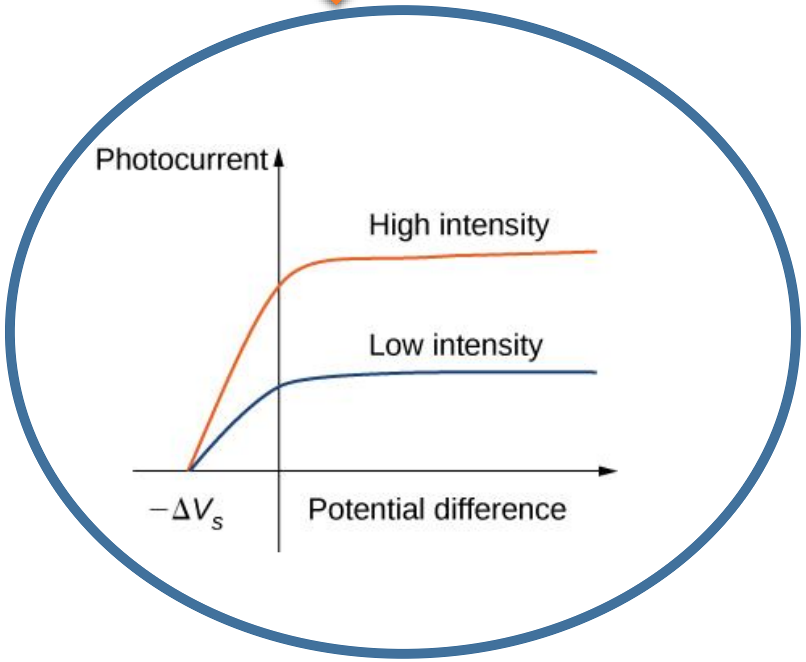
1. Instantaneous
2. Threshold frequency
3. emitted electrons α (intensity)



Total energy of electrons = KE + Pot. energy

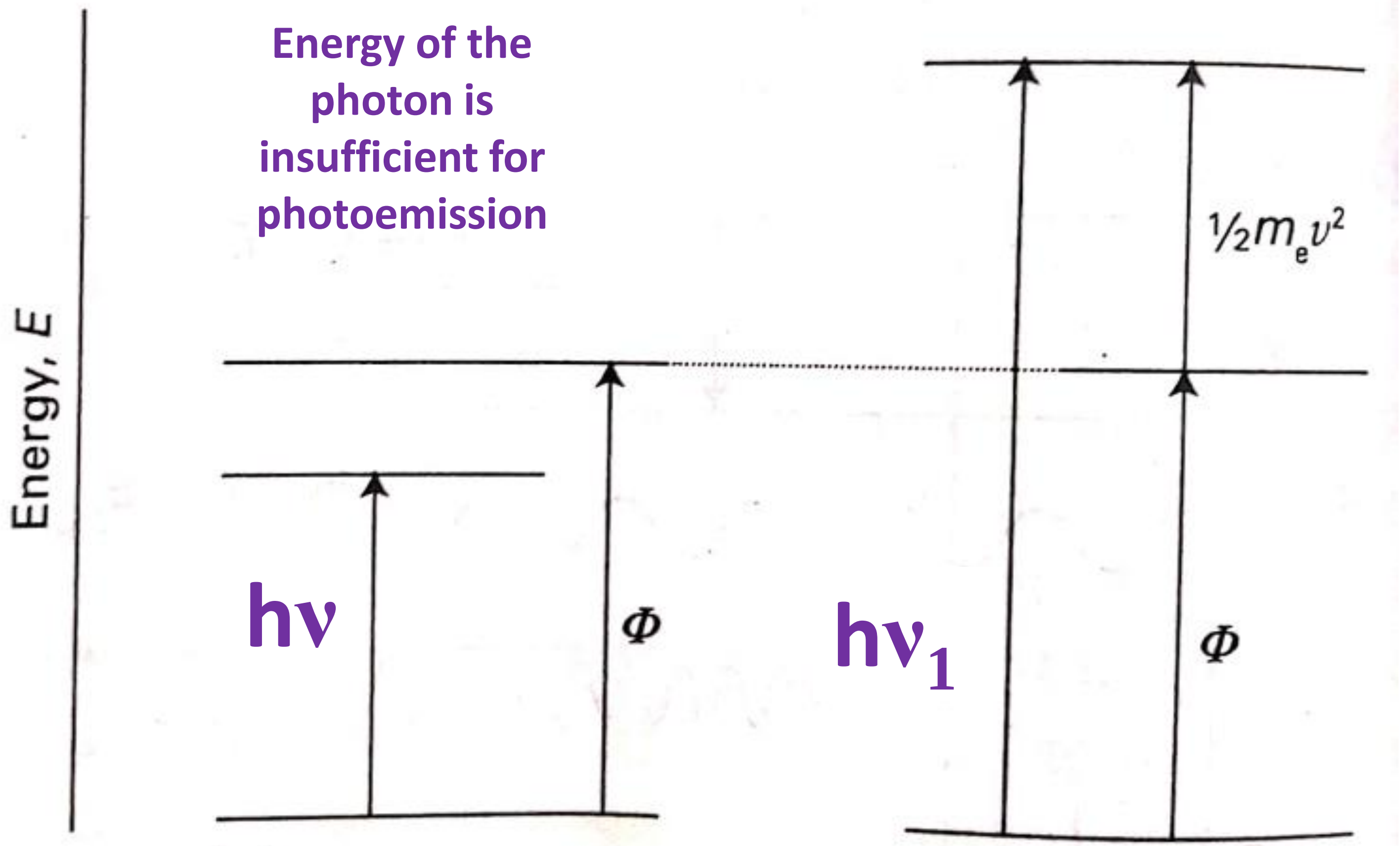
hν = ½ mV²+Work-function





Einstein considered that light wave to be considered in nature with each photon carrying an energy, E=hν

Energy of the photon is insufficient for photoemission



Energy of the photon is sufficient to drive an electron out with kinetic energy

$\nu_{1.} > \nu$

Compton effect (A.H. Compton; 1922)

- When a mono-chromatic beam of 'X-rays' of wavelength (λ) is scattered by a light element (Carbon), it is observed that the scattered X-Rays have maximum intensities at two wavelengths.
- One maximum occurs at the same wavelength λ as the incident beam and other maximum occurs at a slightly higher wavelength (λ').
- Compton's shift: $\Delta\lambda = \lambda - \lambda'$ (dependent on angle of scattering)

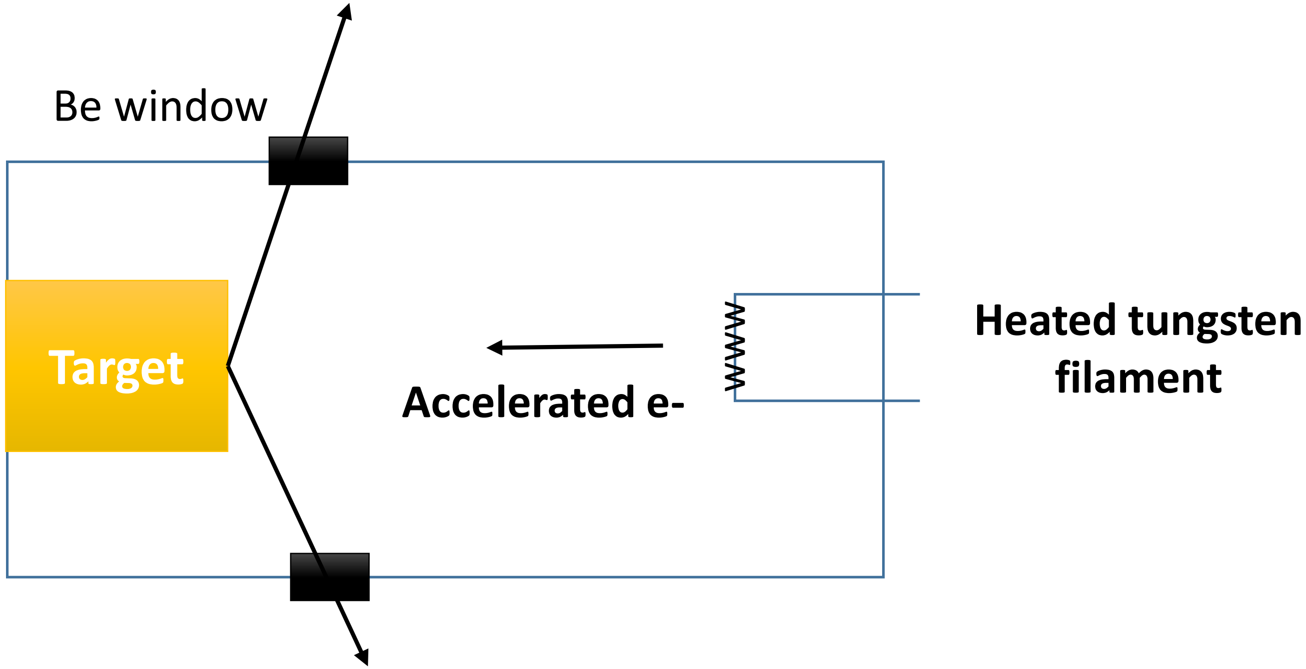
Explanation: Incident photons possess momentum

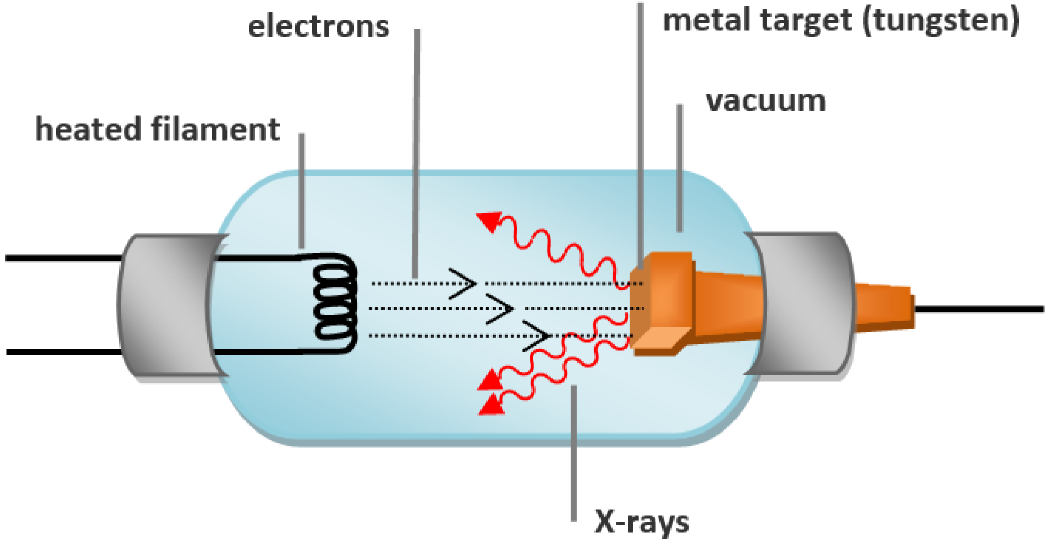
Postulates:

1) **A beam of monochromatic radiation consists of energy $h\nu$, travelling in the direction of the beam with speed of light.**
2) **Scattering by X-ray is by atom is a result of elastic collision between photon and atomic electron.**

Derivation: Wont be done in class!

How X-Rays are generated?





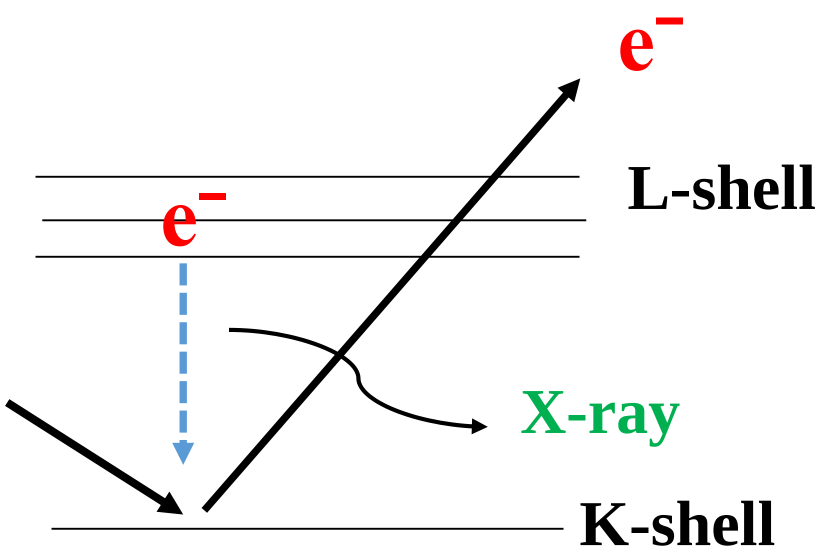
‘Be’ is used as window for exit of X-rays
Pb is used as protector glass as X-rays get absorbed.

- Incoming e⁻ knocks off an electron from inner electronic sub-shells of the target atom.

Ionization process

- This vacancy created in this process is filled by an electron residing in the higher electronic sub-shell

X-ray with definite λ is emitted



The emission of X-ray takes place ≈10^{-4} sec later

Duane- Hunt Law

Maximum frequency of X-ray that can be produced

$$h \times \nu_{x\text{-}ray} = V \times e = hc/\lambda_{x\text{-}ray}$$

where e = electronic charge;

$$\lambda_{x\text{-}ray} = 1239.8/V$$

(Here, V is in volt and $\lambda_{x\text{-}ray}$ in A^{o})

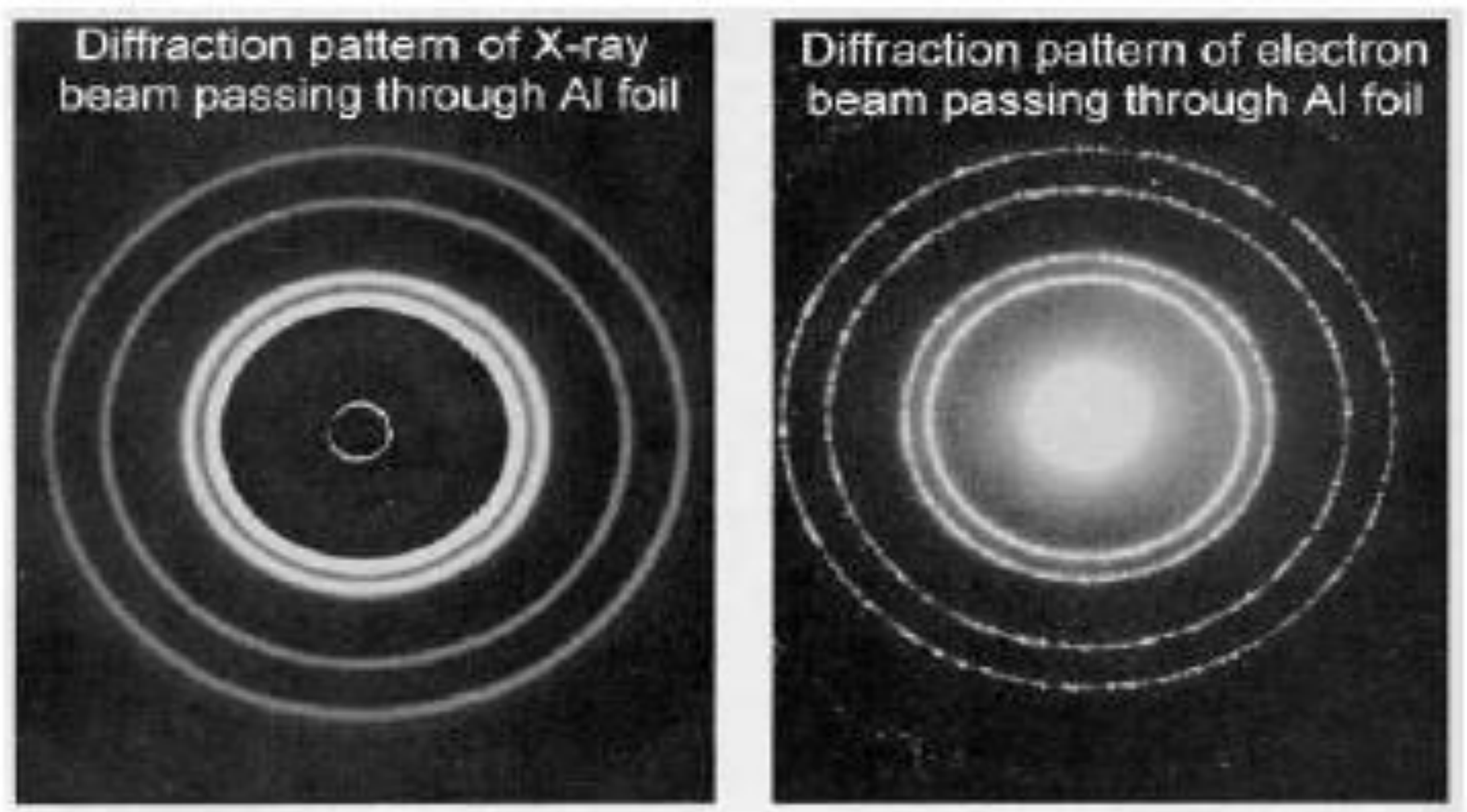
For V= 10 kv

$$\lambda_o \approx 1A^o$$

L3: Objective

1) Dual nature of light (de Broglie's equation)
2) Origin of *Scanning Electron Microscope*
3) Heisenberg's Uncertainty Principle
4) Heisenberg's Microscope
5) Significance of Heisenberg's Uncertainty Principle
6) Concept of a chemical bonding: Electrons as Wave

Wave-particle duality



A similar diffraction pattern is seen from polycrystalline aluminum, regardless of whether it is made with electrons or x-rays.

Wave-particle duality

- The concept of Photo Electric effect can now be well understood by viewing light as a particle.

- However diffraction and interference can be understood only by viewing light as wave and not as wave-packet.

Hence it seems light has a dual nature.

- The situation is contradictory. The contradiction was explained by de Broglie.

- The main aspect of de Broglie's hypothesis is to find out a relationship between wave and particle nature.

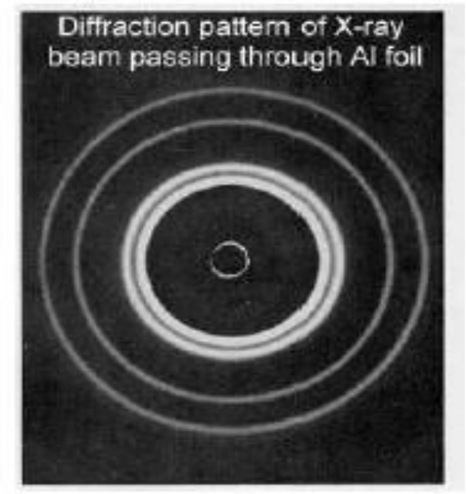
de Broglie's equation

$E = h\nu$

$E=mc^2$

Wave nature of light is characterized by frequency

Diffraction and Interference



Particle nature is characterized by momentum

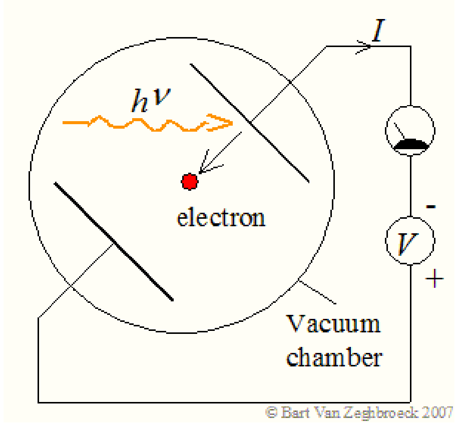
$h\nu=mc^2$

$hc/\lambda=mc^2$

$\lambda=h/P$

$[p=mc]$

Photo-electric effect



Only applicable to sub-atomic word

No significance in real world!!

Calculate de Broglie wavelength of a ball of 140 gm, moving with 40 meter/seconds.

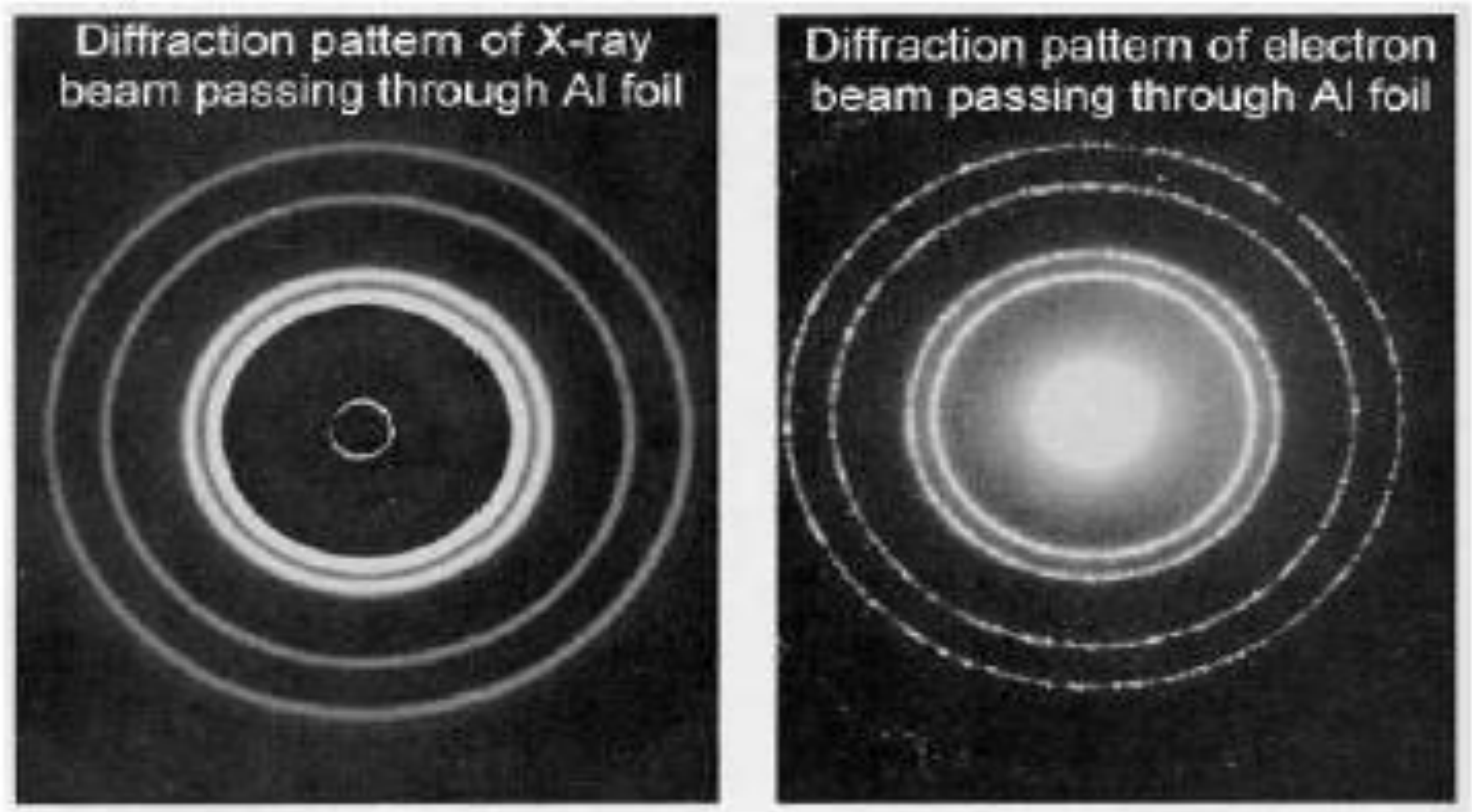
Ans: **1.2×10^{-34} m → undetectable and no practical consequences**

Calculate wavelength of electron, travelling with 1% speed of light.

Ans: **2.43×10^{-10} m=243 pm → In the dimension of X-rays**

Calculation of de Broglie's wavelength for (eliminating velocity term):

- ✓**free particle (potential energy=0 but KE = (1/2)mv^2)**
- ✓**bound particle (Total energy [E]=KE [(1/2)mv^2]+PE [P]**
- ✓**charged particle accelerated with a potential difference V**



A similar diffraction pattern is seen from polycrystalline aluminum, regardless of whether radiation is made with electrons or x-rays.

Electrons shows similar diffraction pattern like X-Rays (aluminum foil diffraction pattern)

Consider an electron is passed through a tube with voltage V_1 with a velocity v

Then,

$$eV_1=(1/2)mv^2$$

$$v = \sqrt{(2eV_1/m)}$$

$$\lambda=h/mv$$

$$\lambda=h/m\sqrt{(2eV_1/m)}$$

$$\lambda=h/\sqrt{(2eV_1m)}$$

$$\lambda \propto 1/\sqrt{V_1}$$

The de Broglie Wavelengths of Various Moving Objects

Particle	*Mass/kg*	*Velocity/m·s⁻¹*	*Wavelength/pm*
Electron accelerated through 100 V	9.11×10^{-31}	5.9×10^{6}	120
Electron accelerated through 10,000 V	9.29×10^{-31}	5.9×10^{7}	12
α particle ejected from radium	6.68×10^{-27}	1.5×10^{7}	6.6×10^{-3}
22-caliber rifle bullet	1.9×10^{-3}	3.2×10^{2}	1.1×10^{-21}
Golf ball	0.045	30	4.9×10^{-22}
Baseball	0.140	25	1.9×10^{-22}

DA McQuarrie, Quantum Chemistry

Relativistic Correction

Remember that when an electron is accelerated through a high potential difference (V_l), then the mass of electron will change as the velocity increases and approaches close to velocity of light. Hence, we need to consider relativistic mass of electrons.

Relativistic momentum:

$$p = mv = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}}$$

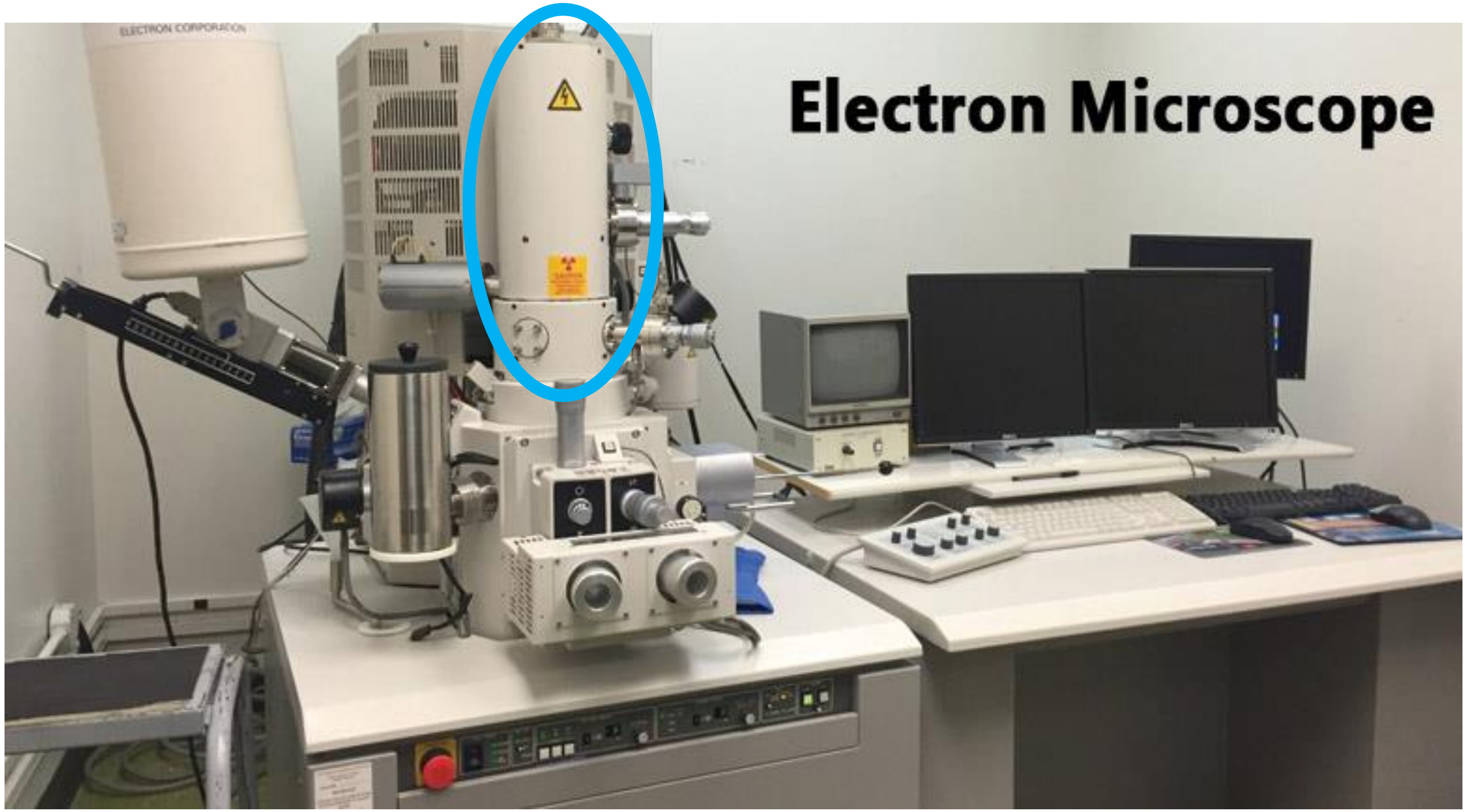
$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{C^2}}}$$

m= relativistic mass
m_0=rest mass
V=velocity
c-=velocity of light

Scanning Electron Microscope

Electron-Mater interaction

Electron mater interaction
-To be discussed later



http://www.hit.ac.il/staff/lapsker/sem/path.html

What is the context for the discussion of SEM?

Particle size < 100 nm → Nanoparticles

1 nm = 10^{-9} m

- **Nanoscale materials are defined as a set of materials where at least one dimension is less than ~100 nm. A nanometer is one millionth of a millimeter - approximately 100,000 times smaller than the diameter of a human hair.**

The term ‘*nano*’ originated from the Greek ‘*nanos*’ means ‘dwarf’.

Relativistic Correction

"Relativistic Correction for kinetic energy"

- Kinetic energy = $eV = (m-m_0)C^2$ [m_0=rest mass of electron]

$$m = m_0 + eV/C^2$$

$$m = m_0(1+eV/m_0C^2)$$

Or, $\sqrt{m} = \sqrt{m_0}\,(1+eV/m_0C^2)^{1/2}$ (1)

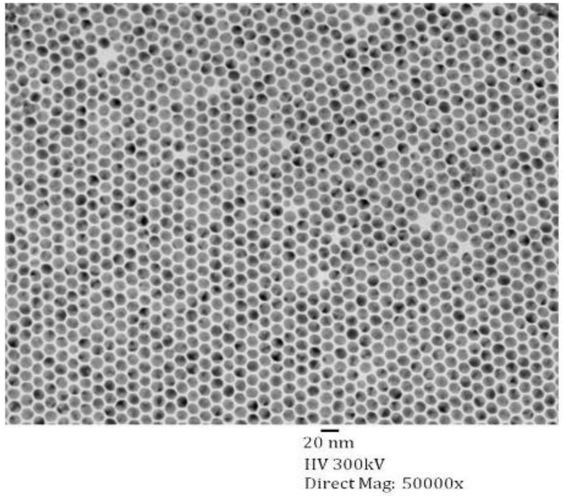
$$\lambda = h/\sqrt{(2eVm)} = h/\sqrt{(2eVm_0)} \times (1+eV/m_0C^2)^{-1/2}$$

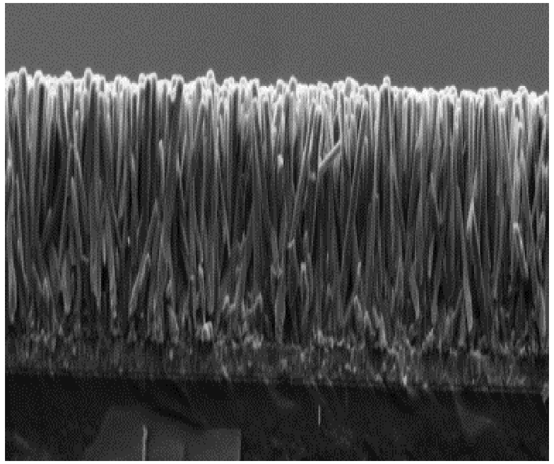
$$\lambda = 12.27/\sqrt{V} \times (1+eV/m_0C^2)^{-1/2}$$

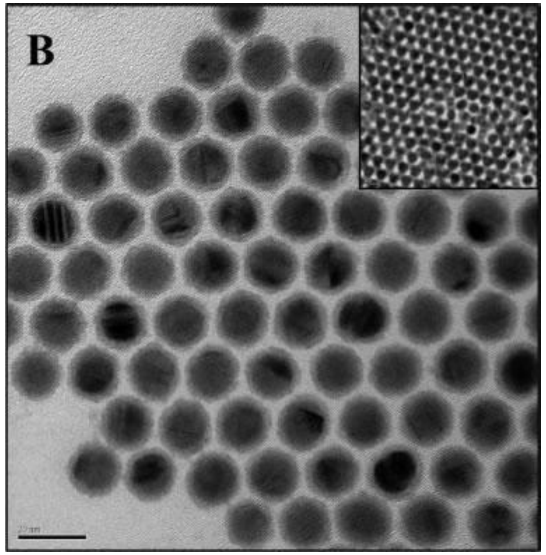
SEM is carried out at lower kV (30 kV)

TEM is carried out at 120-200 kV

Big vs Small







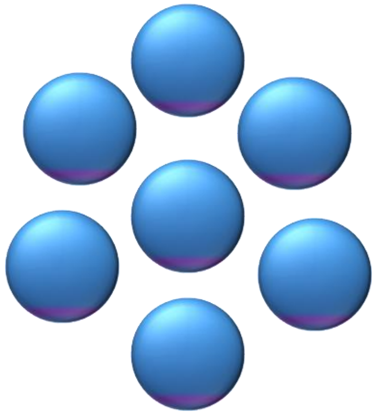
How will you measure the Size?

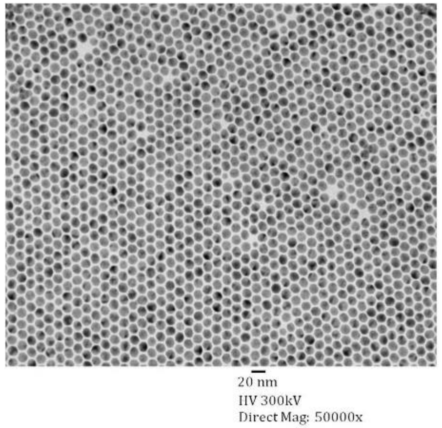
Answer:

1) Scanning Electron Microscope

Classification of Nanomaterials

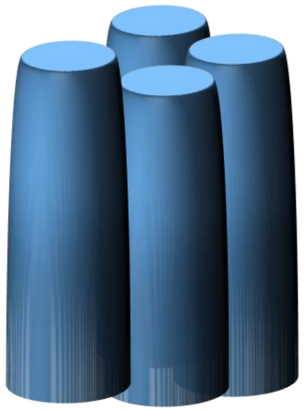
0D spheres/clusters

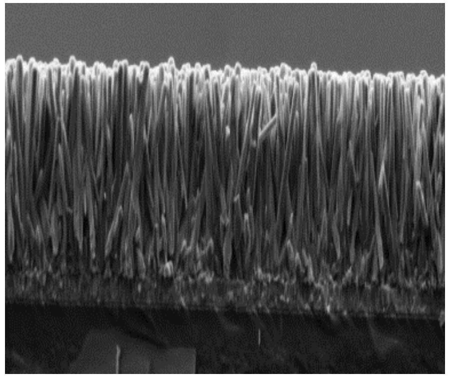




Metal based (Au, Pt, Ag)
Oxide based: TiO_2, ZnO, Al_2O_3

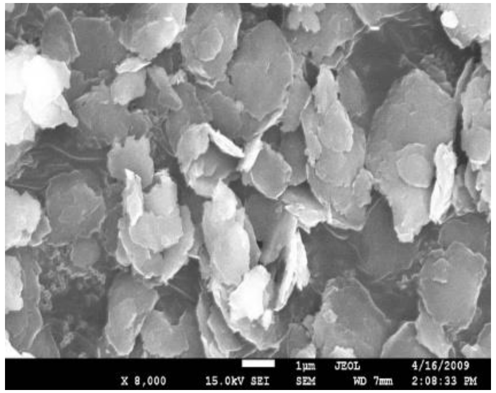
1D nanowires/rods





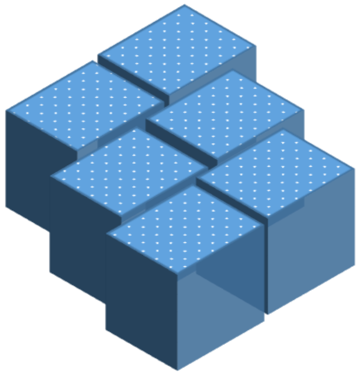
ZnO nano rods
Carbon nanotubes

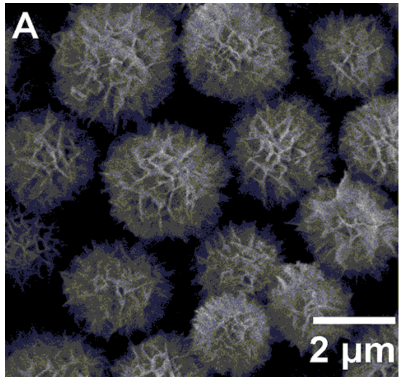
2D nanosheets



Graphene
Clay (aluminosilicates)

3D framework

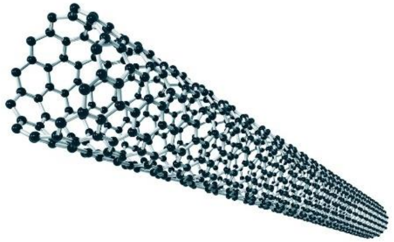


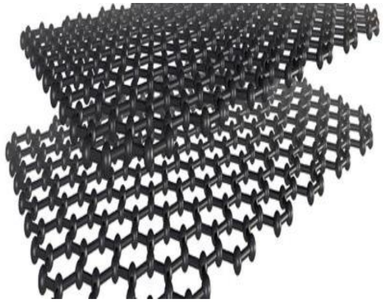


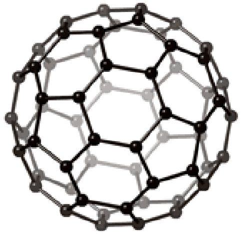
Interconnected
Metal organic framework

List of some different carbon materials along with their likely benefits to light-matter interactions

C-type	Structure
CNTs*,Δ	1D tubular
Graphene/ Reduced Graphene Oxide*,Δ	2D sheet like
Graphene QD*	2D sheet (small graphene fragments, <20 nm)
Fullerenes*,Δ C_{60}, C_{70}	0D Hollow sphere

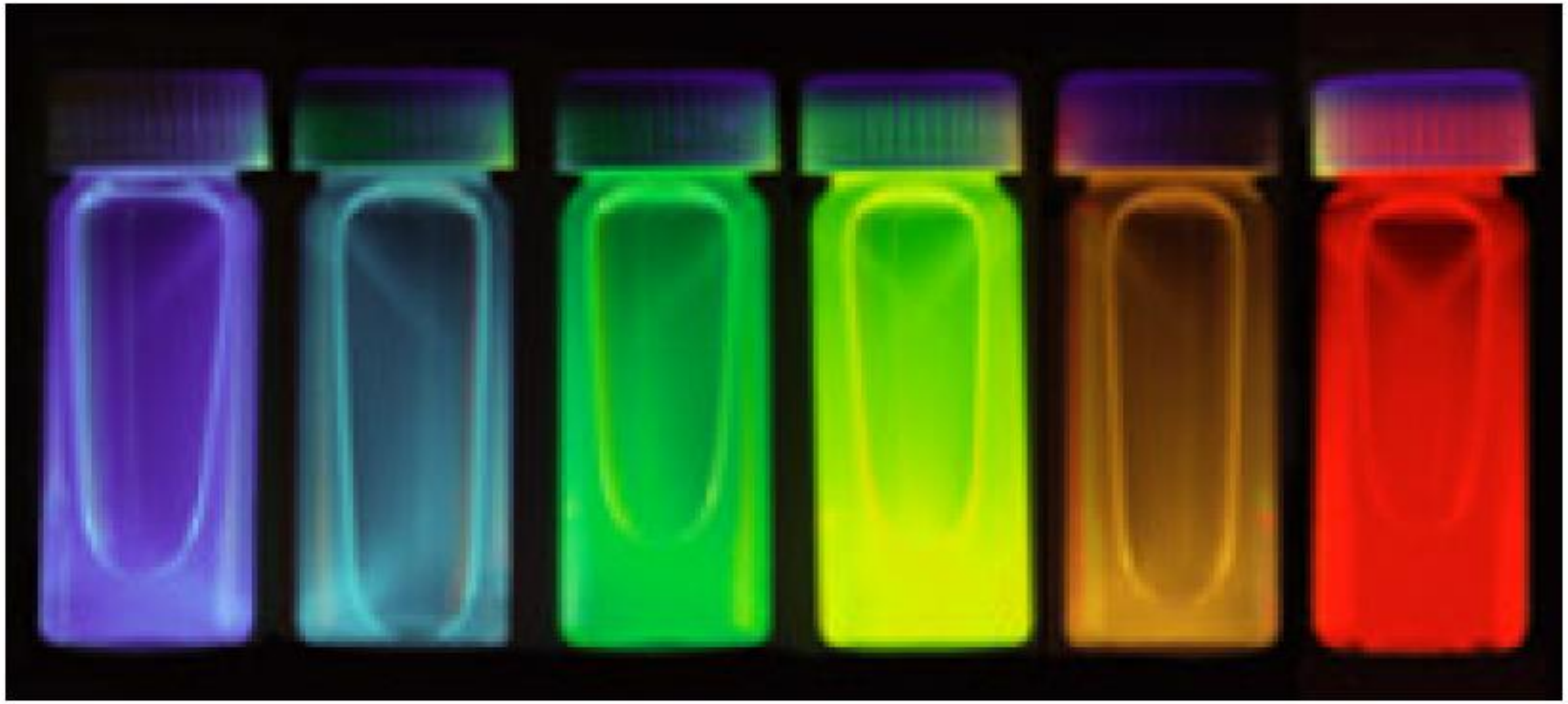




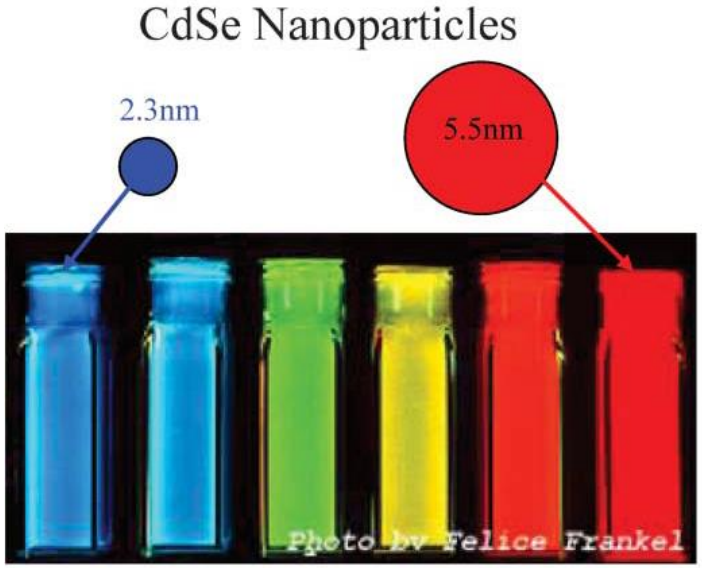


*Photovoltaic (PV) cells, Δ Photo-electrochemical (PEC) cells

Quantum confinement



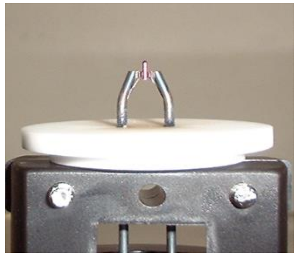
Colloidal CdSe quantum dots dispersed in hexane



Particle in 1D Box?

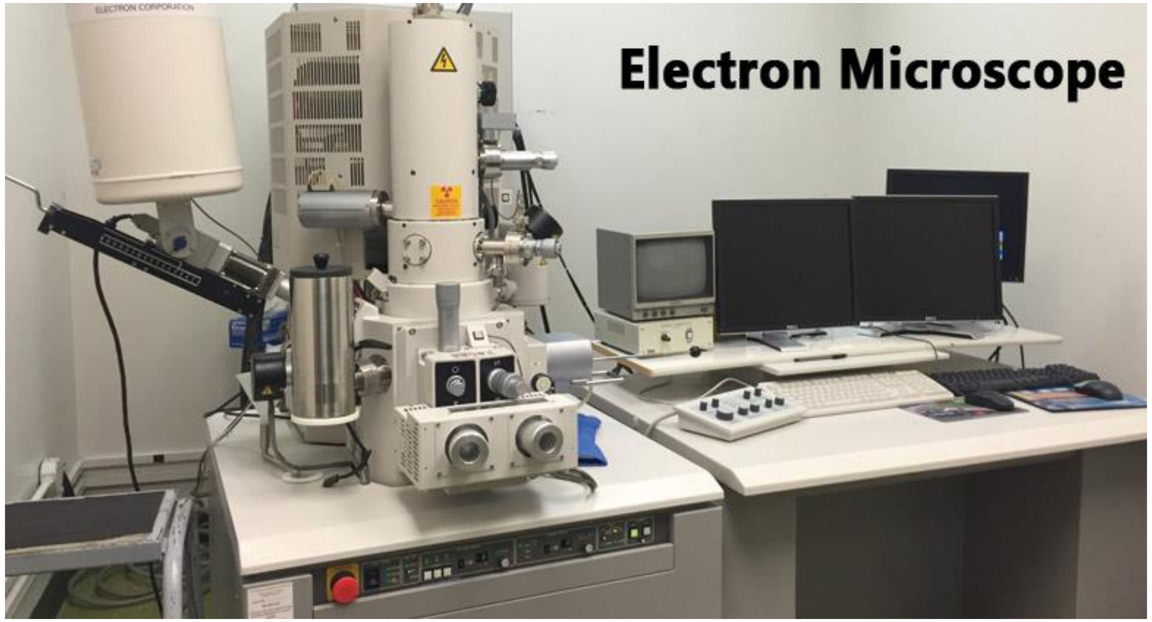
Scanning Electron Microscope

A. Source/electron gun (LaB_6)

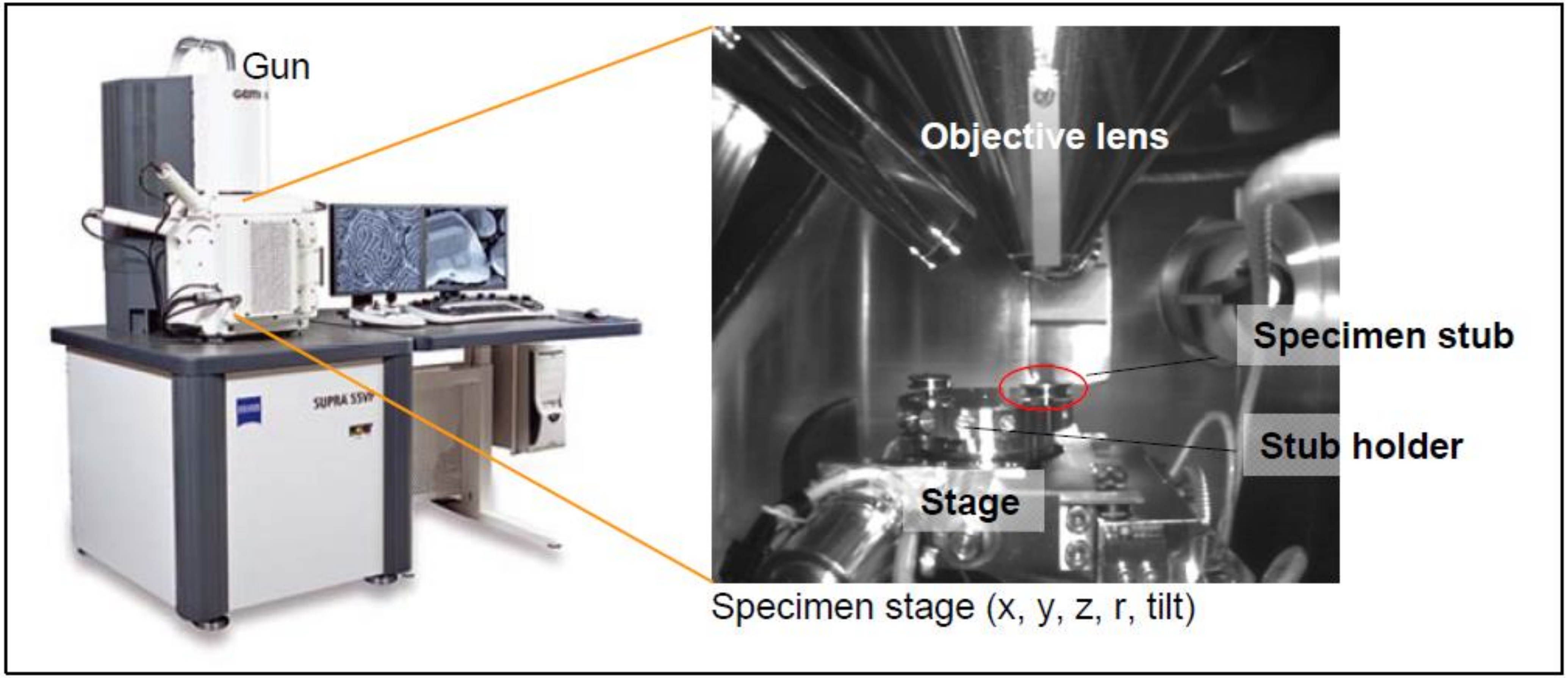


B. Focusing system (Magnetic or Electrostatic Lens)

C. Detection (Electron multiplier tube)



http://www.hit.ac.il/staff/lapsker/sem/path.html

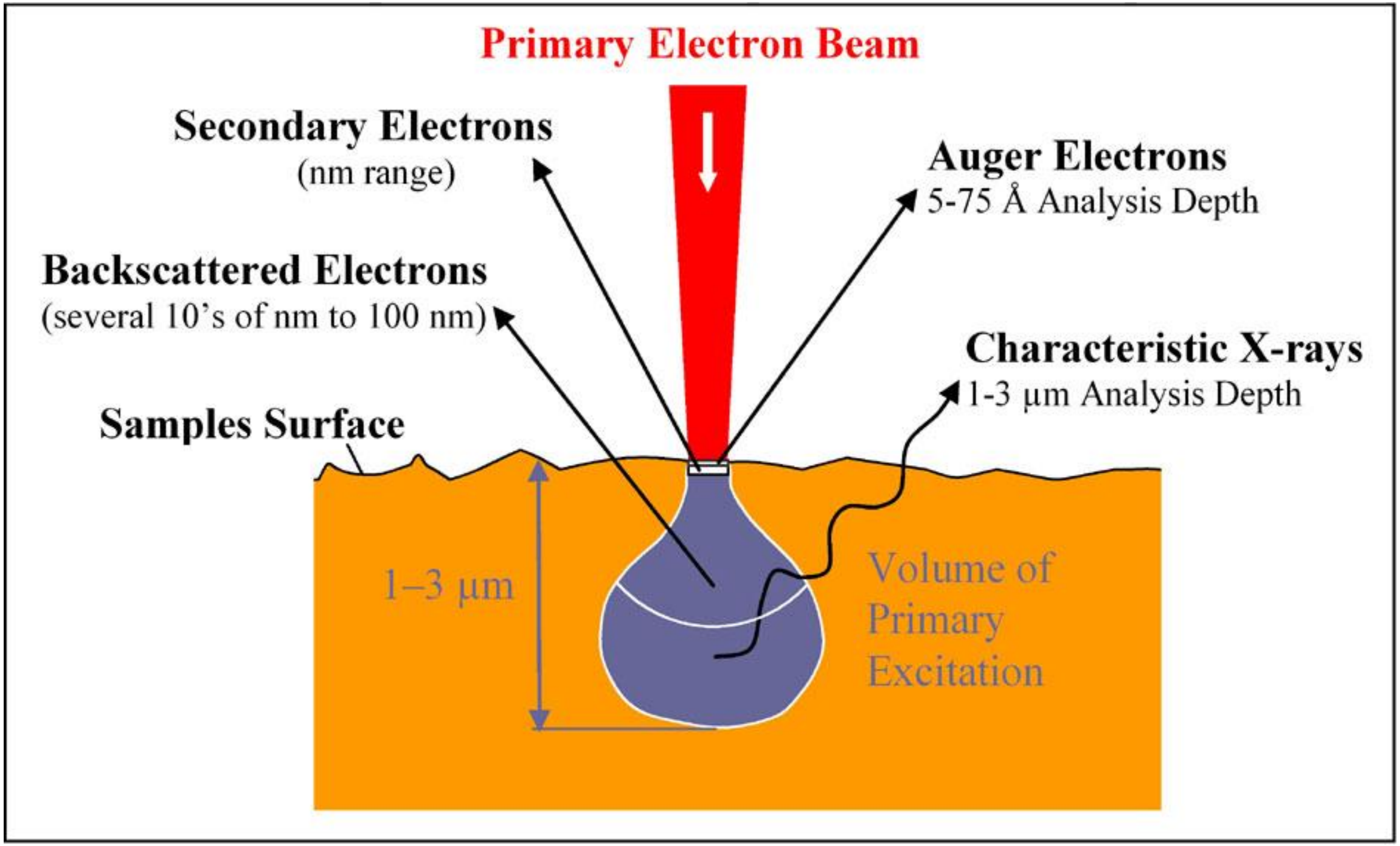

Gun
SUPRA 55VP
Objective lens
Specimen stub
Stub holder
Stage
Specimen stage (x, y, z, r, tilt)

Electron Microscope

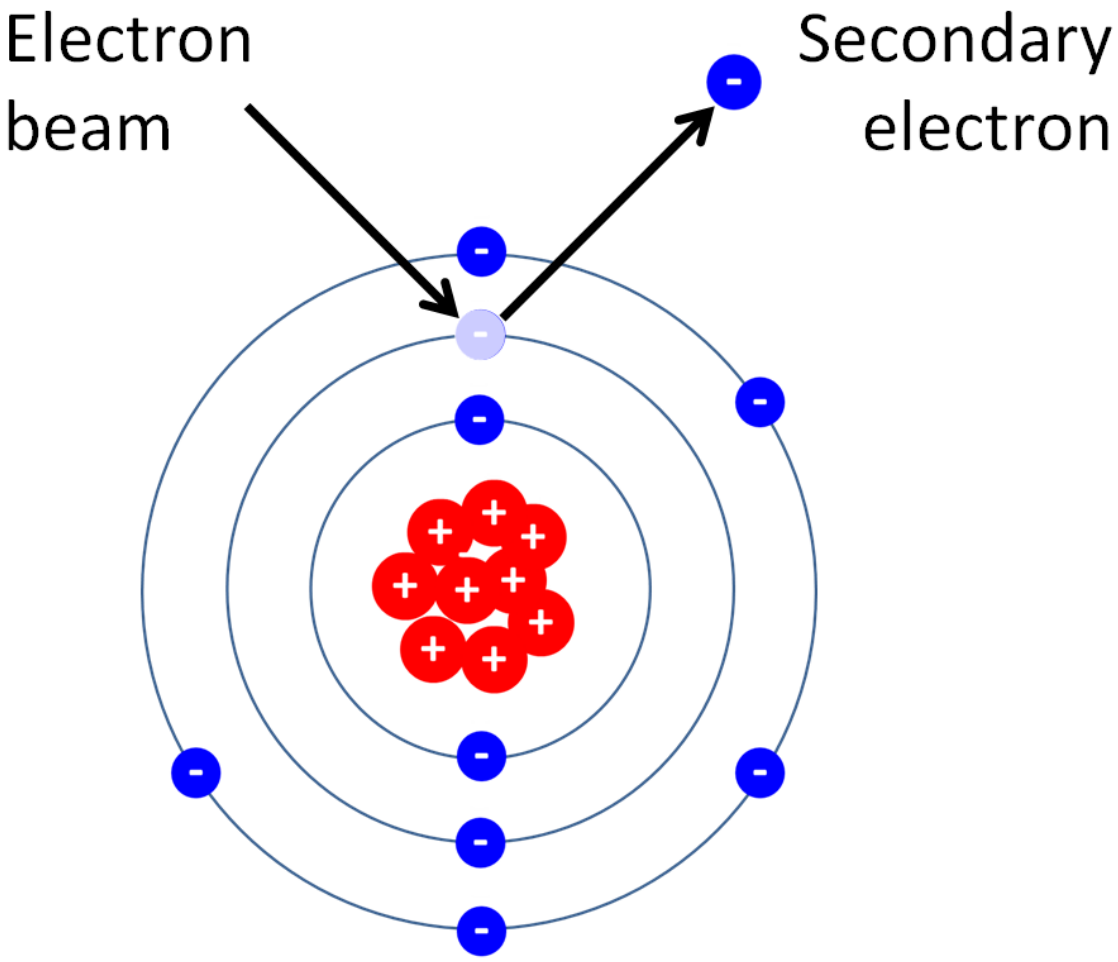
↓

Electron Mater Interaction

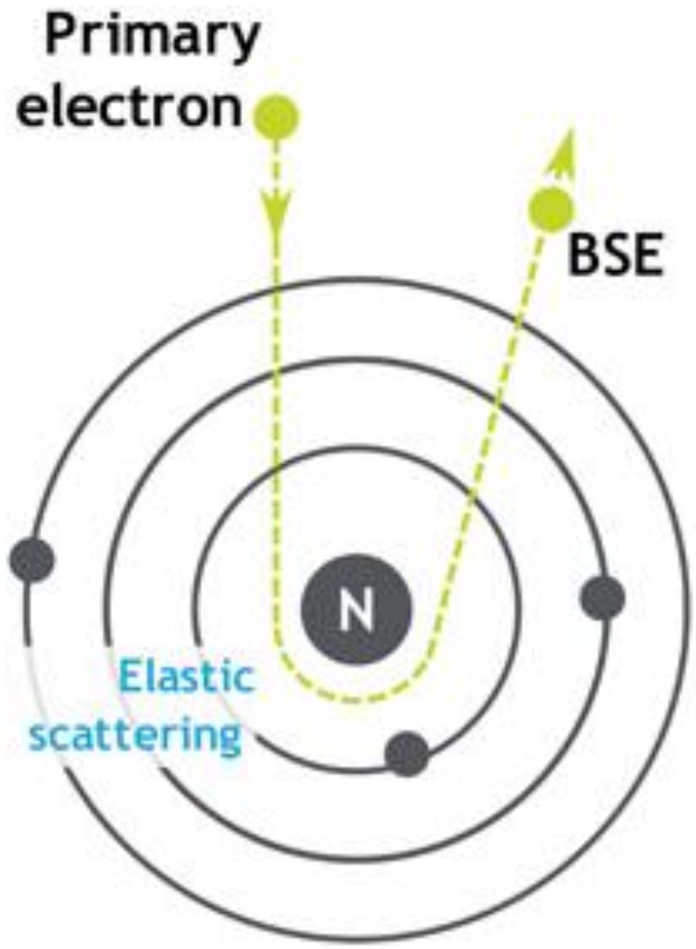
Interactions Between an Incident Electron Beam & Target Material



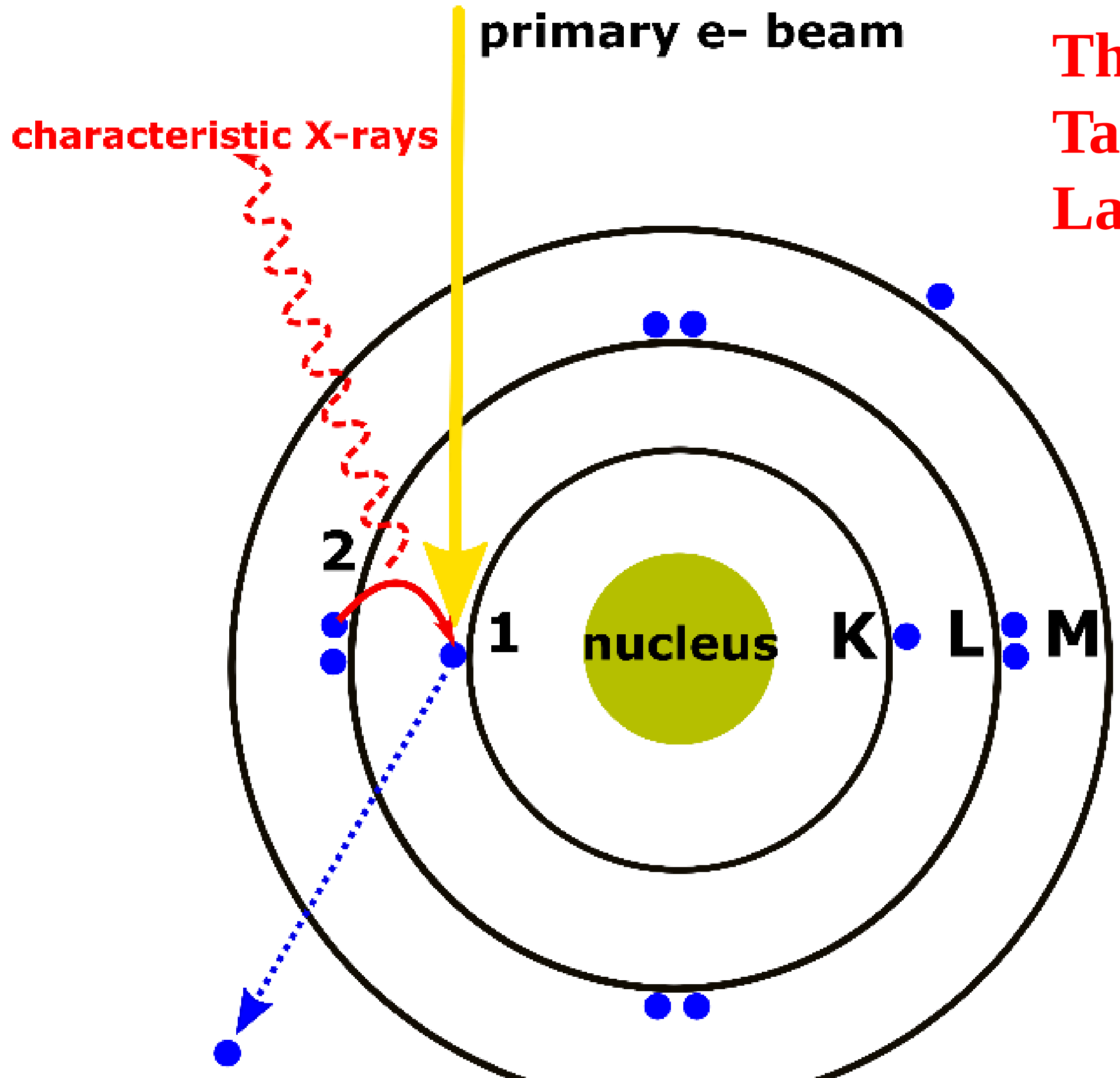
Secondary Electron Emission



Back Scattered Electrons

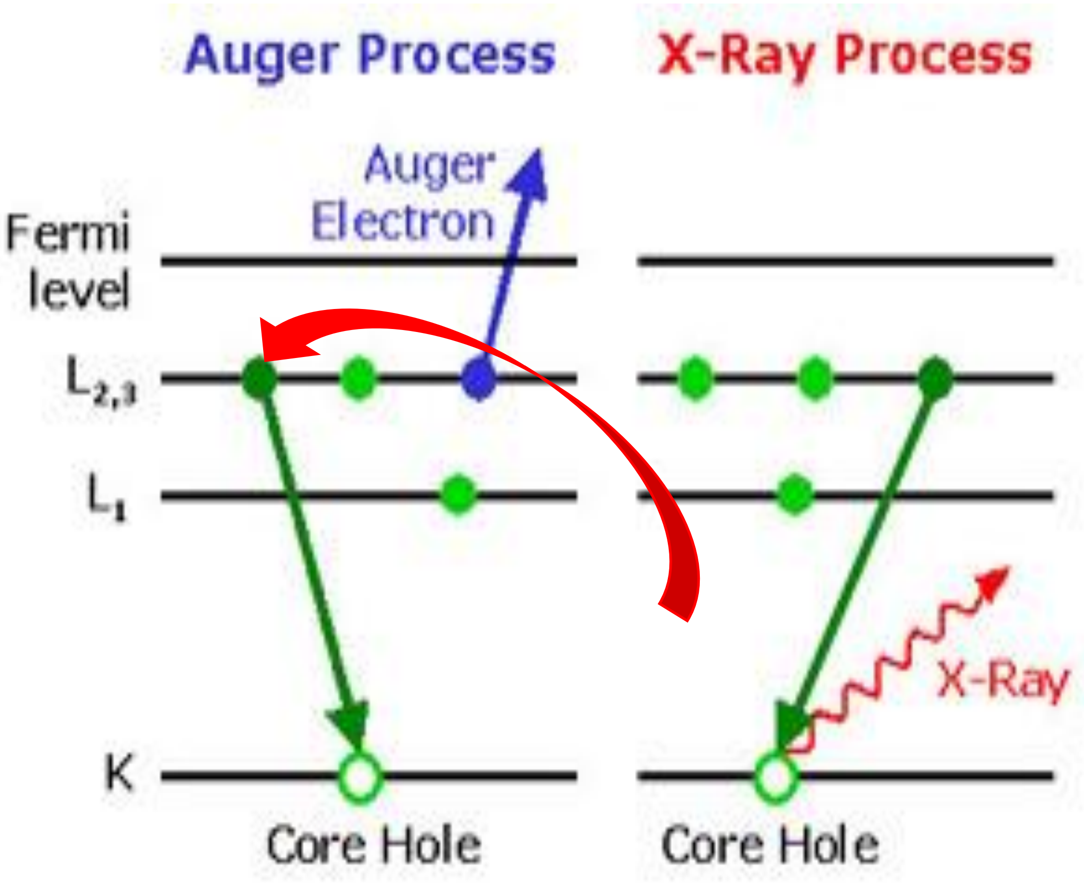


Characteristic X-Ray

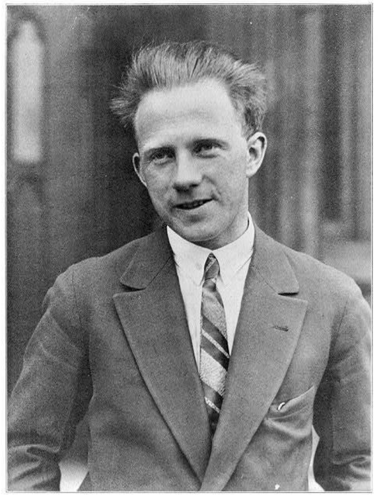


The emission of X-ray Takes place ≈10^{-4} sec Later.

Auger Electron Emission



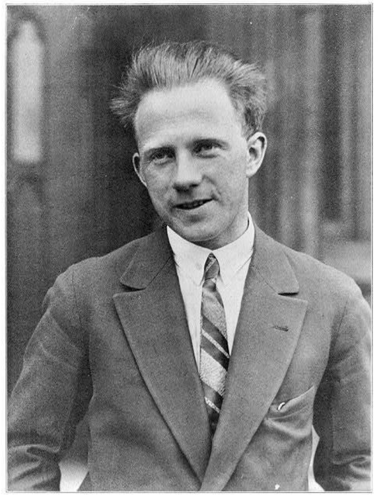
Heisenberg's Uncertainty Principle



It states that **product of uncertainty in determining the position and momentum of a particle is approximately equal to a number in the order of h/2π.**

$$\Delta X \times \Delta P \geq h/2\pi \ (1.055 \times 10^{-34}\ Js)$$

Heisenberg’s Uncertainty Principle



If we wish to locate any particle within a distance ΔX, then we automatically introduce an uncertainty in momentum.

$$\Delta X \times \Delta P \geq h/4\pi$$

Similarly:

$$\Delta t \times \Delta E \geq h/4\pi$$

- If we want to locate an electron within ΔX, using a light having wavelength λ, then λ must be equal to ΔX, so that it interacts with the electron.

However, when the Photon will interact with the electron and transfer its momentum (**as photon is a particle with momentum mv**) and we can’t determine momentum accurately. If we reduce λ further, the momentum of the light will increase further and will be transferred to the electron.

$\downarrow \lambda = h/mv \uparrow$

Likewise, if we want to calculate P (mv) accurately, we have to reduce velocity (v) of the light.
Then ‘**λ will increase’** and will cause uncertainty in position, as it will pass the electron without any interaction.

$\uparrow \lambda = h/mv \downarrow$