Physics –II

UNIT – 1 (Part-II)

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Operators

Operators (O) are those mathematical operations which changes one function (f(x)) into another function (g(x)) i.e. $Of(x) = g(x)$

Ex: $$\frac{d}{dx}(x^3 + 3) = 3x^2$$

Here, $\frac{d}{dx}$ is an Operator (O), (x^3+3) is function f(x) and $3x^2$ is g(x).

Operators corresponding to Energy and Momentum

Let us consider a wave function,

$$\psi = Ae^{\frac{-i}{\hbar}(Et-px)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

Differentiating equation (1) with respect to 't', we get

$$\frac{\partial\psi}{\partial t} = \left(\frac{-i}{\hbar}E\right)Ae^{\frac{-i}{\hbar}(Et-px)}$$

Here $Ae^{\frac{-i}{\hbar}(Et-px)}$ is ψ hence now we have;

$$\frac{\partial\psi}{\partial t} = \left(-\frac{i}{\hbar}E\right)\psi$$

Or $$E\,\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t}$$ [by transferring the terms]

Or $$E\,\psi = i\,\hbar\frac{\partial\psi}{\partial t}$$

Now; if we remove ψ from both sides then we will get

$$\boxed{E \rightarrow i\,\hbar\frac{\partial\psi}{\partial t}}$$

This is Operator corresponding to Energy.

Now again differentiating equation (1) with respect to 'x', we get

$$\frac{\partial\psi}{\partial x} = \left(\frac{i}{\hbar}p\right)Ae^{\frac{-i}{\hbar}(Et-px)}$$

Here $Ae^{\frac{-i}{\hbar}(Et-px)}$ is ψ hence now we have;

$$\frac{\partial\psi}{\partial x} = \left(\frac{i}{\hbar}p\right)\psi$$

Or $$p\,\psi = \frac{\hbar}{i}\frac{\partial\psi}{\partial x}$$ [by transferring the terms]

Or $$E\,\psi = -i\,\hbar\frac{\partial\psi}{\partial x}$$

Now; if we remove ψ from both sides then we will get

$$\boxed{p \rightarrow -i\,\hbar\frac{\partial\psi}{\partial x}}$$

This is Operator corresponding to Momentum.

In three dimensions (3D) the operator corresponding to momentum can be written as

$$\boldsymbol{p} \rightarrow -\boldsymbol{i}\hbar\boldsymbol{\nabla}$$

Eigen Function & Eigen Value

There are a class of functions which when operated by an operator (O) are only multiplied by some constant i.e., O f(x) = λf(x)

Such types of functions are known as **Eigen functions** and the constant value 'λ' is known as **Eigen value.**

Ex: - (i) $\frac{d}{dx}e^{5x} = 5e^{5x}$; Here e^{5x} is termed as Eigen function and 5 is termed as Eigen value

(ii) $\frac{d^2}{dx^2}\sin 4x = -16\sin 4x$; Here $\sin 4x$ is termed as eigen function and -16 is termed as Eigen value.

Application of Schrodinger Wave Equation

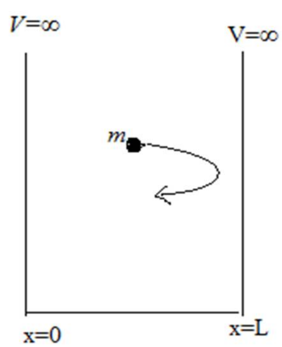
(1) Particle in one dimensional box-

Let us consider that a particle of mass 'm' is trapped with in a one-dimensional box of length 'L'. Let the rigidity of the wall be of infinite order. Let the potential energy corresponding to the height of the wall be of infinite order. Let the potential energy within the box be 0. Thus, potential energy now can be written as,

V= ∞ x=0,

V=0 0<x<L,

V= ∞ x=L



Schrodinger equation in one dimension can be written as ,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \qquad \text{……………….(1)}$$

So, within the box (i.e. for V=0) this equation can be written as,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

Or $$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

Where $$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

The general solution of equation (2) can be written as,

$$\Psi = A \sin kx + B \cos kx \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots..(4)$$

Here,

At $x=0$, $\Psi=0$, and

At $x=L$, $\Psi=0$ …………………..(5)

Let us apply first boundary condition i.e.,

[at $x=0$, $\Psi=0$] in eq^n (4) we get,

$$0 = A\sin k.0 + B\cos k.0$$

$$\Rightarrow B=0$$

Thus, equation (4) now can be written as,

$$\Psi = A \sin kx \qquad \ldots\ldots\ldots\ldots(6)$$

Let us apply second boundary condition in equation (6) we get,

$$0 = A \sin kL$$

$$\text{or } A \sin kL = 0$$

Here, 'A' can't be zero. Thus we are left with

$$\sin KL = 0$$

i.e. $$KL = n\pi$$

So, n can take only the values as n=0,1,2,3,……..

$$\text{or } K = n\pi/L \qquad \ldots\ldots\ldots\ldots\ldots.(7)$$

Thus the wave function can be written as,

$$\Psi = A\sin\frac{n\pi}{L}x \qquad \ldots\ldots\ldots\ldots\ldots(8)$$

Putting these values of k in equation (3) we get,

$$\frac{n\pi}{L} = \sqrt{\frac{2mE}{\hbar^2}}$$

Squaring on both sides,

$$\frac{n^2\pi^2}{L^2} = \frac{2mE}{\hbar^2}$$

Or $$E = \frac{n^2\pi^2\hbar^2}{L^2 2m}$$

Or $$E = \frac{n^2\pi^2 h^2}{2mL^2 4\pi^2}$$

Or $$E = \frac{n^2h^2}{8mL^2} \qquad \ldots\ldots\ldots\ldots(9)$$

This is the expression for energy & represents the quantization of energy due to 'n'.

Since, particle is trapped within the box. Therefore, we must have,

$$\int_0^L [\Psi^2]dx = 1$$

$$\int_0^L [A^2] sin^2 \frac{n\pi}{L} x dx = 1$$

$$\frac{A^2}{2}\int_0^l \left[1 - cos\frac{2n\pi}{L}x\right] dx = 1$$

$$\frac{A^2}{2}\ [\, x - \frac{L}{2\pi n} sin\frac{2n\pi x}{L}\ ]_0^L = 1$$

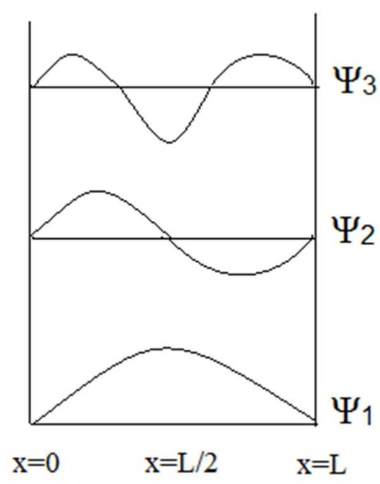
$$\frac{A^2}{2} L = 1$$

$$A = \sqrt{\frac{2}{L}}$$

Thus, wave function can be written as:

$$\boxed{\Psi = \sqrt{\frac{2}{L}}\ sin\frac{n\pi}{L}\ x} \qquad \ldots\ldots\ldots\ldots\ldots..(10)$$

Let us plot the wave function Ψ for different values of n:



For n=1, $\psi_1 = \sqrt{\frac{2}{L}}\ sin\frac{\pi}{L}\ x$

For n=2 $\psi_2 = \sqrt{\frac{2}{L}}\ sin\frac{2\pi}{L}\ x$

For n=3, $\psi_3 = \sqrt{\frac{2}{L}}\ sin\frac{3\pi}{L}\ x$

X-Rays

X-rays are electronegative waves having very short wavelength (0.1 – 100 A^o). X-rays were discovered by W. Roentgen in 1895. Distant galaxies and black holes are natural source of X-rays. In laboratory X-rays are produced by Coolidge tube which is known as modern X-ray tube. X-rays are produced when fast moving electrons are suddenly stopped by a suitable target.

Production of X-rays:

X-rays are produced by Coolidge tube as shown below.

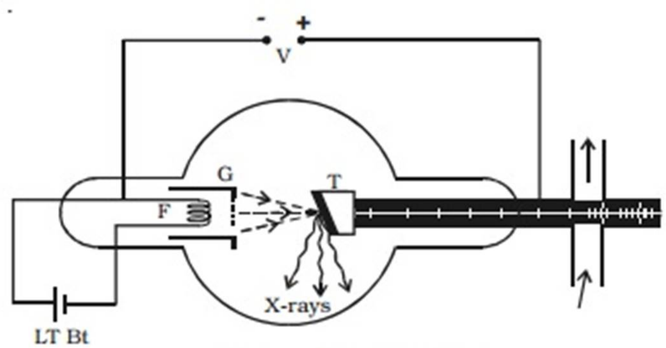


Fig Coolidge tube

Here a glass chamber having very high order vacuum contains the filament F and the target T. As the power is switched on (LT) electrons are emitted by filament F and are focused on the target T (Tungsten & Molybdenum) mounted on a copper anode. When fast moving electrons strikes with the target then 98% of the electron lose their energy in collision with the target & the energy of only 2% electron is converted into X-rays. The anode is heat up too much so that a cooling arrangement is attached with it. The intensity of the produced X-rays is controlled by controlling the filament current and power of X-ray i.e., penetrating power is controlled by the potential difference V(HT) applied to between anode & cathode. On the basis of penetrating power; X-rays are of two types:

(i) Soft X-rays, and
(ii) Hard X-rays.

Soft X-rays and Hard X-rays:

X-rays having low penetrating power are termed as soft X-rays. However, X-rays having high penetrating power are known as hard X-rays. On the basis of origin or spectra X-rays are of two types:

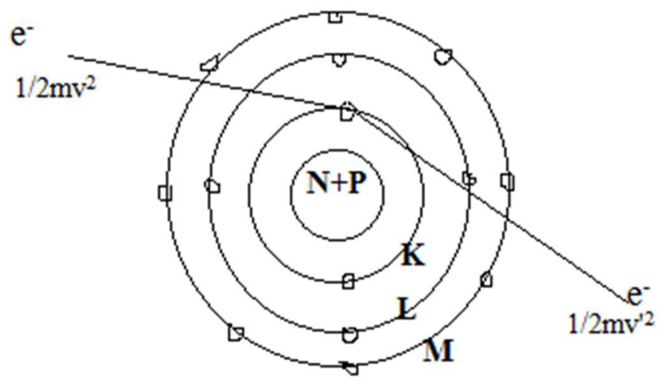
(i) Continuous X-rays, and
(ii) Characteristics X-rays.

Properties of X-rays:

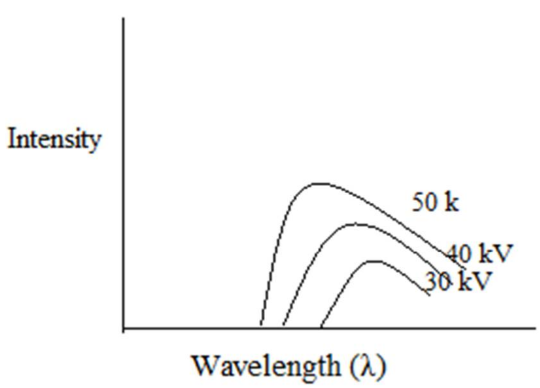
(1) X-rays are electromagnetic waves.
(2) They affect photographic plate.
(3) They produce fluorescence.
(4) They have penetrating power.
(5) X-rays are not deflected by electric & magnetic field
(6) X-rays are reflected and diffracted like other electromagnetic waves.

Continuous X-rays:

When fast moving electrons are passed close to the nucleus of target atom then they experience a strong force of attraction. As a result of which the fast moving electrons are decelerated and deflected from their path as shown below:



According to classical electrodynamics; whenever a charge particle is accelerated or decelerated, it emits electromagnetic radiation. Therefore, the decelerated electron emits electromagnetic radiation in form of X-rays which is known as Bremsstrahlung (Braking Radiation). Since there are large number of electrons and they suffer different deceleration therefore, X-rays of all possible wavelength within a certain limit are emitted which is known as continuous X-rays. The spectra of continuous X- rays are as shown below:



Duane & Hunts Law

As we know that energy due to decelerated electron is emitted in form of X-Ray. Therefore, we must have,

$$\tfrac{1}{2} mv^2 - \tfrac{1}{2}mv'^2 = h\upsilon \qquad \text{---------------(1)}$$

Where, m is mass of the electron, v is initial velocity of electron,

v' is final velocity of electron, h is Planck's constant,

υ is frequency of emitted X-ray.

For maximum frequency we must have v'=0.

Thus,

$$\tfrac{1}{2} mv^2 = h\upsilon_{max} \qquad \text{--------------------(2)}$$

Since electrons are accelerated by the potential difference (V) applied between anode and cathode, therefore, we have

$$\tfrac{1}{2} mv^2 = eV \qquad \text{-----------(3)}$$

From equation (2) and (3),

$$h\upsilon_{max} = eV,$$

or

$$\frac{hc}{\lambda_{min}} = eV$$

or

$$\lambda_{min} = \frac{hc}{eV}$$

Putting values of different constants we get;

$$\lambda_{min} = \frac{6.62\text{x}10^{-34}\text{x}3\text{x}10^{8}}{1.6x10^{-19}\,V}$$

Or

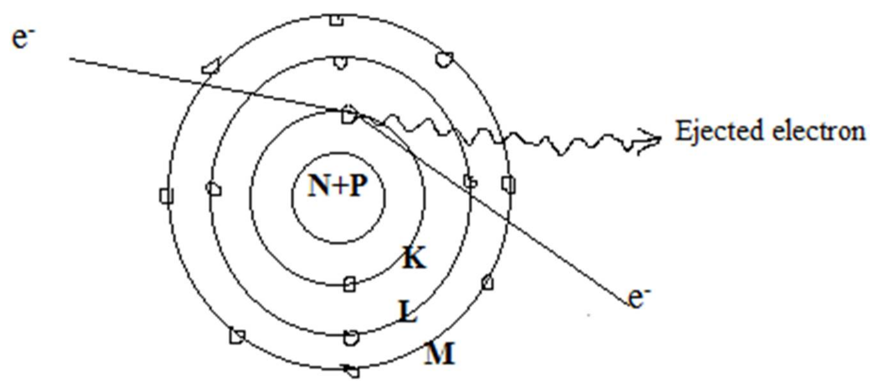
$$\boxed{\boldsymbol{\lambda_{min}} = \frac{\mathbf{12400}}{\boldsymbol{V}}\ \text{Å}} \qquad \text{............(4)}$$

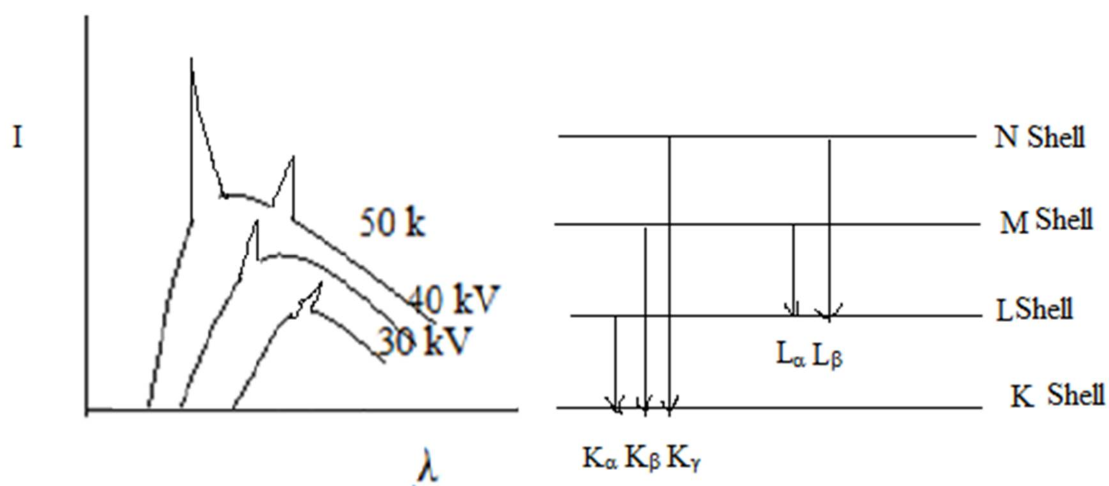
This [i.e. equation (4)] is known as Duane & Hunts law.

If V = 10 kV, Then $\lambda_{min} = \frac{12400}{10000}\ \text{Å} = 1.24\ \text{Å}$

Characteristic X-ray:

When fast moving electron penetrate deeply inside the target atom and knock out (by giving energy in collision) any electron of inner shell (say K) then a vacancy is created there which may be filled by any electron of next higher inner shell. So the difference of the energy of the two shells is emitted or radiated in form of X- rays which is known as characteristic X-ray. These emitted X-rays are known as characteristic X- rays because the emitted frequency represents the characteristic of target atom. The process and characteristic spectra are as shown below.





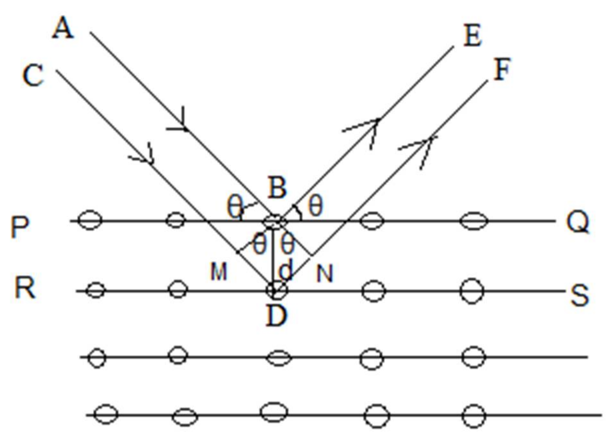
Suppose a vacancy is created in K shell which may be filled by any electron of L shell and K_α line is emitted. Now due to transition of electron in K shell a vacancy will be created in L shell which may be filled by any electron of M shell and L_α line is emitted. This process is continued till the vacancy reaches in the outermost orbit which may be filled by any outermost orbital electron. When the created vacancy in K shell is filled up by any electron of L shell then K_α line is emitted. If the vacancy created in K shell is filled up by any electron of M shell then K_β line is emitted. Similarly if any electron of N shell jumps to fill up the vacancy in K shell then K_γ line is emitted. If the vacancy is created in the L shell and which may be filled by any electron of M shell then L_α is emitted. In the similar process L_β line is emitted as shown in above figure.

Diffraction of X-rays:

For the diffraction of any beam or wave it is required that size of obstacle must be of the order of incident radiation. As we know that the grating element of an optical grating is nearly 16000 A° and the wavelength of X-rays is nearly 0.1 – 100 A°. Since the order of grating element do not match with the wavelength of X- rays therefore, normal optical grating can't diffract X rays. In 1913, Lau suggested that since the order of inter atomic space of a crystal is of the order of wavelength of X-rays therefore, crystal may act as a grating for the diffraction of X-rays.

Bragg's Law:

Let us consider a wave front AB and CD of X-rays is incident on a crystal plane PQ and RS at glancing angle θ. Let the inter planar distance be 'd' and the reflected wave front be BE and DF as shown in figure.



Let us draw perpendicular BM and BN on CD and DF respectively.

The path difference between two wavefront can be calculated as follows,

From ΔBMD,

$$MD = d \sin\theta$$

Similarly, from ΔBDN,

$$DN = d \sin\theta$$

Thus, total path difference can be given by

$$\Delta = MD + DN$$

$$= d \sin\theta + d \sin\theta$$

$$= 2d \sin\theta$$

For maximum intensity,

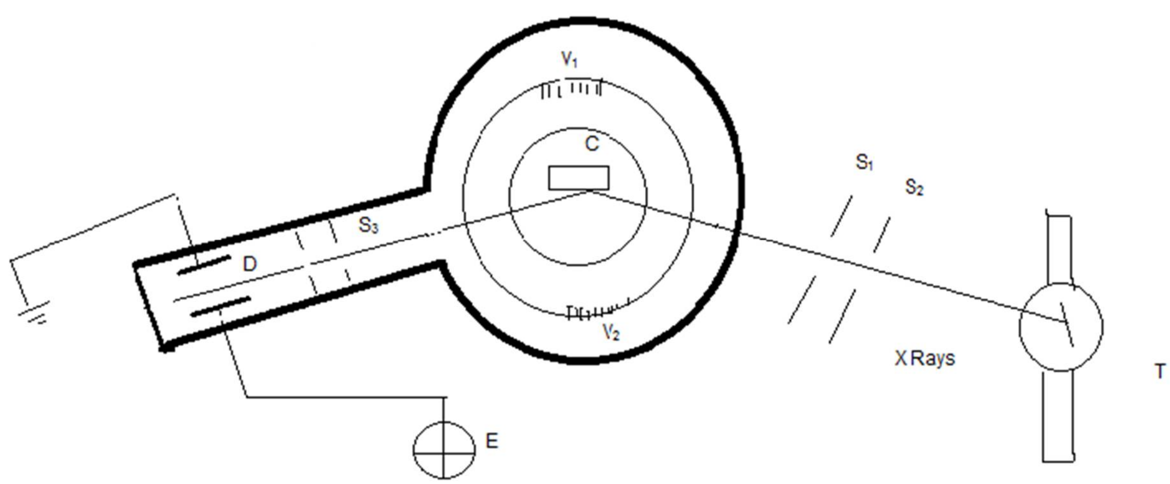
$$\boxed{2d\sin\theta = n\lambda}$$

Where 'n' is order and λ is wavelength of X-Ray.

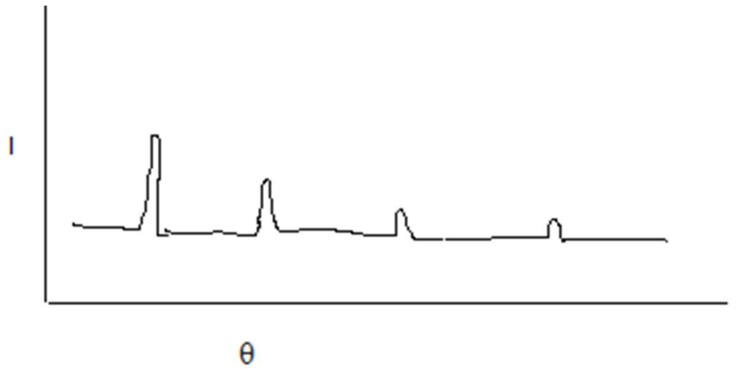
This is known as Bragg's Law.

Bragg’s Spectrometer:

This spectrometer is very much similar to optical spectrometer and was designed by W.L. Bragg and W.H. Bragg. The main parts of this spectrometer are shown below.



X rays from an X ray tube 'T' is incident on crystal 'C' under investigation by passing two slits S_1 and S_2. Let the glancing angle be θ. The reflected rays are sent to an ionization chamber. After crossing slit S_3 the ionization chamber and the prism table at which crystal is mounted can be rotated about the same axis. The mechanical arrangement is such that if the crystal is rotated through an angle of θ, then ionization chamber will rotate through an angle of 2θ. Ionization chamber contains a vapour of methyl bromide (CH_3Br). As the crystal is rotated by certain angle then the reflected X-ray enters ionization chamber and ionizes the vapours of methyl bromide and the resulting current is measured by an electrometer E. A graph between θ and resulting current 'I' (which alternatively measures the intensity of X-Ray) is plotted as shown below.

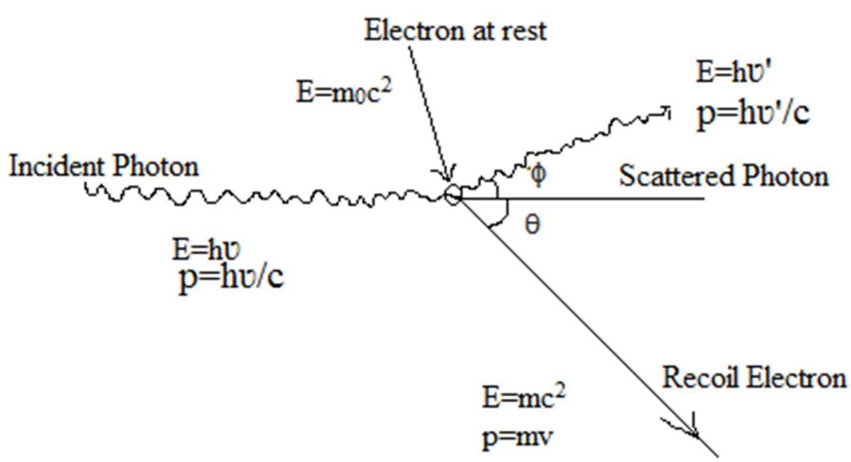


Using Bragg's law the interplanner distance d is calculated and the structure of crystal is investigated.

<u>Compton's Effect:</u>

This effect was discovered by Professor A.H. Compton in 1923. According to this effect when an x-ray Photon strikes with an atom of light element (an electron at rest), then after collision the wavelength of X-Ray is changed (it increased).

Let us consider that an X-ray photon of energy $h\upsilon$ strikes with an electron at rest having rest mass m_0 and energy m_0c^2. Let after the collision the energy of X-Ray Photon be $h\upsilon'$ ($\upsilon'<\upsilon$) and the energy of electron be mc^2 as shown in figure.



Let ϕ and θ be the scattering angle of photon and electron respectively. Let us apply principle of conservation of energy (Energy before collision = Energy after collision).

$$h\upsilon + m_o c^2 = h\upsilon' + mc^2$$

or $$mc^2 = h\upsilon - h\upsilon' + m_o c^2$$

Squaring both sides,

$$m^2c^4 = (h\upsilon - h\upsilon')^2 + 2(h\upsilon - h\upsilon')m_o c^2 + m_o^2 c^4$$

$$m^2c^4 = h^2\upsilon^2 - 2h^2\upsilon\upsilon' + h^2\upsilon'^2 + 2(h\upsilon - h\upsilon')m_o c^2 + m_o^2 c^4 \quad \text{---------(1)}$$

Let us apply principle of conservation of momentum along X-axis.

$$\frac{h\upsilon}{c} + 0 = \frac{h\upsilon'}{c}\cos\phi + mv\cos\theta$$

Or $$mvc\cos\theta = h\upsilon - h\upsilon'\cos\phi \quad \text{------(2)}$$

Let us apply the principle of conservation of momentum along Y-axis.

$$0 + 0 = \frac{h\upsilon'}{c}\sin\phi - mv\sin\theta$$

Or $$mvc\sin\theta = h\upsilon'\sin\phi \quad \text{---------(3)}$$

Squaring and adding equation (2) and (3)

$$m^2v^2c^2(\cos^2\theta + \sin^2\theta) = h^2\upsilon^2 - 2h^2\upsilon\upsilon'\cos\phi + h^2\upsilon'^2\cos^2\phi + h^2\upsilon'^2\sin^2\phi$$

or $$m^2v^2c^2 = h^2\upsilon^2 - 2h^2\upsilon\upsilon'\cos\phi + h^2\upsilon'^2 \quad \text{------(4)}$$

Subtracting equation (4) from (1)

$$m^2c^2(c^2 - v^2) = 2(h\upsilon - h\upsilon')m_o c^2 + m_o^2c^4 - 2h^2\upsilon\upsilon'(1 - \cos\phi) \quad \text{-------(5)}$$

Since, $$m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}} \quad \text{........................(6)}$$

Squaring equation (6) we get, $$m^2 = \frac{m_0{}^2c^2}{c^2 - v^2}$$

Putting this value of m^2 in equation (5) we get,

$$\frac{m_0{}^2c^2c^2(c^2 - v^2)}{c^2 - v^2} = 2(h\upsilon - h\upsilon')m_0c^2 + m_0{}^2c^4 - 2h^2\upsilon\upsilon'(1 - \cos\phi)$$

$$2(h\upsilon - h\upsilon')m_o c^2 = 2h^2\upsilon\upsilon'(1 - \cos\phi)$$

$$(\upsilon - \upsilon')m_o c^2 = h\upsilon\upsilon'(1 - \cos\phi)$$

or $$\frac{\upsilon}{\upsilon\upsilon'} - \frac{\upsilon'}{\upsilon\upsilon'} = \frac{h}{m_0c^2}(1 - \cos\phi)$$

or $$\frac{1}{\upsilon'} - \frac{1}{\upsilon} = \frac{h}{m_0c^2}(1 - \cos\phi)$$

or $$\frac{\lambda'}{c} - \frac{\lambda}{c} = \frac{h}{m_0c^2}(1 - \cos\phi)$$

or $$\boxed{\lambda' - \lambda = \frac{h}{m_0c}(1 - \cos\phi)}$$

Case 1: Let $\phi = 0$, then $\lambda' = \lambda$.

Case 2: Let $\phi = \pi/2$ then $\lambda' - \lambda = \frac{h}{m_0c}$

This is known as Compton wave length.

Note 1- Compton Effect gives the convincing proof of existence of photon.
Note 2- This effect correlates the theory of relativity and quantum mechanics.