## Chapter one: X-ray properties



### 1.1 Introduction

X-rays were discovered in 1895 by the German physicist Wilhelm Röntgen and were so named because their nature was unknown at that time. X-rays are part of the electromagnetic radiation, which have high frequency ranging from $3\times10^{16}$ Hz to $3\times10^{19}$ Hz, short wavelength ranging from 0.1 to 10000 Å and energies in the range 100 eV to 100 keV. X-ray wavelengths are shorter than those of UV rays and typically longer than those of gamma rays. X-rays were invisible and they traveled in straight lines could easily pass through the human body, wood, quit thick pieces of metal and other opaque objects.

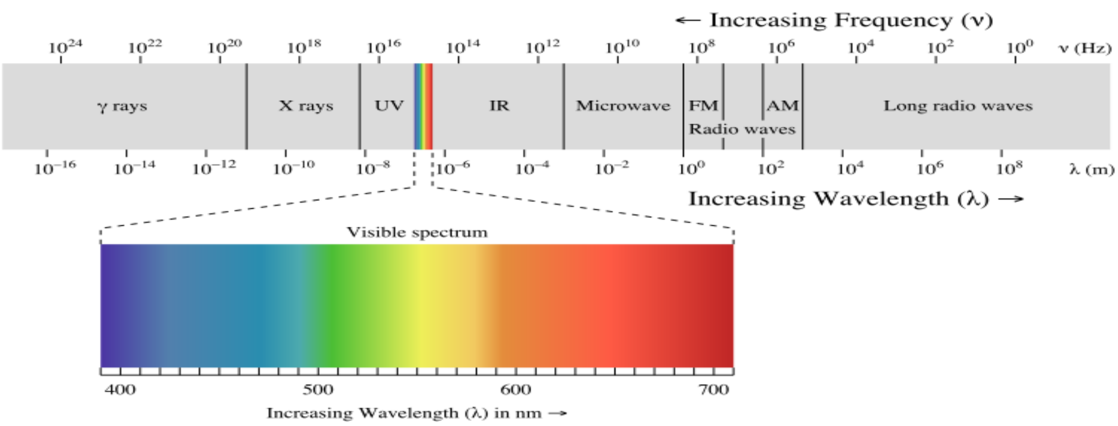


Fig.1

### 1.2 Electromagnetic radiation

To review briefly some properties of electromagnetic waves, suppose a monochromatic beam of x-rays, i.e., x-rays of a single wavelength, is traveling in the x-direction. Then it has associated with it an electric field E in, say, the y direction and, at right angles to this, a magnetic field H in the z direction.

When H=0 , the plan-polarized wave considered (the electric field vector E is confined to the xy-plane as the wave travels along). E is not constant with time t but varies from +y to –y direction and back again

At any particular point x=0, $E = Asin\,(-2\pi vt)$, whereas at any instant time t=o,

$$E = Asin2\pi\frac{x}{\lambda}$$

At both variations E assumed to be sinusoidal, as follows:

$$E = Asin2\pi\,(\frac{x}{\lambda} - vt)$$

Where A= amplitude of the wave, $\lambda$=wavelength and v=frequency.

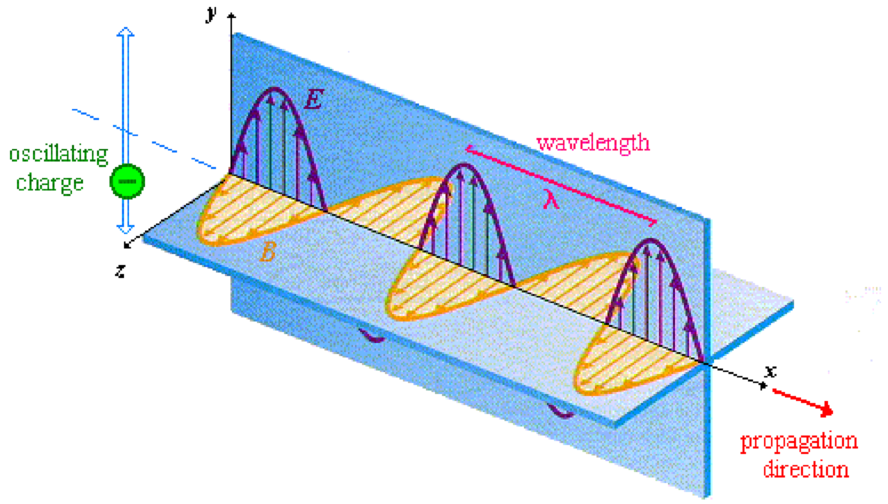


Fig.2

The wavelength and frequency are connected by the relation:

$$\lambda = \frac{c}{v}$$

where c=velocity of light=$3\times10^{10}$cm/sec.

Electromagnetic radiation, such as a beam of x-rays, carries energy, and the rate of flow of this energy through unit area perpendicular to the direction of motion of the wave is called the intensity I. The average value of the intensity is proportional to the square of the amplitude of the wave, i.e., proportional to $A^2$. The x-ray intensity measurements are made on a relative basis in arbitrary units. According to the quantum theory, however, electromagnetic radiation can also be considered as a stream of particles called photons. Each photon has associated with it an amount of energy hv, where h is Planck's constant ($6.63\times10^{-34}$ J.s).

**1.3 Production of X-rays**

X-rays can be generated by an X-ray tube, a vacuum tube that uses a high voltage to accelerate the electrons released by a hot cathode to a high velocity. The high velocity electrons collide with a metal target (the anode) creating the X-rays. The cathode is a filament like the lamp filament is heated by the electric current of about 3 Amp and emits electrons which rapidly drawn to the target (cooling water is circulated through the anode to keep it from melting, i.e., >99% of input power generates heat) by high voltage (up to 60 kV) is across the tube. X-rays are emitted through two or more windows in the tube. The metal target is usually tungsten, molybdenum. In crystallography, a copper target is most common.

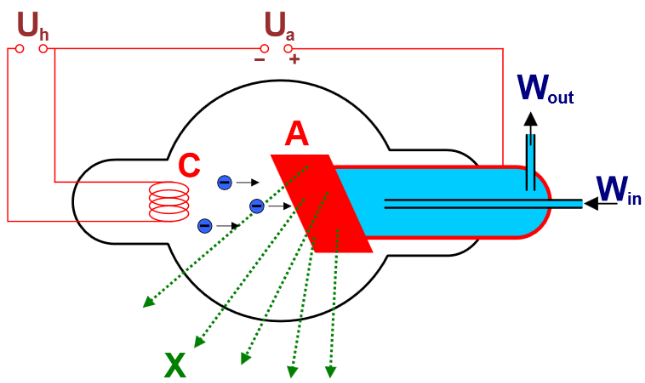


Fig. 3

We can understand the process of X-ray production, from the following: based on the electromagnetic theory. When an electron transfers very quickly near the nucleus of an atom; there is the attraction force between the electron (negatively charged) and nucleus (positively charged), as shown in the figure:

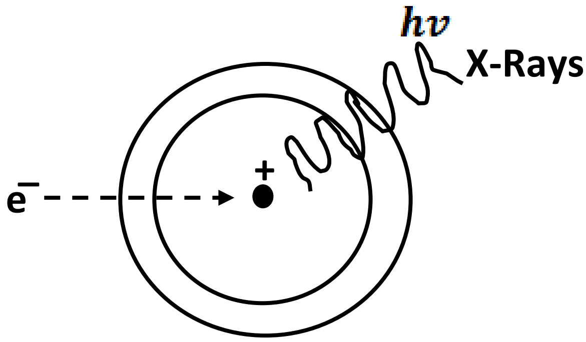


Fig. 4

This force leads to deviation of the electron to the curved path, which producing either deceleration or acceleration of this electron and will emit electromagnetic radiation with an energy equal to $hv$, these radiation is called x-rays.

**1.4 The continuous spectrum**

X-rays are produced when any electrically charged particle of sufficient kinetic energy is rapidly decelerated. Electrons are usually used for this purpose, the radiation being produced in an x-ray tube which contains a source of electrons and two metal electrodes. The high voltage maintained across these electrodes, rapidly draws the electrons to the anode, or target, which they strike with very high velocity. X-rays are produced at the point of impact and radiate in all directions. If e is the charge on the electron ($1.6\times10^{-19}$ C) and V is the voltage across the electrodes, then the kinetic energy (eV) of the electrons on impact is given by the equation:

$$K.E.=eV=\frac{1}{2}mv^2$$

where m is the mass of the electron (9.11×10-31 kg), and v its the electron velocity (m/sec). Most of the kinetic energy of the electrons striking the target is converted into heat, less than 1 % being transformed into x-rays. When the rays coming from the target are analyzed, they are found to consist of a mixture of different wavelengths, and the variation of intensity with wavelength is found to depend on the tube voltage, as shown in Fig. 4.

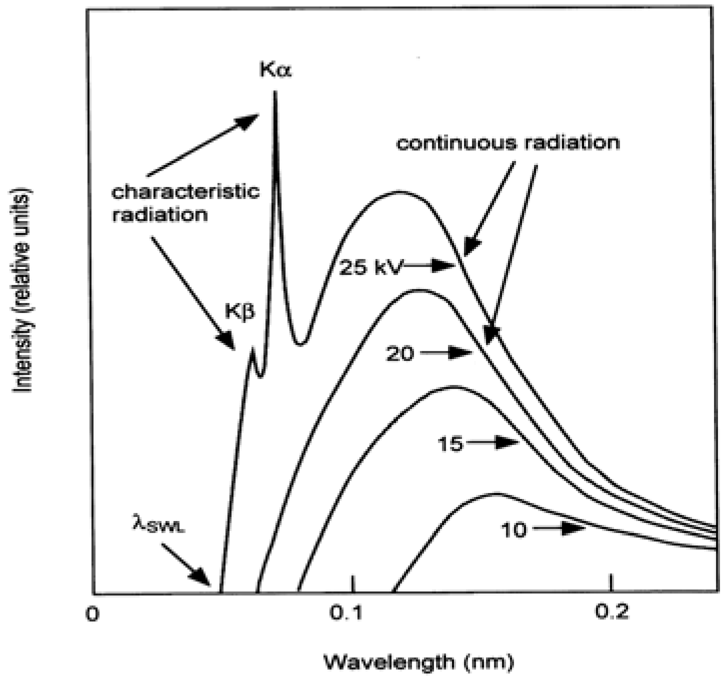


Fig.5

If the applied voltages of 20 kv or less, the intensity is zero up to certain wavelength, called the short-wavelength limit ($\lambda_{SWL}$), increases rapidly to a maximum and then decreases, with no sharp limit on the long wavelength side. This type of radiation is know as *continuous spectrum*, or white radiation, since it is made up, like white light, of rays of many wavelengths.

[***The continuous spectrum*** *is due to the rapid deceleration of the electrons hitting the target and any decelerated charge emits energy*].

Not every electron is decelerated in the same way, however; some are stopped in one impact will give rise to photons of maximum energy, as the following equation:

eV=$hv_{max}$

From the relation between the wavelength and frequency,

$\lambda = \frac{c}{v}$; $\lambda_{SWL} = \frac{c}{v_{max}} = \frac{hc}{eV} = \frac{12400}{V}$

Above equation gives the short-wavelength limit (in angstroms, Å) as a function of the applied voltage V. The total x-ray energy emitted per second, which is depend on the atomic number (Z) of the target and on the tube current (I), the latter being a measure of the number of electrons per second striking the target. This total x-ray intensity is given by:

$I_{continuous\ spectrum} = AIZV^{m}$

where *A* is a proportionality constant and *m* is a constant with a value of about 2. Where large amounts of white radiation are desired, it is therefore necessary to use a heavy metal like tungsten *(Z* = 74) as a target and as high a voltage as possible.

**1.5 The characteristic spectrum**

When the voltage on an x-ray tube is raised to 25 kv or above, sharp intensity maxima appear at certain wavelengths, superimposed on the continuous spectrum. Since they are so narrow and their wavelengths are characteristic of the target metal used, they are called *characteristic lines*. These lines fall into several sets, referred to as K, L, M, etc., in the order of increasing wavelength, all the lines together forming the characteristic spectrum of the metal used as the target.

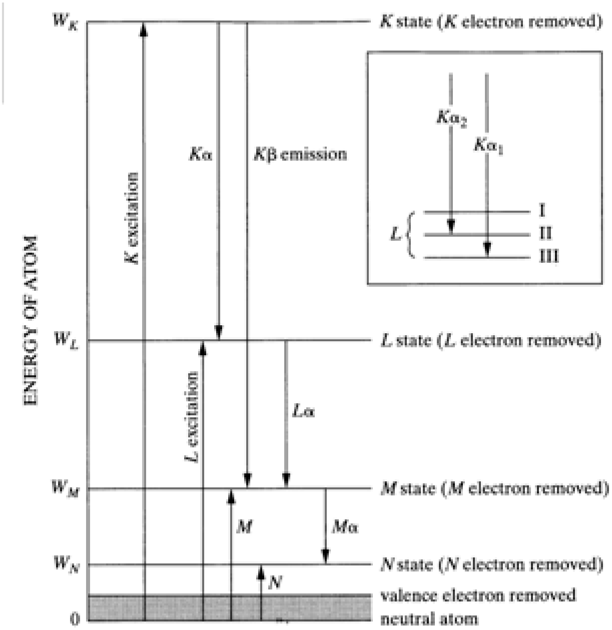


Fig.6

[***The characteristic line*** *is created when a hole in the inner shell, created by a collision event, is filled by an electron from higher energy shell* (*outer shell*)].

Let a K-shell electron be knocked out -- the vacancy can be filled by an electron from the L-shell (Kα radiation) or the M-shell ($K_\beta$ radiation). Usually only the K-lines are useful in x-ray diffraction.

The intensity of any characteristic line, measured above the continuous spectrum, depends both on the tube current I and the amount by which the applied voltage V exceeds the critical excitation voltage for that line. For a K line, the intensity is given by:

$$I_{K\ line} = BI(V - V_K)^n$$

where $B$ is a proportionality constant, $V_K$ the K excitation voltage, and n a constant with a value of about 1.5.

The characteristic x-ray lines were discovered by W. H. Bragg and systematized by H. G. Moseley. The latter found that the wavelength of any particular line decreased as the atomic number of the emitter increased. In particular, he found a linear relation (Moseley's law) between the square root of the line frequency v and the atomic number Z: $\sqrt{v} = C(Z - \sigma)$, where C and $\sigma$ are constants.

**1.6 Absorption**

When x-rays encounter any form of matter, they are partly transmitted and partly absorbed. Experiment shows that the fractional decrease in the intensity I of an x-ray beam as it passes through any homogeneous substance is proportional to the distance traversed, *x*. In differential form,

$$-\frac{dI}{I} = \mu dx$$

where the proportionality constant $\mu$ is called the linear absorption coefficient and is dependent on the substance considered, its density, and the wavelength of the x-rays. Integration of above equation gives

$$I_x = I_o e^{-\mu x}$$

where $I_o$ = intensity of incident x-ray beam and $I_x$ = intensity of transmitted beam after passing through a thickness *x*. The linear absorption coefficient $\mu$ is proportional to the density $\rho$, which means that the quantity $\mu/\rho$ is a constant of the material and independent of its physical state (solid, liquid, or gas). This latter quantity, called the *mass absorption coefficient*, then the above equation can be written as:

$$I_x = I_o e^{-(\mu/\rho)\rho x}$$

The mass absorption coefficient of the substance containing more than one element is a weighted average of the mass absorption coefficients of its constituent elements. Whether the substance is a mechanical mixture, a solution, or a chemical compound, and whether it is in the solid, liquid, or gaseous state, its mass absorption coefficient is simply the weighted average of the mass absorption coefficients of its constituent elements. If $w_1$, $w_2$ , $w_3$ , … are the weight fractions of elements 1, 2, 3, … and $(\mu/\rho)_1$, $(\mu/\rho)_2$ , $(\mu/\rho)_3$ etc., their mass absorption coefficients, then the mass absorption coefficient of the substance is given by

$$\frac{\mu}{\rho} = w_1\left(\frac{\mu}{\rho}\right) + w_2\left(\frac{\mu}{\rho}\right) + \cdots$$

The way in which the absorption coefficient varies with wavelength gives the clue to the interaction of x-rays and atoms. The lower curve of the following Fig,

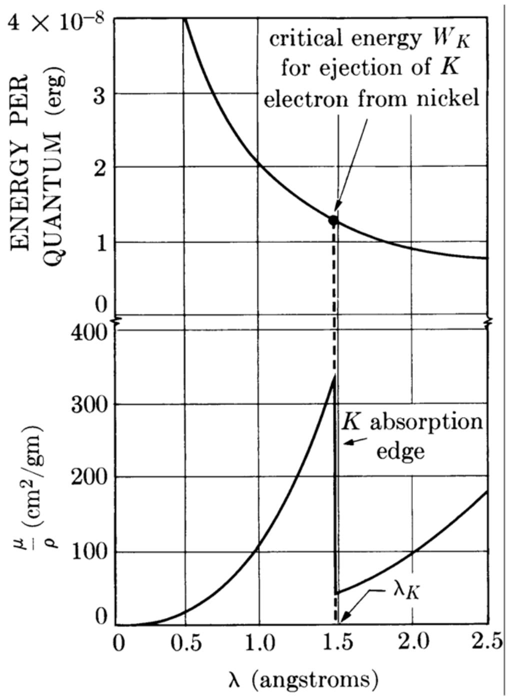


Fig. 7

The curve consists of two similar branches separated by a sharp discontinuity called an absorption edge. Along each branch the absorption coefficient varies with wavelength approximately according to a relation of the form

$$\frac{\mu}{\rho} = k\lambda^3 Z^3$$

where $k$ = a constant, with a different value for each branch of the curve, and Z = atomic number of absorber. Incident x-ray quanta with energy $W_K$ can knock out an electron from K atomic shell. The energy per quantum is $hv$ and wavelength is inversely proportional to frequency. These relations may be written

$$eV_K = W_K = hv_K = \frac{hc}{\lambda_K}$$

where $V_K$ is K excitation voltage, $v_K$ and $\lambda_K$ are the frequency and wavelength, respectively, of the K absorption edge.

**1.7 Filters**

Many x-ray diffraction experiments require radiation which is as closely monochromatic as possible. However, the beam from an x-ray tube contains not only the strong $K_\alpha$ line but also the weaker $K_\beta$ line and the continuous spectrum. The intensity of these undesirable components can be decreased relative to the intensity of the $K_\alpha$ line by passing the beam through a filter made of a material whose K absorption edge lies between the $K_\alpha$ and $K_\beta$ wavelengths of the target metal. A filter so chosen will absorb the $K_\beta$ component much more strongly than the $K_\alpha$ component. The filtration is never perfect. Thicker the filter betters the suppression of $K_\beta$ component but this also results in weaker $K_\alpha$. There is always a compromise. The following Table shows the filters used with the common target metals, the thicknesses required, and the transmission factors for the $K_\alpha$ line.

Filters for Suppression of $K\beta$ Radiation

| Target | Filter | Incident beam* $\frac{I(K\alpha)}{I(K\beta)}$ | Filter thickness for $\frac{I(K\alpha)}{I(K\beta)} = \frac{500}{1}$ in trans. beam | | $\frac{I(K\alpha)\text{ trans.}}{I(K\alpha)\text{ incident}}$ |
|---|---|---|---|---|---|
| | | | mg/cm$^2$ | in. | |
| Mo | Zr | 5.4 | 77 | 0.0046 | 0.29 |
| Cu | Ni | 7.5 | 18 | 0.0008 | 0.42 |
| Co | Fe | 9.4 | 14 | 0.0007 | 0.46 |
| Fe | Mn | 9.0 | 12 | 0.0007 | 0.48 |
| Cr | V | 8.5 | 10 | 0.0006 | 0.49 |

**1.8 Safety precautions**

The radiation hazard is due to the fact that x-rays can:

(1) Kill human tissue. (2) Burns (due to localized high-intensity beams).are painful and may be difficult, if not impossible, to heal. (3) Radiation sickness (due to radiation received generally by the whole body).

The safest procedure for the experimenter to follow is: first, to locate the primary beam from the tube with a small fluorescent screen fixed to the end of a rod and thereafter avoid it; and second, to make sure that he is well shielded by lead or lead-glass screens from the radiation scattered by the camera or other apparatus which may be in the path of the primary beam. Strict and constant attention to these precautions will ensure safety.