$$\cos\delta_1 = \frac{d}{a/h}, \cos\delta_2 = \frac{d}{b/k}, \cos\delta_3 = \frac{d}{c/l},$$

For orthogonal axes, we know that $\cos^2\delta_1 + \cos^2\delta_2 + \cos^2\delta_3 = 1$

Hence $d^2\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right] = 1$ or, $d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$

For cubic system a = b = c (=a say)

$$\boxed{d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}}$$

§ 9.13 X-rays

§ 9.13.1 Production of X-rays on the basis of Quantum theory

X-rays are actually produced from less frequent but more catastrophic encounters of the incoming electrons with the target nuclei. It interacts with the nucleus via coulomb field, transferring momentum to the nucleus. In the process a part of energy of electron is converted into photon. The target nucleus is so heavy that it does not recoil. After encounter the electron moves with remaining energy E'. The frequency or the wavelength λ of the emitted radiation is given by $h\nu = \frac{ch}{\lambda} = E - E'$

The incoming electron suffers many encounters with target nuclei before coming to rest and loses different amount of energy in such collisions. The emitted radiation, therefore, forms a continuous spectrum.

The classical theory provides no explanation for the existence of the short wavelength limit and the characteristic radiation. On the other hand quantum theory provides straightforward explanation of both the experimental observations. As the highly energetic beam passes through the target material, it collisions, which are slow deceleration process, are not responsible for the production of x-rays.

The x-ray photon of shortest wavelength (highest frequency) is emitted when the incident electron loses all of its kinetic energy in a single encounter. In this case $E' = 0$ and hence

$$h\nu_{max} = \frac{ch}{\lambda_{min}} = E \text{ \& where } E = eV$$

where $V \rightarrow$ accelerating voltage. From above relation we have $\frac{ch}{\lambda_{min}} = eV$ So that $\lambda_{min} = \frac{ch}{eV}$ Å

the value of $\frac{hc}{eV} = \frac{6.63\times10^{-34}\times3\times10^{8}}{1.6\times10^{-19}\times V} \approx \frac{12.420\times10^{-7}}{V} \approx \frac{12420}{V}$ Å

So λ_{min} is inversely proportional to accelerating voltage.

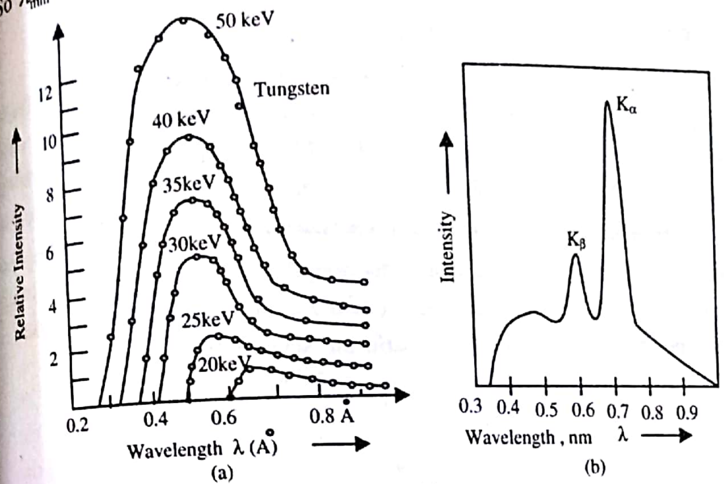

Figure 12:

X-ray spectrum: (a) continuous spectrum emitted by a tungsten target. Note that the short wavelength limits shift to lower wavelength for increasing accelerating potentials; (b) the characteristic line spectrum emitted by a molybdenum target K_α. and K_β lines are seen superposed on the continuous spectrum .

Thus we see that quantum theory provides an easy and convincing explanation for the existence of short wave length limit. If we set h=0 we get $\lambda_{min} = 0$. This means that the existence of λ_{min} is a quantum mechanical phenomenon. The emission of X-ray from deceleration electron is called Bremsstrahlung process. This process is sometimes called inverse photoelectric effect. In a photoelectric process, photon is absorbed; its energy and momentum are transferred to electron. In this process a photon is created, its energy and momentum are derived from the electron-nuclear collision.

Continuous and Characteristic X-ray spectrum The dependence ... intensity of X-rays emitted by a source on wavelength (or frequency) ... known as its X-ray spectrum.

It has been observed that the X-ray spectrum emitted by all the ta... materials consists of a continuous spectrum, having radiations of ... possible wavelength, within a certain range and the lines be... characteristic of the material used as target.

§ 9.13.2 Continuous spectrum

It consists of radiations of all possible wavelengths within a defin... wavelengths range having a definite short wavelength limit. In this ca... intensity varies continuously with all wavelengths as the accelerati... voltage is increased. The shortest wavelength λ_{min} of x-rays emitted ... sharply defined and it depends on voltage applied. Higher the applie... voltage lower is the shortest wavelength. Intensity variation wi... wavelengths of X-rays is independent of the nature of the target material. It is shown in the fig 13 below for different accelerating voltages.

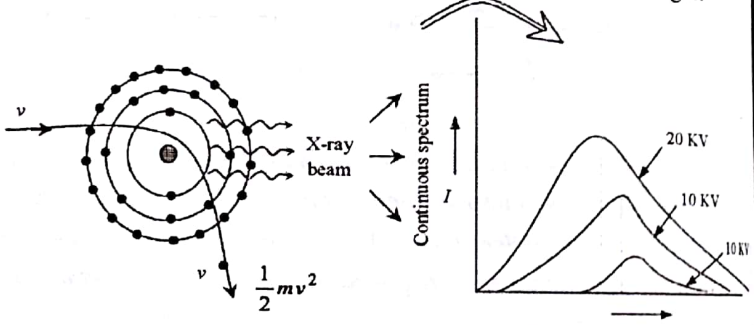

Figure 13:

§ 9.13.2.1 Origin of Continuous Spectrum

When a charged particle is decelerated it radiates energy in terms o... photon, which is known as Bremsstrahlung radiation. The principle behin... the generation of continuous X-ray is also this Bremsstrahlung radiatio... Electrons emitted from the cathode in the X-rays tube are accelerate... towards the target, strike it, penetrate deep into the interior of its atoms an... are attracted by the nuclei due to strong electrostatic interaction. Th... electron therefore deviates from the original path as it shown in th...

diagram. The deviation of the electron from its straight line path is equivalent to its collision with nucleus. So the electron losses some of its energy due to the collision. This energy appears as an X-ray photon. If E_1 is the initial kinetic energy of the electron and E_2 is the final kinetic energy, then the energy of the X-ray photon is $E_1 = E_2$. If is the frequency of the X-ray photon emitted, then $hv = E_1 - E_2$.

The electron may suffer many collisions with various nuclei before coming to rest. Each collision is accompanied by the emission of an X-rays photon. Hence a number of photons of different frequencies are emitted. As there are a large number of electrons in the beam and each electron suffers collision in a different way, we get photons of almost all frequencies or wavelength, thus producing a continuous X-ray spectrum. The production of continuous spectrum is the result of inverse photo-electric effect with electron kinetic energy $E_1 - E_2$ being transformed into photon of energy hv.

§ 9.13.3 Characteristic spectrum

It was found that X-ray radiation emitted by a target consists of a continuous spectrum superimposed with high intensity peaks, as illustrated in the figure 14 below. The peaks occur at wavelengths characteristic of the target material. They occur only at specific wavelengths and hence the characteristic radiation has a line spectrum.

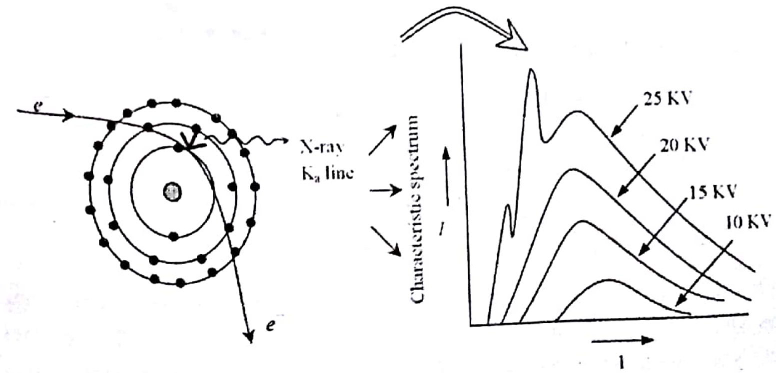

Figure 14:

The origin of x-ray line spectra could not be explained on the basis of classical theories. For detailed theory of the origin of the spectrum refer question and answer section.

§ 9.13.3.1 Origin of Characteristic Spectrum

The origin of X-ray line spectrum was explained on the basis of Bohr's model of atom. According to the model, electrons in an atom are organized into various shells called K, L, M, N.... etc. An atom radiates energy when an electron jumps from one allowed orbit to another allowed orbit. Optical radiation is emitted when a valence electron performs such a transition. The energy involved in such a transition is only a few electron volts. Normally, electron transitions cannot take place from the outermost orbits to the innermost orbits because the inner orbits are occupied. However, such a transition can occur when a very high energy electron knocks off an inner core electron belonging to K, L, ... shells. An electron from an outer orbit jumps to fill up the vacated inner orbit and the energy difference appears in the form of x-ray photon. To give an example, the binding energy of an electron in K-shell of sodium atom is 1041eV. The binding energy of an electron (2s) in L shell is 63eV. If a high energy electron dislodges 1s electron, the 2s electron jumps into 1s level and the energy difference of 1041-63eV=978eV is emitted in the form of an X-ray photon.

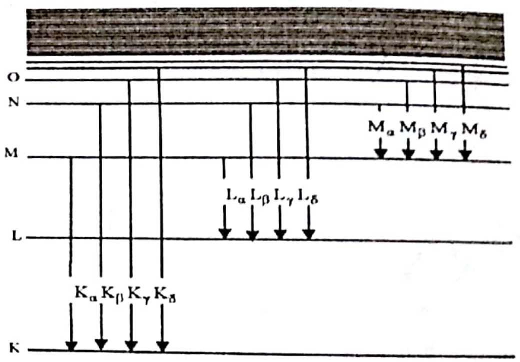

Figure 15: Electronic transition produce characteristic X-ray lines

The characteristic spectrum consists of a series of discrete lines. The group of lines having the shortest wavelength is called K-series. These lines occur when an electron from the K-shell is knocked away and the resulting vacancy is filled by an electron from the next higher shells L, M...... etc. If an electron from L-shell jumps into K-shell, the energy difference

$\Delta E = E_K - E_L$ is emitted in the form of K_α radiation. If an electron from M-shell falls into K-shell, $\Delta E = E_K - E_M$ is emitted as K_β radiation. The transition of N-shell electron to K-shell produces K radiation as illustrated in figure. Usually, only two lines namely K_α and K_β are observed. The K_α line is always the strongest and has shorter wavelength compared to other lines in the K-series. In a similar way the L-series (L_α, L_β....etc.) is produced when vacancies in L-shell are filled by electrons jumping from next higher shells. In case of the lightest elements only K-series is observed while K, L, M-series can be detected in case of heaviest elements.

It is now easy to understand why all X-ray characteristic spectra are similar. According to Bohr model, the structure of the innermost shells is the same for all atoms. Therefore, when electrons are knocked off from the inner shells, identical transitions occur in all atoms and the resulting line spectra are found to be similar. The inner shells in a heavier atom are tightly bound and are of lower energy. It causes larger energy changes during corresponding transitions. The resulting X-rays are of shorter wavelength. It is for this reason that the spectrum shifts to shorter wavelength side as we proceed from lightest to heaviest atoms.

§ 9.13.4 Absorption of X-rays

When a X-ray beam is passing through a material of thickness x, intensity of transmitted. X-ray beam is reduced to some extent. The intensity (I) of the transmitted beam is proportional to the intensity of the incident beam (I_0) as well as thickness of the material (Δx). Mathematically we can write $\Delta I \propto I$ or, $\Delta I \propto \Delta x$ or $\Delta I = \mu I \Delta x$

where μ is absorption coefficient $\therefore \frac{dI}{I} = -\mu dx \rightarrow I = I_0 e^{-\mu x}$

$$\therefore \frac{I_0}{2} = I_0 e^{-\mu x_{1/2}} \text{ or, } \therefore \mu x_{1/2} = \ln 2 \Rightarrow \mu = \frac{\ln 2}{x_{1/2}} = \frac{0.693}{x_{1/2}}$$

§ 9.13.5 Applications of X-rays

Research applications:

X-rays are used

1. for investigating the structure of the matter
2. for studying the structure of complex organic molecules
3. for identification of chemical elements

[The identification of chemical elements and the investigation of structure of matter are explained in the chapter on crystallography.]

Industrial applications:

1. The X-ray radiography are used to detect internal flaws and blow holes in metal castings and welded joints (Refer x-ray radiography in the chapter on Non destructive testing).
2. The X-rays are used to study the molecular structure of engineering materials like rubber, plastics, etc.
3. The X-rays are used to study the effect of heat treatment and the formation of alloys.

Medical applications:

1. The X-ray is used for diagnostic purposes (radiography). Using X-ray radiography, one can detect fractures, presence of foreign bodies like bullet embedded in limb, abscess at the roots of teeth etc., by means of differential absorption of X-rays between bones, tissues and metals.
2. The X-rays are also used for curative purposes (X-rays therapy). X-rays are widely used for treating certain types of skin diseases such as cancer, tumour etc., if the affected part is superficial, soft X-rays are applied and for deep seated affected organs hard X-rays are used.

X-rays in Forensic science:

X-ray examination screening and radiographs can be used in crime detection:

1. The nature of internal injuries sustained by a person as a result of any quarrel and whether the injuries have been caused recently could be found.
2. The sex and approximate age of the body in a charred or highly decomposed condition could be determined.
3. The causes of death can be found out.

4. If a person is suspected to have swallowed jewel, the object would be revealed in a radiograph.
5. The hidden gold in a luggage can be identified using X-rays with a fluorescent screen.

Very soft X-rays called Grenz rays are used for the detection of counterfeit current and forgery in documents.

§ 9.14 X-ray diffraction and Bragg's law

A simplified way of looking at the process by a crystal was proposed by W.L. Bragg. He suggested that through any crystal a set of equidistant parallel planes might be imagined through all atoms of the crystal. These planes are called Bragg planes and their spacing as Bragg spacing as shown in the figure.

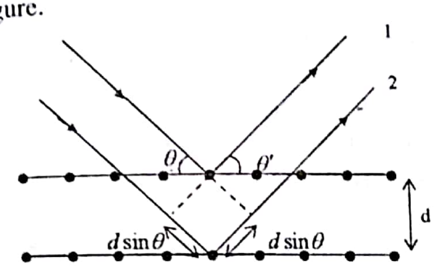

Figure 16:

Let us consider a beam of monochromatic X-rays is incident at these planes. Let the incident rays make angle θ with these planes. This angles is called the glancing angle. The incident rays 1 and 2 will be scattered by atoms of the upper plane, These scattered waves reinforce in the direction $\theta = \theta'$, which is the condition of specular reflection. Thus the atomic planes act as a mirror. Now consider the condition of reinforcement of waves reflected from successive planes that are parallel to the crystal plane. The requirement to be satisfied for the constructive interference is that the path difference for rays reflected from successive planes be equal to integral number of wavelength.

Hence the condition for constructive interference is

$$2d \sin \theta = n\lambda \quad When\ n = 1,2,3,....$$

The above equation is known as Bragg's equation, which should be used in determining the de-Broglie wavelength in crystal diffraction to get the correct result.

Actually Davission and Germer used this equation to determine in their experiment.

§ 9.14.1 Lattice constant measurement:

Bragg's law i.e., $2d\sin\theta = n\lambda$ can be applied in two ways in X-ray diffraction experiments. If the lattice constant i.e., d in the crystal is known, the above said equation permits us the calculation of the wavelength of the X-rays. The crystal can then be used to analyse the spectrum of the X-rays, just as an optical grating is used to analyse the optical spectrum. On the other hand if the wavelength of the X-rays is known, then Bragg's law permits the calculation of the distance between the atoms. This has led to the most precise measurements of atomic distances. The analysis of crystal structure by means of X-rays consists in the demonstration of the actual existence of the space patterns and the determination of their arrangement by the measurement of the size and shape of the unit cell. There are various methods for determining the lattice constants, such as Laue spot, Bragg X-ray spectrometer, rotating crystal, powdered crystal etc.

§ 9.14.2 Relation between crystal density (ρ) and unit cell (a) of a cubic crystal

As we know volume= $\left[\dfrac{\text{mass}}{\text{density}}\right]$. So volume of 1 mole of the substance

$=\left[\dfrac{M_A}{\rho}\right]$ where M_A is the atomic mass of the element. If Avogadro's number be (N_A) then volume of a single atom $=\left[\dfrac{M_A}{N_A\rho}\right]$. The volume of the unit cell of cell length a will be a^3. So equating the cell volume and elemental volume occupied in the unit cell we have

$$\therefore a^3 = \frac{nM_A}{N_A\rho} \quad \text{or} \quad a = \left[\frac{nM_A}{N_A\rho}\right]^{1/3} \quad \text{or, } \therefore \rho = \left[\frac{nM_A}{a^3 N_A}\right]$$

which is the desired relation between density and cell length of a cubic crystal.

Review Questions

Question 1

Find out the packing fraction for F. C. C. structure. Find out the expression for the separation between the planes with Miller indices h, k, l and lattice constant *a* for a simple cubic structure.

[WBUT 2008 (June), 2009 (June)]

Answer:

For packing fraction of FCC refer to article **9.11 (3)**.

The required relation is $d_{hkl} = \dfrac{a}{\sqrt{h^2+k^2+l^2}}$ refer **9.12.2.**

Question 2

How are continuous X-rays produced? Find out the relation between the accelerating voltage of the X-ray tube and the minimum wavelength of X-ray produced.

[WBUT 2008 (June), 2010 (June)]

Answer:

Refer to article **9.13.2** and and then establish the relation $\lambda_{\min} = \dfrac{hc}{eV} \approx \dfrac{12400}{V}\,\text{Å}$ for which refer to **9.13.1**

Question 3

Distinguish between continuous and characteristic x-ray spectra.

[WBUT 2005 (June)]

Answer:

Continuous spectrum:

(i) Consisting of all possible wavelength with a lower wavelength limit