

## UNIT IV

# CRYSTAL STRUCTURE, X-RAYS AND ELECTRODYNAMICS

### 4.1 INTRODUCTION TO CRYSTAL STRUCTURE AND X-RAYS

- The atomic nature of matter has now been established. Nature, however, is never perceived in the atomic form but manifests itself in either of the following forms : (i) Solid, (ii) Liquid, (iii) Gas, (iv) Plasma. The first three occur very commonly while plasma is assumed at elevated temperatures.
- Solid, liquid and gaseous states can be differentiated, superficially, upon certain features exhibited by them. For example, solids possess definite shape, structure and volume, while liquids are devoid of a definite shape but possess a definite volume. Gases possess neither definite shape nor volume.
- It can also be seen that the forms can be differentiated on the basis of their interatomic distance. In the solid state, distances are of the order of a few Angstroms and there is some kind of order, whereas in liquid state there is a transition to a less ordered state. In gaseous state, there is extreme disorder.
- When the atoms or molecules in a solid are arranged in a regular fashion then it is known as **Crystalline**, otherwise it is **Amorphous**. A crystal is a solid composed of a periodic array of atoms. Actual materials are composed of an aggregate of single crystals.
- The study of **Solid State Physics** aims at interpreting the macroscopic properties in terms of the microscopic properties of the minute particles of which the crystal is composed. The study of the geometric forms and physical properties of crystalline solids using X-rays, electron neutron beams etc. constitute the science of **Crystallography**.

### 4.2 UNIT CELL

#### 4.2.1 Space Lattice

- A **Space Lattice** or a **Lattice** is defined as a regular three dimensional periodically repetitive arrangement of points in space, which is infinite in extent.
- Consider an array of points in such a way that the environment around any one point is identical with the environment about any other point. Such an array of

points in two dimensions (See Fig. 4.1) is called the **Plane Lattice**.

- In order to construct the two dimensional lattice, choose any two convenient axes OA and OB. The points lie at equal intervals say 'a' along OA and 'b' along OB.

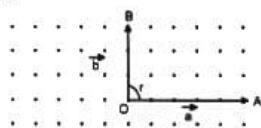


Fig. 4.1

- On extending this array of points in three dimensions, we get a space lattice. The points are arranged at equal intervals say 'c' in the third direction.
- The position vector of any lattice point in two dimensional lattice by choosing any lattice point as origin is

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b}$$

Here  $n_1, n_2$  are integral values representing the number of lattice points along OA and OB and  $\vec{a}$  and  $\vec{b}$  are called the primitive vectors.  $\vec{T}$  is a translation vector connecting two lattice points.

- Similarly  $\vec{T}$  in three dimensions is expressed as

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$$

#### 4.2.2 Unit Cell

[May 19]

- The parallelepiped formed by using the translations  $\vec{a}, \vec{b}, \vec{c}$  as edges is called the **Unit Cell** of the space lattice or the **Primitive Cell**.

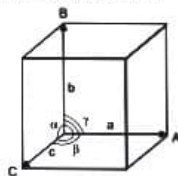


Fig. 4.2 : Unit cell in space lattice

- The angles between primitives (b, c), (c, a) and (a, b) are denoted by  $\alpha$ ,  $\beta$ , and  $\gamma$ .
- Given a lattice work several unit cells are possible. All primitive cells have equal volume which is the minimum possible volume among all unit cells.
- Thus, a **Lattice** is defined as a parallel arrangement of points provided the environment about any point is identical with the environment about any other point.
- A **Non-Primitive Unit cell** contains additional lattice points, either on face or within the unit cell.
- There are two distinct type of unit cells, **Primitive** and **Non-Primitive**.
- The primitive unit cells contain only one lattice point, while non-primitive unit cell contain additional points. The additional lattice point may be in face of the unit cell or within the unit cell.
- The number of additional lattice point per unit cell may be more than one.
- The Fig. 4.3 show the primitive and non-primitive unit cell.



Fig. 4.3

### 4.3 CUBIC SYSTEMS

- The crystals are classified into seven systems on the basis of the shape of unit cell as given in the Table 4.1.

Table 4.1

No.	Name of the Crystal System	Lattice Symbol	Number of Different Lattices in the System	Relation of Axes and the Angles Defining the Cells
1.	Cubic	P (simple cubic) I (Body centred) F (Face centred)	3	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$
2.	Tetragonal	P, I	2	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
3.	Hexagonal	P	1	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$
4.	Trigonal	R (rhombohedral)	1	$a = b = c$ $\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$
5.	Orthorhombic	P, I, F C (base centred)	4	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
6.	Monoclinic	P, C	2	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ, \neq \beta$
7.	Triclinic	P	1	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
Total			14	

- The cubic system is the simplest and the commonest while the triclinic crystals are least symmetrical.

For a cubic system, there exist three types of lattices :

- There is one lattice point at each of the eight corners of the unit cell. This type is called the **Primitive or Simple Cubic Cell (P)** of the system.
- There is one lattice point at each of the eight corners and one lattice point at the centre of the cubic cell. This is a body **Centred Cubic Cell (I)** (bcc type).
- There is one lattice point at each of the eight corners and one lattice point at the centres of each of the six faces of the cubic cell. This is a **Face Centred Cubic Cell (F)** (fcc type) (See Fig. 4.4).

The corresponding Bravais lattices are displayed below in Fig. 4.4.

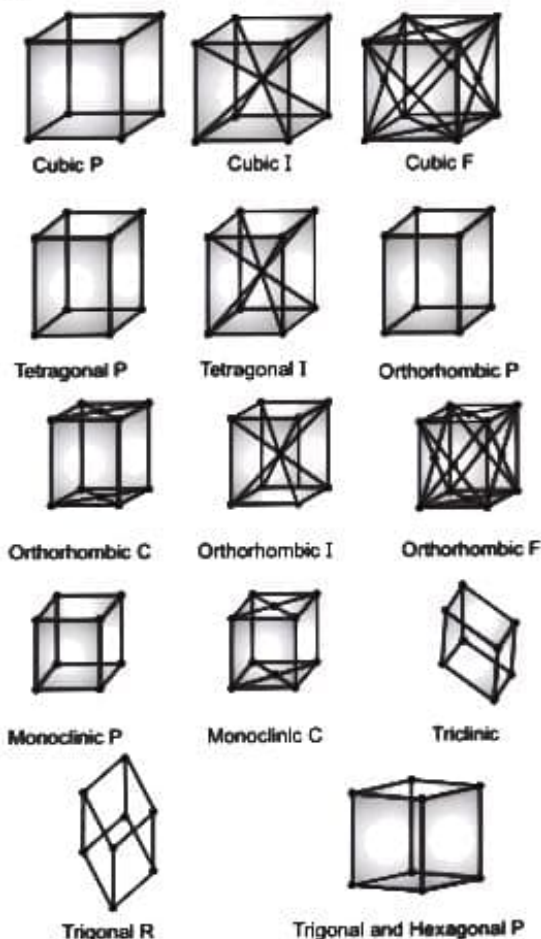


Fig. 4.4 : Bravais space lattice types in three dimensions

### 4.5 NUMBER OF ATOMS PER UNIT CELL



- As each lattice point is shared by eight cubes, we have  $\frac{1}{8}$  of a point (of an atom situated at the lattice point) contributing to the cell. The 8 such corners contribute  $8 \times \frac{1}{8} = 1$ . On repeating the lattice points by identical atoms, this structure therefore has **One Atom per Unit Cell**.



Fig. 4.5 : Simple cubic primitive cell

## 2. Body Centred Cubic (BCC) Lattice :

- As shown in Fig. 4.6 there are eight atoms at the corners and one at the body centre.
- The central atom is totally shared by the unit cell and the contribution due to the 8 corner atoms is  $\frac{1}{8}$  each giving 1 atom in total. Hence, there are **Total 2 Atoms per Unit Cell** for this structure. Alkali metals like Li, Na, K occur naturally in this form. See Fig. 4.6.

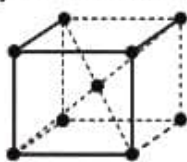


Fig. 4.6 : BCC unit cell

## 3. Face Centred Cubic Lattice (FCC) :

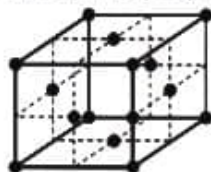


Fig. 4.7 : FCC unit cell

- Each unit cell consists of eight corner atoms each being a member of eight cells. In addition to this there are atoms situated at the centres of the six faces of the cube. Each face is shared by two adjoining cubes.
- Hence there are  $\frac{8}{8} + \frac{6}{2} = 4$  **Atoms per Unit Cell** for this lattice.

Noble metals like gold, silver and copper occur in this group.

## 4.6 CO-ORDINATION NUMBER

- The co-ordination number is defined as the number of nearest neighbours to a given atom in a crystal lattice.

### 1. Simple Cubic Lattice :

- This crystal has one atom at each of the eight corners of the cube. Taking the atom at one corner as the origin and the X, Y, Z axes along the three edges passing through that corner, the positions of nearest neighbours are  $\pm a\hat{i}$ ,  $\pm a\hat{j}$ ,  $\pm a\hat{k}$ . i, j, k being unit vectors along X, Y and Z axes.
- The atoms nearest to the origin having co-ordinates  $(\pm a, 0, 0)$ ,  $(0, \pm a, 0)$ ,  $(0, 0, \pm a)$  are six in number. Hence co-ordination number of a simple cubic lattice is 6. The distance between two neighbours is 'a'.

### 2. BCC Lattice :

- In this lattice there is one atom at each corner of the cube and one atom at the body centre. Taking the central atom as the origin, the positions of nearest neighbours are  $(\pm \frac{a}{2}\hat{i}, \pm \frac{a}{2}\hat{j}, \pm \frac{a}{2}\hat{k})$
- The nearest neighbours are eight in number. Hence co-ordination number of BCC lattice is 8. The distance between the two nearest neighbours is

$$\sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2} = a\sqrt{\frac{3}{2}}$$

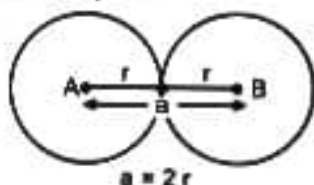
(half the diagonal of the cube)

### 3. FCC Lattice :

- In this lattice, there is one atom at each of the eight corners of the cube and one atom at the centre of each of the six faces of the cube. Taking any one of the lattice points as the origin, the positions of the nearest neighbours are  $(\pm \frac{a}{2}\hat{i}, \pm \frac{a}{2}\hat{j})$ ,  $(\pm \frac{a}{2}\hat{j}, \pm \frac{a}{2}\hat{k})$ ,  $(\pm \frac{a}{2}\hat{k}, \pm \frac{a}{2}\hat{i})$
- The atoms nearest to the origin are 12 in number. Hence co-ordination number of FCC lattice is 12.
- The distance between two nearest neighbours (of the same kind of ions) is

$$\sqrt{\left(\frac{a}{2}\right)^2 + (0)^2 + \left(\frac{a}{2}\right)^2} = \frac{a}{\sqrt{2}}$$

The distance between the centres of two nearest neighbouring atoms is called as **Nearest Neighbour Distance**. It is denoted by 'a'.



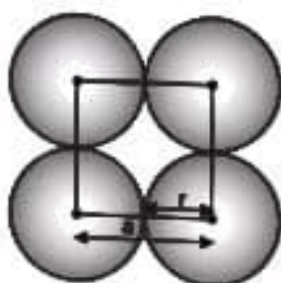
**Fig. 4.8 : Nearest neighbour distance**

If 'r' is considered to be radius of atom, then  $a = 2r$  i.e. the nearest neighbour distance is twice of the radius of atoms.

Let us calculate the radii of different Bravais lattices of a cubical crystal.

### (i) Simple Cube Cell :

A simple cube cell in two-dimensional space can be represented as -



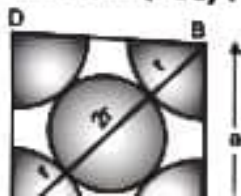
**Fig. 4.9 : Radius of simple cube unit cell**

$$a = 2r$$

$$r = \frac{a}{2}$$

Hence for a simple or primitive cube unit cell, the radius of the atom is half of the distance between centres of the two nearest neighbouring atoms.

### (ii) Face Centered Cubic Cell (FCC) :



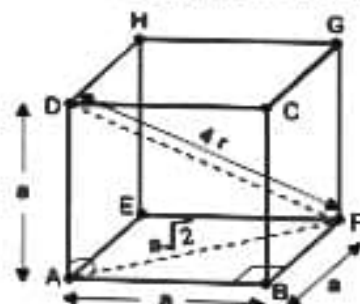
$$r^2 = \frac{2a^2}{16}$$

$$r = \frac{a\sqrt{2}}{4}$$

$\therefore$

### (iii) Body Centered Cubic Cell (BCC) :

In a body centered cubical unit cell, one of the atoms is present inside the unit cell, so it can be shown in Fig. 4.11. It should be noted that the line BC passes through the atom that is present at the centre of the unit cell.



**Fig. 4.11 : Radius of body centered cubical unit cell**

Consider right angled  $\triangle ABF$ ,  $\angle ABF = 90^\circ$

$$\begin{aligned} \therefore AF^2 &= AB^2 + BF^2 \\ &= a^2 + a^2 \\ &= 2a^2 \end{aligned}$$

$$AF = a\sqrt{2} \quad \dots (4.1)$$

Consider right angled  $\triangle DAF$ ,  $\angle DAF = 90^\circ$

$$\therefore DF^2 = AD^2 + AF^2 \quad \dots (4.2)$$

Substituting equation (4.1) in (4.2),

$$\begin{aligned} (4r)^2 &= a^2 + (a\sqrt{2})^2 \\ 16r^2 &= a^2 + 2a^2 \\ 16r^2 &= 3a^2 \end{aligned}$$

$$r = \frac{a\sqrt{3}}{4}$$

Side of the unit cell ' $a$ ' =  $2r$

Volume of the unit cell =  $a^3$

$$\therefore \text{Packing density} = \frac{\frac{4}{3}\pi r^3}{a^3} = \frac{\frac{4}{3}\pi r^3}{(2r)^3} = \frac{\pi}{6}$$

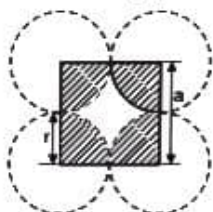


Fig. 4.12 : Simple cubic lattice

## 2. Body Centred Cube :

Number of atoms  
per unit cell = 2

$$\text{Volume of two atoms} = 2 \times \frac{4}{3}\pi r^3$$

$$\text{Side of the unit cell 'a'} = \frac{4r}{\sqrt{3}}$$

$$\text{Volume of the unit cell} = a^3$$

$$\therefore \text{Packing density} = 2 \times \frac{\frac{4}{3}\pi r^3}{a^3} = \frac{\sqrt{3}\pi}{8}$$

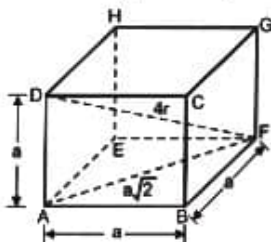


Fig. 4.13 : BCC lattice

## 3. Face Centred Cube :

Number of atoms  
per unit cell = 4

$$\text{Volume of 4 atoms} = 4 \times \frac{4}{3}\pi r^3$$

$$\text{Side of the unit cell 'a'} = \frac{4r}{\sqrt{2}}$$

$$\text{Volume of the unit cell} = a^3$$

$$\therefore \text{Packing fraction} = \frac{4 \times \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} = \sqrt{2} \frac{\pi}{6}$$

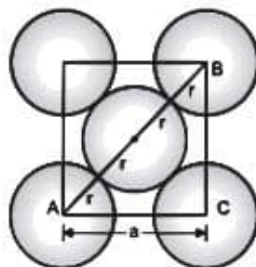


Fig. 4.14 : FCC lattice

## 4.9 RELATION BETWEEN LATTICE CONSTANT AND DENSITY

[May 18]

- Consider a cubic lattice of lattice constant ' $a$ '.  
If  $\rho$  is the density of the crystal then,  
 $\therefore$  Mass in each unit cell =  $a^3\rho$  ... (4.3)  
where  $a^3$  = volume of unit cell
- If  $M$  is the molecular weight,  $N$  the Avogadro number (the number of molecules per kg. mole of the substance) then mass of each molecule =  $\frac{M}{N}$
- If  $n$  is the number of molecules (lattice points) per unit cell, then

$$\text{Mass in each unit cell} = \frac{nM}{N} \quad \dots (4.4)$$

$$\text{From (4.3) and (4.4), } a^3\rho = \frac{nM}{N}$$

$$\text{Or} \quad a = \left(\frac{nM}{N\rho}\right)^{1/3} \quad \dots (4.5)$$

From this relation, the lattice constant ' $a$ ' can be calculated.

## 4.10 LATTICE PLANES AND MILLER INDICES

- A crystal lattice can be considered as an aggregate of a set of parallel equidistant planes passing through the lattice points, which are known as **Lattice Planes**.
- For a particular lattice, these planes may be chosen in different ways as shown, for example, in Fig. 4.15. The problem is that how to designate these planes in crystal Miller developed a method to designate a set of parallel planes in a crystal by three numbers ( $h, k, l$ ) known as **Miller Indices**.



Fig. 4.15



- The steps in determination of Miller indices is given below:

- Consider that the intercepts by the given lattice plane on the three crystal axes X, Y and Z are in the ratio  $pa : qb : rc$  where  $a, b, c$  are the primitives or lattice constants along X, Y, Z axes.  $p, q, r$  may be either small integers or simple fractions.
- Take the reciprocals of  $p, q, r$  i.e.  $\frac{1}{p}, \frac{1}{q}, \frac{1}{r}$ .
- Determine the smallest possible integers  $h, k, l$  such that

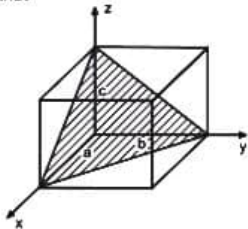


Fig. 4.16

$$h : k : l = \frac{1}{p} : \frac{1}{q} : \frac{1}{r}$$

$$\text{where } h = \frac{L}{p}, k = \frac{L}{q}, l = \frac{L}{r}$$

and  $L$  is the L.C.M. of  $p, q, r$

- The numbers  $h, k, l$  are called the **Miller Indices** of a given set of planes and the plane is specified by  $(h k l)$ .

**To Illustrate the Concept of Miller Indices:** Let a given plane cut intercepts on the axes  $\overline{a}, \overline{b}, \overline{c}$  as  $3a, 6b$  and  $8c$ .

$$\begin{aligned} \text{Then } p &= 3 \\ q &= 6 \\ r &= 8 \end{aligned}$$

$$\text{Hence, } \frac{1}{p} = \frac{1}{3}, \frac{1}{q} = \frac{1}{6}, \frac{1}{r} = \frac{1}{8}$$

$$\text{LCM} = 24$$

$$h = \frac{24}{3} = 8, k = \frac{24}{6} = 4, l = \frac{24}{8} = 3$$

Thus this plane will be represented by the **Miller Indices**  $(8, 4, 3)$ .

#### 4.11 INTERPLANNER SPACING FOR CUBIC SYSTEM

[Dec. 17]

- The spacing between lattice planes of crystals in which the edges of the unit cell are perpendicular can be found as follows:
- Consider the case of plane ABC of a cubic crystal as shown in Fig. 4.17. Let OA, OB and OC be orthogonal axes. Consider any set of parallel planes defined by the

Miller indices  $(h k l)$ . Consider the plane passing through the origin as the reference plane.

- Let line ON be the normal to the plane passing through the origin, the length of which represents the interplanar spacing  $d$ . Let  $\alpha, \beta$  and  $\gamma$  be the angles between co-ordinate axes X, Y, Z and ON respectively. [See Fig. 4.18 (a)].

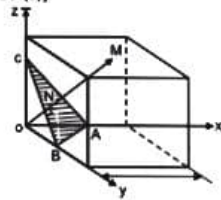


Fig. 4.17

- The intercepts of the plane on the three axes are

$$OA = \frac{a}{h}, OB = \frac{a}{k} \text{ and } OC = \frac{a}{l} \quad \dots (4.6)$$

where 'a' is the cube edge

From Fig. 4.18 (a), we have

$$\cos \alpha = \frac{d}{OA}$$

$$\cos \gamma = \frac{d}{OB} \text{ and } \cos \beta = \frac{d}{OC} \quad \dots (4.7)$$

From Fig. 4.18 (b),

$$ON = [x^2 + y^2 + z^2]^{1/2}$$

$$d = [d^2 (\cos^2 \alpha) + d^2 (\cos^2 \beta) + d^2 (\cos^2 \gamma)]^{1/2}$$

$$\text{i.e. } \cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1 \quad \dots (4.8)$$

Substituting the values of  $\cos \alpha, \cos \beta$  and  $\cos \gamma$  from equation (4.7) in equation (4.8), we get

$$\left(\frac{d}{OA}\right)^2 + \left(\frac{d}{OB}\right)^2 + \left(\frac{d}{OC}\right)^2 = 1$$

$$\text{i.e. } \left(\frac{dh}{a}\right)^2 + \left(\frac{dk}{a}\right)^2 + \left(\frac{dl}{a}\right)^2 = 1$$

$$\text{i.e. } \frac{d^2 h^2}{a^2} + \frac{d^2 k^2}{a^2} + \frac{d^2 l^2}{a^2} = 1$$

$$\frac{d^2}{a^2} (h^2 + k^2 + l^2) = 1 \quad (\text{as } a = b = c \text{ for a cube})$$

$$\text{Or } d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad \dots (4.9)$$

This gives the relation between interplanar spacing 'd' and the edge of the cube 'a'.

For general lattice structures,

$$d_{hkl} = \left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right)^{-1/2}$$

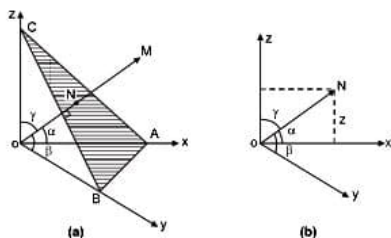


Fig. 4.18

**SOLVED PROBLEMS**

**Problem 4.1 :** Calculate the lattice constant for potassium bromide, given density of potassium bromide is  $2700 \text{ kg/m}^3$  and belongs to FCC lattice. Molecular weight of potassium bromide is 119 and Avogadro number is  $6.02 \times 10^{26} \text{ kg mol}^{-1}$ .

**Data :**  $n = 4$ ,  $M = 119$ ,

$$N = 6.02 \times 10^{26}, \rho = 2700$$

**Formula :**  $a = \left( \frac{nM}{N\rho} \right)^{1/3}$

**Solution :**  $a = \left( \frac{4 \times 119}{6.02 \times 10^{26} \times 2700} \right)^{1/3}$   
 $= (2.928 \times 10^{-28})^{1/3}$   
 $= 6.64 \times 10^{-10} \text{ m}$

**Problem 4.2 :** NaCl crystal has a lattice constant of  $5.643 \text{ \AA}$ . Given molecular weight of NaCl is 58.45 and Avogadro number is  $6 \times 10^{26}$  per kg mole. Find its density.

**Data :**  $n = 4$ ,  $a = 5.643 \text{ \AA}$ ,  $M = 58.45$ ,  $N = 6 \times 10^{26} \text{ kg mol}^{-1}$

**Formula :**  $\rho = \frac{nM}{Na^3}$

**Solution :**  $\rho = \frac{nM}{Na^3}$   
 $= \frac{4 \times 58.45}{6 \times 10^{26} \times (5.643 \times 10^{-10})^3}$   
 $= 2168.51 \text{ Kg/m}^3$

**Problem 4.3 :** Find the Miller indices of a plane making intercepts  $3a$ ,  $5b$ ,  $7c$  on oblique axes  $\bar{a}$ ,  $\bar{b}$ ,  $\bar{c}$ .

**Solution :**

Taking reciprocals of the intercepts,

$$\frac{1}{p_1} : \frac{1}{p_2} : \frac{1}{p_3} = \frac{1}{3} : \frac{1}{5} : \frac{1}{7}$$

Multiplying by the LCM 105

$$\frac{105}{3} : \frac{105}{5} : \frac{105}{7}$$

Then  $h = \frac{105}{3} = 35$ ;

$$k = \frac{105}{5} = 21; L = \frac{105}{7} = 15$$

Miller indices are  $(35, 21, 15)$

**Problem 4.4 :** Calculate the interplanar spacing for  $(3, 2, 1)$  plane in a simple cubic lattice where lattice constant is  $4.2 \times 10^{-10} \text{ m}$ .

**Data :**  $(h k l) = (3, 2, 1)$ ,  $a = 4.2 \times 10^{-10} \text{ m}$

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

**Solution :**  $d_{hkl} = \frac{4.2 \times 10^{-10}}{\sqrt{9 + 4 + 1}} = \frac{4.2}{\sqrt{14}} \times 10^{-10}$   
 $= 1.1225 \times 10^{-10} \text{ m}$

**Problem 4.5 :** A FCC crystal has an atomic radius of  $1.246 \text{ \AA}$ . What are  $d_{200}$ ,  $d_{230}$  and  $d_{111}$  spacings?

**Solution :** For FCC crystal the interatomic distance

$$a = \frac{4r}{\sqrt{2}}$$

$$= 2\sqrt{2} r$$

**Given :** Atomic radius  $r = 1.246 \text{ \AA}$

$$a = 2\sqrt{2} \times 1.246$$

$$a = 3.524 \text{ \AA}$$

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

(i)  $d_{200} = \frac{3.524}{\sqrt{2^2 + 0 + 0}} = \frac{3.524}{2}$

$\therefore d_{200} = 1.762 \text{ \AA}$

(ii)  $d_{220} = \frac{3.524}{\sqrt{4 + 4 + 0}} = 1.245 \text{ \AA}$

(iii)  $d_{111} = \frac{3.524}{\sqrt{1 + 1 + 1}}$   
 $= 2.034 \text{ \AA}$

**Problem 4.6 :** Find out the number of atoms per square millimeter on a plane  $(100)$  of lead whose interatomic distance is  $3.499 \text{ \AA}$ . Lead has face-centred cubic structure.

**Solution :**



Fig. 4.19

For Fig. 4.19 represents (100) plane. The shaded portion shows the portion of the atom.

For FCC structure,

$$r = \frac{\sqrt{2} a}{4}$$

$$\therefore a = \frac{4r}{\sqrt{2}} = 2\sqrt{2} r$$

Interatomic distance = 3.499

$$\therefore 2r = 3.499$$

$$\text{Now, } a = \sqrt{2} (3.499) = 4.95 \text{ \AA}$$

$$\text{area of plane} = a^2$$

where, a is side of given plane

$$= (4.95 \times 10^{-7})^2 \text{ mm}^2$$

Number of atoms in the plane = 2

$$\begin{aligned} \text{Atoms/mm}^2 &= \frac{2 \times 1}{(4.95 \times 10^{-7})^2} \\ &= 8.2 \times 10^{12} \text{ atoms/mm}^2 \end{aligned}$$

**Problem 4.7 :** Calculate the number of atoms per unit cell of metal having a lattice parameter of  $2.9 \text{ \AA}$  and density  $7.87 \text{ gram/cc}$ . Atomic weight of the metal is  $55.85$  and Avogadro constant is  $6.023 \times 10^{23}$ .

**Solution :** Density of crystal  $\rho = \frac{nM}{a^3 N_A}$

$$\text{Given : } a = 2.9 \text{ \AA} = 2.9 \times 10^{-8} \text{ cm, } M = 55.85,$$

$$N_A = 6.023 \times 10^{23}, \rho = 7.87 \text{ gm/cc.}$$

$$\begin{aligned} n &= \frac{\rho a^3 N_A}{M} \\ &= \frac{7.87 \times (2.9 \times 10^{-8})^3 \times 6.023 \times 10^{23}}{55.85} \end{aligned}$$

$$n = 2 \text{ atoms}$$

Hence, unit cell may be body centred cubic.

**Problem 4.8 :** Sketch (112) plane in simple cubic cell.

**Solution :** A plane whose Miller indices are (112) has the following intercepts on the three axes.

$$\frac{1}{1}, \frac{1}{1}, \frac{1}{2}$$

This plane is shown in Fig. 4.20.

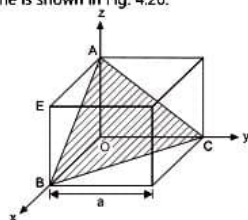


Fig. 4.20

Here,

$$OB = OC = a$$

$$\text{and } OA = \frac{a}{2}$$

**Problem 4.9 :** Sketch (110), (010), (001), (200),  $(\bar{1}10)$  and (112) planes in simple cubic cell.

**Solution :** (i) A plane whose Miller indices are (100) has intercepts  $\frac{1}{1}, \frac{1}{0}, \frac{1}{0}$

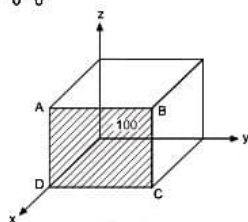


Fig. 4.21

(ii) A plane whose Miller indices are (101) has intercepts

$$\frac{1}{1}, \frac{1}{0}, \frac{1}{1}$$

i.e.

$$1, \infty, 1$$

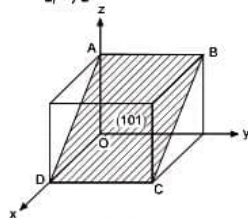


Fig. 4.22



(iii) A plane whose Miller indices are (110) has intercepts

$$\frac{1}{1}, \frac{1}{1}, \frac{1}{0}$$

i.e.  $1, 1, \infty$

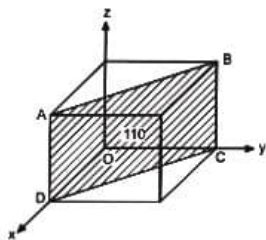


Fig. 4.23

(iv) A plane whose Miller indices are (010) has intercepts.

$$\frac{1}{0}, \frac{1}{1}, \frac{1}{0}$$

i.e.  $\infty, 1, \infty$

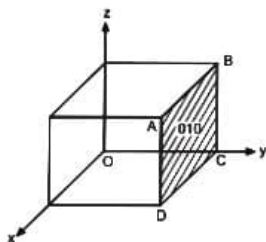


Fig. 4.24

(v) A plane whose Miller indices are (001) has intercepts

$$\frac{1}{0}, \frac{1}{0}, \frac{1}{1}$$

i.e.  $\infty, \infty, 1$

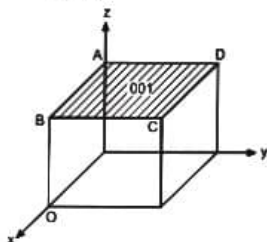


Fig. 4.25

(iv) A plane whose Miller indices are (2, 0, 0) has intercepts

$$\frac{1}{2}, \frac{1}{0}, \frac{1}{0}$$

i.e.  $\frac{1}{2}, \infty, \infty$

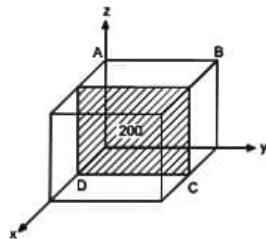


Fig. 4.26

(vii) A plane whose Miller indices are  $(\bar{1}, 0, 0)$  has intercepts

$$\frac{-1}{1}, \frac{1}{0}, \frac{1}{0}$$

i.e.  $-1, \infty, \infty$

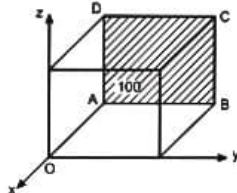


Fig. 4.27

#### 4.12 X-RAY DIFFRACTION

- Because of the short wavelength of X rays ( $\approx 10^{-10}$  m), the ordinary ruled grating with approximately  $6 \times 10^5$  Lines per meter, used with ordinary light, cannot produce any appreciable diffraction.
- But a crystal in which, the atoms arranged in a regular pattern correspond to the grating lines and the atomic spacing (of the order of the X-ray wavelength), forms the grating element exhibits diffraction. The crystal differs from an optical grating in that the former is a **Three Dimensional Space Grating** while the latter is a two dimensional plane grating.
- According to Laue if a narrow pencil of X-rays was made to pass through a thin crystal, a diffraction pattern can be obtained. This symmetrical pattern of spots is known as Laue pattern and it proves that X-rays are electromagnetic waves.

Prof. W. L. Bragg gave a simple interpretation of the diffraction pattern obtained when a beam of monochromatic X-rays was made to pass through a crystal.

- The atoms in a crystal are arranged in a regular three dimensional manner in such a way that there are sets of parallel layers rich in atoms in different planes, each plane having its own spacing between layers, some planes richer in atoms than others.
- When a beam of X-rays falls on the crystal, each atom acts as a scattering centre and emits secondary wavelets whose envelope gives rise to the reflected wavefront (by Huygen's theory). Hence scattering of X-rays can be looked upon as Bragg reflections from planes called the **Bragg Planes**.
- At certain glancing angles, reflections from these set of parallel planes are in phase (to give maximum intensity). At other angles, reflections from different planes are out of phase (to give minimum or zero intensity).

#### 4.13.1 Bragg's Law

[Dec. 18]

- Consider a crystal consisting of a set of parallel planes separated by a distance  $d$ .
- Let a narrow monochromatic beam of X-rays of wavelength  $\lambda$  be incident on this plane at a glancing angle  $\theta$ .
- Consider two parallel rays ABC and DFH which are reflected by two atoms B and F in adjacent layers, F being vertically below B.
- Ray DFH has a longer path than ray ABC and the path difference between them is given by  $(EF + FG)$  where E and G are the feet of the perpendiculars drawn from B on DF and DH respectively.
- This path difference will decide whether the two reflected rays will be in phase or out of phase.
- When the path difference is equal to  $n\lambda$  ( $n$ -an integer), the reflected rays will reinforce each other to produce an intense beam.

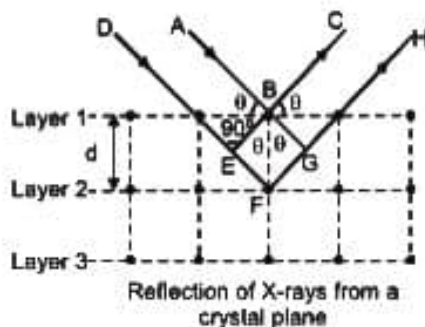


Fig. 4.28

$$EF + FG = n\lambda \quad \dots (4.10)$$

From Fig. 4.28,

$$EF = FG = d \sin \theta \quad \dots (4.11)$$

Substituting (4.11) in (4.10),

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

- This relation is known as **Bragg's Law**. It indicates that, for given values of  $n$ ,  $\lambda$  and  $d$  there is reflection only in a particular direction defined by  $\theta$ .
- Destructive interference occurs in other directions.
- By making  $n$  equal to 1, 2, 3 etc. successively, a series of values are obtained for  $\theta$  for which sharp reflections occur.
- These are called as first order ( $n = 1$ ), second order ( $n = 2$ ), etc. maximum. As the order of the spectrum increases, the intensity decreases.

#### 4.13.2 Bragg's X-Ray Spectrometer

- It consists of three parts : (1) a source of X-rays suitably collimated, (2) a circular table graduated and provided with a vernier to hold the crystal and (3) a deflecting device.
- X-rays from an X-ray tube are collimated into a fine beam by two narrow slits  $S_1$  and  $S_2$ .
- The beam is made to be incident at a glancing angle  $\theta$  on the face of a crystal C (of calcite, rock salt, mica, NaCl etc.), which is mounted on a circular table T. This table can rotate about a vertical axis and its position can be read by the graduated scale and vernier V.
- Rotating about the same axis is an arm R carrying an ionization chamber I, provided with a vernier to fix its position.
- The intensity of the X-ray beam (i.e. degree of ionisation in the chamber) that enters the chamber is measured by an electrometer E.

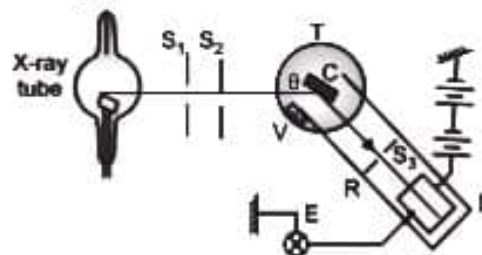


Fig. 4.29

- The turn table T and arm R are so linked that when the T, and hence the crystal, rotates through an angle  $\theta$ , the R and hence the ionization chamber 'I' turns through  $2\theta$ .
- Therefore, whatever be the incident angle of the beam at the crystal surface, it is always reflected into I. If the reflected beam is to be recorded on a photographic film, I can be replaced by a camera.
- The ionization current is measured for different values of  $\theta$  and a plot is obtained.

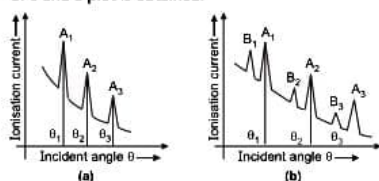


Fig. 4.30

- From the graph, the glancing angles  $\theta_1, \theta_2, \theta_3$  for first, second and third order reflections are measured. Knowing the values of  $d$  and  $n$ , wavelength  $\lambda$  of X-rays can be calculated using Bragg's equation i.e.  $2d \sin \theta = n\lambda$ .
- Fig. 4.30 (a) is the spectrum when the X-ray beam is monochromatic while Fig. 4.30 (b) represents the case when the X-ray beam consists of two wavelengths  $\lambda_1$  and  $\lambda_2$ .
- In this way, Bragg's spectrometer can be used to find the wavelength of X-rays. Conversely  $d$  can be computed if  $\lambda$  of X-rays is known from some other experiment.

**Problem 4.10:** Using Bragg's X-ray spectrometer, the glancing angle for first order spectrum was observed to be  $8^\circ$ . Calculate the wavelength of X-rays if  $d = 2.82 \times 10^{-10} \text{ m}$ .

**Data :**  $\theta = 8^\circ$ ,

$$d = 2.82 \times 10^{-10} \text{ m}, n = 1$$

**Formula :**  $2d \sin \theta = n\lambda$

$$\begin{aligned} \text{Solution : } \lambda &= \frac{2d}{n} \sin \theta \\ &= \frac{2 \times 2.82 \times 10^{-10} \sin 8^\circ}{1} \\ &= 2 \times 2.82 \times 10^{-10} \times 0.1392 \text{ m} \\ &= \boxed{0.7857 \text{ \AA}} \end{aligned}$$

**Problem 4.11 :** X-rays of wavelength  $1.6 \text{ \AA}$  are diffracted by a Bragg crystal spectrometer at an angle  $14.2^\circ$  in the first order. What is the spacing of atomic layers in the crystal ?

**Data :**  $\lambda = 1.6 \text{ \AA} = 1.6 \times 10^{-10} \text{ m}$ ,  $\theta = 14.2^\circ$ ,  $n = 1$

**Formula :**  $2d \sin \theta = n\lambda$

$$\text{i.e. } d = n \frac{\lambda}{2 \sin \theta}$$

$$\begin{aligned} \text{Solution : } d &= 1 \times 1.6 \times \frac{10^{-10}}{2 \times \sin 14.5^\circ} \\ &= \frac{1.6 \times 10^{-10}}{2 \times 0.2454} = \boxed{3.26 \text{ \AA}} \end{aligned}$$

**Problem 4.12 :** Calculate the longest wavelength that can be analysed by a crystal with an interplanar spacing of  $3 \text{ \AA}$  in first order.

**Data :**  $d = 3 \text{ \AA}$ ,  $n = 1$ ,  $\sin \theta = 1$  (maximum)

$$\text{Formula : } \lambda = \frac{2d}{n} \sin \theta$$

$$\begin{aligned} \text{Solution : } \lambda &= 2 \times 3 \text{ \AA} \\ &= \boxed{6 \text{ \AA}} \end{aligned}$$

**Problem 4.13 :** The unit cell dimension 'a' of NaCl lattice is  $5.63 \text{ \AA}$ . If an X-ray beam of  $\lambda = 1.1 \text{ \AA}$  falls on a family of planes with a separation of  $\frac{a}{\sqrt{5}}$ , how many orders of diffraction are observable ?

**Data :**  $\lambda = 1.1 \text{ \AA}$ ,  $a = 5.63 \text{ \AA}$ ,  $d = \frac{a}{\sqrt{5}}$

$$\text{Formula : } n = \frac{2d \sin \theta}{\lambda}$$

**Solution :** For maximum observable orders,  $\theta = 90^\circ$

$$\begin{aligned} \therefore n &= \frac{2d}{\lambda} = \frac{2 \times 5.63}{\sqrt{5}} \times \frac{1}{1.1} \\ &= \boxed{4.585 < 5} \end{aligned}$$

Four orders of diffraction are observable.

**Problem 4.14 :** When a nickel target is used in a X-ray tube, the two shortest wavelengths emitted are found with a Bragg's crystal spectrograph to be diffracted at an angle of  $15.1^\circ$  and  $17.1^\circ$  respectively. Find their wavelength assuming crystal spacing of  $2.81 \text{ \AA}$ .

**Data :**  $d = 2.81 \text{ \AA}$ ,  $\theta_1 = 15.1^\circ$ ,  $\theta_2 = 17.1^\circ$ ,  $n = 1$

$$\text{Formula : } \lambda = \frac{2d \sin \theta}{n}$$



**Solution :**  $\lambda_1 = \frac{2d \sin \theta}{n} = 2 \times 1.81 \times \sin 15.1^\circ$   
 $= 1.464 \text{ \AA}$   
 $\lambda_2 = \frac{2d \sin \theta}{n} = 2 \times 1.81 \times \sin 17.1^\circ$   
 $= 1.652 \text{ \AA}$

#### 4.13.3 Crystal Structure using X-Rays Diffraction

- Atoms of different elements in a crystal have definite orderly arrangement in the space. When X-rays are incident on the crystal, they are scattered by each atom of the crystal. Definite arrangement of atoms represent sets of parallel planes which are rich in these atoms.
- Combined effect of scattering of X-rays by these sets of planes can be considered as reflection of X-rays by these planes.
- The scattering caused by the atoms is called **Bragg's Scattering** or **Bragg's Reflection**. The planes which cause these reflections are called **Bragg's Planes**.
- Due to the presence of sets of parallel planes rich in certain types of atoms, the crystal acts like diffraction grating for X-rays.
- X-ray reflections from these sets of parallel planes are in phase with each other for certain glancing angle. Hence, different reflected X-rays combine together to give a very strong effect. As a result the ionisation current produced by these is very large. If the angles of incidence are other than the above angle, X-ray reflections are antiphase with each other. So the resultant reflection is zero or extremely weak.

#### 4.14 LINE AND CONTINUOUS SPECTRUM OF X-RAY

- The X-rays are produced when high velocity electrons strike the target material of high atomic number, such as tungsten or molybdenum. About 99 % of electrons striking solid matter targets are wasted in heating the target and increasing the kinetic energy of the particles hit. The remaining 1 % collisions produce two types of X-rays, the characteristic X-rays and continuous X-rays, by losing their energy in the following two ways.
- Some of the incident electrons transfer their energy to the target atoms. The target atoms retain this energy temporarily as excitation energy and then emit it shortly as X-rays which are characteristic of the target material. So they are called **Characteristic X-Rays**.

- Other electrons are stopped by the target and their energy is directly converted into X-rays. There is continuous loss in kinetic energy of incident electrons and X-rays are emitted continuously. So they are called **Continuous X-Rays**.

- The basic requirements of X-ray production are : (i) A source of electrons (ii) Effective means of accelerating electrons and (iii) A target of suitable material of high atomic number.
- There are two types of X-ray tubes. (i) The gas filled or Roentgen X-ray tube and (ii) The Coolidge hot cathode X-ray tube.
- In Coolidge X-ray tube, it is possible to achieve separate control of the intensity and quality of X-rays independent of each other. So we describe it here.

#### 4.14.1 Coolidge Hot-Cathode X-Ray Tube

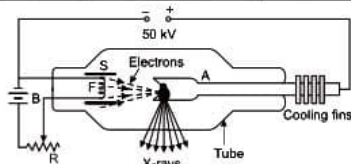


Fig. 4.31 : Coolidge tube

- This tube is widely used for commercial and medical purposes. The essential elements of a modern Coolidge X-ray tube are shown in Fig. 4.31.
- A tungsten filamentary cathode F is heated by a low voltage battery and electrons are produced thermionically. These electrons are focused on the target T by a cylindrical shield S which surrounds F. The shield S is maintained at a negative potential. The electrons are accelerated to very high speeds by the d.c. voltage of 50 kV to 100 kV applied between the cathode F and the anode.
- This high d.c. voltage is obtained from a step up transformer whose output is converted into d.c. voltage by a full wave rectifier.
- The target T consists of a copper block in which a piece of tungsten or molybdenum is fitted. The face of the copper anode is sloped at  $45^\circ$  to the electron beam.
- The copper block conducts heat efficiently to the external cooling fins. The anode should be of a metal of high melting point, so that, it will not melt under the bombardment of electrons.

- To produce hard X-rays and for their abundant yield, the anode should be of a metal of high atomic number.
- When the accelerated electrons strike the target and are stopped by it, they give up their kinetic energy and thereby produce X-rays.
- The intensity of X-rays depends on the number of electrons striking the target. This number depends on the temperature of the filament and so on the filament current. So, by controlling the filament current by a rheostat R, the thermionic emission and hence intensity of X-rays can be controlled.
- The quality of X-rays is measured in terms of their penetrating power. It depends on the p.d. between the cathode and the anode.
- Greater the accelerating voltage, higher is the speed of the striking electrons and consequently, more penetrating are the X-rays produced.
- High penetrating X-rays are called hard X-rays and low penetrating X-rays are called soft X-rays. Thus the quality of X-rays in Coolidge tube can be controlled by varying the p.d. between the cathode and the anode.

#### 4.14.2 Continuous X-Rays

[Dec. 17, May 19]

- When fast moving electrons are obstructed by solid metal targets, X-rays are produced. Some of the high velocity electrons penetrate deep into the interior of the atoms of the target material and are attracted by their positively charged nuclei. As an electron passes close to the nucleus, it is deflected from its path as shown in Fig. 4.32.
- The electron experiences deceleration during its deflection in the strong field of the nucleus. The energy lost during its retardation is given out in the form of X-rays of continuously varying wavelength.
- These X-rays produce a continuous spectrum having a sharply defined short wavelength limit  $\lambda_{\min}$  (or high frequency limit  $\nu_{\max}$ ) which corresponds to the maximum energy of the incident electron.
- As shown in Fig. 4.32, if the striking electron of mass  $m$  has its velocity reduced from  $v$  to  $v'$  due to deflection or due to collision, then loss of its energy is  $\left(\frac{1}{2}mv^2 - \frac{1}{2}mv'^2\right)$  and this must be equal to the energy  $h\nu$  of the emitted X-ray photon,

$$\therefore h\nu = \frac{1}{2} m (v^2 - v'^2)$$

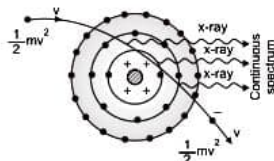


Fig. 4.32

- When the electron is completely stopped, i.e. when  $v' = 0$ , X-rays of maximum frequency are emitted. In that case,

$$h\nu_{\max} = \frac{1}{2} mv^2 \quad \dots (4.12)$$

- If kinetic energy is imparted to the electron by accelerating it through a p.d. of  $V$  volts, then

$$eV = \frac{1}{2} mv^2 \quad \dots (4.13)$$

From equations (4.12) and (4.13)

$$h\nu_{\max} = eV$$

$$\text{i.e. } h \frac{c}{\lambda_{\min}} = eV \quad (\because \lambda_{\min} \nu_{\max} = c)$$

$$\therefore \lambda_{\min} = \frac{hc}{eV} \quad \dots (4.14)$$

where  $c$  is the velocity of light.

- Equation (4.14) gives the short-wavelength limit of the continuous X-ray spectrum.

Substituting for the constants

$$c = 3 \times 10^8 \text{ m/s, } e = 1.6 \times 10^{-19} \text{ C, } h = 6.63 \times 10^{-34} \text{ J-s,}$$

we get,

$$\begin{aligned} \lambda_{\min} &= \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-19} V} \text{ metres} \\ &= \frac{1.24 \times 10^{-6}}{V} \text{ m} \\ \therefore \lambda_{\min} &= \frac{12400}{V} \text{ \AA} \quad \dots (4.15) \end{aligned}$$

- Such radiations are called **Braking Radiations**, because they are due to braking or slowing down of high velocity electrons in the positive field of a nucleus. These X-rays consist of a series of uninterrupted wavelengths having a sharply defined short wavelength limits  $\lambda_{\min}$  and they form the continuous spectrum.

- They are determined by the p.d. between the cathode and the anode of the X-ray tube and are independent of the nature of the target material.

#### 4.14.3 Characteristic of X-Rays

- When fast moving electrons are suddenly stopped by solid metal targets, X-rays are produced. Some of the high velocity electrons knock out the tightly bound electrons in the innermost shells (like K, L, M... etc. shells) of the atoms, while penetrating the interior of the atoms of the target material.
- When electrons from outer orbits jump to fill up the vacancy so produced, the energy difference is given out in the form of X-rays of definite wavelength.
- These wavelengths form the line spectrum which is characteristic of the material of the target. So it is called **Characteristic X-Ray spectrum**.

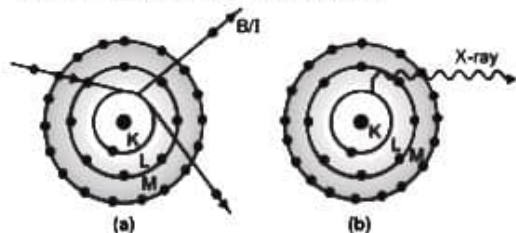


Fig. 4.33

- Fig. 4.33 (a) shows the case when the high velocity incident electrons knock out one electron from the K-shell of the atom. As shown in Fig. 4.33 (b), this K-shell vacancy is filled up by an electron from a nearby L-shell.
- During this jump an X-ray photon of frequency  $\nu$ , such that  $E_K - E_L = h\nu$  is emitted, where  $E_K$  is the energy required to dislodge a K-shell electron and  $E_L$  is the energy required to dislodge an L-shell electron.
- As this energy difference ( $E_K - E_L$ ) is comparatively very large, the emitted X-rays have very large energy and hence they are highly penetrating.

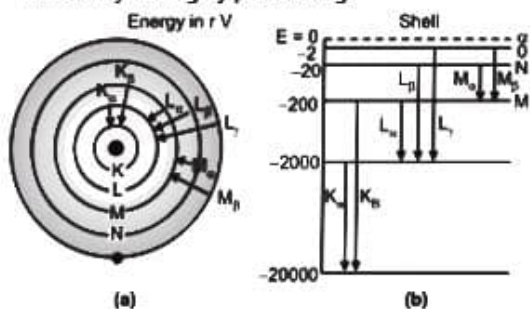


Fig. 4.34

- If, however, the K-shell vacancy is filled up by an electron jumping from the M-shell, the emitted X-rays would be still more energetic and would possess still higher frequency because  $(E_K - E_M) > (E_K - E_L)$ . Such X-rays arising from millions of atoms produce the K-lines of the characteristic spectrum as shown in Fig. 4.34 (a). Usually,  $K_\alpha$  and  $K_\beta$  lines of this series are detected although there are many more.

Similarly, when the incident electron has somewhat lesser energy, it dislodges an L-shell electron. This L-shell vacancy is filled up by an electron jumping from M-shell to other outer shells, and X-rays of frequency lower than that of K-series are produced. This gives the  $L_\alpha$ ,  $L_\beta$ , and  $L_\gamma$  lines of the L-series of the characteristic spectrum, as shown in Fig. 4.34 (a) and (b).

- Spectral lines of M-series are produced when incident electron knocks out an M-shell electron and this M-shell vacancy is filled up by electrons jumping from outer shells. The characteristic X-ray lines are shown in energy level diagram in Fig. 4.34 (a) and (b).
- These K-series, L-series and M-series constitute the line spectra of the X-rays, which are characteristic of the material of the target used in the X-ray tube.
- So, the X-rays produced by an X-ray tube consist of two parts,
  1. One part consists of a series of uninterrupted wavelengths having a short cut off  $\lambda_{\min}$ . This constitutes the continuous spectrum.
  2. The other part consists of a number of distinct and discrete wavelengths. They constitute the line or the characteristic X-ray spectrum.
- The characteristic spectrum is superposed on the continuous spectrum. X-ray spectrum of molybdenum is shown in Fig. 4.35.

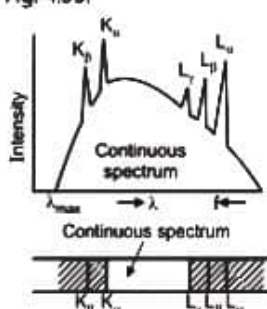


Fig. 4.35



**4.15 MOSELEY'S LAW****[May 18]**

- A systematic study of characteristic X-ray spectra of different metallic elements was carried out by Moseley in 1913 - 14 by using them as targets in the X-ray tube. He used Bragg's spectrometer for this study.

- His observations are :

➤ The characteristic X-ray spectra of different elements are similar, as characteristic spectrum of any element consists of K-series, L-series and M-series.

➤ The frequency of lines (in every series) produced from an element of higher atomic number is greater than that produced by an element of lower atomic number. This is so because the binding energy of electrons increases as we go from one element to another of higher atomic number, i.e. larger amount of energy is required to liberate an electron from K-shells, L-shells and M-shells of atoms of an element of higher atomic number.

- Thus, say for  $K_{\alpha}$  line, the higher the atomic number of the target material, higher is the frequency of the  $K_{\alpha}$  line. Mathematically,

$$\nu \propto (Z - a)^2$$

$$\text{or } \nu = b(Z - a)^2 \quad \dots (4.16)$$

where  $\nu$  = frequency of characteristic radiation.

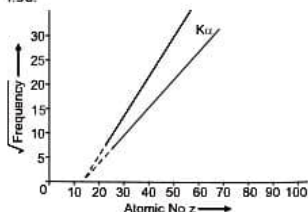
$b$  = constant, which is different for different series.

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

$Z$  = Atomic number of the target material.

- Equation (4.16) is called Moseley's law. It may be stated as, "The frequency of a spectral line in characteristic X-ray spectrum varies directly as the square of the atomic number of the element emitting it".

- Moseley's diagram for  $K_{\alpha}$  and  $K_{\beta}$  lines, obtained by plotting  $\sqrt{\nu}$  versus  $Z$  of different elements is shown in Fig. 4.36.

**Fig. 4.36**

- For  $K_{\alpha}$  line, it was found that  $b = \frac{3}{4} R$ , where  $R$  is Rydberg constant, and  $a = 1$ .

Hence for  $K_{\alpha}$  line,

$$\nu_{K_{\alpha}} = \frac{3}{4} R (Z - 1)^2 \quad \dots (4.17)$$

**Importance of Moseley's Law :**

- As per this law, the atomic number of an element determines its physical and chemical properties, and not its atomic weight. So the basis of periodic table is now taken as to arrange elements according to their increasing atomic number and not as their increasing atomic weights as was done earlier.

- Mandeleev's basis of the periodic table was to arrange elements in ascending atomic weights. So, Potassium  ${}_{19}\text{K}^{39}$  was placed before Argon  ${}_{18}\text{Ar}^{40}$  and Nickel  ${}_{28}\text{Ni}^{58.7}$  was placed before Cobalt  ${}_{27}\text{Co}^{58.9}$ . However, Mandeleev observed that to maintain the periodicity of chemical and physical properties their orders should be reversed. This difficulty was removed by Moseley's law, because as per their atomic numbers, their order should be just opposite.

- Moseley's law also led to the discovery of some new elements like Hafnium ( $Z = 72$ ), Promethenium ( $Z = 61$ ), Technitium ( $Z = 43$ ), Rhenium ( $Z = 75$ ) etc.

**Problem 4.15 :** An X-ray tube operating at 20 kV emits a continuous spectrum with shortest wavelength limit of 0.62 Å. Calculate Planck's constant.

**Solution :** Short wavelength limit

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

$$\therefore h = \frac{eV \lambda_{\min}}{c}$$

$$= \frac{1.6 \times 10^{-19} \times 2 \times 10^4 \times 0.62 \times 10^{-10}}{3 \times 10^8}$$

$$\therefore h = 6.72 \times 10^{-34} \text{ Js}$$

**Problem 4.16 :** A Coolidge tube operates at 50 kV. Find (i) the maximum velocity of the electrons striking the anticathode (ii) minimum wavelength of X-rays generated.

Given  $e = 1.6 \times 10^{-19} \text{ C}$ ,  $m = 9.1 \times 10^{-31} \text{ kg}$ .

**Data :**  $V = 50 \text{ kV} = 50 \times 10^3 \text{ V}$ ,  $e = 1.6 \times 10^{-19} \text{ C}$ ,  $m = 9.1 \times 10^{-31} \text{ kg}$

**Formula :** (i)  $v_{\max} = \sqrt{\frac{2eV}{m}}$

(ii)  $\lambda_{\min} = \frac{12400}{V} \text{ Å}$

**Solution :** (i)  $v_{\max} = \sqrt{\frac{2 \times 1.6 \times 10^{-19} \times 50 \times 10^3}{9.1 \times 10^{-31}}}$   
 $= 1.326 \times 10^8 \text{ m/sec}$   
 (ii)  $\lambda_{\min} = \frac{12400}{50 \times 10^3}$   
 $= 0.248 \text{ \AA}$

**Problem 4.17 :** In an X-ray tube, electrons bombarding the anode produce X-rays of wavelength  $1 \text{ \AA}$ . Taking Planck's constant as  $h = 6.6 \times 10^{-34} \text{ J-sec}$ , calculate the energy of the electrons as it hits the anode (in Joules) and the voltage of the X-ray tube.

**Data :**  $\lambda_{\min} = 1 \text{ \AA} = 10^{-10} \text{ m}$ ,  $h = 6.6 \times 10^{-34} \text{ J-sec}$ ,  $e = 1.6 \times 10^{-19} \text{ C}$ ,  $m = 9.1 \times 10^{-31} \text{ kg}$ ,  $c = 3 \times 10^8 \text{ m/sec}$ .

**Formula :** (i)  $E = \frac{hc}{\lambda_{\min}}$  (ii)  $V = \frac{E}{e}$

**Solution :** (i)  $E = \frac{6.6 \times 10^{-34} \times 3 \times 10^8}{10^{-10}}$   
 $= 19.8 \times 10^{-16} \text{ J}$   
 (ii)  $V = \frac{19.8 \times 10^{-16}}{1.6 \times 10^{-19}}$   
 $= 12.375 \times 10^3$   
 $= 12375 \text{ volts}$

**Problem 4.18 :** What is the frequency of an X-ray photon whose momentum is  $1.1 \times 10^{-23} \text{ kg-m/sec}$ .

**Data :**  $p = 1.1 \times 10^{-23} \text{ kg-m/sec}$ ,  $c = 3 \times 10^8 \text{ m/sec}$ ,  $h = 6.6 \times 10^{-34} \text{ J-sec}$ .

**Formula :**  $E = pc = hu$

**Solution :**  $u = \frac{pc}{h}$   
 $= \frac{1.1 \times 10^{-23} \times 3 \times 10^8}{6.6 \times 10^{-34}}$   
 $= 5 \times 10^{18} \text{ Hz}$

**Problem 4.19 :** What is the wavelength of electrons emitted when  $100 \text{ keV}$  electrons strike a target ? What is their frequency.

**Data :**  $E = 100 \text{ KeV} = 100 \times 10^3 \times 1.6 \times 10^{-19} \text{ J}$ ,  $c = 3 \times 10^8 \text{ m/sec}$ ,  $h = 6.6 \times 10^{-34} \text{ J-sec}$ .

**Formula :** (i)  $\lambda_{\min} = \frac{hc}{E}$

(ii)  $u = \frac{E}{h}$

**Solution :**

(i)  $\lambda_{\min} = \frac{6.6 \times 10^{-34} \times 3 \times 10^8}{100 \times 10^3 \times 1.6 \times 10^{-19}}$   
 $= 12.375 \times 10^{-10} \text{ m}$   
 (ii)  $u = \frac{100 \times 10^3 \times 1.6 \times 10^{-19}}{6.6 \times 10^{-34}}$   
 $= 0.24 \times 10^{20} \text{ C/sec}$

**Problem 4.20 :** If the p.d. applied across an X-ray tube is  $25 \text{ kV}$  and the current through it is  $10 \text{ mA}$ , calculate the number of electrons striking the target per second and the short wavelength limit of the X-rays generated.

**Data :**  $V = 25 \text{ kV} = 25 \times 10^3 \text{ V}$ ,  $I = 10 \text{ mA} = 10 \times 10^{-3} \text{ Amp}$ ,  $e = 1.6 \times 10^{-19} \text{ C}$

**Formula :** (i)  $I = ne$

(ii)  $\lambda_{\min} = \frac{12400}{V} \text{ \AA}$

**Solution :**

(i)  $n = \frac{I}{e} = \frac{10 \times 10^{-3}}{1.6 \times 10^{-19}}$   
 $= 0.625 \times 10^{23} / \text{sec}$   
 (ii)  $\lambda_{\min} = \frac{12400}{25 \times 10^3} \text{ \AA}$   
 $= 0.496 \text{ \AA}$

**Problem 4.21 :** An X-ray tube operated at  $50 \text{ kV}$  emits a continuous spectrum with a short wavelength limit of  $0.24 \text{ \AA}$ . Calculate Planck's constant.

**Data :**  $V = 50 \times 10^3 \text{ V}$ ,  $\lambda_{\min} = 0.24 \text{ \AA}$ ,  
 $c = 3 \times 10^8 \text{ m/sec}$ ,  $e = 1.6 \times 10^{-19} \text{ C}$ .

**Formula :**  $\lambda_{\min} = \frac{hc}{eV}$

**Solution :**

$h = \frac{e \cdot V \cdot \lambda_{\min}}{c}$   
 $= \frac{1.6 \times 10^{-19} \times 50 \times 10^3 \times 0.24 \times 10^{-10}}{3 \times 10^8}$   
 $= 6.4 \times 10^{-34} \text{ J-sec}$

#### 4.16 INTRODUCTION TO ELECTRODYNAMICS

- The space is filled with two things, matter and radiation. The matter is constituted by electrons, protons, neutrons etc. where as radiations are electromagnetic, phonon, gravitons etc.

- Ordinary matter is made up of atoms which have positively charged nuclei and negatively charged electrons orbiting around them.
- The charge of an atom is quantized in terms of the electronic charge  $-e$  whose value is  $1.6 \times 10^{-19}$  coulomb. When two charges are separated a distance, would experience a force due to the electric field produced by them.
- On the other hand the motion of charges generate current and hence magnetic field. When these fields are time varying they produce electromagnetic waves are coupled with each other by Maxwell's equation.
- With the help of Maxwell's equations, we can derive wave equation, based on which the propagation of electromagnetic waves can be investigated in different media.

#### 4.17 INTRODUCTION OF MAXWELL'S EQUATION

[Dec. 18]

- When the charges are in motion, the electric and magnetic fields are associated with them which will change in both the space and time. Thus, the electric and magnetic fields are interrelated with each other. This phenomenon is called **Electromagnetism** which are mathematically explained by **Maxwell's Equations**. We can write Maxwell's equations in differential or integral form.

##### 4.17.1 Differential form of Maxwell's Equation

[May 19]

In differential form, the Maxwell's equations are as given below (S.I. Units)

$$\nabla \cdot \vec{D} = \rho \text{ or } \nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0} \text{ Gauss's law ... (4.18)}$$

$$\nabla \cdot \vec{B} = 0 \text{ Monopoles do not exist ... (4.19)}$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \text{ Faraday's law ... (4.20)}$$

$$\nabla \times \vec{H} = \vec{J} \text{ Ampere's circuital law ... (4.21)}$$

These are the Maxwell's four equations which govern electromagnetism.

- **Displacement Current :**

[Dec. 18]

- The first three of these are general equations and are valid for static as well as dynamic fields.
- But the fourth equation is derived for steady state, for time-varying fields take the divergence on both sides.

$$\nabla \cdot (\nabla \times \vec{H}) = \nabla \cdot \vec{J} = 0 \quad \dots (4.22)$$

The above equation is incompatible with the principle of conservation of charge in the equation of continuity.

$$\text{i.e. } \nabla \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0 \quad \dots (4.23)$$

This is due to incomplete definition of current density. Thus the total current density can be written as

$$\nabla \times \vec{J} = -\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial t} (\nabla \cdot \vec{D})$$

$$\nabla \times \vec{J} = \nabla \times \left( -\frac{\partial \vec{D}}{\partial t} \right)$$

$$\therefore \nabla \times \left( \vec{J} + \frac{\partial \vec{D}}{\partial t} \right) = 0 \quad \dots (4.24)$$

Maxwell replaced  $\vec{J}$  in Ampere's law by  $\vec{J} + \frac{\partial \vec{D}}{\partial t}$ .

Therefore, the Ampere's law takes the form

$$\nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \quad \dots (4.25)$$

- The above equation is valid for steady state phenomenon and is also compatible with the equation of continuity for time dependent fields.
- The term  $\vec{J}$  is called **Conduction Current Density** and  $\frac{\partial \vec{D}}{\partial t}$  is called **Displacement Current Density**.

##### 4.17.2 Integral Form of Maxwell's Equation

[Dec. 18]

The Maxwell's equations in integral form are

$$(i) \oint_S \vec{D} \cdot d\vec{S} = q \quad \dots (4.26)$$

$$(ii) \oint_S \vec{B} \cdot d\vec{S} = 0 \quad \dots (4.27)$$

$$(iii) \oint \vec{E} \cdot d\vec{l} = -\frac{\partial}{\partial t} \int_S \vec{B} \cdot d\vec{S} \quad \dots (4.28)$$

$$(iv) \oint \vec{H} \cdot d\vec{l} = \int_S \left[ \vec{J} + \frac{\partial \vec{D}}{\partial t} \right] \cdot d\vec{S} \quad \dots (4.29)$$

#### 4.18 ELECTROMAGNETIC WAVE IN FREE SPACE

[Dec. 17]

The Maxwell's equations for free space are given by,

$$\nabla \times \vec{E} = 0 \quad \dots (4.30)$$

$$\nabla \times \vec{H} = 0 \quad \dots (4.31)$$



$$\nabla \times \vec{E} = -\mu_0 \frac{\partial \vec{H}}{\partial t} \quad \dots (4.32)$$

$$\text{and } \nabla \times \vec{E} = \epsilon_0 \frac{\partial \vec{E}}{\partial t} \quad \dots (4.33)$$

Taking Curl of equation (4.32)

$$\nabla \times (\nabla \times \vec{E}) = -\mu_0 \frac{\partial}{\partial t} (\nabla \cdot \vec{H})$$

$$\text{or } \nabla \times (\nabla \times \vec{E}) - \nabla^2 \vec{E} = -\mu_0 \frac{\partial}{\partial t} \left[ \epsilon_0 \frac{\partial \vec{E}}{\partial t} \right]$$

$$\text{But } \nabla \cdot \vec{E} = 0$$

$$\therefore \nabla^2 \vec{E} = -\mu_0 \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \quad \dots (4.34)$$

This is the wave equation governing the field  $\vec{E}$ .

We can write this as

$$\nabla^2 \vec{E} - \frac{1}{v^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \quad \dots (4.35)$$

$$\text{where, } v = \frac{1}{\sqrt{\mu_0 \epsilon_0}} \quad \dots (4.36)$$

Similarly the curl of equation (4.33) gives the wave equation for the field  $\vec{H}$ .

$$\text{i.e. } \nabla^2 \vec{H} - \mu_0 \epsilon_0 \frac{\partial^2 \vec{H}}{\partial t^2} = 0 \quad \dots (4.37)$$

$$\text{if } v = \frac{1}{\sqrt{\mu_0 \epsilon_0}} \quad \dots (4.38)$$

$$\text{then } \nabla^2 \vec{H} - \frac{1}{v^2} \frac{\partial^2 \vec{H}}{\partial t^2} = 0 \quad \dots (4.39)$$

The solution of equations (4.35) and (4.36) is written as

$$\vec{E}(\vec{r}, t) = \vec{E}_0 e^{i(\vec{k} \cdot \vec{r} - \omega t)} \quad \dots (4.40)$$

$$\text{and } \vec{H}(\vec{r}, t) = \vec{H}_0 e^{i(\vec{k} \cdot \vec{r} - \omega t)} \quad \dots (4.41)$$

where,  $\omega$  is the angular frequency of variation of the fields  $\vec{E}$  and  $\vec{H}$ .

$\vec{k}$  is the wave vector which tells the direction of propagation of the wave.

The ratio  $\omega/k$  gives the phase velocity of the wave which is equal to the speed of light  $c$  in the free space or vacuum.

In free space (vacuum)

$$\mu_0 = 4\pi \times 10^{-7} \text{ H/m}$$

$$\epsilon_0 = 8.854 \times 10^{-12} \text{ F/m}$$

From equ. (4.38),

$$\therefore c = 2.99 \times 10^8 \text{ m/s,}$$

which is the velocity of light.

### SUMMARY

- **Space Lattice** : It is defined as a regular 3-dimensional periodically repetitive arrangement of points in space, which is infinite in extent.
- **Basis** : It is a group of atoms or molecules.
- **Crystal Structure** : It is formed by the addition of basis to every lattice point of space lattice.
- **Unit Cell** : The parallelepiped formed by using primitive vectors ( $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$ ) as edge is called unit vector.
- **Bravais Lattice** : Common nomenclature given to the 14 different lattices under the seven systems of the crystals.
- **Co-Ordination Number** : It is the number of nearest neighbours to a given atom in a crystal lattice.
- **Lattice Constant** : The distance between two neighbouring atoms,  $a = \left( \frac{nM}{N\rho} \right)^{1/3}$ .
- **Packing Factor** : The ratio of the volume of the atoms per unit cell to the total volume of the unit cell.
- **Lattice Plane** : A set of parallel equidistant planes passing through the lattice points.
- **Miller Indices** :  $h : k : l = \frac{1}{p} : \frac{1}{q} : \frac{1}{r}$ .

The numbers  $h, k, l$  are called the Miller indices of a given set of planes and the plane is specified by  $(hkl)$ .

- **Relation between Interplanar Distance and Miller Indices**:

$$d_{(hkl)} = \left( \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right)^{1/2}$$

- **Symmetry** : There exists certain operations which when operated upon a given structure, carry the structure into itself. The structure is said to possess symmetry under that operation.
- The main symmetry elements of a crystalline solid are :
  - Axes of symmetry.
  - Planes of symmetry.
  - Centre of symmetry.

- **Axis of Symmetry** : When a crystal is rotated about a vertical axis.
- **Plane of Symmetry** : When a crystal is cut along a certain plane and the mirror image of one half reproduces the other half of the crystal, then the plane along which it is cut, is called as plane of symmetry.
- **Centre of Symmetry** : It is a point in a crystal such that if a line is drawn from any point on the crystal through this point and produced an equal distance on the other side of this centre, it meets an identical point.
- **Bragg's Law** :  $2d \sin \theta = n\lambda$ .
- **Bragg's X-Ray Spectrometer** : Experimental arrangement for verification of Bragg's law.
- The X-rays are produced when high energy electrons are stopped by material having high atomic number.
- The X-ray beam contains continuous and characteristics X-rays.
- The frequency of an spectral line in characteristic X-ray spectrum varies directly as the square of the atomic number of the element emitting it.
- The time changing electric and magnetic fields are governed by Maxwell's equation.
- An electromagnetic wave travels with velocity  $C$  in vacuum.

### IMPORTANT FORMULAE

- Lattice Constant,  $a = \left( \frac{nM}{N_p} \right)^{1/3}$
- Interplaner distance,  

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$
- Bragg's Law,  $2d \sin \theta = n\lambda$
- For continuous X-rays,  

$$\lambda_{\min} = \frac{hc}{eV} = \frac{12400}{V} \text{ \AA}$$
- Moseley's law,  

$$\nu \propto (Z - a)^2$$
- Maxwell's equations are
  - $\nabla \cdot \vec{D} = \rho$
  - $\nabla \cdot \vec{B} = 0$
  - $\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$
  - $\nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t}$

### UNSOLVED PROBLEMS

1. If density of NaCl is 2.163 g/cc and molecular weight is 58.45, find the spacing between planes parallel to the cubic lattice faces of NaCl crystal. [Ans. 2.83 Å]
2. A substance with fcc lattice has a density of 6250 kg/m<sup>3</sup> and molecular weight of 60.2. Calculate the lattice constant  $a$ . Given Avogadro number as  $6.02 \times 10^{26}$  per kg-mole. [Ans. 4 Å]
3. Find Miller indices of a set of parallel planes making intercepts in the ratio  $3a : 4b$  on X, Y axes and being parallel to Z-axis,  $a, b, c$ , being primitive vectors of the lattice. [Ans. (4, 3, 0)]
4. Calculate interplanar spacing between (327) planes in a cubic crystal of lattice constant  $4.2 \times 10^{-8}$  cm. [Ans.  $1.1 \times 10^{-8}$  cm]
5. Calculate the wavelength of an X-ray beam incident at  $12^\circ$  for the first order reflection from calcite crystal if the grating constant of the crystal is 3.035 Å. [Ans. 1.26 Å]
6. Monochromatic X-rays of wavelength 1.5 Å are incident on a crystal whose interplanar spacing is 1.6 Å. Find the various orders in which Bragg's reflections take place.

[Ans. 1<sup>st</sup> and 2<sup>nd</sup> order maxima]

### EXERCISE

1. Define crystal lattice, basis and crystal structure.
2. What is meant by a space lattice ? How do we associate a crystal structure to the lattice ?
3. Describe the seven systems of crystals. Explain with examples the types of lattices in cubic systems.
4. What is co-ordination number ? Calculate co-ordination number for simple bcc and fcc lattices.
5. What is packing factor ? Show that the packing factor for simple cubic, bcc and fcc lattices are  $\frac{\pi}{6}$ ,  $\sqrt{3} \frac{\pi}{8}$  and  $\sqrt{2} \frac{\pi}{6}$ .
6. What is lattice constant ? Calculate for fcc and bcc lattices in terms of atomic radius.
7. What are Miller indices of a crystal ? Obtain an expression for the spacing between consecutive planes.
8. What are symmetry operations ? Enumerate the different types with examples.

9. Show the symmetry elements of an equilateral triangle and a square.
10. Explain and deduce Bragg's law in X-ray diffraction. Describe a Bragg's spectrometer and explain how it is used to determine the wavelength of X-rays.
11. What is X-ray diffraction ?
12. What are the types of X-rays? How they are produced?
13. Explain method of producing continuous spectra. Derive the formula for minimum wavelength of the X-rays.
14. State and explain Moseley's Law.
15. Write the Maxell's equation in different form.
16. Derive the formula for electromagnetic wave in free space.

### UNIVERSITY QUESTIONS

**December 2017**

1. Define atomic radius. Calculate atomic radii in SC, BCC and FCC lattices with suitable diagrams. **[4+2]**  
Lead exhibits FCC structure. Each side of unit cell is of  $4.95 \text{ \AA}$ . Calculate radius of lead atom.
2. Derive the relation between interplaner spacing 'd' defined by Miller Indices (hkl) and lattice parameter 'a'. **[4+2]**  
Calculate the interplaner spacing for (220) plane where the lattice constant is  $4.938 \text{ \AA}$ .
3. What is X-ray? How do we get the continuous spectrum in X-rays explain. **[4+2]**
4. Derive an expression for electromagnetic wave in free space and hence calculate the value of velocity of light in free space. **[6]**

**May 2018**

1. Define Packing Density. Find the packing density in SC, BCC, and FCC lattices. **[6]**
2. Derive the relation between crystal density ' $\rho$ ' and lattice parameter 'a'.  
The density of copper is  $8980 \text{ Kg/ m}^3$  and unit cell dimension is  $3.61 \text{ \AA}$ . Atomic weight of copper is 63.54. Determine crystal structure. **[6]**
3. State and Derive Moseley's law for characteristics X-ray spectrum. **[6]**
4. What is displacement current? Write Maxwell's equations in differential and integral form. **[6]**

**December 2018**

1. What is primitive and nonprimitive unit cells? Find the number of atoms per unit cell in SC, BCC, FCC lattices. **[6]**
2. Define atomic radius. Find the atomic radius in SC, BCC, FCC lattices. **[6]**
3. State and Derive Bragg's law of X-ray diffraction. An X-ray is operated at 20 kV. Calculate the minimum wavelength of X-rays emitting from it. **[6]**
4. What is displacement current? Write Maxwell's equations in differential and integral form. **[6]**

**May 2019**

1. Define primitive and non-primitive unit cells. Calculate the lattice constant of iron which has BCC structure. Given  $\rho = 7.86 \text{ gm/cc}$ ,  $M = 55.85$  **[6]**
2. Explain continuous X-ray spectrum with neat diagram. An X-ray is operated at 18 kV. Calculate the minimum velocity of electron bombarded at the anode. **[6]**
3. What is displacement current? Write Maxwell's equation in integral and differential form. **[6]**