CHAPTER 2

Unit II

Crystallography

Syllabus

(Prerequisites : Crystal physics (unit cell, space lattice, crystal structure, simple cubic, body centered cubic, face centered cubic, diamond structure, production of x-rays), Miller indices, interplanar spacing, x-ray diffraction and Bragg's law, determination of crystal structure using Bragg's diffractometer

Learning Objectives :

After reading this chapter, learner should be able to

- Understand Miller indices for planes and direction
- Understand x-ray diffraction
- Derive Bragg's law
- Determine crystal structure using X - ray diffractometer

2.1 Introduction

Matter occurs in three states – solid, liquid and gaseous. Different solids have different structures such as crystalline and amorphous.

Table 2.1.1

Sr. No.	Crystalline solids	Amorphous solids
1.	Form a regular, repeated three dimensional pattern of atoms, ions or molecules of which they are made up	No such regular or repeated pattern or arrangement is observed
2.	Since the atoms or molecules are arranged in a regular manner over a long distance, a long range order prevails in crystals.	Atoms or molecules are not arranged in regular manner hence no such order exists. Only a short range order is exhibited.
3.	Mathematics involved to analyze is simpler	Mathematics involved is more complicated

More about crystal structure

- In a crystalline solid, each atom or molecule is fixed at a definite point in space and at a definite distance from and in a definite angular orientation to other atoms or molecules surrounding it.
- Hence, a perfect crystal is considered to be made up of infinite regular repetition of identical structural units called **unit cells.**
- Crystals can further be divided into two main categories *viz.* single crystal and polycrystalline.
- Single crystal is the one where orientation of atoms or molecules is uniform throughout the entire crystal.

- Polycrystalline is the one where whole crystal is made up of smaller crystallites. Each small crystallite is called **grain**. The grains form the whole crystal, for example,*quartz*.
- For a given grain, orientation of atoms is always uniform, but grains are generally oriented randomly. Due to this reason single crystals are preferred.

2.2 Miller Indices

MU - Dec. 18, May 19

Q. Draw (123), (321), $(\bar{1}02)$. **(Dec. 18, 3 Marks)**

Q. Draw the following for a cubic unit cell – $(\overline{123})$, (200), $(\overline{23}\,0)$. **(May 19, 3 Marks)**

2.2.1 Crystal Planes and Miller Indices

"Identification of a plane"

- The crystal structure may be regarded as made up of an aggregate of a set of parallel equidistant planes passing through at least one lattice point or a number of lattice points. In a given crystal a plane may be selected in a number of ways.
- **The position of a crystal plane can be specified in terms of three integers called Miller indices**. Miller developed a method by which one can find three integers (hk*l*). This method is universally employed.

  The procedure is as follows:

1. Find the intercepts of the plane with the crystal axes along the basic vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$. Let the intercepts be m, n and p respectively.
2. Express m, n and p in terms of the respective basic vectors, as fractional multiples we get, $\frac{m}{a}, \frac{n}{b}, \frac{p}{c}$.
3. Take the reciprocals of the three fractions, i.e. $\frac{a}{m}, \frac{b}{n}, \frac{c}{p}$.
4. Find the LCM of the denominator by which the above three ratios are multiplied. This operation reduces them to a set of three integers h, k and *l*. The resultant three integers are called Miller indices of the given plane, denoted by (hk*l*).

- While finding Miller indices of a plane, following points should be kept in mind:
  - (i) When a plane is parallel to one of the axes it is said to have intercept at ∞ and its reciprocal is zero.
  - (ii) When the intercept of a plane is on the negative part, the corresponding Miller index is distinguished by a bar over it.
  - (iii) Parallel planes have same Miller indices.
  - (iv) Miller indices, in practice do not define a particular plane but a set of parallel planes.
  - (v) A plane passing through the origin is defined in terms of a parallel plane having non-zero intercept.

Ex. 2.2.1 : Find the Miller indices of planes given in Fig. P. 2.2.1.

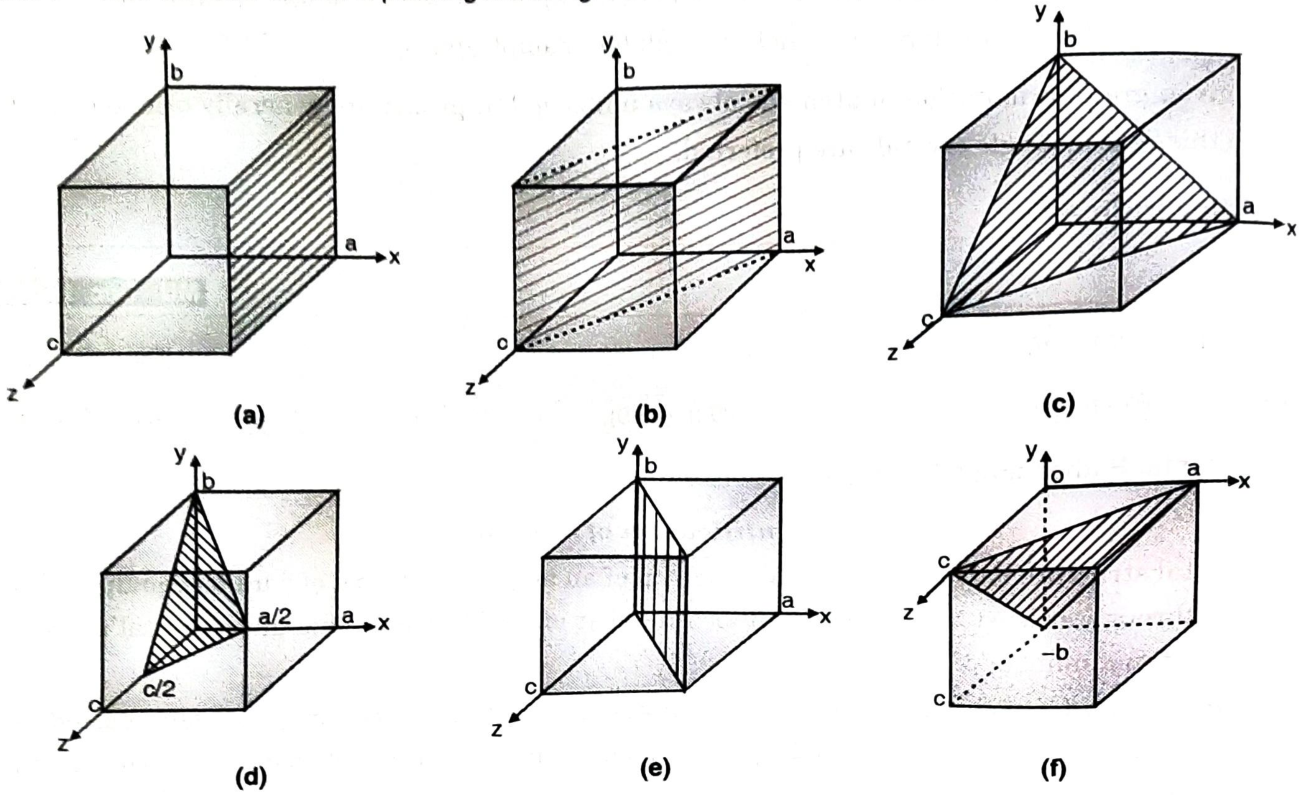


Fig. P. 2.2.1

Soln. :

(a) Here m = a, n = ∞, p = ∞

$$\therefore \frac{m}{a}, \frac{n}{b}, \frac{p}{c} :: \frac{a}{a}, \frac{\infty}{b}, \frac{\infty}{c}$$

∴ Reciprocals

$$\frac{a}{m}, \frac{b}{n}, \frac{c}{p} :: \frac{a}{a}, \frac{b}{\infty}, \frac{c}{\infty} :: 1, 0, 0$$

Since they are integers, no LCM is needed. The three integers are (1, 0, 0).

$$\therefore (hkl) = (1\ 0\ 0)$$

(b) Here m = a, n = ∞, p = c

$$\frac{a}{m}, \frac{b}{n}, \frac{c}{p} :: \frac{a}{a}, \frac{b}{\infty}, \frac{c}{c} :: 1, 0, 1$$

$$\therefore (hkl) = (1\ 0\ 1)$$

(c) Here m = a, n = b, p = c

∴ Reciprocals

$$\frac{a}{m}, \frac{b}{n}, \frac{c}{p} :: \frac{a}{a}, \frac{b}{b}, \frac{c}{c} :: 1, 1, 1$$

$$\therefore (hkl) = (1\ 1\ 1)$$

(d) Here $m = \frac{a}{2}$, n = b, $p = \frac{c}{2}$

∴ Reciprocals

$$\frac{a}{m}, \frac{b}{n}, \frac{c}{p} :: \frac{a}{a/2}, \frac{b}{b}, \frac{c}{c/2} :: 2, 1, 2$$

$$\therefore (hkl) = (2\ 1\ 2)$$

(e) Since the plane is passing through the origin, consider a plane which is parallel to it and not passing through the origin.

Here m = – a, n = ∞, p = c

∴ Reciprocals

$$\frac{a}{m}, \frac{b}{n}, \frac{c}{p} :: \frac{a}{-a}, \frac{b}{\infty}, \frac{c}{c} :: -1, 0, 1$$

Taking negative intercept in consideration

$$(hkl) = (\bar{1}\ 0\ 1)$$

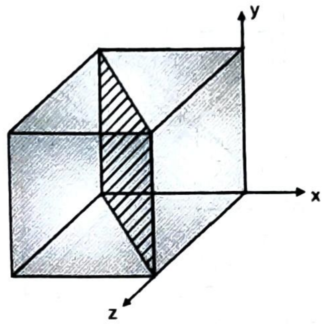


Fig. P. 2.2.1(g) : Shifting of plane

(f) Here m = a, n = – b, p = c

∴ Reciprocals

$$\frac{a}{m}, \frac{b}{n}, \frac{c}{p} :: \frac{a}{a}, \frac{b}{-b}, \frac{c}{c} :: 1, -1, 1$$

$$\therefore \quad (hkl) = (1\ \bar{1}\ 1)$$

Ex. 2.2.2 : Obtain the Miller indices of a plane which intercepts a, $\frac{b}{3}$, 2 c in a simple cubic unit cell.

Soln. :

Intercepts $m : n : p :: a : \frac{b}{3} : 2c$

∴ Intercepts interms of respective basic vector

$$\left(\frac{m}{a}, \frac{n}{b}, \frac{p}{c}\right) = \left(\frac{a}{a}, \frac{b/3}{b}, \frac{2c}{c}\right)$$

Reciprocals

$$\left(\frac{a}{m}, \frac{b}{n}, \frac{c}{p}\right) = \left(\frac{a}{a}, \frac{b}{b/3}, \frac{c}{2c}\right)$$

$$\text{As, } a = b = c = \left(1, 3, \frac{1}{2}\right)$$

$$\text{Taking LCM} = (2\ 6\ 1)$$

$$\therefore (hkl) = (2\ 6\ 1)$$

It is also meaningful to learn how to draw a plane if Miller indices are provided.

Let us follow a simple procedure:

(i) Take the reciprocals of indices

(ii) These represent intercepts on corresponding axes

(iii) Join the intercepts

Ex. 2.2.3 : Draw the following planes.

(i) $(1\ 1\ 0)$ (ii) $(1\ \bar{1}\ 0)$ (iii) $(2\ 3\ 1)$ (iv) $(\bar{2}\ 3\ \bar{1})$

(v) $(\bar{2}\ 0\ \bar{1})$ (vi) $(3\ 0\ 0)$ (vii) $(1\ 2\ \bar{1})$ (viii) $(1\ \bar{2}\ 3)$ (ix) $(\bar{1}\ 1\ \bar{1})$

Soln. :

*Only simple cubic structures where a = b = c are to be considered.

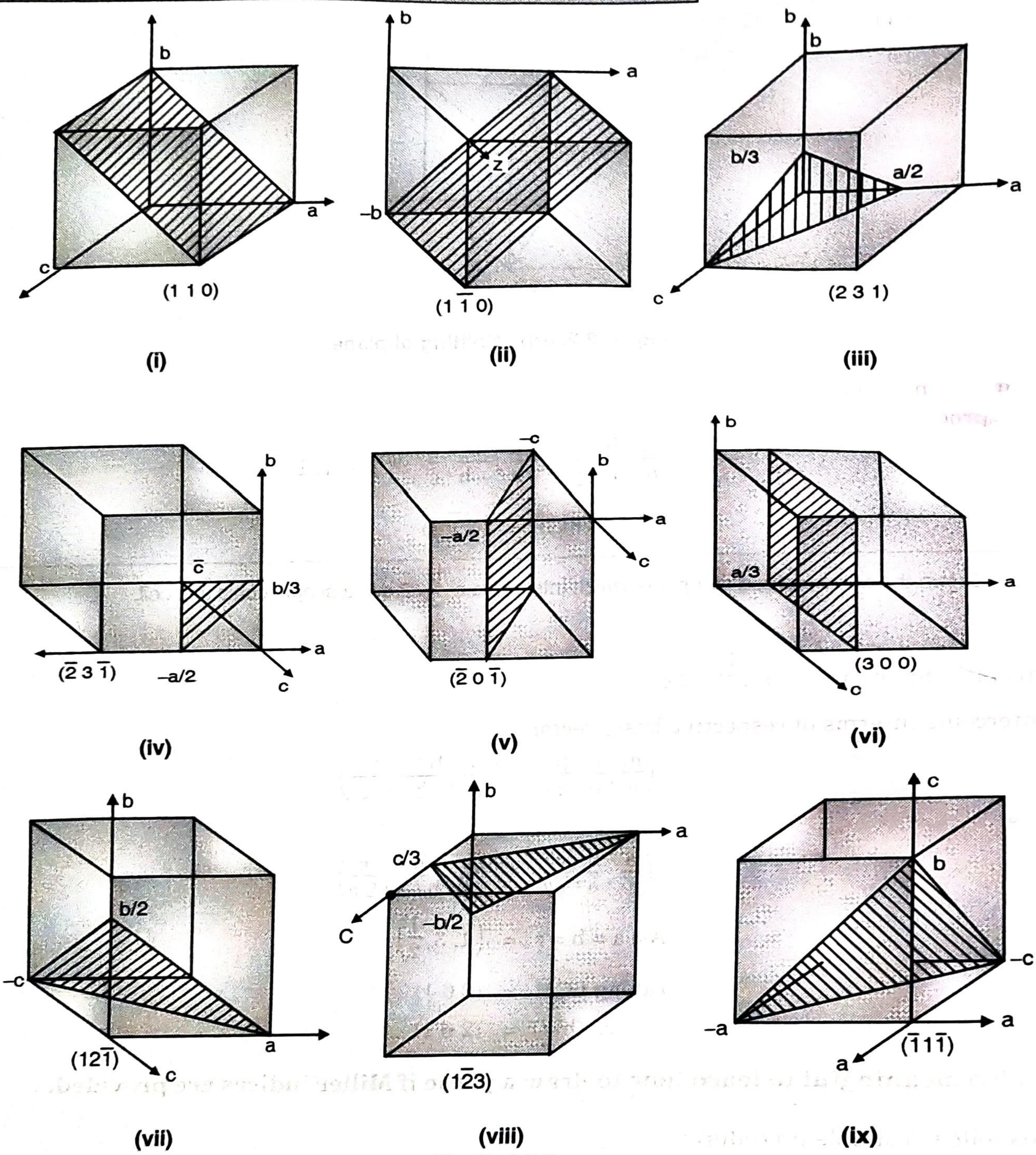


Fig. P. 2.2.3

2.2.2 Interplanar Spacing

- It is clear that parallel planes have same Miller indices.
- At the same time spacing between such parallel planes is an important parameter.
- It is denoted by d_{hkl} i.e. the interplanar spacing between planes with same Miller indices (hk*l*).
- In the Fig. 2.2.1, we have plane ABC with Miller indices (hk*l*). Other plane with same Miller indices is assumed to pass through point 'O' (which is not shown in the diagram). The perpendicular spacing between these two planes is ON = d.

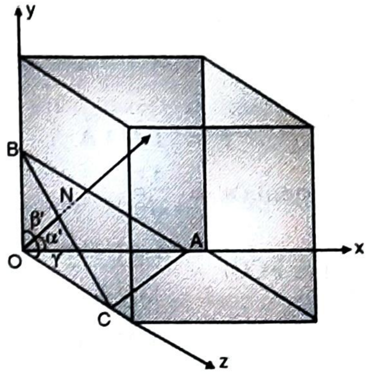


Fig. 2.2.1 : Interplanar spacing

- Let $\overrightarrow{ON}$ make an angle α' with X axis, β' with Y axis and γ' with Z axis.

$$\left.\begin{aligned} \therefore \cos\alpha' &= \frac{ON}{OA} = \frac{d}{OA} \\ \cos\beta' &= \frac{ON}{OB} = \frac{d}{OB} \\ \cos\gamma' &= \frac{ON}{OC} = \frac{d}{OC} \end{aligned}\right\} \quad ...(2.2.1)$$

$$\left.\begin{aligned} \text{But } OA &= \frac{a}{h} \\ OB &= \frac{a}{k} \\ OC &= \frac{a}{l} \end{aligned}\right\} \text{Intercepts of plane ABC} \quad ...(2.2.2)$$

$$\left.\begin{aligned} \therefore \cos\alpha' &= \frac{d}{a/h} = \frac{dh}{a} \\ \cos\beta' &= \frac{d}{a/k} = \frac{dk}{a} \\ \cos\gamma' &= \frac{d}{a/l} = \frac{dl}{a} \end{aligned}\right\} \quad ...(2.2.3)$$

Using relation of space geometry,

$$\cos^2\alpha' + \cos^2\beta' + \cos^2\gamma' = 1$$

$$\therefore \left(\frac{dh}{a}\right)^2 + \left(\frac{dk}{a}\right)^2 + \left(\frac{dl}{a}\right)^2 = 1$$

$$\therefore \frac{d^2}{a^2}(h^2 + k^2 + l^2) = 1$$

$$\therefore d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad ...(2.2.4)$$

This is the expression for interplanar spacing in terms of lattice constant **a** and Miller indices **(h k *l*)**.

Ex. 2.2.4 : Silver has FCC structure and its atomic radius is 1.414 Å. Find the interplanar spacing for (2 0 0) and (1 1 1) planes.

Soln. :

Given : Structureis FCC.

$$r = 1.414 \text{ Å}$$

Step 1:

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

$$(\text{For FCC}) = \frac{4 \times 1.414}{\sqrt{2}}$$

$$= 3.999 \text{ Å}$$

Step 2:

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

$$\text{For } (2\ 0\ 0) d_{200} = \frac{3.999}{\sqrt{2^2 + 0^2 + 0^2}} = 1.999 \text{ Å}$$ ...Ans.

$$\text{For } (1\ 1\ 1) d_{111} = \frac{3.999}{\sqrt{1^2 + 1^2 + 1^2}} = 2.309 \text{ Å}$$ ...Ans.

2.2.3 Directions

"A correct path to reach a plane"

- The direction in crystallography is a line joining any two points of the lattice. The indices of direction are the vector components of direction resolved along each of the axes. The vector components are again multiples of lattice constants.
- Therefore, the indices of the lattice site are simultaneously the indices of direction, assuming that the directions are through the origin. The directions are denoted by square brackets i.e. [hk*l*]. Some of the directions are shown below in Fig. 2.2.2(a).

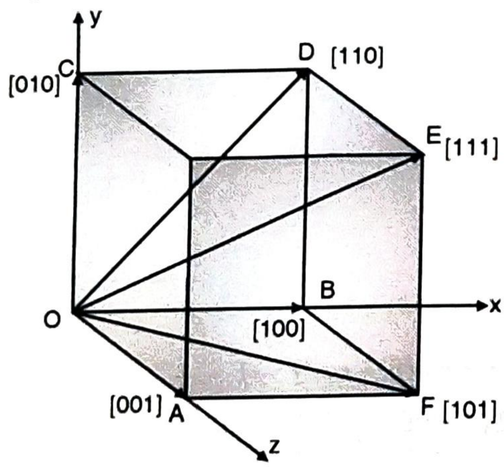


Fig. 2.2.2(a)

$\overrightarrow{OA}$ represents [0 0 1], $\overrightarrow{OB}$ represents [1 0 0], $\overrightarrow{OC}$ represents [0 1 0].

$\overrightarrow{OD}$ represents [1 1 0], $\overrightarrow{OE}$ represents [1 1 1], $\overrightarrow{OF}$ represents [1 0 1].

If there is any negative component, it is denoted by a bar placed above it.

For example, in Fig. 2.2.2(a).

$\overrightarrow{BO}$ represents $[\bar{1}\ 0\ 0]$, $\overrightarrow{AO}$ represents $[0\ 0\ \bar{1}]$, $\overrightarrow{FO}$ represents $[\bar{1}\ 0\ \bar{1}]$, and so on.

- As far as a plane with Miller indices 0 and 1 is considered, drawing a direction is simple. But when indices are other than 0 and 1, it has been observed that students draw a plane and a normal to it from origin.
- Students draw a direction on a 2-D paper using a picture of 3-D model. This technique does not have any precision regarding the normal.
- Consider Fig. 2.2.2(b) which has direction [1 2 0] plotted on it.

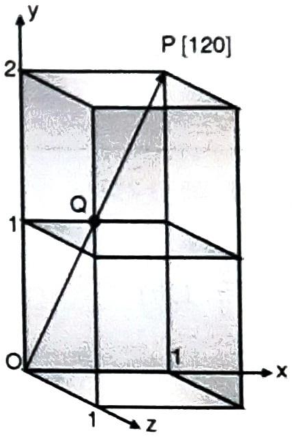


Fig. 2.2.2(b)

- Here, $\overrightarrow{OP}$ represents [1 2 0], co-ordinates of point P are (1, 2, 0). Careful observation reveals that, co-ordinates of point Q are $\left(\frac{1}{2}, 1, 0\right)$. Using this information, we can adopt a method to scale down the co-ordinates.
- The main advantage of this method is removal of the difficulty faced by students when they draw a plane and draw a normal to it from origin to express direction. The normal in such cases is simply assumed to be just a normal, but it does not have any mathematical support.
- The procedure to draw a direction is explained through following steps (with an example [1 2 0])
  1. Divide all the indices by the highest index.

     (For [1 2 0], highest index is 2. $\therefore \left[\frac{1}{2}, 1, 0\right]$).
  2. At least one index will be unity (here it is corresponding to Y axis).
  3. Select this particular axis as shown in Fig. 2.2.2(b) for better visualization.

     (Advantage of this is any point taken on plane ABCD (Fig. 2.2.3) will have its Y co-ordinates unity).

4. Plot other two co-ordinates on remaining axes (draw x co-ordinate = $\frac{1}{2}$ and Z co-ordinate = 0)

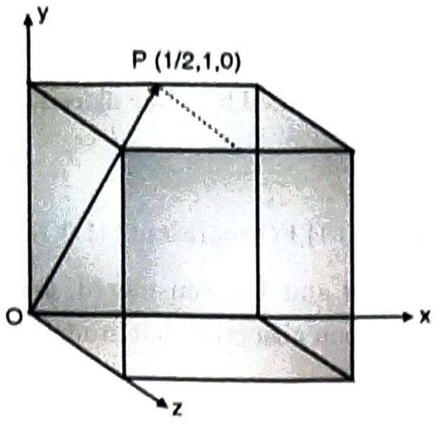


Fig. 2.2.3

5. Find the point with co-ordinates obtained in step 1 above (co-ordinates of P are $\left(\frac{1}{2}, 1, 0\right)$)

6. Join that point with the origin, the resultant vector in the desired direction $\vec{OP}$ is [1 2 0].

Compare Figs. 2.2.3 and 2.2.2(b).

Ex. 2.2.5 : Draw the following : (i) [1 2 1],(ii) [2 3 1], (iii) [1 $\bar{2}$ 0]

Soln. :

(i) [2 3 0] divide by 3, $\left(\frac{2}{3}, 1, 0\right)$ draw a point $\left(\frac{2}{3}, 1, 0\right)$

$\vec{OQ}$ **represents [2 3 0]**

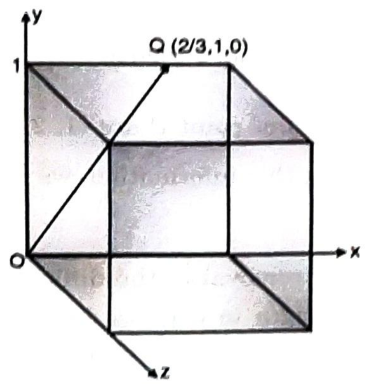


Fig. P. 2.2.5(a)

(ii) [1 2 1] divide it by 2

$\left(\frac{1}{2}, 1, \frac{1}{2}\right)$

draw a point $\left(\frac{1}{2}, 1, \frac{1}{2}\right)$

$\therefore \vec{OR}$ **represents [1 2 1]**

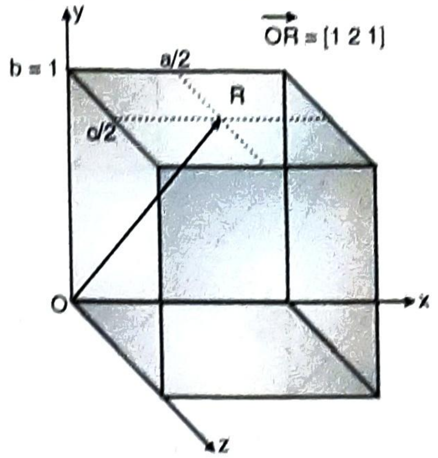


Fig. P. 2.2.5(b)

(iii) [2 3 1] divide it by 3, we get

$\left(\frac{2}{3}, 1, \frac{1}{3}\right)$,

draw this point

$\therefore \overrightarrow{OS}$ **represents [2 3 1]**

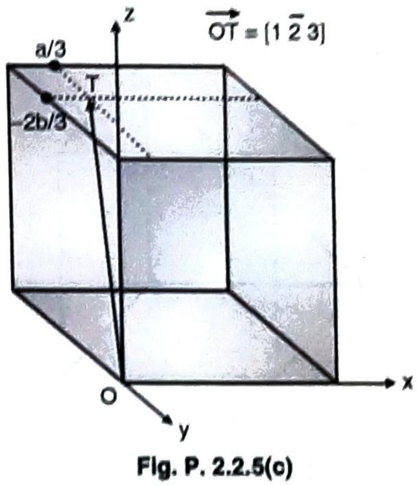


Fig. P. 2.2.5(c)

(iv) [1 $\bar{2}$ 3]

(Note that one of the indices is negative.)

Divide by 3, we get $\left(\frac{1}{3}, \frac{-2}{3}, 1\right)$

Draw the point $\left(\frac{1}{3}, \frac{-2}{3}, 1\right)$.

$\therefore \overrightarrow{OT}$ **represents [1 $\bar{2}$ 3]**

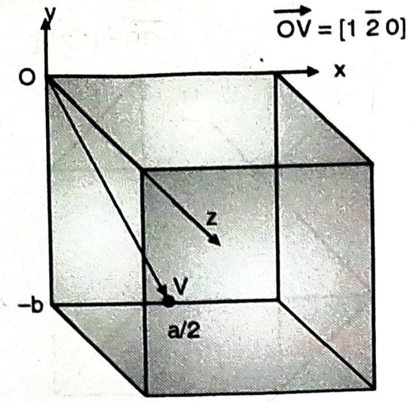


Fig. P. 2.2.5(d)

(v) $[1\ \bar{2}\ 0]$

(Note that one of the indices is negative.)

Divide by 2, we get $\left(\frac{1}{2}, -1, 0\right)$

Draw the point $\left(\frac{1}{2}, -1, 0\right)$.

$\therefore \overrightarrow{OV}$ represents $[1\ \bar{2}\ 0]$

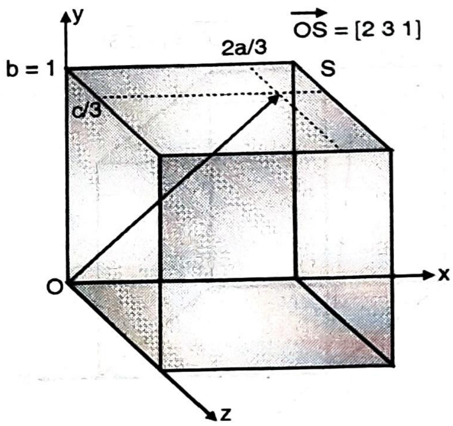


Fig. P. 2.2.5(e)

2.3 X-ray Diffraction

MU - May 13, May 16, Dec. 17, May 18

Q. Derive Bragg's law. Explain why x-rays and not γ-rays are used for crystal structure analysis. What data about the crystal structure can be obtained from the x-ray diffraction pattern of a crystal? **(May 13, 7 Marks)**

Q. Explain the statement "crystal act as three dimensional grating with x-rays". **(May 16, Dec. 17, 2 Marks)**

Q. Why X-rays are used to study the crystal structure? **(May 18, 3 Marks)**

"Because of periodicity"

– **Diffraction** is defined as the bending of a ray of light when it encounters an object whose dimensions are of the order of the wavelength.

- The explanation needs support of interference also.
- Secondary wavelets originate at the location of the object and spread in all directions. The constructive and destructive interference of such waves results in increase and decrease of intensity at the corresponding regions which is known as **diffraction pattern**.
- If the diffracting objects are located in random fashion, the superposition of individual diffraction effects due to various objects leads to a pattern which will not have any particular distribution of intensity. Whereas, if the diffracting objects are distributed in a regular pattern, then the diffraction pattern will also have regularity.
- One essential aspect of diffraction is the availability of objects whose dimensions are extremely small, i.e. of the order of the wavelength of light incident on it.
- In crystals we have seen that atoms are arranged in a perfectly ordered manner. Also the dimensions of atoms are 10^{-8} cm which is nearly of the same order of x-ray wavelength.
- Hence, when x-rays are made incident upon crystals, we get an ordered, regular diffraction pattern or one can say that a **crystal act as a three-dimensional reflection grating with x-rays.**

2.4 Bragg's Law

MU - May 12, Dec. 12, May 14, May 19

Q. Derive Bragg's equation. Explain construction and working of Bragg's spectrometer. **(May 12, May 14, 4/8 Marks)**

Q. Derive Bragg's law. **(Dec. 12, 3 Marks)**

Q. Derive Bragg's equation for x-ray diffraction in crystals. Calculate the glancing angle on a plane (1 0 0) of rock slat having lattice constant 2.814Å corresponding to first order Bragg's diffraction maximum for x-rays of wavelength 1.541Å. **(May 19, 8 Marks)**

- Before one starts the derivation of Bragg's law, it is necessary to understand Bragg's diffraction. W.L. Bragg and W.H. Bragg (father and son) put forward a novel idea for studying x-ray diffraction in crystals.
- They emphasised on the planes with same Miller indices i.e. parallel planes.
- It is possible to identify families of such planes. They addressed component plane of the said family as **Bragg planes.**
- When a monochromatic x-ray beam is made incident on them at an angle θ,* which is called as glancing angle, it is shown that constructive interference takes place between the rays scattered by the atoms only when a condition called Bragg's law as shown below is satisfied.

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

where, d = Interplanar spacing

n = Integer

Bragg's law

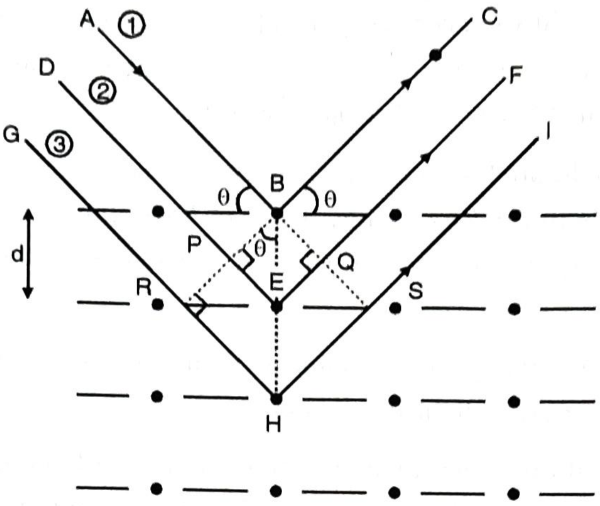


Fig. 2.4.1 : Bragg's law

- *Here, the angle θ is measured with respect to the horizontal and not from the normal as we do in optics.
- When the condition for constructive interference is satisfied, a sudden jump in the intensity is observed. Now let's take a look at Bragg's law.
- In the Fig. 2.4.1 we have Bragg planes with atoms shown with dots.
- An ordered or regular arrangement of atoms has been depicted. Let the interplanar spacing be d. A monochromatic and parallel beam of x-rays at glancing angle θ is made incident on planes. Ray AB will be scattered at point B on the first plane. Rays DE and GH which are parallel to AB will also experience scattering at points E and H respectively at second and third plane. The scattering due to atoms on crystal plane is in all directions.
- Among the scattered rays select rays BC and EF which are parallel to each other. It is assumed that they have path difference $\Delta = n\lambda$ and produce **constructive interference.** Bragg's law provides the condition at which $\Delta = n\lambda$. Lets obtain value of path difference Δ.
- Draw perpendiculars BP and BQ to the rays DE and EF. One can say that upto BP, path covered by both the incident rays is the same. So BQ onwards parallel rays BC and EF cover the same distance.

  ∴ Path difference between rays 1 and 2 is

$$\Delta = PE + EQ$$

From Δ BPE and Δ BQE,

$$PE = BE \sin\theta \text{ and,}$$

$$EQ = BE \sin\theta$$

$$\therefore \Delta = BE \sin\theta + BE \sin\theta$$

$$= 2\,BE \sin\theta$$

$$= 2\,d \sin\theta \qquad (BE = d)$$

- As we have already assumed that constructive interference is taking place Δ nλ

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

- The logic can be extended for rays 2 and 3 in the Fig. 2.4.1. Hence if rays 1 and 2 give constructive interference and rays 2 and 3 also give constructive interference, then rays 1 and 3 will also provide the same. In this case path difference between rays 1 and 3 will be

$$\Delta' = 4\, d \sin\theta = 2\,(2\, d \sin\theta) = 2\,(\Delta)$$

i.e. integral multiple of Δ.

Ex. 2.4.1 : Calculate the glancing angle on a plane (100) of rock salt having lattice constant 2.814A° corresponding to first order Bragg's diffraction maximum for X-rays of wavelength 1.641A°. **May 19, 8 Marks**

Soln. :

Given :

$$\text{Lattice constant } a = 2.814 A^\circ$$

$$\text{Crystal} = \text{Rock salt}$$

$$\text{Order of diffraction} = 1$$

For rock salt interplanar spacing

$$D = \frac{a}{z} = \frac{2.814}{2} = 1.407 A^\circ$$

Using Bragg's law

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

$$\therefore \sin\theta = \frac{n\lambda}{2d}$$

$$= \frac{1 \times 1.541}{2 \times 1.407}$$

$$= 0.5476$$

$$\therefore \theta = \sin^{-1}(0.5476) = 33.2^\circ$$

... Ans.

2.5 Bragg's Spectrometer

MU - Dec. 13, Dec. 15, Dec. 16, Dec. 17, May 18, May 19

Q. Explain with neat diagram : Construction of Bragg's x-ray spectrometer. Write the procedure to determine crystal structure. **(Dec. 13, 4 Marks)**

Q. Explain analysis of crystal structure using Bragg's X-ray spectrometer. **(Dec. 15, Dec. 16, Dec. 17, 5 Marks)**

Q. Explain with example how to determine crystal structure by Bragg's x-ray spectrometer. **(May 18, 5 Marks)**

Q. Write a short note on Bragg's spectrometer. **(May 19, 5 Marks)**

- Based upon Bragg's law an instrument called as Bragg's spectrometer was designed. **This is a modified form of ordinary spectrometer to suit the use of x-rays.**

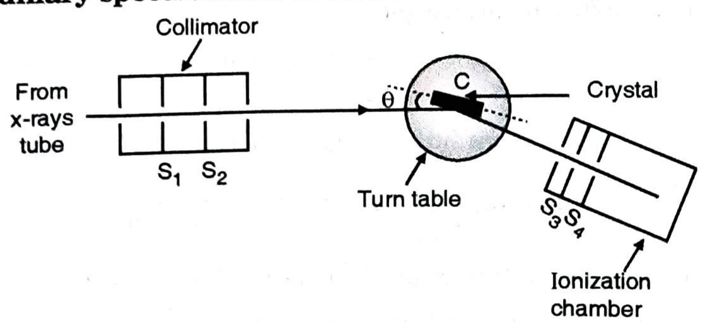


Fig. 2.5.1 : Schematic diagram of Bragg's spectrometer

1X10 A/m

- A monochromatic x-ray beam obtained from x-ray tube is made to pass through slits S_1 and S_2 which are made up of lead. The fine beam is then made to fall on the crystal C fixed on a crystal mount exactly at the centre of circular turn table.
- The x-rays reflected are collected by ionization chamber. Since ionization chamber is sturdy, the turn table is rotated till we get a sharp increase in the intensity.
- The sudden increase in the intensity of x-ray suggests that Bragg's law is satisfied at the given angle θ of the incident beam.
- The peak in ionisation current which represents the intensity occurs more than once as θ is varied because Bragg's law states $n\lambda = 2d \sin\theta$ i.e. for $n = 1, 2, 3, \ldots$ we have $\theta_1, \theta_2, \theta_3, \ldots$.
- If the intensity (or ionization current) is plotted against glancing angle then we get the graph as shown in Fig. 2.5.2.
- Using graph shown above we find the angles $\theta_1, \theta_2, \ldots$ where the peak occurs.

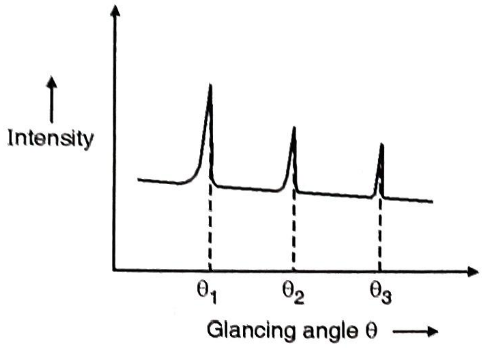


Fig. 2.5.2 : Variation of ionisation current

Determination of crystal structure (for cubic crystals)

Here the crystal face used for reflecting the x-rays can be so cut that it remains parallel to one set of planes, then to another and so on when placed at the centre of the turn table on Bragg's spectrometer with x-rays of known λ incident upon it. For a given plane used as reflecting surface, find the corresponding d using

$$n\lambda = 2\, d \sin\theta \quad \text{(take n = 1)}$$

Similarly, find value of d for other planes as well.

For cubic structure we select three planes *viz*. (100), (110), (111).

As λ is same throughout the experiment, we get,

$$\lambda = 2d_{100} \sin\theta_1 = 2d_{110} \sin\theta_2 = 2d_{111} \sin\theta_3 \qquad \ldots(2.5.1)$$

$$\therefore d_{100} : d_{110} : d_{111} :: \frac{1}{\sin\theta_1} : \frac{1}{\sin\theta_2} : \frac{1}{\sin\theta_3} \qquad \ldots(2.5.2)$$

where θ_1, θ_2 and $\theta_3$are obtained from the graph. Intensity $\rightarrow\theta$ i.e. where the peak occurs. The reason for selection of planes (100), (110) and (111) is that these are the planes rich enough in terms of atoms.

Studies have found out ratios of d_{100}, d_{110} and d_{111} for SC, BCC and FCC as follows,

$$\left.\begin{array}{lccccc} \text{SC} & 1 & : & \frac{1}{\sqrt{2}} & : & \frac{1}{\sqrt{3}} \\ \text{BCC} & 1 & : & \frac{2}{\sqrt{2}} & : & \frac{1}{\sqrt{3}} \\ \text{FCC} & 1 & : & \frac{1}{\sqrt{2}} & : & \frac{2}{\sqrt{3}} \end{array}\right\} \quad \text{...(2.5.3)}$$

Experimentally obtained values of θ_1, θ_2 and θ_3 will provide us d_{100}, d_{110} and d_{111}. By comparing their ratio with equation (2.5.3), one can determine crystal structure.

Ex. 2.5.1 : Find the Miller indices of a set of a parallel planes which make the intercepts in the ratio 3 a : 4 b on X and Y axes and are parallel to Z axis. a, b and c are basic vector. **MU - May 14, 3 Marks**

Soln. :

Given : Intercepts of the plane are in the proportion

3 a : 4 b : ∞ (Plane is parallel to Z-axis)

As a, b and c are basic vectors, the proportion of intercepts 3 : 4 : ∞

∴ Reciprocal $\frac{1}{3} \; \frac{1}{4} \; \frac{1}{\infty} = \frac{1}{3}, \frac{1}{4}, 0$

Taking LCM and converting to the integers, 4, 3, 0

∴ Miller indices (430) **...Ans.**

Ex. 2.5.2 : In an orthorhombic crystal lattice, a plane cuts intercepts of lengths 3 a, – 2 b and 3c/2 along three axes. Find Miller indices of the plane, where a, b, c are primitive vectors of the unit cell.

Soln. :

As a, b and c are primitive vectors, intercepts are 3, – 2, $\frac{3}{2}$

∴ Reciprocal $\frac{1}{3}, \frac{-1}{2}, \frac{2}{3}$

Taking LCM and converting them to integers 2, – 3, 4

$$\therefore \quad (hkl) = (2\,\bar{3}\,4)$$ **...Ans.**

Ex. 2.5.3 : In a simple cubic crystal, find the ratio of intercepts on the three axes by (1 2 3) plane.

Soln. :

If a plane cuts intercepts at length m, n, p on the three crystal axes, then

$$m : n : p = xa : yb : zc$$

Where a, b and c are primitive vectors of the unit cell and numbers x, y and z are related to the Miller indices (hk*l*) of the plane by the relation.

$$\frac{1}{x} : \frac{1}{y} : \frac{1}{z} = h : k : l$$

Since a = b = c (crystal is simple cubic)

$$\text{and } (hkl) = (1\,2\,3)$$

m || Th. H. - ,

$$\frac{1}{x} : \frac{1}{y} : \frac{1}{z} = 1:2:3$$

$$\therefore x:y:z = \frac{1}{1} : \frac{1}{2} : \frac{1}{3}$$

Multiply RHS by LCM = 6

$$x:y:z = 6:3:2$$

$$\therefore m:n:p = 6:3:2$$

...Ans.

Ex. 2.5.4 : A crystalwhose primitive vectors are 1.2 Å, 1.8 Å and 2 Å for a plane (2 3 1) cuts an intercept 1.2 Å along X axis. Find the length of Y and Z intercepts along Y and Z axes.

Soln. :

Primitive vectors a = 1.2 Å, b = 1.8 Å, c = 2 Å

Miller indices of the plane (2 3 1)

$\therefore$ Intercepts are $\frac{a}{2}, \frac{b}{3}, \frac{c}{1}$

i.e. $\frac{1.2}{2}, \frac{1.8}{3}, \frac{2}{1}$ ...(A)

This gives the intercept along X axis as $\frac{1.2}{2}$ Å = 0.6 Å. But it is given that plane cuts X-axis at 1.2 Å. This shows that the plane under consideration is another plane which is parallel to it (to keep Miller indices same).

In the statement A,

$$\text{X intercept is } 1.2\ \text{Å} = 2 \times 0.6\ \text{Å}$$

$\therefore$ Multiply other intercepts by 2

$$\therefore \text{Y intercept} = 2\left(\frac{1.8}{3}\right) = 1.2\ \text{Å}$$

$$\text{And, Z intercept} = 2\left(\frac{2}{1}\right) = 4\ \text{Å}$$

...Ans.

Ex. 2.5.5 : The interplanar spacing of (1 1 0) plane is 2 Å for a FCC crystal. Find the atomic radius.

Soln. :

Given : $(hkl) = (1\ 1\ 0)$, $d = 2$ Å

Formula :

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$\therefore a = d \times \sqrt{h^2 + k^2 + l^2}$$

$$= 2 \times \sqrt{1^2 + 1^2 + 0^2} = 2.828\ \text{Å}$$

For FCC structure,

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

$$= \frac{\sqrt{2} \times 2.828}{4}$$

$$\therefore \text{Radius } r = 1\ \text{Å}$$

...Ans.

Ex. 2.5.6 : Consider the density of Cu as 8930 kg / m^3 and its atomic weight 63.546. If the average number of electrons contributed per atom is 1.23, calculate the free electron concentration in Cu.

Soln. :

Given :

$$\text{Density} = 8930 \text{ kg / m}^3,$$

$$\text{Atomic weight} = 63.546$$

$$\text{Number of e}^- \text{/ atom} = 1.23$$

$$\text{Density} = \frac{\text{Mass}}{\text{Volume}}$$

$$\therefore \frac{1}{\text{Volume}} = \frac{\text{Density}}{\text{Mass}}$$

Since e$^-$ concentration is needed, let us find number of $\frac{\text{Atoms}}{\text{Volume}}$.

$$\therefore \frac{\text{Number of atoms}}{\text{Volume}} = 6.023 \times 10^{26} \times \frac{\text{Density}}{\text{Mass}}$$

$$= \frac{6.023 \times 10^{26} \times 8930}{63.546}$$

$$= 8.464 \times 10^{28} \frac{\text{Atoms}}{\text{m}^3}$$

Now, one atom contributes 1.23 e$^-$

$\therefore$ 8.464 × 10^{28} atoms will contribute

$$1.23 \times 8.464 \times 10^{28} = 1.041 \times 10^{29}$$

$\therefore$ Free e$^-$ concentration

$$= 1.041 \times 10^{29} \frac{\text{electrons}}{\text{m}^3}$$ ...**Ans.**

Ex. 2.5.7 : A crystal lattice plane (326) makes an intercept of 1.5 Å on X -axis in a crystal having lattice constant 1.5 Å, 2 Å and 4 Å on X, Y and Z axis respectively. Find Y and Z -axes intercepts.

Soln. :

Here a = 1.5 Å, b = 2Å, c = 4Å

Miller indices : (326)

$\therefore$ Intercepts are $\frac{a}{3}, \frac{b}{2}, \frac{c}{6}$ i.e. $\frac{1.5}{3}, \frac{2}{2}, \frac{4}{6}$

This gives the intercept along X-axis as $\frac{1.5}{3}$ Å = 0.5 Å

But it is given that plane cuts X-axis at 1.5 Å. This shows that the plane under consideration is another plane which is parallel to it and its x - intercept is 3 × 0.5 = 1.5 Å i.e. multiple of 2

$$\therefore \text{Y- intercept} = 3\left(\frac{2}{2}\right) = 3 \text{ Å}$$

$$\text{Z - intercept} = 3\left(\frac{4}{6}\right) = 2 \text{ Å}$$ ...**Ans.**

Ex. 2.5.8 : Sodium is a BCC crystal. It's density is 9.6×10^2 kg/m^3 and atomic weight is 23. Calculate the lattice constant for sodium crystal.

Soln. :

Given : n = 2 (BCC), $\rho = 9.6 \times 10^2$ kg/m^3, A = 23

Formula :

$$a^3\rho = \frac{nA}{N}$$

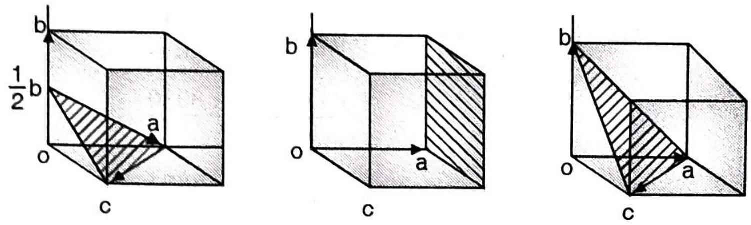
$$\therefore \quad a = \sqrt[3]{\frac{nA}{N\rho}} = \sqrt[3]{\frac{2 \times 23}{9.6 \times 10^2 \times 6.023 \times 10^{26}}}$$

$$= 4.3 \times 10^{-10} \text{ m} = 4.3 \text{ Å}$$

...**Ans.**

Ex. 2.5.9 : Draw the following planes (121), (100), (111).

Soln. :



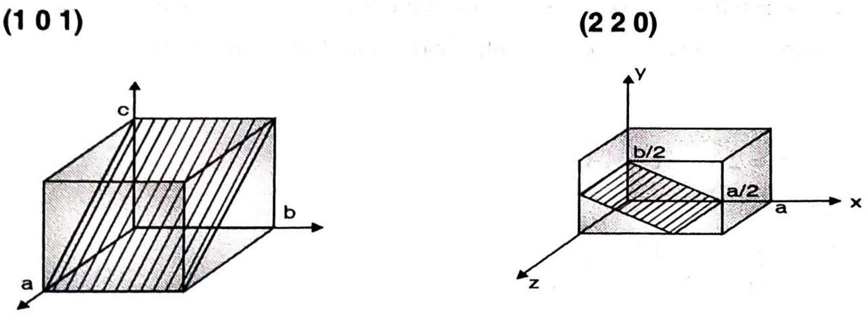
(a) (b) (c)

Fig. P. 2.5.9

Ex. 2.5.10 : Draw the following : (1 0 0), (2 2 0), (1 0 1)

Soln. :

(1 0 0)→Please refer solved Fig. P. 2.5.10(b)



(a) (b)

Fig. P. 2.5.10

Ex. 2.5.11 : Calculate the wavelength of X-rays reflected from the face of FCC crystal with lattice constant of 2.82 nm if the second order Bragg reflection occurs at a glancing angle of 17.167 deg.

Soln. :

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

Data given : $d = 2.82 \times 10^{-9}$ m (assume reflection in 100 plane),

$n = 2, \quad \theta = 17.167°$

$$\text{Because, } d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$= \frac{a}{\sqrt{1^2 + 0 + 0}}$$

$$= a$$

$$\lambda = \frac{2 \times 2.82 \times 10^{-9} \times \sin(17.167^\circ)}{2}$$

$$= 8.32 \times 10^{-10} m$$

$$= \mathbf{8.32\ A^\circ}$$ **...Ans.**

Possible solutions (100), (010), (001), because all of them provide d = a

Ex. 2.5.12 : Find out the intercepts made by the planes (10 1) and (4 1 4) in a cubic unit cell. Draw $[1\ \bar{2}\ 1]$ and [1 2 4] in a cubic unit cell. **MU - May 13, 5 Marks**

Soln. :

Let basic vectors be a, b, c and intercepts m, n, p respectively.

∴ On expressing m, n and p in terms of fractional multiples of a, b, c

$$\frac{m}{a}, \frac{n}{b}, \frac{p}{c}$$

As Miller indices are reciprocal of these fractions

$$(h\,k\,l) :: \left(\frac{a}{m}, \frac{b}{n}, \frac{c}{p}\right)$$

∴ For (101) :
$$\frac{a}{m} = 1, \frac{b}{n} = 0, \frac{c}{p} = 1$$

∴ w.r.t lattice parameters a, b, c the intercepts are

$$\frac{1}{1} = m = 1; \frac{1}{0} = n = \infty;$$

$$\frac{1}{1} = p = 1$$

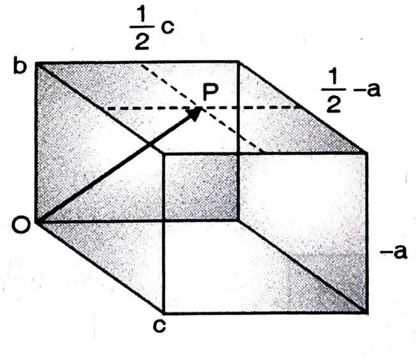


Fig. P. 2.5.12(a)

Similarly for (4 1 4)

$$m = \frac{1}{4}, n = 1, p = \frac{1}{4}$$

To draw $[\bar{1}\,2\,1]$ Draw points $\left[\frac{\bar{1}}{2}, 1, \frac{1}{2}\right]$

$$\vec{OP} = [\bar{1}\,2\,1]$$

[1 2 4] Draw points $\left[\frac{1}{4}, \frac{1}{2}, 1\right]$

$$\vec{OQ} = [1\,2\,4]$$

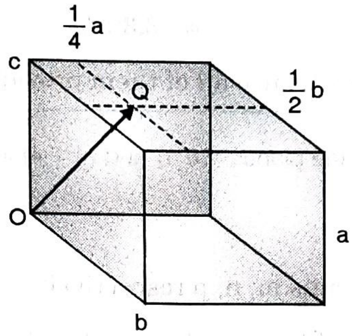


Fig. P. 2.5.12(b)

Ex. 2.5.13 : Find the interplanar spacing between the family of planes (111) in crystal of lattice constant 3 Å.

MU - Dec. 13, 3 Marks

Soln. :

Given :

$$a = 3,$$
$$(h\,k\,l) = (111)$$

Formula :

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

$$\therefore \quad d_{111} = \frac{3}{\sqrt{1^2 + 1^2 + 1^2}}$$

$$= \frac{3}{\sqrt{3}} = \sqrt{3}\ \text{Å}$$ ...Ans.

Ex. 2.5.14 : Represent the following in the unit cell. $(1\,\bar{1}\,2)\,(0\,0\,2)\,[1\,2\,1]$

MU - Dec. 13, 3 Marks

Soln. :

(1) $(1\,\bar{1}\,2)$

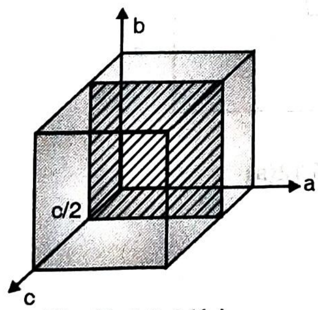


Fig. P. 2.5.14(a)

(2) $(0\,0\,2)$

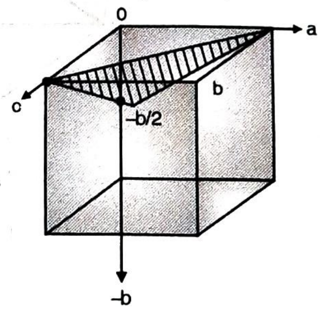


Fig. P. 2.5.14(b)

(3) [1 2 1] (Refer Solved Ex. 2.2.5)

Ex. 2.5.15 : Draw in cubic unit cell (021), (123), [121]

MU - May 14,3 Marks

Soln. : (a) (021)

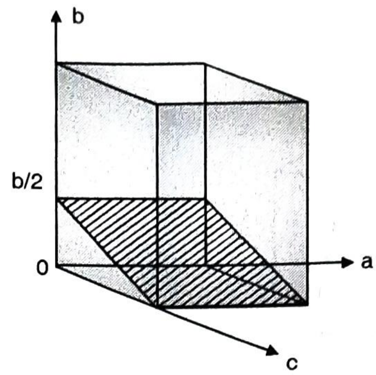


Fig. P. 2.5.15(a)

(b) (123)

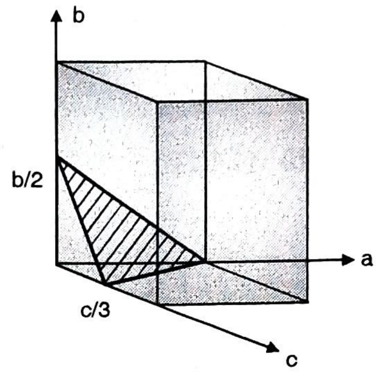


Fig. P. 2.5.15(b)

(c) [121] : Refer solved Ex. 2.2.5

Ex. 2.5.16 : Miller indices of a plane whose intercepts are, 4a and a where a is lattice constant. Draw (102), [201] and $(0\bar{4}0)$ in a cubic unit cell.

MU - Dec. 14, 5 Marks

Soln. : As intercepts area, 4 as and a with a as lattice constant.

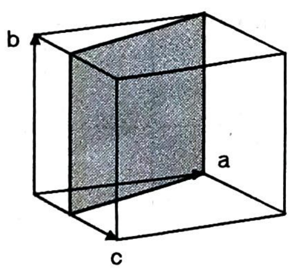
$\therefore$ Actual plane intercept are 1, 4 and 1.

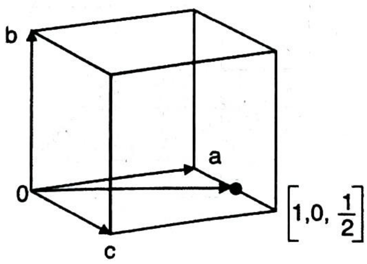
Take reciprocals : $\frac{1}{1}, \frac{1}{4}, \frac{1}{1}$

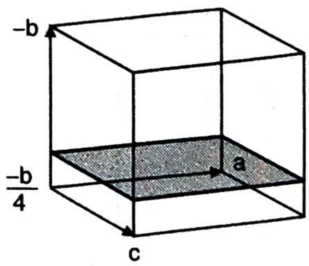
Taking LCM : (4 1 4)

$\therefore$ MI are (4 1 4) **...Ans.**

Draw (1) (1 0 2) (2) (2 0 1) (3) $(0\,\bar{4}\,0)$



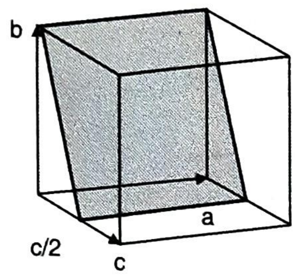


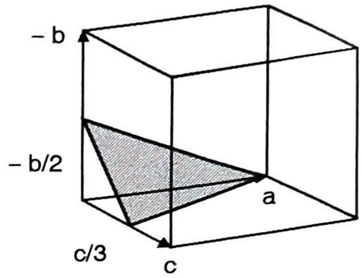


Ex.2.5.17 : Draw the following : (a) (0 1 2) (b) (1 $\bar{2}$ 3) (c) [1 2 1]

MU - May 15, 3 Marks

Soln. : **(a)(0 1 2)** **(b)(1 $\bar{2}$, 3)**



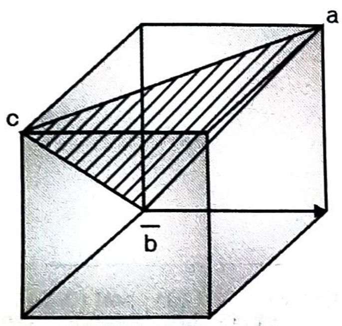


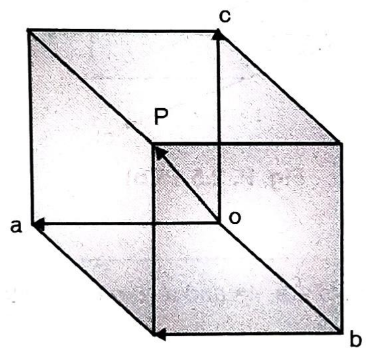
(c) [121] : Refer solved Ex. 2.2.5

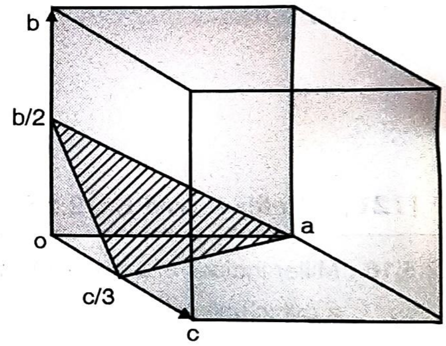
Ex. 2.5.18 : Draw the following w.r.t. a cubic unit cell : (1$\bar{1}$1) [$\bar{1}$11] (123)

MU - Dec. 15, 3 Marks

Soln. : **(a) (1 $\bar{1}$1)** **(b) [$\bar{1}$ 1 1]** **(C) (123)**







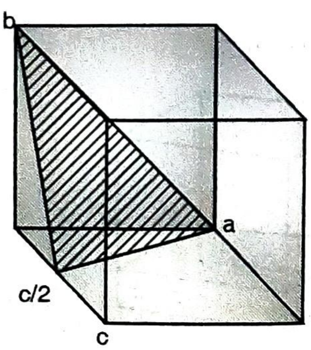
Ex. 2.5.19 : Draw (a) (112) (b) (040) (c) [040] with reference to a cubic unit cell.

MU - May 16, 3 Marks

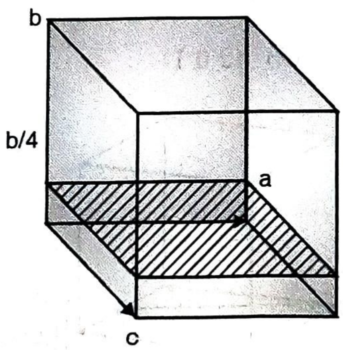
Soln. :

(a) (112) **(b) (040)** **(c) [040]**

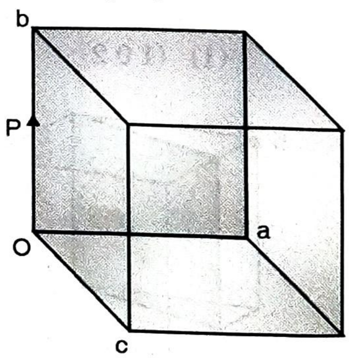
(112)



(040)



[040]



2.6 Solved Problems on X-rays

Ex. 2.6.1 : Calculate the smallest glancing angle at which x-ray of 1.549 Å will be reflected from crystal having spacing of 4.255 Å. What is the highest order of reflection that can be observed?

MU - May 14, 5 Marks

Soln. :

Consider Bragg's law,

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

(i) **For smallest glancing angle, n = 1**

$$\therefore \theta = \sin^{-1}\left(\frac{\lambda}{2d}\right) = \mathbf{10.488°} \quad \text{...Ans.}$$

(ii) **For highest order,** we know that always

$$\sin\theta \leq 1$$

∴ Find n which satisfies this condition using relation

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

for $n = 1$, $\sin\theta = \frac{\lambda}{2d} = 0.18$

for $n = 2$, $\sin\theta = 0.36$

for $n = 3$, $\sin\theta = 0.54$

for $n = 4$, $\sin\theta = 0.72$

for $n = 5$, $\sin\theta = 0.9$

for $n = 6$, $\sin\theta = 1.087 > 1$

As $\sin\theta$ cannot be greater than 1, the highest order possible is n = 5 **...Ans.**

Other way possible to solve this is by taking maximum $\sin\theta = 1$

$$\therefore n\lambda = 2d$$

$$\therefore n = \frac{2d}{\lambda} = \frac{2 \times 4.255}{1.549} = 5.49$$

Now n is a fraction, and to convert it into integer remove fractional part.

Ex. 2.6.2 : Calculate the glancing angle on the plane (100) for a crystal of rock salt(a = 2.125 Å). Consider the case of 2nd order maximum and wavelength 0.592 Å.

MU - Dec. 12, 4 Marks

Soln. :

(i) Calculate d for rock salt

$$d = \frac{a}{2} = 1.0625\ \text{Å}$$

(ii) Use Bragg's law for n = 2

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

$$\therefore 2 \times 0.592 \times 10^{-10} = 2 \times 1.0625 \times 10^{-10} \times \sin\theta$$

$$\sin\theta = 0.557$$

$$\therefore \theta = \mathbf{33.86°} \quad \text{...Ans.}$$

Ex. 2.6.3 : Monochromatic high energy x-rays are incident on a crystal. If first order reflection is observed at an angle 3.4°, at what angle would second order reflection be expected?

Soln. :

Data : For order

$$n = 1, \quad \theta_1 = 3.4°]$$

Use Bragg's law

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

$$\text{for } n = 1$$

$$\lambda = 2\,d \sin (3.4°)$$

$$\therefore\ d = \lambda/2 \sin (3.4°)$$

∴ For order n = 2

$$2\lambda = 2\,d \sin \theta_2$$

$$\therefore\ \sin \theta_2 = \frac{\lambda}{d} \quad ...(1)$$

Replace value of d from equation (1)

$$\sin \theta_2 = \frac{\lambda}{\lambda / 2 \sin (3.4)}$$

$$= 2 \sin 3 \cdot 4 = 0.1186$$

$$\therefore \theta_2 = \sin^{-1} (0.1186) = 6.811°$$

...Ans.

Ex. 2.6.4 : The radiation of an x-ray tube operated at 50 kV are diffracted by a cubic KCl, FCC crystal of molecular weight 74.6 and density 1.99×10^3 kg/m^3. Calculate:

Glancing angle for first order reflection from the reflecting planes of the crystal for wavelength, 0.248A°.

Soln. :

Given :

$V = 50 \times 10^3$ volts, $M = 74.6$, $\rho = 1.99 \times 10^3$ kg/m^3,

n = number of atoms/unit cell = 4 (FCC), $\lambda = 0.248$A°

Step 1 :

$$\text{Now } a^3\rho = \frac{nM}{N}$$

$$\therefore\ a = \sqrt[3]{\frac{nM}{N} \cdot \frac{1}{\rho}}$$

$$= \sqrt[3]{\frac{4 \times 74.6}{6.023 \times 10^{26}} \times \frac{1}{1.99 \times 10^3}}$$

$$= 6.29 \times 10^{-10} \text{ m}$$

Since KCl is ionic crystal,

$$\therefore\ d = a/2 = \frac{6.29}{2} \times 10^{-10} = 3.145 \times 10^{-10} \text{ m}$$

Step 2 : Using Bragg's law

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

Consider

$$n = 1 \text{ for } \lambda = \lambda_{min}$$

$$\therefore \sin\theta = \frac{1\times\lambda}{2d} = \frac{1\times 0.248\times 10^{-10}}{2\times 3.145\times 10^{-10}} = 0.0394$$

$$\therefore \theta = \sin^{-1}(0.0394) = \mathbf{2.26^\circ}$$ ...Ans.

Ex. 2.6.5 : Monochromatic x-rays of wavelength 0.82 Å undergo first order Bragg reflection from a crystal of cubic lattice with lattice constant 3 Å, at a glancing angle of 7° 51′ 48″. Identify the possible planes which give rise to this reflection in terms of their Miller indices.

Soln. :

Data : $\lambda = 0.82\times 10^{-10}$ m, $n = 1$, $\theta = 7^\circ\, 51'\, 48''$,

$a = 3\times 10^{-10}$ m

Use Bragg's law

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

$$\therefore d = \frac{n\lambda}{2\sin\theta} = \frac{1\times 0.82\times 10^{-10}}{2\times\sin(7^\circ\, 51'48'')}$$

$$= 3\times 10^{-10}\text{ m}$$

$$\text{Now, } d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$\text{Here we have } d = a$$

$$\therefore \sqrt{h^2+k^2+l^2} = 1$$

∴ Possible solutions (100), (010), (001) because for all of them,

Where, $\sqrt{\mathbf{h^2+k^2+l^2}} = 1$ ...Ans.

Ex. 2.6.6 : The glancing angle of reflection for the first order K_α x-rays from palladium are 5.4° from (100) planes, 7.6° from (110) planes and 9.4° from (111) planes. From the above mentioned data determine the cubic lattice structure of the crystal.

Soln. :

Using Bragg's law,

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

$$\therefore d = \frac{\lambda}{2\sin\theta} \quad (n = 1)$$

or

$$\text{for (100)}, d_1 = \frac{\lambda}{2\sin 5.4^\circ} = \frac{\lambda}{0.1882}$$

$$\text{for (110)}, d_2 = \frac{\lambda}{2\sin 7.6^\circ} = \frac{\lambda}{0.2645}$$

$$\text{for (111)}, d_3 = \frac{\lambda}{2\sin 9.4^\circ} = \frac{\lambda}{0.3266}$$

$$d_1 : d_2 : d_3 = \frac{\lambda}{0.1882}\, [1 : 0.711 : 0.576]$$

$$d_1 : d_2 : d_3 :: [1 : \sqrt{2} : \sqrt{3}\,] \therefore \text{ it is SC}$$ ...Ans.

Ex. 2.6.7 : Bragg's reflection of the first order was observed at 21.7° for parallel planes for a crystal under test. If the wavelength of x-rays used is 1.54 Å find the lattice constant of the crystal.

Soln. :

$$n = 1,$$

$$\theta = 21.7^\circ \text{ (Assume it is glancing angle)}$$

$$\lambda = 1.54\ \text{Å},$$

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

$$d = \frac{n\lambda}{2\sin\theta} = \frac{1 \times 1.54 \times 10^{-10}}{2 \times \sin(21.7°)}$$

$$= 2.083 \times 10^{-10}\ \text{m}$$

$$\mathbf{d = 2.083\ \text{Å}}$$ **...Ans.**

Ex. 2.6.8 : Calculate the glancing angle on the cube (100) of a rock salt (a = 2.814 Å) corresponding 2^{nd} order diffraction maximum for x-rays of wavelength 0.714 Å.

Soln. :

$$d_{nkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{2.814}{\sqrt{1^2 + 0^2 + 0^2}} = 2.814\ \text{Å}$$

For 2^{nd} order Bragg reflection

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

$$2(0.714) = 2(2.814)\sin\theta$$

$$\therefore\ \sin\theta = 0.2537$$

$$\therefore \theta = \mathbf{14° 41'}$$ **...Ans.**

Ex. 2.6.9 : The spacing between the principal planes in a crystal of NaCl is 2.82 Å. It is found that first order Bragg's reflection occurs at 10°.

(a) What is the wavelength of x-ray?

(b) At what angle does the second order reflection occur?

(c) What is the highest order of reflection seen?

Soln. :

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

(a)

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

$$\therefore \lambda = 2(2.82 \times 10^{-10})(\sin 10°)$$

$$= 9.79 \times 10^{-11}\ \text{m}$$

$$\therefore \lambda = \mathbf{0.979\ \text{Å}}$$ **...Ans.**

(b) For n = 2 find θ

Using

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

$$\therefore\ 2 \times (0.979 \times 10^{-10}) = 2(2.82 \times 10^{-10})\sin\theta$$

$$\therefore\ \sin\theta = 0.347$$

$$\therefore \theta = \mathbf{20° 18'}$$ **...Ans.**

(c) For highest order

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

$$\therefore\ \sin\theta = \frac{n\lambda}{2d}$$

As sinθ cannot exceed one,

for various values of n i.e. n = 1, 2, 3,... find sinθ.

The value of n which yields

$\sin\theta > 1$ is not possible.

here for $n = 6$ we get, $\sin\theta = 1.041$

i.e. $\sin\theta > 1$

∴Highest order possible is 5. **...Ans.**

Ex. 2.6.10 : In comparing the wavelengths of two monochromatic x-ray lines, it is found that line A gives a 1st order Bragg reflection maximum at a glancing angle of 30° to the smooth face of a crystal. Line B of known wavelength of 0.97 Å gives a 3rd order reflection maximum at a glancing angle of 60° with the same face of the same crystal. Find the wavelength of the line A.

Soln. :

For line – Aorder $n = 1$

$\theta = 30°, \lambda = ?$

Using Bragg's law for line – A

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

$$1\lambda_A = 2d\sin 30 = 2d \times \frac{1}{2} = d$$

$$\therefore \lambda_A = d \qquad ...(1)$$

For line – B

$$\lambda = 0.97\ \text{Å} \quad n=3$$

$$\theta = 60° \quad d=\lambda_A$$

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

$$3(0.97) = 2(\lambda_A)\cdot\sin 60°$$

$$3(0.97) = 2(\lambda_A)\cdot\frac{\sqrt{3}}{2} = \sqrt{3}\lambda_A$$

$$\therefore \lambda_A = \frac{3\times 0.97}{\sqrt{3}} = \mathbf{1.68\ \text{Å}} \qquad \text{...Ans.}$$

Ex. 2.6.11 : A 10 keV electrons are passed through a thin film of a metal for which atomic spacing is 5.5×10^{-11} m. What is the angle of deviation of the first order diffraction minimum?

Soln. :

(1)

$$\text{Energy} = 10\ \text{keV} = 10 \times 10^3 \times 1.6 \times 10^{-19}\ \text{J}$$

$$\therefore \lambda = \frac{h}{\sqrt{2mE}}$$

$$= \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 10^4 \times 1.6 \times 10^{-19}}}$$

$$= 1.23 \times 10^{-11}\ \text{m}$$

Using Bragg's law (for $n = 1$)

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

$$\therefore \sin\theta = \frac{1 \times 1.23 \times 10^{-11}}{2 \times 5.5 \times 10^{-11}} = 0.118$$

$$\therefore \theta = \mathbf{6.42°} \qquad \text{...Ans.}$$

Ex. 2.6.12 : Calculate the glancing angle on cube (100) of rock salt having lattice constant 2.814 Å corresponding to first order diffraction maximum for x-rays of wavelength 1.541 Å.

Soln. :

Given : Plane (100)

$$a = 2.814\ \text{Å} = 2.814 \times 10^{-10}\ \text{m}$$

$$\lambda = 1.541\text{Å} = 1.541 \times 10^{-10}\ \text{m}$$

$$n = 1$$

Bragg's law,

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

For rock salt

$$d = \frac{a}{2} = 1.407 \times 10^{-10}\ \text{m}$$

$$\therefore \theta = \sin^{-1}\left(\frac{n\lambda}{2d}\right)$$

$$= \sin^{-1}\left(\frac{1 \times 1.541 \times 10^{-10}}{2 \times 1.407 \times 10^{-10}}\right)$$

$$\theta = \sin^{-1}(0.5476) = \mathbf{33.20°}$$ ...Ans.

Ex. 2.6.13 : Calculate the maximum order of diffraction if x-rays of wavelength 0.819 Å are incident on a crystal of lattice spacing 0.282 nm. **MU - Dec. 13, 4 Marks**

Soln. :

Given : $\lambda = 0.819$ Å , $d = 0.282$ nm

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

for the given values of λ and d, $n \alpha \sin \theta$

for n to be maximum, $\sin \theta = 1$

$$\therefore\ n = \frac{2d}{\lambda} = \frac{2 \times 0.282 \times 10^{-9}}{0.819 \times 10^{-10}} = 6.88$$

$\therefore$ As order cannot be a fraction and n is maximum,

$$\mathbf{n = 6}$$ ...Ans.

Ex. 2.6.14 : Calculate Bragg angle if (200) planes of a BCC crystal with lattice parameter 2.814 Å give second order reflection with X-rays of wavelength 0.71 Å. **MU - Dec. 14, 4 Marks**

Soln. :

Given:

$$a = 2.814$$

$$(hkl) = (200)$$

$$\therefore d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$= \frac{2.814}{\sqrt{2^2 + 0 + 0}}$$

$$= 1.407\ \text{Å}$$

Using Bragg's law

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

$$\therefore \quad 2 \times 0.71 = 2 \times 1.407 \times \sin\theta$$

$$\therefore \quad \sin\theta = \frac{0.71}{1.407} = 0.5046$$

$$\therefore \theta = \mathbf{30.30^\circ}$$ **...Ans.**

Ex. 2.6.15 : X-rays of unknown wavelength give first order Bragg's reflection at glancing angle 20° with (212) planes of copper having FCC structure. Find wavelength of x-rays if the lattice constant for copper is 3.615 Å. **MU - May 15, 7 Marks**

Soln. :

Using formula

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$= \frac{3.615}{\sqrt{2^2 + 1^2 + 2^2}} \text{ Å}$$

$$= 1.205 \text{ Å}$$

Using Bragg's law

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

Here,

$$n = 1$$

$$\theta = 20^\circ$$

$$\therefore 1 \times \lambda = 2 \times 1.205 \times \sin 20$$

$$\therefore \lambda = \mathbf{0.824 \text{ Å}}$$ **...Ans.**

Ex. 2.6.16 : Monochromatic x-ray beam of wavelength λ = 5.8189 A° is reflected strongly for a glancing angle of θ = 75.86° in first order by certain planes of cubic of lattice constant 3A°. Determine Miller indices of the possible reflecting planes. **MU - May 16, 3 Marks**

Soln. :

Problem :

$\lambda = 5.8189$ A°, $\theta = 75.86^\circ$, $n = 1$, $a = 3$ A°

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

$$d = \frac{n\lambda}{2\sin\theta} = 3 \text{ A}^\circ$$

$$\text{as} \quad a = 3\text{A}^\circ \quad \text{(given)}$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$\therefore d = a$$

$\therefore$ Possible planes (1 0 0), (0 1 0), (0 0 1) **... Ans.**

Ex. 2.6.17 : An electron is accelerated through 1200 volts and is reflected from a crystal. The second order reflection occurs when glancing angle is 60°. Calculate the interplanar spacing of the crystal. **MU - May 17, 8 Marks**

Soln. :

Data : V = 1200 volt, order n = 2,

glancing angle = 60°

To find : Interplanar spacing d.

T = ?

Using relation

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2m\,(eV)}} = 6.63 \times 10^{-34}$$

$$= \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 1200}}$$

$$= 3.547 \times 10^{-11} \text{ m}$$

Using Bragg's law

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

$$d = \frac{n\lambda}{2 \sin\theta} = \frac{2 \times 3.547 \times 10^{-11}}{2 \times \sin 60^\circ}$$

$$= 4.09 \times 10^{-11} \text{ m}$$

$\therefore$ Interplanar spacing $=$ **4.09×10^{-11} m** ...**Ans.**