4.2 A substance with *fcc* lattice has density 6250 kg/m^3 and molecular weight 60.2. Calculate the lattice constant a.

Hint : $$a = \left[\frac{nM}{\rho N}\right]^{1/3} = \left[\frac{4 \times 60.2}{6250 \times 60.23 \times 10^{26}}\right]^{1/3} = 4 \times 10^{-10}\,\text{m} = 4\,\text{Å}$$

4.3 Zinc has *hcp* structure. The height of unit cell is 4.9 Å, the nearest neighbour distance is 2.7 Å. Calculate the volume of the unit cell.

Hint : $$a = 2r = 2.7\,\text{Å},$$

$$V = \frac{3\sqrt{3}a^2c}{2} = \frac{3\sqrt{3} \times (2.7 \times 10^{-10}\,\text{m})^2 \times (4.9 \times 10^{-10}\,\text{m})}{2} = 9.4 \times 10^{-29}\,\text{m}^3$$

4.4 Calculate the lattice constant of NaCl crystal. The density of NaCl crystal is 2189 kg/m^3 and Avogadro's number N is 6.02×10^{26} kg/molecule.

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

$$= \left(\frac{4 \times 58.5}{6.02 \times 10^{26} \times 2189}\right)^{1/3} = (177 \times 10^{-30})^{1/3} = 5.61 \times 10^{10}\,\text{m} = 5.61\,\text{Å}.$$

4.5 Obtain lattice constant and radius of the atom having simple lattice and volume density of $3 \times 10^{22}/\text{cm}^3$ assuming that the atoms are hard sphere with each atom touching its nearest neighbour.

Hint : $$a = \left[\frac{\text{no. of lattice points}}{\text{volume density}}\right]^{1/3}, \text{ no. of lattice points } (sc) = 8 \times \frac{1}{8} = 1$$

$$= \left[\frac{1}{3 \times 10^{22}}\right]^{1/3} = 0.322 \times 10^{-7}\,\text{cm} = 3.22\,\text{Å}$$

4.6 An element of atomic weight 60 has density 6.23 gm/cc. What is the radius of its atom of it has *fcc* structure ?

Hint : $$\rho_a = \left[\frac{nM}{N\rho}\right]^{1/3} = \left[\frac{4 \times 60}{6.023 \times 10^{23} \times 6.23}\right]^{1/3} = 4.0 \times 10^{-8}\,\text{cm}$$

Then $$r = \frac{a\sqrt{2}}{4} = 1.414\,\text{Å}$$

4.7 Calculate packing factor for chromium metal having *bcc* structure if its density = 5.96 g/cc and atomic weight = 50.

[GGSIPU, May 2019 (2.5 marks)]

Hint : $$a = \left(\frac{nM}{N\rho}\right)^{1/3} = 5.496 \times 10^{-8}\,\text{cm},$$

$$r = \frac{a\sqrt{3}}{4} = 2.38 \times 10^{-8}\,\text{cm}$$

$$\text{Packing factor} = \frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}} = \frac{2 \times \frac{4}{3}\pi r^3}{a^3} = 0.68$$

4.8 Sodium is a *bcc* crystal. Its density is $9.6 \times 10^2\ kg/m^3$ and atomic weight is 23. Calculate the lattice constant a for sodium crystal.

Hint : $$a = \left(\frac{nM}{N\rho}\right)^{1/3} = \left[\frac{2\times 23}{6.023\times 10^{26}\times 9.6\times 10^2}\right]^{1/3} = 4.3\ Å$$

4.9 The nearest neighbour distance in a silver crystal is 2.87 Å. Silver crystallizes in *fcc* form, determine its density.

Hint : $$a = \sqrt{2}r = \sqrt{2}\times 2.87\times 10^{-10}\ m$$

$$\rho = \frac{n\times M}{N\times a^3}$$

$$= \frac{4\times 107.68}{6.023\times 10^{26}\times(4.06\times 10^{-10})^3} = 1.068\times 10^4\ kg/m^3$$

4.10 Sodium chloride has *fcc* structure. Its density is $2.18\times 10^3\ kg/m^3$. The atomic weights of sodium and chloride are 23 and 35.5, respectively. Calculate the interatomic separation.

Hint : $a = \left(\frac{nM}{N\rho}\right)^{1/3} = 5.63$ Å, the interatomic distance

$$r = \frac{a}{2} = 2.81\ Å.$$

4.11 Copper has *fcc* structure and its atomic radius is 1.278 Å. Calculate its density. Atomic weight of copper = 63.5, Avogadro's number 6.023×10^{23}.

[GGSIPU, May 2014 (2 marks) ; May 2018 (2.5 marks)]

Hin : $$\rho = \frac{n}{a^3}\frac{M}{N}$$

$$= \frac{nM}{\left(\frac{4r}{\sqrt{2}}\right)^3 N} = \frac{4\times 63.54}{\left(\frac{4\times 1.278\times 10^{-8}}{\sqrt{2}}\right)^3\times(6.02\times 10^{23})} = 8.98\ gm/cc$$

4.12 Rubidium (at. mass = 85.5) crystallizes into *bcc* structure. If its density is $1510\ kg/m^3$ and radius of the rubidium atom is 2.48 Å, determine Avogadro's number.

Hint : $$N = \frac{nM}{\rho a^3},$$

$$a = \frac{4r}{\sqrt{3}} = \frac{4\times 2.48\times 10^{-10}}{\sqrt{3}}\ Å$$

$$N = \frac{2\times 85.5(\sqrt{3})^3}{1510\times(4\times 2.48\times 10^{-10})^3} = 6.019\times 10^{26}$$

4.13 Lithium crystallizes in *bcc* structure. Calculate the lattice constant, given that the atomic weight and density for lithium are 6.94 and $530\ kg/m^3$ respectively.

Hint. We know $a^3 = \frac{nM}{\rho N} = \frac{2\times 6.94}{530\times 6.023\times 10^{26}} = 43.50\times 10^{-30}$

$\therefore a = 3.517\times 10^{-10}\ m = 3.517\ Å$

4.14 Germanium crystallizes in diamond (form) structure with 8 atoms per unit cell. If lattice constant is 5.62 Å, calculate its density. **[GGSIPU, May 2016 (2.5 marks)]**

Hint : We know, $a^3 = \dfrac{nM}{\rho N}$

or
$$\rho = \frac{nM}{Na^3}$$

$$= \frac{8 \times 72.59}{(5.62 \times 10^{-10})^3 \times 6.023 \times 10^{26}} = 5434.5 \text{ kg/m}^3 = 5.435 \text{ g/cc}$$

4.15 Calculate the density of diamond crystal, given that its lattice parameter 'a' is 3.57 Å and atomic mass $A = 12$

Hint : The effective number of atoms in the diamond cubic unit cell is 8

$$\rho = \frac{Mn}{Na^3}$$

where N = Avogadro's number

$$\therefore \quad \rho = \frac{8 \times 12}{6.023 \times 10^{26} \times (3.57 \times 10^{-10})^3} = 3540 \text{ kg/m}^3 = 3.54 \text{ g/cc}$$

Example 5.8 *Calculate the smallest glancing angles at which the X-rays of wavelength ($\lambda = 1.449$ Å) will be reflected from a quartz crystal, which has the atomic spacing $d = 4.255$ Å*

[GGSIPU, April 2014 (2 marks)]

Solution. Since we know Bragg's relation

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

Here $\lambda = 1.449$ Å and $d = 4.255$ Å.

For *first reflection i.e.,* $n = 1$

$$2d \sin\theta_1 = \lambda$$

or
$$\sin\theta_1 = \frac{\lambda}{2d} = \frac{1.449 \text{ Å}}{2 \times 4.255 \text{ Å}} = 0.170$$

$$\theta_1 = \sin^{-1}(0.170) = 9.78°$$

Similarly, for *second reflection i.e.,* $n = 2$.

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

$$\sin\theta_2 = \frac{2 \times 1.449 \text{ Å}}{2 \times 4.255 \text{ Å}} = 0.340$$

$$\theta_2 = \sin^{-1}(0.340) = 19.88°.$$

Problem 5.1 *Find the set of Miller indices for a plane cutting of intercepts 3a,2b,4c*

Solution. From the law of rational indices, we may write

$$3a : 2b : 4c = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$

where h, k, l are the Miller indices.

$$\therefore \quad \frac{1}{h} : \frac{1}{k} : \frac{1}{l} = 3 : 2 : 4 \quad \text{or} \quad h : k : l = \frac{1}{3} : \frac{1}{2} : \frac{1}{4}$$

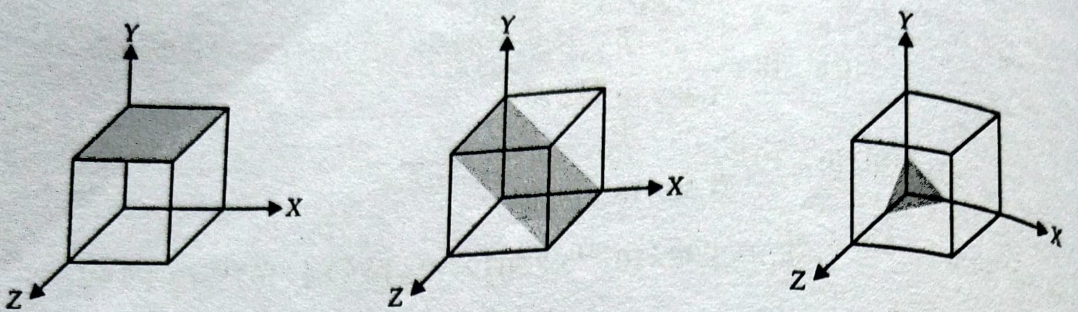
Converting to smallest whole numbers having the same ratios, we have

$$h : k : l = \frac{4}{12} : \frac{6}{12} : \frac{3}{12} = 4 : 6 : 3$$

Thus, the Miller indices of the planes are 4, 6 and 3 or the plane is (463).

Problem 5.2 *Draw (010), (110) and (222) planes in a cubic crystal.*

Solution.



(010) Plane (110) Plane (222) Plane

Fig. 5.27

Problem 5.3 *A certain crystal has lattice constant of 4.24 Å, 10 Å and 3.66 Å on the x, y and z axes respectively. Determine the Miller indices of the plane of this crystal having 4.24 Å, 5 Å and 1.83 Å as its x, y and z intercepts respectively.* **[GGSIPU, May 2018 (3 marks)]**

Solution. Lattice parameters are = 4.24 Å, 10 Å and 3.66 Å

The intercepts of the given plane = 2.12 Å, 10 Å and 1.83 Å *i.e.*, the intercepts are 0.5, 1 and 0.5.

Step 1. The intercepts are $\frac{1}{2}$, 1 and $\frac{1}{2}$.

Step 2. The reciprocals are 2, 1 and 2.

Step 3. The least common denominator (lcd) is 2.

Step 4. Multiplying the lcd by each reciprocal we get, 4, 2 and 4.

Step 5. By writing them in parenthesis we get (4 2 4).

Therefore the Miller indices of the given plane is (4 2 4) or (2 1 2).

Problem 5.4 *Deduce the Miller indices of a plane which cuts off intercepts in the ratio $1a : 3b : -2c$ along the three axes.* **[GGSIPU, May 2016 (2 Marks)]**

Solution. From the law of rational indices, we may write

$$1a : 3b : -2c = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$

where h, k, l are the Miller indices

$$\frac{1}{h} : \frac{1}{k} : \frac{1}{l} = 1 : 3 : -2 \quad \text{or} \quad h : k : l = 1 : \frac{1}{3} : -\frac{1}{2} = 6 : 2 : -3$$

Thus, $h = 6$, $k = 2$, $l = -3$. Hence, the plane is $(62\bar{3})$.

Problem 5.5 *Find the Miller indices of a set of parallel planes which make intercepts in the ratio of $3a : 4b$ on the x and y axes and are parallel to the z-axis.*

Solution. The parallel planes are parallel to the z-axis, that is, their intercepts on the z-axis are infinite. From the law of rational indices, we may write

$$3a : 4b : \infty c = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$

or
$$\frac{1}{h} : \frac{1}{k} : \frac{1}{l} = 3 : 4 : \infty$$

or
$$h : k : l = \frac{1}{3} : \frac{1}{4} : \frac{1}{\infty} = 4 : 3 : 0$$

The Miller indices are [430].

Problem 5.6 *X-rays of wavelength 2×10^{-11} m suffer first order reflection from (111) crystal plane at an angle of 45°. What is interatomic spacing of the crystal ?*

[GGSIPU, May 2007 (2.5 Marks)]

Solution. We know that $d_{hkl} = \dfrac{a}{\sqrt{h^2 + k^2 + l^2}}$

where a = interatomic distance, d = interplanar distance, h, k, l = Miller indices

According to problem $h = k = l = 1$ (being d_{111})

$$\theta = 45°, \quad \lambda = 10^{-11} \text{ m}, \quad n = 1$$

From Bragg's law $\quad 2d \sin\theta = n\lambda,$

We have $\quad 2\dfrac{a}{\sqrt{3}} \times \sin 45° = 2 \times 10^{-11}$

$$a = \sqrt{6} \times 10^{-11} = 2.45 \times 10^{-11} \text{ m} = 0.25 \text{ Å}$$

Problem 5.7 *A beam of X-ray $\lambda = 0.842$ Å is incident on a crystal at a grazing angle of 8°35′ when the first order Bragg's reflection occurs. Calculate the glancing angle for 3rd order reflection.*

Solution. According to Bragg's equation,

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

For first order,

$$2d \sin 8°35' = 1 \times 0.842 \times 10^{-10} \quad \text{...}(i)$$

and *for third order,*

$$2d \sin\theta_3 = 3 \times 0.842 \times 10^{-10} \quad \text{...}(ii)$$

From Eqs. (*i*) and (*ii*),

$$\frac{\sin\theta_3}{\sin 8°35'} = 3$$

or
$$\sin\theta_3 = 3 \sin 8°35' = 3 \times 0.15$$

or
$$\theta_3 = \sin^{-1}(0.45) = 26.5°$$

Problem 5.8 *Calculate the glancing angle of the (110) plane of simple cubic crystal (a = 2.814 Å) corresponding to second order diffraction maxima for the X-rays of wavelength 0.710 Å.*

[GGSIPU, May 2006 (4.5 Marks) ; May 2019 (3.5 marks)]

Solution. For n^{th} order diffraction maximum for X-rays of wavelength λ from lattice planes of spacing d, the glancing angle θ is given by ...(*i*)

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

The distance between consecutive lattice planes defined by Miller indices (*hkl*) in a cubic lattice

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

Here $a = 2.814$ Å, $h = 1$, $k = 1$, $l = 0$

then
$$d_{110} = \frac{2.814}{\sqrt{1^2 + 1^2 + 0}} = \frac{2.814}{\sqrt{2}} \text{ Å} = 1.989 \text{ Å}$$

Also we have $n = 2$ and $\lambda = 710$ Å

Substituting these values in Eq. (*i*)

$$2 \times 1.989 \sin\theta = 2 \times 0.710$$

$$\sin\theta = \frac{0.710}{1.989} = 0.3569$$

$$\theta = \sin^{-1}(0.3569)$$

$$\theta = 20°55'$$

Problem 5.9 *From a powder camera of diameter 114.6 mm using an X-ray beam of wavelength 1.54 Å, the following S values in mm are obtained for material : 86, 100, 148, 130, 188, 232 and 272. Determine the structure and lattice parameter.*

Solution. Given, radius of camera $= \frac{114.6}{2} = 57.3$ mm

The Bragg's angles in degrees at which reflections are observed are equal to 5/4 and are : 21.5°, 25°, 37°, 47°, 58° and 68°.

The $\sin^2\theta$ values are in the ratio 0.1346 : 0.1788 : 0.3620 : 0.5003 : 0.5352 : 0.7195 : 0.8596 within experimental error, these values can be expressed in the ratio of integral numbers

3 : 4 : 8 : 11 : 12 : 16 : 19.

From the extinction rules, the structure is *fcc*. The lattice parameter calculated from highest angle is 3.62 Å

5.2 X-rays with 1.54 Å are used for calculation of the d_{100} plane of a cubic crystal. The Bragg's angle of first order reflection is 10°. What is the size of unit cell ?

Hint : $d_{100} = \frac{a}{\sqrt{h^2+k^2+l^2}} = a\,\text{Å}$

$$2d_{100}\sin\theta = n\lambda \quad \Rightarrow \quad 2a\sin\theta = n\lambda \quad \Rightarrow \quad a = 4.43\ \text{Å}$$

5.3 For a cubic lattice, calculate the distance of (1 2 3) and (2 3 4) planes from a plane passing through the origin.

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

$$\Rightarrow \quad d_{123} = \frac{a}{\sqrt{1+4+9}} = \frac{a}{14} \quad \text{and} \quad d_{234} = \frac{a}{\sqrt{4+9+16}} = \frac{a}{\sqrt{29}}$$

5.4 Deduce the Miller indices for the plane having intercepts a, b and c at $-2, \infty, -2$. Also draw the plane.

[GGSIPU, May 2019 (2.5 marks)]

Hint : Intercept are $-2, \infty, -2$

The reciprocal are : $\frac{1}{-2}, \frac{1}{\infty}, \frac{1}{-2}$

LCD $\quad -2,\ 0,\ -2$

Miller indices for the plane is $(\bar{2}0\bar{2})$

5.5 Deduce the Miller indices of a set of parallel which make intercepts in the ratio of $a:2b$ on the x and y axes are parallel to z-axis, a, b, c *being primitive vectors of lattice. Also calculate the interplanar distance d of the plane taking the lattice to be cube with* $a = b = c = 5\,\text{Å}$.

[GGSIPU, May 2015 (5 marks)]

Hint : $a:2b:\infty = \frac{a}{h}:\frac{b}{k}:\frac{c}{l}; h:k:l = 1:\frac{1}{2}:\frac{1}{\infty} = 2:1:0$

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{5}{\sqrt{4+1+0}}\,\text{Å} = \sqrt{5}\,\text{Å}$$

5.6 In a simple cubic crystal (*i*) find the ratio of intercepts of three axes by (123) plane and (*ii*) find the ratio of spacing of (110) and (111) planes.

[GGSIPU, May 2015 (4 marks)]

Hint : Ratio of intercepts : $\frac{a}{1}:\frac{a}{2}:\frac{a}{3} = 1:\frac{1}{2}:\frac{1}{3}$

$$d_{110} = \frac{a}{\sqrt{1^2+1^2+0}} = \frac{a}{\sqrt{2}};\ d_{111} = \frac{a}{\sqrt{1^2+1^2+1^2}} = \frac{a}{\sqrt{3}}$$

$$d_{110}/d_{111} = \frac{\sqrt{3}}{\sqrt{2}} = 1.225$$

5.7 What is the difference between (111) and $\langle 111 \rangle$ for Miller indices ? [GGSIPU, May 2016 (2.5 marks)]

Hint : (111) → plane and $\langle 111 \rangle$ → direction.

5.8 Sodium crystallizes in bcc structure. If the radius of the sodium atom is 1.55 nm, compute the spacing between the (111) planes.

[GGSIPU, May 2018 (2 marks)]

Hint : $a = \frac{4}{\sqrt{3}}r = \frac{4}{\sqrt{3}} \times (1.55\times10^{-9})\text{m}$. The spacing $d_{111} = \frac{a}{\sqrt{h^2+k^2+l^2}}$

$$d_{111} = \frac{4}{\sqrt{3}} \times \frac{1.55\times10^{-9}}{\sqrt{3}} = \frac{6.20}{3}\times10^{-9}\text{m} = 3.1\times10^{-9}\text{m}.$$

5.9 Find the Miller indices of a plane that makes intercepts 1 on a-axis, 2 on b-axis and is parallel to c-axis.

Hint : Intercepts 1, 2, ∞ ; reciprocal 1, $\frac{1}{2}$, 0 ; smallest integer having same ratio 2, 1, 0, Miller indices (2 1 0).

5.10 Obtain the Miller indices of planes have intercepts $\frac{a}{2}$, b and $2c$ in a simple cubic cell. Draw Miller indices.

Hint : $\frac{1}{2}$, 1, 2 ; Reciprocal 2, 1, $\frac{1}{2}$; LCM 2 and Miller Indices (4 2 1)

5.11 Copper has fcc structure and atomic radius is 0.127 nm. Find the ratio of the spacing of (111) and (123) planes. **[GGSIPU, May 2017 (2.5 marks)]**

Hint : $a = 2\sqrt{2}r = 2\sqrt{2} \times (0.127 \times 10^{-9})\text{m} \quad \Rightarrow \frac{d_{111}}{d_{123}} = \sqrt{\frac{(1+4+9)}{(1+1+1)}} = \sqrt{\frac{14}{3}} = 2.16$

5.12 If a, b and c are the primitive vectors of the unit cell a plane of Miller indices (310) cut the crystal lattice, find the intercepts of the plane along the three axes. **[GGSIPU, May 2017 (3 marks)]**

Hint : LCD = 3 ; Reciprocal : 1, $\frac{1}{3}$, 0 and Intercepts : 1, 3, 0

5.13 Lead has fcc structure and its body diagonal is 0.86 nm. When X-rays of wavelength 0.71 Å undergoes diffraction from (110) plane to produce second order maxima, calculate the glancing angle. **[GGSIPU, May 2017 (2.5 marks)]**

Hint : $4r = 0.86 \times 10^{-9}\,\text{m}, \quad r = 0.215 \times 10^{-9}\,\text{m}$;

$$d_{110} = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{2\sqrt{2} \times 0.215 \times 10^{-9}}{\sqrt{1^2+1^2+0}} = 0.43 \times 10^{-9}\,\text{m} \; ; \; 2d\sin\theta = n\lambda$$

$$\Rightarrow \quad \sin\theta = \frac{n\lambda}{2d} = \frac{2 \times (0.71 \times 10^{-10})}{0.86 \times 10^{-9}} = 0.65 \quad \Rightarrow \theta = \sin^{-1}\left(\frac{2 \times (0.71 \times 10^{-10})}{0.86 \times 10^{-9}}\right) = 9.49°$$

5.14 The first order maxima in Bragg's diffraction patterns by a crystal is observed at 28° when X-rays of wavelength of 0.32 nm are used. Find the distance between atomic planes.

Hint : $n = 1, \quad \theta = 28°, \quad \lambda = 0.32\,\text{nm}$

$$2d\sin\theta = n\lambda \quad \Rightarrow d = \frac{n\lambda}{2\sin\theta} = \frac{1 \times 0.32 \times 10^{-9}}{2 \times \sin 28°} = 0.34 \times 10^{-9} = 0.34\,\text{Å}$$

5.15 If X-rays of wavelength 0.5 Å are diffracted at an angle of 5° in the first order, what is the spacing between the adjacent planes of the crystal ? At what angle will second maximum occur ?

Hint : $2d\sin\theta = n\lambda \quad \Rightarrow d = \frac{n\lambda}{2\sin\theta} = 2.87\,\text{Å} \; ; \; 2d\sin\theta' = 2\lambda$

$$\Rightarrow \quad \theta' = \sin^{-1}\frac{\lambda}{d} = 10.03°$$

5.16 An electron initially at rest is accelerated through a p.d. of 5000 V. Calculate (*i*) momentum, (*ii*) de-Broglie wavelengths (*iii*) wave number. Also calculate the Bragg's angle for first order reflection from (111) plane which are 0.2 nm apart.

[GGSIPU, May 2014-reappear (6 marks)]

Hint :

(i) $p^2 = 2meV \quad \Rightarrow \quad p = \sqrt{2\times 9.1\times 10^{-31}\times 1.6\times 10^{-19}\times 5000} = 3.816\times 10^{-23}\,\text{kg m/s}$

(ii) $\lambda = \dfrac{h}{p} = \dfrac{6.623\times 10^{-34}}{3.186\times 10^{-23}} = 1.735\times 10^{-11} = 0.1735\ \text{Å}$

(iii) $k = \dfrac{2\pi}{\lambda} = \dfrac{2\times 3.14}{0.1735\times 10^{-10}} = 3.62\times 10^{11}\,/\text{m}$

(iv) $2d\sin\theta = n\lambda \quad \Rightarrow \quad \theta = \sin^{-1}\left(\dfrac{n\lambda}{2d}\right) = \sin^{-1}\left[\dfrac{1\times 0.01735}{0.2}\right] = 4.9°$

5.17 From the following data, calculate the wavelength of neutron beam and its speed. Spacing between successive (100) planes = 3.84Å ; grazing angle 30° ; order of the Bragg's reflection = 1

Hint : $2d\sin\theta = n\lambda \quad \Rightarrow \lambda = \dfrac{2d\sin\theta}{n} = \dfrac{2\times 2.84\times 10^{-10}\sin 30°}{1} = 3.84\times 10^{-10}\ \text{m}$

As per de-Broglie relation, $\dfrac{h}{mv} = \lambda \Rightarrow v = \dfrac{h}{m\lambda} = \dfrac{6.623\times 10^{-34}}{1.67\times 10^{-27}\times 3.84\times 10^{-10}} = 1.03\times 10^{3}\ \text{m/s}$

5.18 Calculate the glancing angles on the cube (100) of a rock salt ($a = 2.814$Å) corresponding to 2nd order diffraction maxima for X-rays of wavelength 0.710 Å.

Hint : $2d\sin\theta = n\lambda$ and $d_{hkl} = \dfrac{a}{\sqrt{h^2+k^2+l^2}}$

We have, $\dfrac{2a}{\sqrt{h^2+k^2+l^2}}\sin\theta = n\lambda$

$$\frac{2\times 2.814}{\sqrt{1}}\sin\theta = 2\times 0.710 \quad \Rightarrow \quad \sin\theta = 0.2523 \quad \Rightarrow \theta = 14°36'40''$$

5.19 For a certain *bcc* crystal the (110) planes have a separation 1.81 Å. These (110) planes are indicated with X-rays of wavelength 1.54 Å. How many order of Bragg's reflection can be ?

Hint : $n = \dfrac{2d\sin\theta}{\lambda} = \dfrac{2\times 1.81\times 10^{-10}\times\sin 90°}{1.54\times 10^{-10}} = 1.53 \approx 1.$

5.20 The powder of *BCC* structure crystal is studied with X-rays of wavelength 2 Å. The (210) reflection is observed at Bragg's angle 35°. Calculate lattice parameter.

Hint : $2d\sin\theta = n\lambda \quad \Rightarrow \quad d = \dfrac{n\lambda}{2\sin\theta}$

$$a = d\sqrt{h^2+k^2+l^2} = \frac{n\lambda}{2\sin\theta}\sqrt{h^2+k^2+l^2} = 3.89\ \text{Å}$$

5.21 Calculate the glancing angle of the (111) plane of simple cubic structure (atomic radius 1.404 Å) corresponding to second order diffraction maxima for X-rays of wavelength 1 Å.

[GGSIPU, May 2014 (3.5 marks)]

Hint : $2d\sin\theta = n\lambda,\ d_{hkl} = \dfrac{a}{\sqrt{h_2+k^2+l^2}} = \dfrac{2.808}{\sqrt{3}}\text{Å}$

Then $\theta = \sin^{-1}\left(\dfrac{n\lambda}{2d}\right) = \sin^{-1}\left(\dfrac{2\times 1\times 10^{-10}\times\sqrt{3}}{2.808\times 10^{-10}}\right) = \sin^{-1}(1.23)$

Note. Answers is wrong, it will be correct for $n = 1$