Q.1) In Certain BCC Structure the volume/unit cell is $61.72 \times 10^{-30} / m^3$. Calculate the lattice parameter.

Ans → ~~Total~~ Volume = $61.72 \times 10^{-30}\ m^3$

free volume = volume of unit cell − volume of atoms in unit cell

$$61.72 \times 10^{-30} = a^3 - n\frac{4}{3}\pi r^3$$

$$a^3 = 61.72 \times 10^{-30} + 2 \times \frac{4}{3}\pi \left(\frac{a\sqrt{3}}{4}\right)^3$$

$$a^3 = 61.72 \times 10^{-30} + \frac{8\pi}{3} \cdot \frac{a^3\, 3\sqrt{3}}{216 \times 4}$$

$$a^3 - \frac{\sqrt{3}\pi\, a^3}{8} = 61.72 \times 10^{-30}$$

$$a^3 - 0.68\, a^3 = 61.72 \times 10^{-30}$$

$$0.32\ \cancel{0.616}\ a^3 = 61.72 \times 10^{-30}$$

$$a^3 = \frac{61.72 \times 10^{-30}}{\cancel{0.616}\ 0.32}$$

$$a = \cancel{4.645\ A^0}\ 5.778\ A^0$$

Q.2) Identify the Crystal structure If its density is $9.6 \times 10^2\ kg/m^3$. Lattice Constant is $4.3 A^0$ and atomic weight is 23.

Ans → $\rho = 9.6 \times 10^2\ kg/m^3 = 9.6 \times 10^2 \times 10^3\ g/cm^3$

$M = 23$

$$\rho = \frac{nM}{N_A a^3}$$

$$9.6 \times 10^5 = \frac{n \times 23}{6.023 \times 10^{23} \times (4.3 \times 10^{-10})^3}$$

$$n = \frac{9.6 \times 10^5 \times 6.023 \times 10^{23} \times (4.3 \times 10^{-10})^3}{23}$$

$$n = 1.999$$

$$n = 2$$

$\therefore$ Crystal structure is BCC.

Q.3) Pottasium bromide has FCC crystal structure with lattice constant 6.6 A°. If it's molecular weight is 119, calculate it's density.

Ans → $a = 6.6\ A^0 = 6.6 \times 10^{-10}\ m$

$M = 119$

$n = 4$

$\rho = ?$

$$\rho = \frac{nM}{N_A a^3}$$

$$\rho = \frac{4 \times 119}{6.023 \times 10^{23} \times (6.6 \times 10^{-10})^3}$$

$$\rho = 2.75 \times 10^{-3}\ g/m^3$$

$$\rho = 2.75\ g/cm^3$$

Q.4) An elementral Crystal has a density of 8570 kg/m³ and packing fraction 0.68. Determine the mass of the atom, nearest neighbor distance is 2.86 A°.

Ans → $\rho = 8570 \ kg/m^3 = 8570 \times 10^{-3} \ g/cm^3$

$$\rho = \frac{n \cdot M}{N_A a^3}$$

$$8570 \times 10^{-3} = \frac{n \times M}{6.023 \times 10^{23} \times a^3}$$

Packing fraction is 0.68 thus the given crystal is in Bcc structure

$$n = 2$$

$$\text{neighbour distance} = \frac{a\sqrt{3}}{2}$$

$$2.86 \times 10^{-8} = \frac{a \times \sqrt{3}}{2}$$

$$\frac{2 \times 2.86 \times 10^{-8}}{\sqrt{3}} = a$$

$$3.30 \times 10^{-8} = a$$

$\therefore$ $$8570 \times 10^{-3} = \frac{2 \times M}{6.023 \times 10^{23} \times (3.3 \times 10^{-8})^3}$$

$$\frac{8570 \times 10^{-3} \times 6.023 \times 10^{23} \times (3.3 \times 10^{-8})^3}{2} = M$$

$$92.75 = M$$

Q.5) Lithium crystallizes in BCC structure. calculate the lattice constant, given that the atomic weight and density for Li are 6.94 and 530 kg/m³ respectively.

Ans → Given →

BCC ∴ $n = 2$

$M = 6.94$

$\rho = 530 \ kg/m^3 = 0.53 \ g/cm^3$

Solution →

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

$$0.53 = \frac{2 \times 6.94}{a^3 \times 6.023 \times 10^{23}}$$

$$a^3 = \frac{2 \times 6.94}{0.53 \times 6.023 \times 10^{23}}$$

$$a^3 = 43.48 \times 10^{-24}$$

$$a = 3.5 \ A^0$$

Q.6.) Silicon has same structure as that of diamond. If it's density is $2.33 \times 10^3 \ kg/m^3$ and atomic weight is 28.9. calculate the lattice constant and the atomic radius of silicon.

Ans →

$\rho = 2.33 \times 10^6 \ g/m^3$

$A = 28.9$

$n = 8$

Ans →
$$\rho = \frac{nM}{N_A a^3}$$

$$a^3 = \frac{nM}{N_A \rho} = \frac{8 \times 28.9}{6.023 \times 10^{23} \times 2.33 \times 10^3}$$

$$a^3 = 16.4747 \times 10^{-26}$$
$$a = 5.482 \times 10^{-9} \, m$$

Atomic radius of silicon $= \frac{a\sqrt{3}}{8} = 5.482 \times 10^{-9} \times \frac{\sqrt{3}}{8}$

$$r = 1.1864 \times 10^{-9} \, m$$

Q.7) Diamond structure has its cube edge 3.75 A^0 and atomic weight 12.01, calculate its density.

Ans → Given: $a = 3.75 \, A^0 = 3.75 \times 10^{-10} \, m$

$A = 12.01$

$\rho = ?$

$$\rho = \frac{nM}{N_A a^3}$$

$$\rho = \frac{8 \times 12.01}{6.023 \times 10^{23} \times (3.75 \times 10^{-10})^3}$$

$$\rho = 3 \times 10^{-3} \, g/m^3$$

$$\rho = 3 \, g/cm^3$$

Q.8). A crystal plane makes intercept at a length a, 2b, $-\frac{3}{2}c$. Find the miller indices of the planes

Ans → Given → Intercepts = $a, 2b, -\frac{3}{2}c$

Solution :-

let $A = [a, 2b, -\frac{3}{2}c]$

Resiprocal of $A = \left[\frac{1}{a}, \frac{1}{2}b, -\frac{2}{3}c\right]$

by taking LCM,

considering $a = b = c = -1$

$A = [6, -3, -4]$

Hence Miller Indices = (6, -3, -4)

Q.9) A certain Crystal has lattice constant of 4.24 A°, 10 A° and 3.66 A° on x, y, z axis respectively. Determine the miller indices of the lattice planes having intercepts of

(i) 2.12 A°, 10 A°, 1.83 A°

Ans → let A be the intercepts

$A = \left[\frac{2.12}{4.24} \quad \frac{10}{10} \quad \frac{3.66}{1.83}\right]$

$A = \left[\frac{1}{2}, 1, \frac{1}{2}\right]$

taking resiprocal

$A = [2 \quad 1 \quad 2]$

$\therefore$ Miller Indices $\equiv (2 \quad 1 \quad 2)$

(ii) $4.24 A^0$, ∞, $1.22 A^0$

let $B = \left[\frac{4.24}{4.24} \quad \frac{\infty}{10} \quad \frac{1.22}{3.66}\right]$

$B = \left[1 , \frac{\infty}{10} , \frac{1}{3}\right]$

Taking resiprocol

$B = \left[1 \quad \frac{10}{\infty} \quad 3\right]$

$B = [1 \quad 0 \quad 3]$

$\therefore$ Miller Indices $\equiv (1, 0, 3)$

Q.10) If the x-rays of Wavelength $1.549 A^0$ will be reflected from a crystal with interplanar spacing $4.255 A^0$ Calculate the smallest glancing angle and the highest Order of reflection that can be observed.

Ans → Wavelength (λ) = $1.549 A^0 = 1.549 \times 10^{-10} m$

Interplanar Spacing = $4.255 A^0 = 4.255 \times 10^{-10} m$

by Bragg's law,

$n = 1$

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

$$\sin\theta = \frac{n\lambda}{2d} = \frac{1 \times 1.549 \times 10^{-10}}{2 \times 4.225 \times 10^{-10}}$$

$\sin\theta = 0.183$

$\theta = \sin^{-1}(0.183)$

$\theta = 10.544^0$

for highest, $\sin\theta = 1$

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

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

$$n = \frac{2 \times 4.255 \times 10^{-10} \times 1}{1.549 \times 10^{-10}}$$

$n = 5.49$

i.e $n = 5$

$\therefore$ highest order is 5

Q.11) An x-ray beam of wavelength $0.71 A^0$ is diffracted by a FCC crystal of density 1.99×10^3 kg/m³. Calculate the interplanar spacing for [200] planes and the glancing angle for the 2nd order reflection from these planes if the molecular weight of the crystal is 74.6

Ans → wave length $(\lambda) = 0.71 A^0 = 0.71 \times 10^{-10}$ m

no. of atomic unit = 4 (fcc crystal)

Density $(\rho) = 1.99 \times 10^3$ kg/m³

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

$$a^3 = \frac{4 \times 74.6}{6.023 \times 10^{26} \times 1.99 \times 10^3}$$

$$a^3 = 2.4896 \times 10^{-30}$$

$$a = 6.29 \times 10^{-10}$$

$$a = 6.29\ A^0$$

As we know, $d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

$h = 2,\ k = 0,\ l = 0$

$$d = \frac{6.29 \times 10^{-10}}{\sqrt{2^2 + 0^2 + 0^2}}$$

$$d = 3.14 \times 10^{-10}$$

$$d = 3.14\ A^0$$

Now

for glancing angle 2^{nd} order

$\therefore n = 2$

By bragg's law

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

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

$$\sin\theta = 0.2251$$
$$\theta = 13.04^0$$

Q.12) In comparing the wavelengths of two monochromatic x-ray lines it is found that line A gives 1st order Bragg's maximum at a glancing angle of 30° to the smooth face of crystal line B of known wavelength of 0.97 A° gives 3rd order reflection maximum at a glancing angle of 60° with the same ~~fre~~ face of crystal. find the wavelength of line A

Ans →

for line A
$n_1 = 1$
$\theta_1 = 30^0$

for line B
$n_2 = 3$
$\theta_2 = 60^0$

$$2d\sin\theta_1 = n_1\lambda_1 \quad \text{--- (i)}$$

$$2d\sin\theta_2 = n_2\lambda_2 \quad \text{--- (ii)}$$

$$\therefore \frac{\sin\theta_1}{\sin\theta_2} = \frac{n_1}{n_2} = \frac{\lambda_1}{\lambda_2}$$

$$\therefore \lambda_1 = \lambda_2 \times \frac{\sin\theta_1}{\sin\theta_2} \times \frac{n_2}{n_1}$$

$$\lambda_1 = 0.97\times10^{-10} \times \frac{\sin 30}{\sin 60} \times \frac{3}{1}$$

$$\lambda_1 = 1.68\times10^{-10}m$$

$$\lambda_1 = 1.68\ A^0$$