Assignment-4

PHYSICS-II

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Q.1 Define lattice points, Bravais lattice, primitive cell, coordination number and atomic packing fraction. Calculate packing fraction for SC, BCC and FCC structures.

Answer- Lattice Point

It is the position in the unit cell or in a crystal where the probability of finding an atom is the highest.

Bravais Lattice

When the discrete points are atoms, ions or polymer (strings of solid matter), the Bravais Lattice concept is used to formally define a crystalline arrangement & its frontiers.

Primitive Cell

The smallest possible unit cell of a lattice, have lattice points at each of its eight vertices only.

Coordination Number

The number of atoms or ions immediately surrounding a central atom in a complex crystal.

Atomic Packing Fraction

It is the percentage of total space filled by the particles.

$$ATF = \frac{\text{volume occupied by all spheres in unit cell}}{\text{Total volume}} \times 100$$

Simple Cubic -

$a = 2r$

No. of spheres per unit cell $= \frac{1}{8} \times 8 = 1$

Atomic Packing Fraction $= \frac{4/3\,\pi r^3}{8r^3} = 0.524$

$\therefore$ Percentage of ATF $= 52.4\,\%$

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Body centred cubic unit cell (BCC) -

No. of spheres = 2 ; $a = \frac{4r}{\sqrt{3}}$

Atomic Packing fraction $= \frac{2\times\frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} \times 100$

$= \frac{2\times \cancel{4}}{\cancel{3}} \cdot \pi \times \cancel{100}^{50} \times \frac{\cancel{3}}{\cancel{16}}$

$= 68\%$

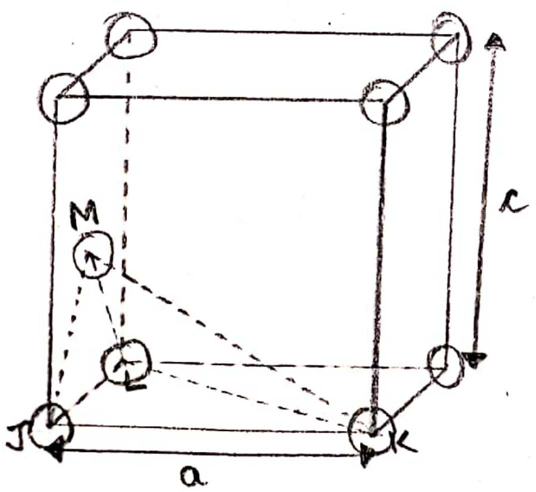
Face centered cubic unit cell -

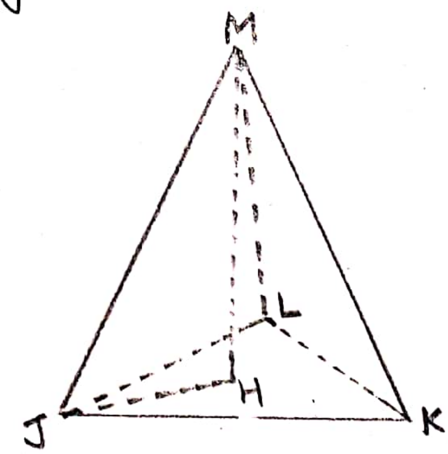
No. of spheres = 4 ; $a = 4/\sqrt{2}\, r$

Atomic Packing fraction $= \frac{4\times\frac{4}{3}\pi r^3 \times 2}{4\times 4 \cdot r^3} = 74\%$

$= 74\%$

Q.2: Calculation of (c/a) ratio and packing fraction for an ideal Hexagonal closed packing (hcp) structure.





The atom at point M is midway between the top and bottom faces of the unit cell.

i.e. $\overline{MH} = c/2$

Also, $\overline{JM} = \overline{JK} = 2R = a$, R is atomic radius

From triangle JHM →

$(\overline{JM})^2 = (\overline{JH})^2 + (\overline{MH})^2$

$a^2 = (\overline{JH})^2 + (c/2)^2$ ..... (1)

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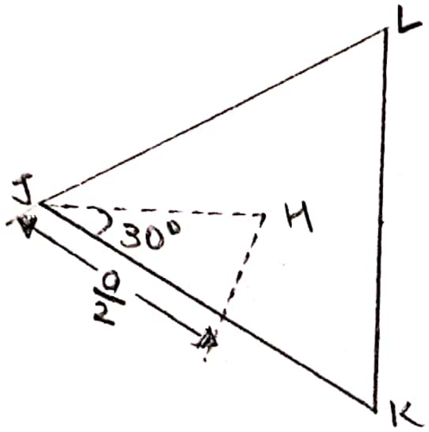
Now, determining JH by triangle JKL →



$$\cos 30° = \frac{a/2}{JH} = \frac{\sqrt{3}}{2}$$

and $JH = \frac{a}{\sqrt{3}}$

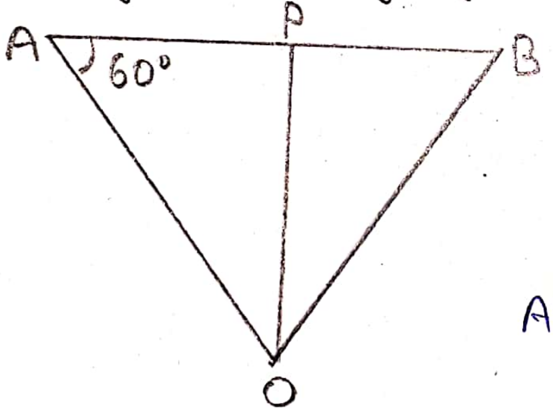
Substituting value for JH in eqn (1) we get -

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

Now, solving for $\left(\frac{c}{a}\right)$ →

$$\frac{c}{a} = \sqrt{\frac{8}{3}} = \boxed{1.633}$$

Packing Efficiency of HCP-



Area of $\Delta OAB = 0.5 \times AB \times OP$

$= \frac{1}{2} \times a \times a \sin 60°$

$= \frac{\sqrt{3}}{4} a^2$

Area of Basal plane $= 6 \times \frac{\sqrt{3}}{4} a^2$

$= \frac{3\sqrt{3}}{2} a^2$

Given: $a = 2R$, $\frac{c}{a} = 1.633 \Rightarrow c = 1.63a = 3.26R$

Volume of unit cell →

$V_c = c \times$ base area

$= 3.26R \times 10.392R^2 = 33.878R^3$

Atomic Packing Fraction $= \frac{8\pi R^3}{33.878} = 0.74$

$= 0.74$

∴ Percentage of ATF $= \boxed{74\%}$

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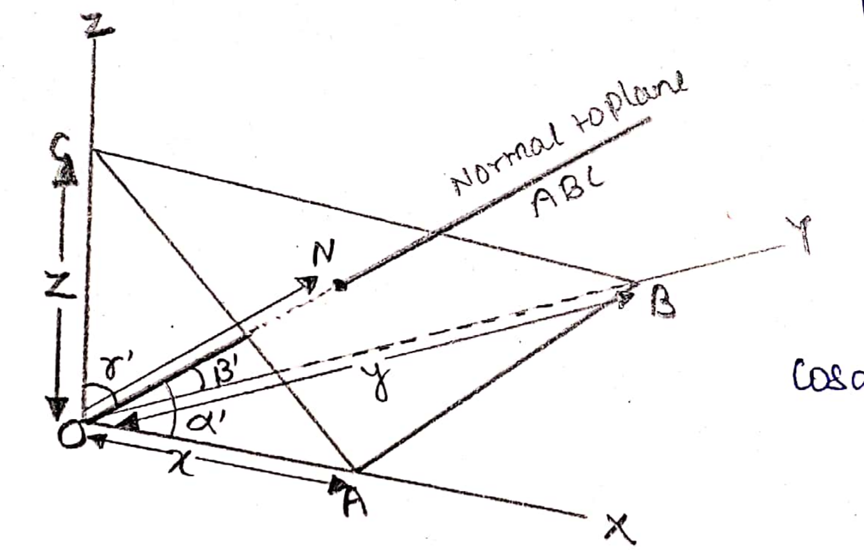
Q.3: Explain Miller Indices and how Miller Indices are derived. Derive an expression for inter planar spacing of a crystal in terms of Miller Indices.

Answer– Miller Indices form a notation system in crystallography for planes in Bravais lattices. In particular, a family of lattice planes is determined by three integers h, k and l.

Miller Indices are determined by intersection of plane with the axes. The reciprocal of these intercepts are completed and fractions are cleared to give h, k and l.

Derivation:



Intercepts of plane on the three axes are:

$OA = a/h \qquad OB = a/k$

$OC = a/l$

$a \rightarrow$ length of cube edge

$\cos\alpha' = \frac{dh}{a} \qquad \cos\beta' = \frac{dk}{a}$

$\cos\gamma' = \frac{dl}{a}$

$ON = (x^2+y^2+z^2)^{1/2}$

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

Also, $[\cos^2\alpha' + \cos^2\beta' + \cos^2\gamma' = 1] \rightarrow$ for orthogonal coordinates

Substituting the respective values $\rightarrow$

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

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

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

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