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Crystallography

Crystal : | **Amorphous**

regular, periodic arrangement
↓
atoms / molecules / ions

1) shape of size
2) anisotropic → directly dependent
3) BP & MP fixed
4) Homogeneous chemical comp.

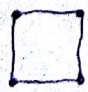
Crystal → single crystal
Crystal → poly crystal

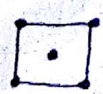
Basis + Lattice = Crystal

L.C

Unit cell : translation

Smallest geometric fig. by translating which in a particular direction the whole crystal can be achieved is known as unit cell.

 → primitive unit cell

 → non primitive unit cell

All primitive cell are unit cell but all unit cell are not primitive cell.

In 2D : 4 types of Bravias lattices.

2D - 4 sys → 5 types

3D - 7 sys → 14 types.

Co-ordination No : Equidistant nearest neighbour to a particular atom.

Simple cubic : 6

BCC : 8

FCC : 12

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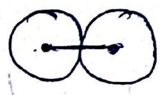
Relation b/w atomic radius and lattice const.

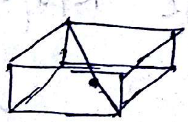
Simple cubic : $2r = a$

$r = a/2$



BCC : $4r = \sqrt{3}a$

$r = \sqrt{3}/4\, a$



FCC : $4r = \sqrt{2}a$

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

Atomic Packing fraction

$$\frac{\text{Vol. of total no. of atoms inside unit cell}}{\text{Vol. of unit cell.}}$$

$$SC : \frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{a^3} = 52.3\%$$

$$BCC : \frac{2 \cdot \frac{4}{3} \cdot \pi\left(\frac{\sqrt{3}}{4}a\right)^3}{a^3} = 68\%$$

$$FCC : \frac{4 \times \frac{4}{3}\pi\left(\frac{a}{2\sqrt{2}}\right)^3}{a^3} = 74\%$$

Relation b/w lattice const. and the density of the material.

L.c $= a$ $\quad \rho =$ density

vol $= a^3$.

Mass of unit cell $= \rho a^3$

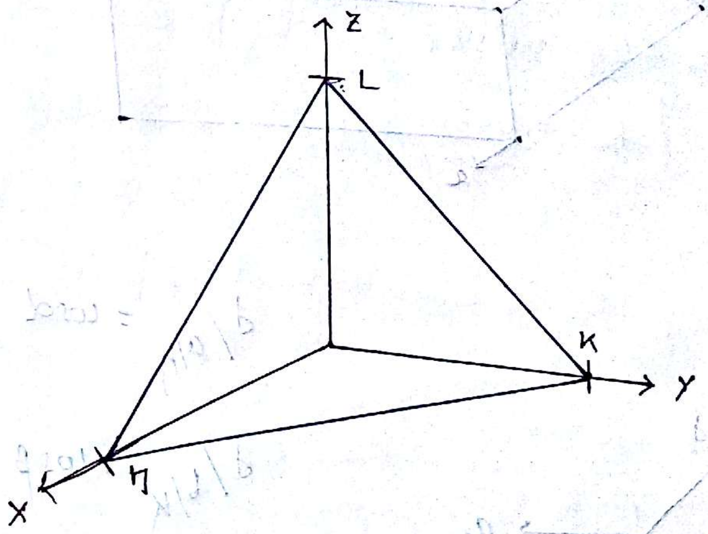
If M is Molecular weight then mass of one atom M/N ; $N =$ Avg no.

If there is n no. of eff atoms in unit cell then mass of unit cell $= \frac{M}{N} \cdot n$

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

$$\Rightarrow a = \left(\frac{M}{N} \cdot \frac{n}{\rho} \right)^{1/3}$$

Miller indices :



Steps :

1) Choice of origin.

2) Cal. the intercept in 3 diff axes (X, Y, Z dirn.)

3) Then take the reciprocal of the intercepts.

(e.g $1/h$, $1/k$, $1/l$)

4) Take the LCM of the intercepts h, k, l.

5) Convert $\frac{1}{H} \times LCM$, $\frac{1}{K} \times LCM$, $\frac{1}{L} \times LCM$

$\Rightarrow (H, K, L) \rightarrow$ (say) //.

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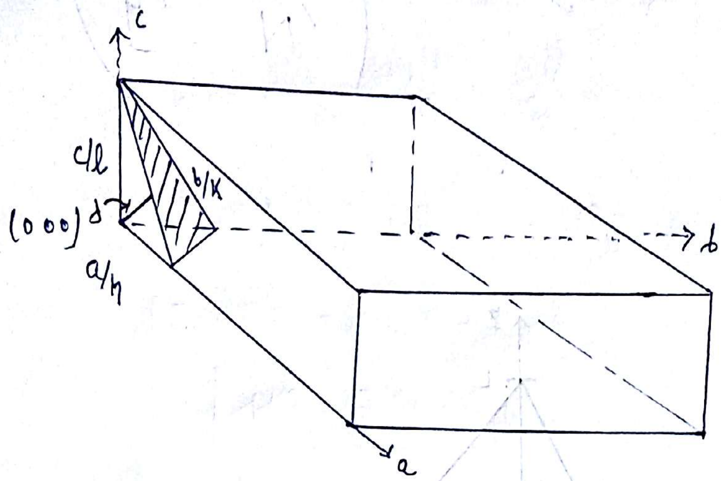
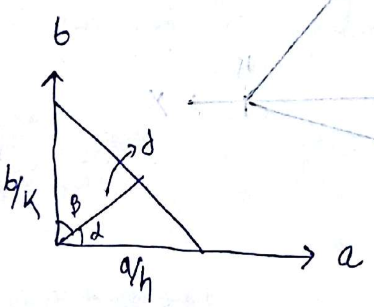
Interplanar spacing / dist b/w two adjacent planes.





$$\frac{d}{a/h} = \cos\alpha$$

$$\frac{d}{b/K} = \cos\beta$$

$$\frac{d}{c/l} = \cos\gamma$$

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

$$\frac{d^2}{(a/h)^2} + \frac{d^2}{(b/K)^2} + \frac{d^2}{(c/l)^2} = 1$$

$$d^2\left[\frac{1}{(a/h)^2} + \frac{1}{(b/K)^2} + \frac{1}{(c/l)^2}\right] = 1$$

or $$d = \sqrt{\frac{1}{h^2/a^2 + K^2/b^2 + l^2/c^2}}$$

Case I: Simple cubic

$a = b = c = a$

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

Q) Find the M.I of a plane that makes intercept of 3Å, 4Å, 5Å respectively on the co-od axis of an orthorombic cell with $a:b:c = 1:2:5$

Intercept : $3/1$, $4/2$, $5/5$

$= 3, 2, 1$

Reciprocal $= 1/3, 1/2, 1/1$

LCM of reciprocal : 6

$\therefore$ MI : 2, 3, 6

Q) For an element bragg's first order reflection occur at $\sin\theta = .225, .317, .389$ for reflection from (1,0,0), (1,1,0), (1,1,1) plane respectively. The wavelength of X-ray used is .154nm. Show that the unit cell is cubic and also calculate the length of side of unit length.

$\Rightarrow$ $n\lambda = 2d_1\sin\theta$ $\qquad$ $n\lambda = 2d_2\sin\theta$

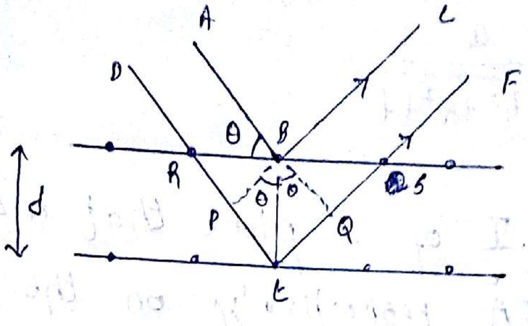
$\Rightarrow$ $d_1 = \dfrac{.154\times10^{-9}}{2\times.225}$ $\qquad$ $d_2 = \dfrac{.154\times10^{-9}}{2\times.317}$ $\qquad$ $d_3 = \dfrac{.154\times10^{-9}}{2\times.389}$

$= .342$ $\qquad$ $= .242$ $\qquad$ $= .198$

$a = d_1 = .342$ nm $\qquad$ $b = .342$ nm $\qquad$ $c = .342$ nm

X-rays

Bragg's law



$$PE + EQ = d\sin\theta + d\sin\theta$$

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

Determination of Lattice Constant

Bragg's X-ray spectrometer

for order $n=1$

$$\therefore \frac{1}{d} = \frac{2\sin\theta}{\lambda}$$

Note:

$$\frac{1}{d_{100}} : \frac{1}{d_{110}} : \frac{1}{d_{111}} = \sin\theta_1 : \sin\theta_2 : \sin\theta_3$$

Simple cubic : $\sqrt{1} : \sqrt{2} : \sqrt{3}$

BCC : $1 : 1/\sqrt{2} \; 1 : \sqrt{3}$

FCC : $1 : \sqrt{2} : \sqrt{3}/2$