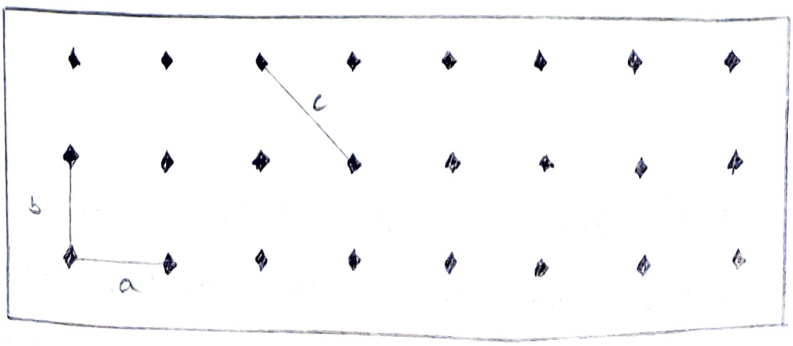
Module - I : Crystal Structures

→ **Amorphous** : In a solid, if atoms are arranged irregularly and the environment of each item is not the same then its called amorphous. Inter-atomic distance is different. Its also called non-crystalline.

→ **Crystals** : In a solid, if atoms are arranged regularly in 3d and if the environment of each atom is same then its called a crystalline structure. Inter-atomic distance is constant. crystalline type includes mono- and poly-crystalline structure.

→ **Space lattice** : Infinite array of points in three dimensional in which every point has the surroundings identical to that of any other point in the array.

- Each lattice point in space represents an atom.
- Atomic arrangement in a crystal is called crystal structure.



Repeated translations of $\vec{a}$ and $\vec{b}$ generates a square array, magnitude of a and b = unity, angle b/w a and b is 90°. $\vec{a}$ and $\vec{b}$ are called fundamental translation vectors.

Let n_1 be the no. of translations of magnitude $\vec{a}$ in direction x-axis, then its translation vetor $\vec{T_1} = n_1 \vec{a}$.

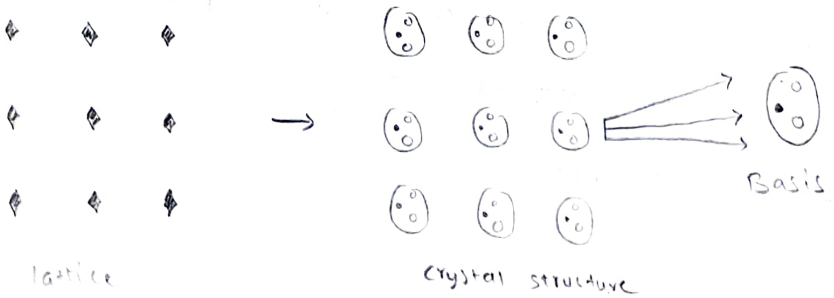
Let n_2 be the no. of translations of magnitude $\vec{b}$ in direction of y-axis, then its translation vector $\vec{T_2} = n_2 \vec{b}$.

Resultant translation vector, $\vec{T} = \vec{T_1} + \vec{T_2}$.

$\vec{T} = n_1\vec{a} + n_2\vec{b}$. In 3D, $\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$.

→ Basis : Assembly of atoms or molecules or ions in identical composition, arrangement and orientation present at every ~~point~~ lattice point in the space lattice, thereby forming the crystal structure. [14 sept]

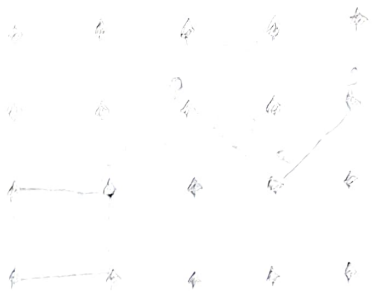
Lattice + Basis = Crystal Structure



→ Unit cell : Smallest geometrical figure which is repeated to give the actual crystal struc.

The choice of a unit cell may be of different types.

2D unit cell is called a parallelogram whereas in 3D, its called a parallelepiped.



- Primitive cell – simple unit cell
- multiple cell – contains more than one lattice point. In the fig, PQRS has points at corners and centre.

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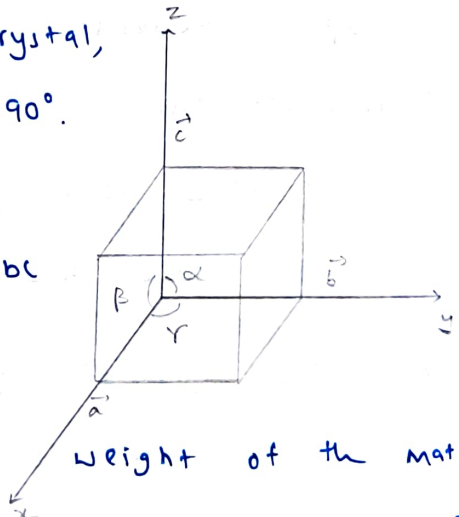
* Lattice Parameters

$\vec{a}, \vec{b}, \vec{c}$ are 3 vectors defined along 3 axes.

α, β, γ are 3 interfacial angles b/w ($\vec{b}$ and $\vec{c}$), ($\vec{c}$ and $\vec{a}$) and ($\vec{a}$ and $\vec{b}$) respectively.

A crystal structure is based on $\vec{a}, \vec{b}, \vec{c}$ and α, β, γ.

If we consider a cubic crystal, then $\vec{a} = \vec{b} = \vec{c}$ and $\alpha = \beta = \gamma = 90°$.



Let ρ be the density of the molecules and volume $V = abc$

$V = a^3$. $\boxed{\text{Mass} = \rho . a^3}$ —— (1)

Let 'M' be the molecular weight of the material

N_a be the avagadro's number $= 6.023 \times 10^{23}$/mol

Mass of each molecule $= \frac{M}{N_a}$. If there are 'n' no. of atoms or molecules in unit cell,

$\therefore \boxed{\text{mass of unit cell} = \frac{nM}{N_a}}$ - (2)

from equations ① and ②,

$$\rho a^3 = \frac{nM}{N_a} \Rightarrow a^3 = \frac{nM}{\rho N_a} \Rightarrow \boxed{a = \left[\frac{nM}{\rho N_a}\right]^{1/3}}$$

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* Crystal Lattice [15 Sept]

1. **Bravais lattice**

All atoms are the same kind.

All lattice points are equivalent.

2. **Non-Bravais lattice**

Atoms are of different kinds.

Some atoms lattice points are not equivalent.

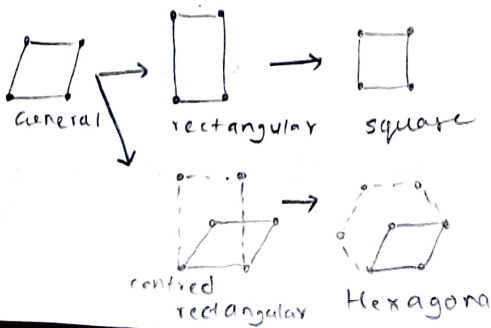
→ Bravais lattice

3D space generated by repeated translation of 3 non-coplanar vectors a, b, c. There are 14 distinguishable ways of arranging lattice points in 3D space. These are called Bravais Lattices.

14 possible types of space lattice are categorised in seven different crystal systems.

1 - Triclinic
2 - Monoclinic
1 - Hexagonal
1 - Trigonal
4 - orthorhombic
2 - tetragonal
3 - cubic

In the case of 2D, there are five bravais lattices.



→ 4 types of unit cells :

P = Primitive cell

I = Body centred cubic unit cell

F = face centred cubic unit cell

C = Side centred cubic unit cell

Primitive

Body centred

side centred

face centred

A unit cell consists of only one full atom.

A primitive cell got points or atoms only at corners.

If a unit cell containst more than one atom, then it is not a primitive cell.

→ Seven Crystal Systems

1. Cubic (3)

$a = b = c$

$\alpha = \beta = \gamma = 90°$

2. Tetragonal (2)

$a = b \neq c$

$\alpha = \beta = \gamma = 90°$

3. Orthorhombic (4)

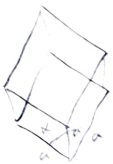
$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$

4. Rhombohedral (1)

$a = b = c$

$\alpha = \beta = \gamma \neq 90°$



5. Hexagonal (1)

$a = b \neq c$

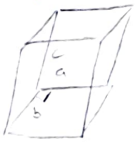
$\alpha = \beta = 90°$

$\gamma = 120°$

6. Monoclinic (2)

$a \neq b \neq c$

$\alpha = \beta = 90° \neq \gamma$



7. Triclinic (1)

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90°$

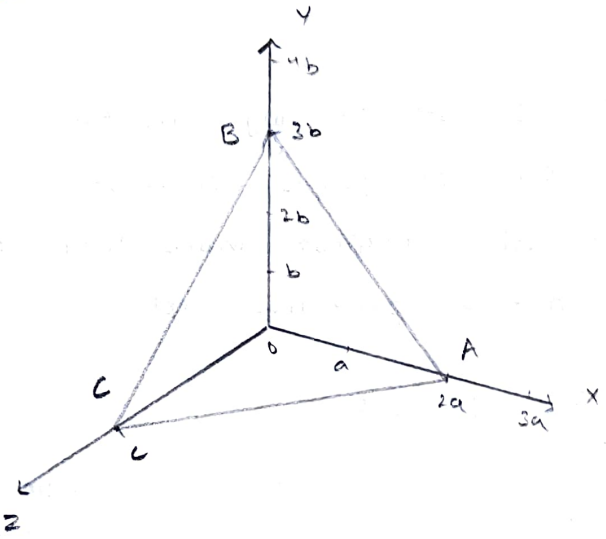
* Miller Indices

10 oct

Plane makes intercepts 2a, 3b, c along x, y, z directions. reciprocals of the intercepts are cleared by fractions upon multiplication with LCM.

$\frac{1}{2} \times 6 \;,\; \frac{1}{3} \times 6 \;,\; \frac{1}{1} \times 6 \;\Rightarrow\; 3, 2, 6$

∴ The miller indices are (3, 2, 6)



→ Procedure for finding miller indices.

Step 1: Determine the intercepts of the plane along the axis

Step 2: Determine the reciprocals of these numbers.

Step 3: Find the LCM and multiply each by this LCM.

Step 4: Write it in paranthesis in the form (h, k, l)

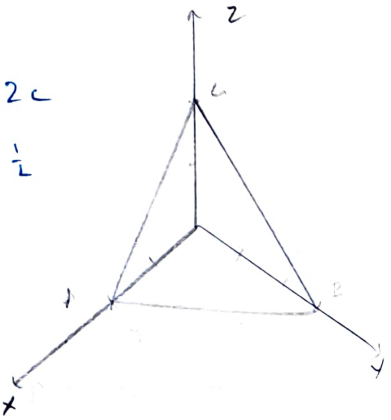
Example –

Step: 1 intercepts are 2a, 3b & 2c

Step: 2 reciprocals are $\frac{1}{2}, \frac{1}{3}, \frac{1}{2}$

Step 3: LCM - 6 ∴ ⇒ 3, 2, 3

Step 4: Miller indices (3, 2, 3)



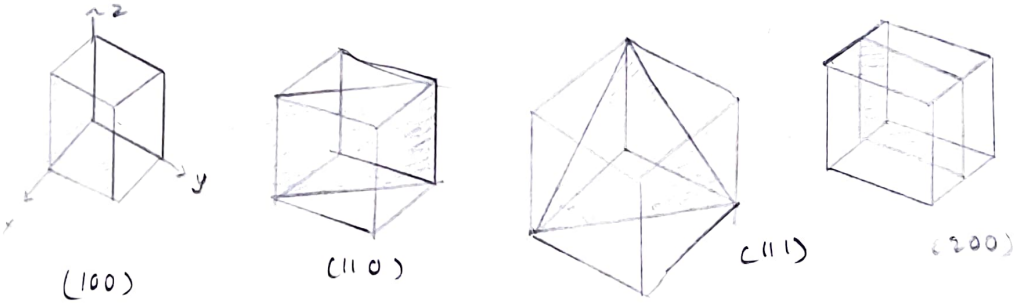
→ Important features of Miller Indices :

All the parallel and equidistant planes have the same (h,k,l) values. So, Miller Indices (h,k,l) defines a set of paralled planes.

If any plane is parallel to one of the axes, then its intercept may be taken as infinity.

The plane passing through the origin is defined in terms of a parallel planes having non-zero intercept.

If the miller Indices of two planes are having the same ratio. for example (844), (422) and (211) are three planes, and then the planes are parallel to eachother.



(100) (110) (111) (200)

→ Miller conventions

Generally a notation allows for distinction between a specific direction or plane or families of such

[] - to identify specific direction

<> - to identify a family of equivalent directions

() - to identify a family of equivalent planes

{} - to identify a family of equivalent planes

→ Coordination number

Defined as the number of equidistant nearest neighbours that an atom has in a given structure. More closely packed structures greater coordination number.

Simply, coordination number of an atom number of atoms which it touches.

Coordination nos. of :

SC - 6 , BCC - 8 , FCC - 12 , HCP - 12 , diamond - 4

→ Lattice points per cell

It represents the no. of atoms per unit cell.

SC - 1 , BCC - 2 , FCC - 4 , HCP - 6 , diamond - 8

→ Nearest neighbour distance

distance between the centers of two nearest neighbour atoms.

formula : $d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$

for cubic system $a = b = c$,

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

SC - a BCC - $\frac{\sqrt{3}a}{2}$ FCC - $\frac{a}{\sqrt{2}}$ HCP - a diamond - $\frac{\sqrt{3}a}{4}$

BCC

no. of atoms - 2

Atomic radius - $\frac{\sqrt{3}a}{4}$

Coordination no - 8

APF - $\frac{3\pi}{8}$ or 0.68