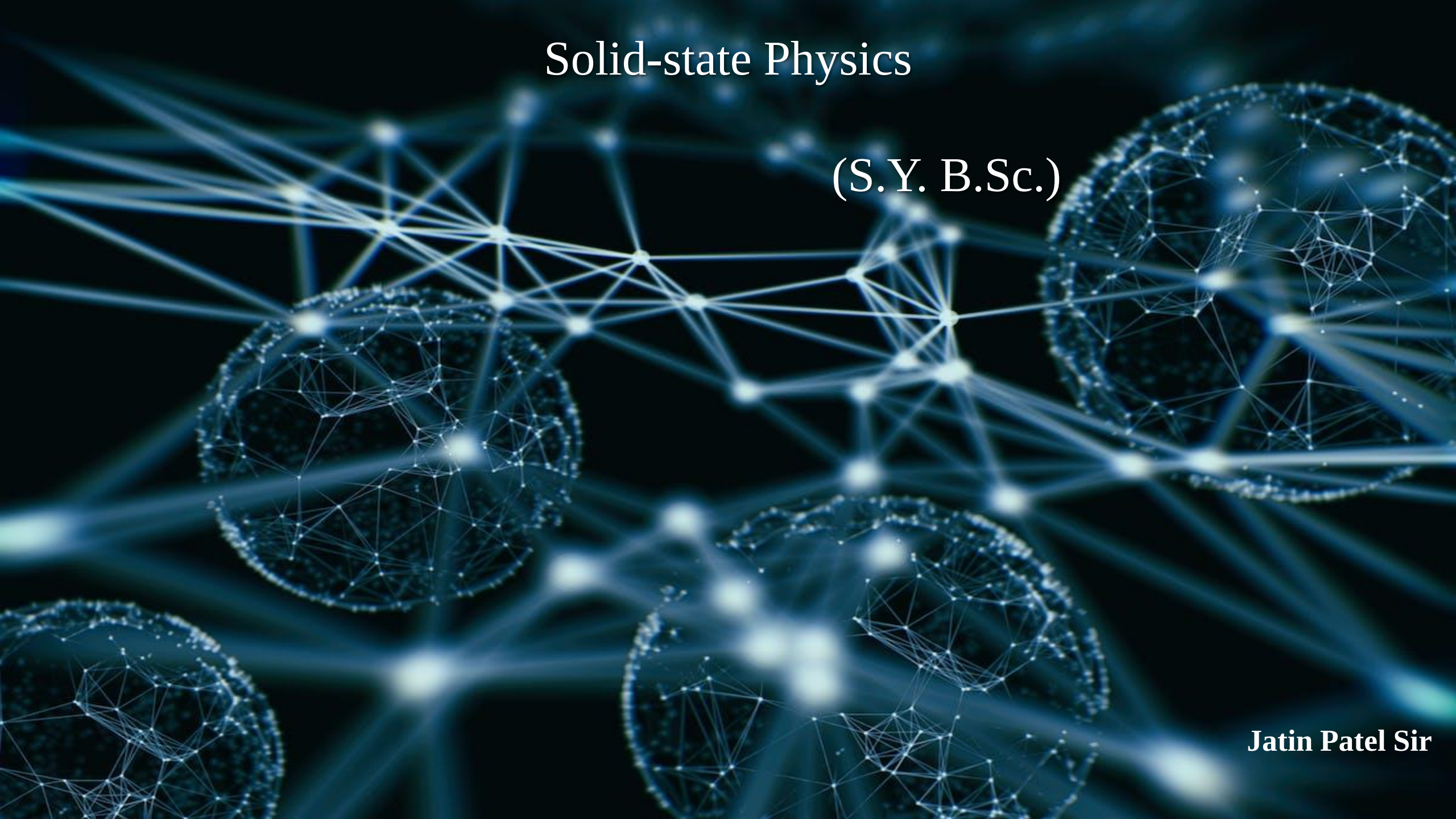


Solid-state Physics

(S.Y. B.Sc.)

Jatin Patel Sir

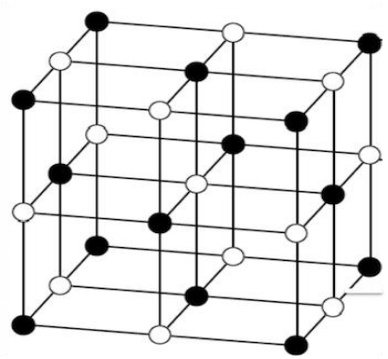
Solid-state Physics

- ✓ Condensed-matter physics is the study of substances in their solid state. This includes the investigation of both crystalline solids in which the atoms are positioned on a repeating three-dimensional lattice, such as diamond, and amorphous materials in which atomic position is more irregular, like in glass.

- ✓ In a single crystalline solid, the regular order extends over the entire crystal. In a polycrystalline solid, however, the regular order only exists over a small region of the crystal, ranging from a few hundred angstroms to a few centimeters.

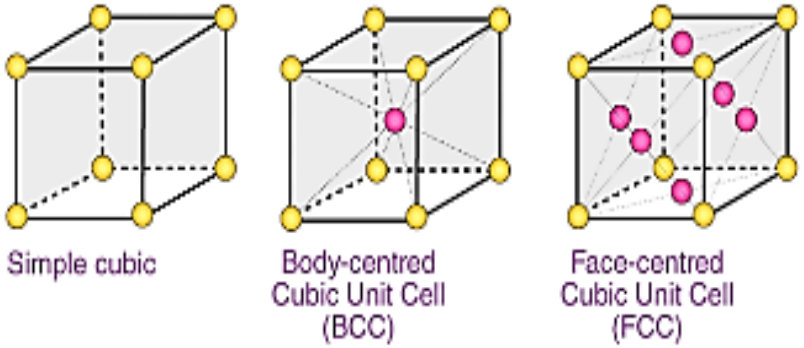
- ✓ A crystal lattice is the regular three-dimensional arrangement of identical points in space that represents how the atoms, ions, and molecules of a crystal are structured.

- ✓ Unit cell is the smallest component of a crystal lattice, which when repeated in different orientations creates the entire crystal lattice.

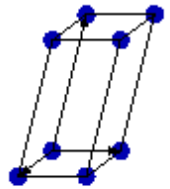
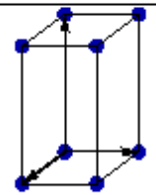
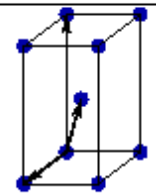
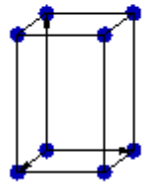
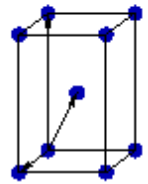
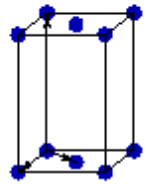
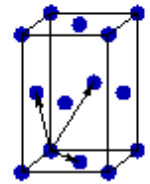
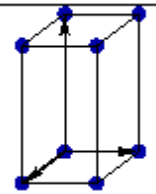
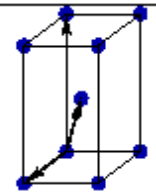
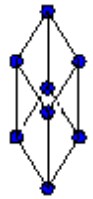
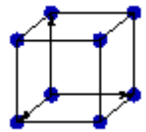
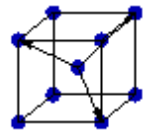
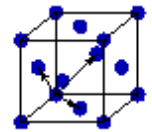
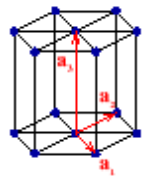


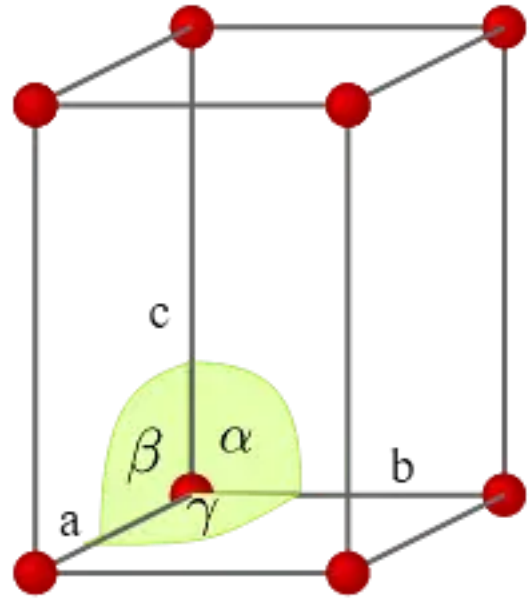
• The unit cell, or building block of a crystal, is the smallest repeating unit in the crystal lattice and the primitive cell is a unit cell corresponding to a single lattice point, it is the smallest possible unit cell.

• It can be of different types: Simple cubic (S.C.), body-centered cubic (B.C.C.), or face-centered cubic (F.C.C.)



- The basis is the arrangement of atoms associated with each lattice point.
- Lattice + Basis = Crystal
- Bravais Lattice is a system of arrangement of atoms inside a unit cell observed by Auguste Bravais. There are a total of 7 Crystal System which has different possible combinations leading to 14 possible Bravais lattices.

Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				



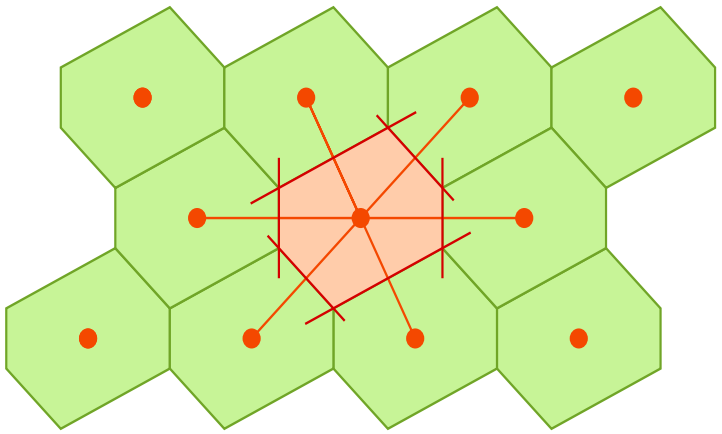
primitive

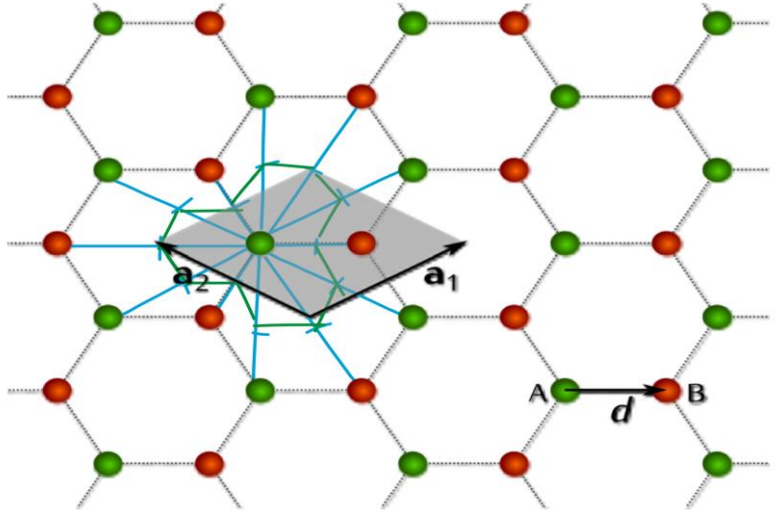
- Miller Indices are the mathematical representation of the crystal planes. Miller indices, group of three numbers that indicates the orientation of a plane or set of parallel planes of atoms in a crystal.

- For example, a plane parallel to two axes but cutting the third axis at a length equal to one edge of a unit cell has Miller indices of (100), (010), or (001), depending upon the axis cut; and a plane cutting all three axes at lengths equal to the edges of a unit cell has Miller indices of (111). It is denoted by (h k l).

- If you have h+k+l = Even number , it is BCC. However if h, k, & l are all even, it is FCC, all even numbers added together give an even number.

- The Wigner-Seitz cell is obtained by connecting a lattice point to all other lattice points and drawing the planes perpendicular to these connecting lines and passing through their midpoints





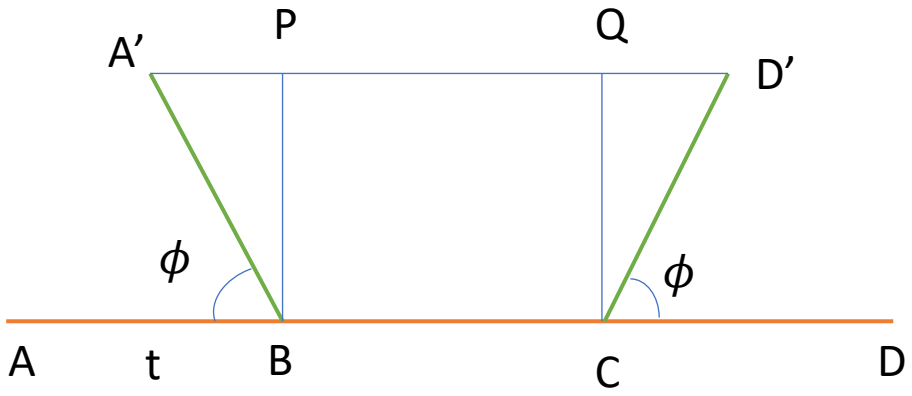
- Symmetry Operations :

✓ Symmetry is used to determine the internal crystal structure of a crystal.

✓ If the shape of the crystal after the process (Rotations) looks similar to the above, then it is symmetry operations.

✓ the shape of the crystal after the process $T = n_1 a + n_2 b + n_3 c$ looks similar to the above, then it is Translational symmetry operations. Where n_1, n_2, n_3 = Integer Numbers and a,b,c = Primitive fundamental vector

✓ the shape of the crystal after the rotation $\theta = \frac{2\pi}{n}$ looks similar to the above, then it is rotational symmetry operations. and rotational axis is called Fold denoted by n.



- 5 Fold not possible

m = 0, $\cos\phi = \frac{-1}{2}$, $\phi = 120^0$, $n = \frac{360^0}{\phi} = 3$

m = 1, $\cos\phi = 0$, $\phi = 90^0$, $n = \frac{360^0}{\phi} = 4$

m = -1, $\cos\phi = -1$, $\phi = 180^0$, $n = \frac{360^0}{\phi} = 2$

m = 2, $\cos\phi = \frac{1}{2}$, $\phi = 60^0$, $n = \frac{360^0}{\phi} = 6$

m = -2, $\cos\phi = \frac{-3}{2}$, Not in cosine function

m = 3, $\cos\phi = 1$, $\phi = 360^0$, $n = \frac{360^0}{\phi} = 1$

m = 4, $\cos\phi = \frac{3}{2}$, Not in cosine function

A'D' = mt, m = integer

A'D' = A'P + PQ + QD' = mt
A'P + t + QD' = mt

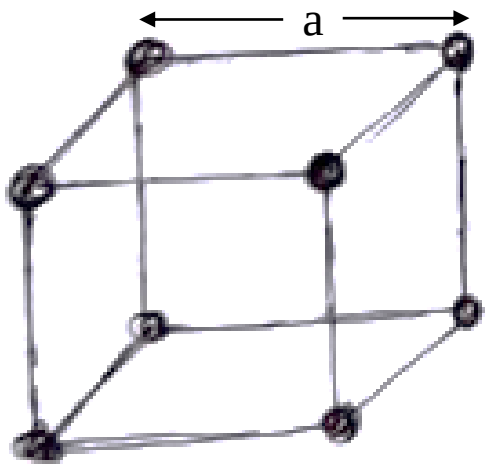
Angle PBA' = $90^0 - \phi$
$\sin(90^0 - \phi) = \frac{A'P}{A'B}$
$\cos\phi = \frac{A'P}{t}$
A'P = $t\cos\phi$, lly, QD' = $t\cos\phi$

$t\cos\phi + t + t\cos\phi = mt$
$m = 2\cos\phi + 1$

$\cos\phi = \frac{m-1}{2}$

n = 1 fold then it is Identity axis.
n = 2 fold then it is diad axis.
n = 3 fold then it is triad axis.
n = 4 fold then it is tetrad axis.
n = 6 fold then it is hexad axis.

✓ **Simple Cubic -**



- Vertex – 08, Face – 00, In - 00
- Atoms per Unit cell, $N = \frac{N_c}{8} + \frac{N_F}{2} + N_i$

$$N = 1$$

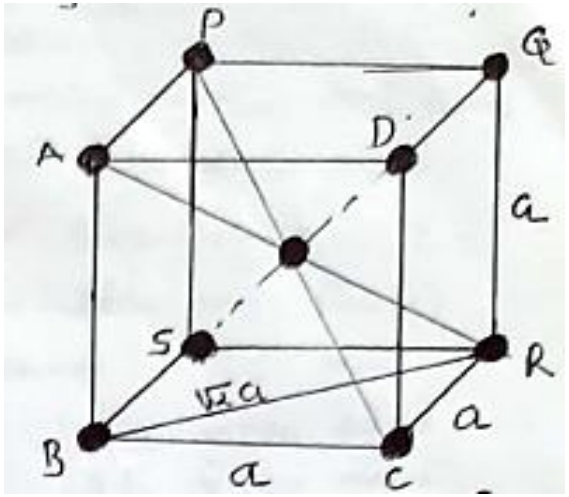
✓ a = 2r ; Where, r = Radius of Sphere (Atom)

$$r = \frac{a}{2}$$

✓ Packing Fraction = $\frac{Volume\ of\ an\ Atom}{Volume\ of\ unitcell} = \frac{1\ X\ \frac{4}{3}\pi r^3}{a^3} = 0.52$

❖ 52 % Atoms and 48 % Space in S.C. Unit cell

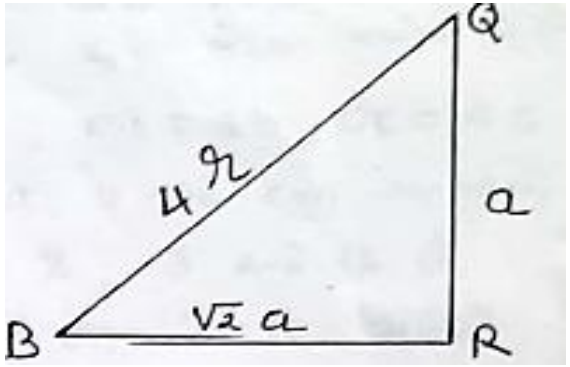
✓ Body Centered Cubic -



- Vertex – 08, Face – 00, In - 01
- Atoms per Unit cell, $N = \frac{N_c}{8} + \frac{N_F}{2} + N_i$

$$N = 2$$

✓ Surface Diagonal - $\sqrt{2}a$, Diagonal in Unit cell – 4r, Distance between two consecutive Lattice point - a



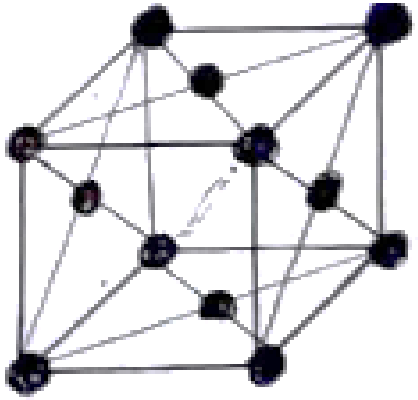
$$4r^2 = a^2 + \left(\sqrt{2}a\right)^2$$

$$r = \frac{\sqrt{3}}{4}a$$

✓ Packing Fraction = $\frac{Volume\ of\ an\ Atom}{Volume\ of\ unitcell} = \frac{2 \times \frac{4}{3}\pi r^3}{a^3} = 0.68$

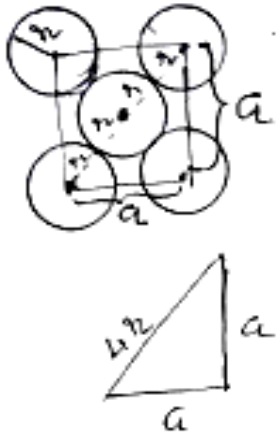
❖ 68 % Atoms and 32 % Space in B.C.C. Unit cell

✓ Face Centered Cubic -



- Vertex – 08, Face – 06, In - 00
- Atoms per Unit cell, $N = \frac{N_c}{8} + \frac{N_F}{2} + N_i$

N = 4



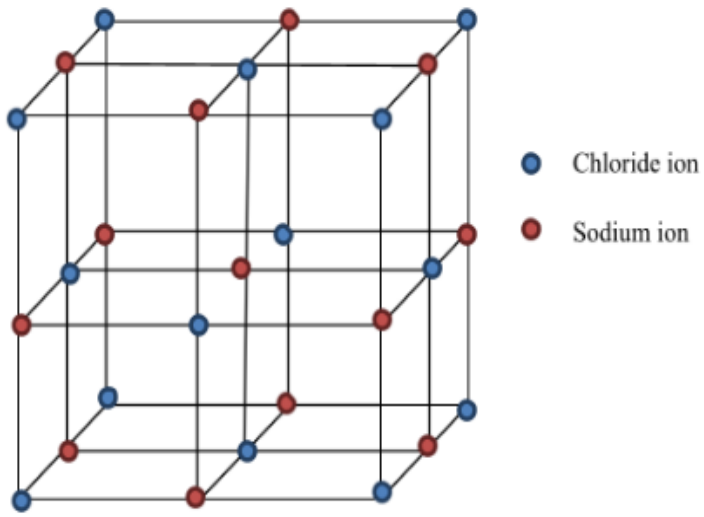
$4r^2 = a^2 + a^2$

$r = \frac{\sqrt{2}}{4}\, a$

✓ Packing Fraction = $\frac{Volume\ of\ an\ Atom}{Volume\ of\ unitcell} = \frac{4\ X\ \frac{4}{3}\pi r^3}{a^3} = 0.74$

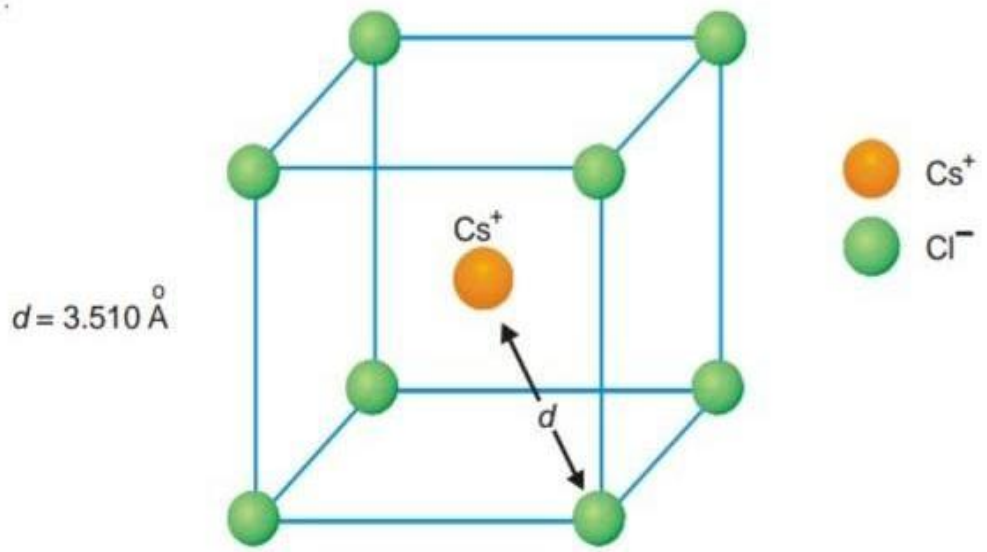
❖ 74 % Atoms and 26 % Space in B.C.C. Unit cell

- NaCl Structure -



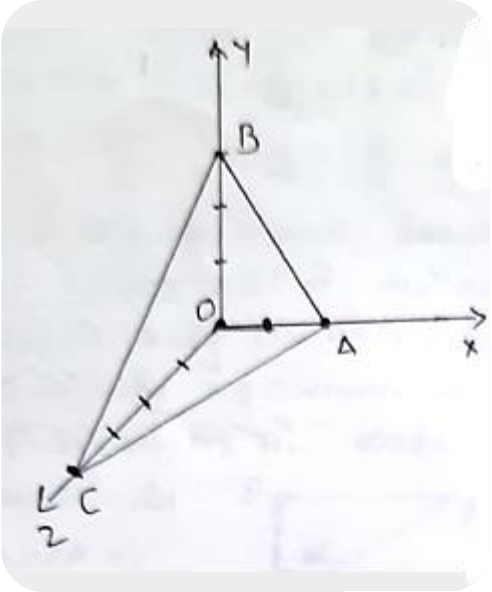
- Type – F.C.C.

- CsCl Structure -



- Type – B.C.C.

- Miller Indices -



- Suppose, Plane ABC cuts the X axis at a distance of 2a, cuts the Y axis at a distance of 3b & cuts the Z axis at a distance of 4c.
- Least Common Multiple of 2,3 and 4 is 12.
- Now, $\{ \frac{1}{2} \text{ X } 12, \ \frac{1}{3} \text{ X } 12, \ \frac{1}{4} \text{ X } 12 \} = (6\ 4\ 3) = (h\ k\ l)$
- If plane is parallel to axis than its intersect the axis and $\frac{1}{\infty} = 0$.\
- If –ve axis, than its denoted by Bar symbol on indices.
- <h k l> = Equivalent Miller indices, [h k l] = Direction of crystal.