

8. Solid State

Unit Cell	Corners	Body	Face	Total No. of atoms per unit cell
SCC	$1/8 \times 8 = 1$	----	----	1
BCC	$1/8 \times 8 = 1$	1	----	2
FCC/CCP	$1/8 \times 8 = 1$	----	$6 \times 1/2 = 3$	4
End Centred	$1/8 \times 8 = 1$	----	$2 \times 1/2 = 1$	2

Seven Primitive cells their Possible variations as centred unit cells			
Crystal system	Possible variations	Axial distances or edge lengths	Axial angles
Cubic	Primitive Body-centred	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$
Tetragonal	Primitive, Body-centred	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
Orthorhombic	Primitive, Body-centred, Face-centred, End-centred	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
Rhombohedral or Trigonal	Primitive	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$
Hexagonal	Primitive	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$
Monoclinic	Primitive, End-centred	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ, \beta \neq 120^\circ$
Triclinic	Primitive	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$

	S.C.	B.C.C.	F.C.C.	H.C.P.
No. of atom	1	2	4	6
P.E.	52.4%	68%	74%	74%
Void space	47.6%	32%	26%	26%
C.N.	6	8	12	12
No. of T.V.	0	0	8	12
No. of O.V.	0	0	4	6
Relationship between edge length and radius	$r = \frac{a}{2}$	$r = \frac{\sqrt{3}a}{4}$	$r = \frac{a}{2\sqrt{2}}$	$r = \frac{a}{2}$
Type of Packing	AAA Type		ABCABC Type	ABAB AB type

$$d = \frac{Z \times M}{N_A \times a^3}$$

d = density z = number of atom in a unit cell.

$$N_A = 6.022 \times 10^{23}$$

Square Close Packing

- The spheres in the adjacent row lie just one over & show a horizontal & vertical alignment
- Co-ordⁿ 4**
- Packing fraction = 78.5%

Hexagonal Close Packing

- The spheres in every second row are seated in the depression.
- Co-ordⁿ 6**
- Packing fraction = 90.75% (91%)

Tetrahedral Void

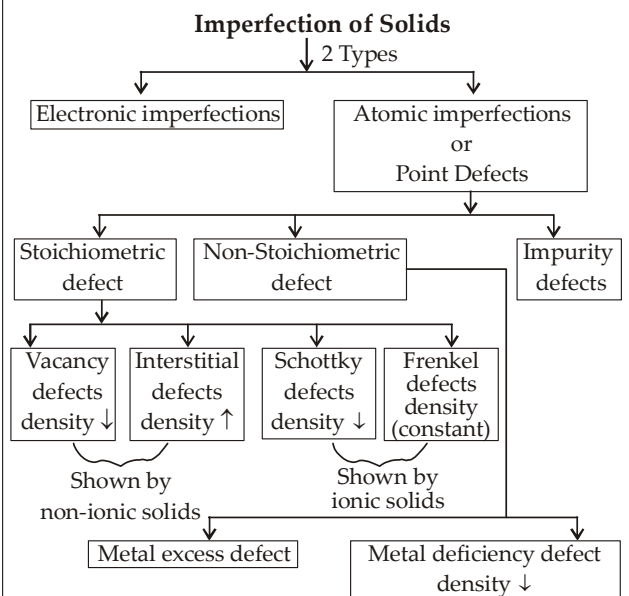
- Co-ordⁿ = 4**
- Radius Ratio** = $\frac{r_{\text{void}}}{r_{\text{sphere}}} = 0.225$
- T.V.'s. Location at body diagonal**
- Max No. of T.V. in one body diagonal = 2**
- 1st Nearest distn betn two T.V. = $\frac{a}{2}$**
- 2nd Nearest distn betn two T.V. = $\frac{a}{\sqrt{2}}$**
- 3rd Nearest distn betn two T.V. = $\frac{\sqrt{3}a}{2}$**
- Distn betn Corner atom & T.V. = $\frac{\sqrt{3}a}{4}$**
- Ratio betn T.V. & O.V. = 2 : 1**
- Ratio betn T.V. & O.V. at 1 body diagonal = 2:1**
- Distance Between O.V. & T.V. = $\frac{\sqrt{3}a}{4}$**

Octahedral Void

- Co-ordⁿ = 6**
- Radius Ratio** = $\frac{r_{\text{void}}}{r_{\text{sphere}}} = 0.414$
- O.V.'s. Location at body center & as well as edge center**

- Max No. of O.V. in one body diagonal = 1**
- 1st Nearest distn betn two O.V. = $\frac{a}{\sqrt{2}}$**
- Distn betn edge center's O.V. & Body center's O.V. = $\frac{a}{\sqrt{2}}$**
- Diamond = $\frac{\pi\sqrt{3}}{6} = 0.34$**

Defects in Crystal Structure :



➤ Radius ratio and co-ordination number (CN)

Limiting radius ratio	CN	Geometry
[0.155 – 0.225]	3	[Plane triangle]
[0.255 – 0.414]	4	[Tetrahedral]
[0.414 – 0.732]	6	[Octahedral]
[0.732 – 1]	8	[bcc]

- Relationship between radius of void (r) and the radius of the sphere (R): r (tetrahedral) = $0.225 R$; r (octahedral) = $0.414 R$
- Paramagnetic : Presence of unpaired electrons [attracted by magnetic field]
- Ferromagnetic : Permanent magnetism [↑ ↑ ↑ ↑]
- Antiferromagnetic : Net magnetic moment is zero [↑ ↓ ↑ ↓]