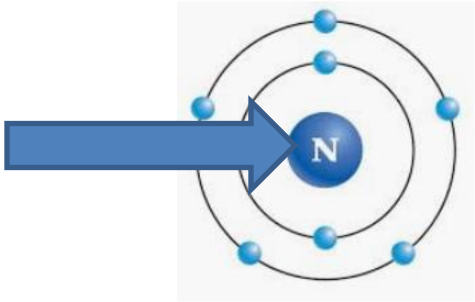
N is nitrogen (N≅N)

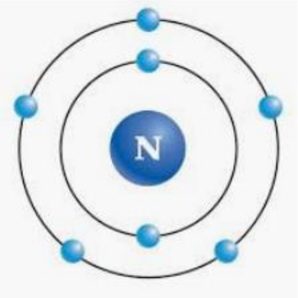


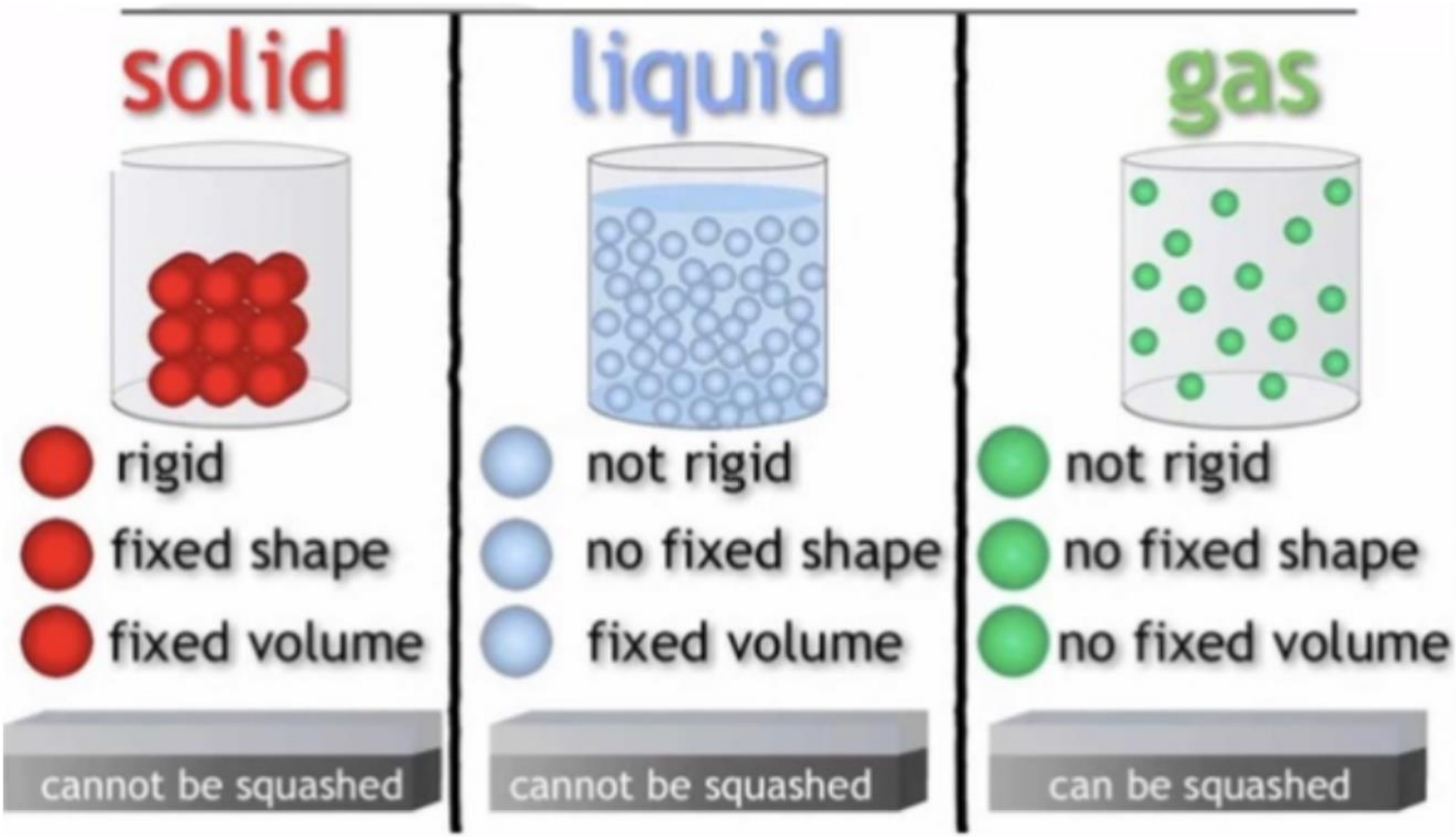
Presentation by

NAGENDAR NUTHALAPATI(N≅N)
about

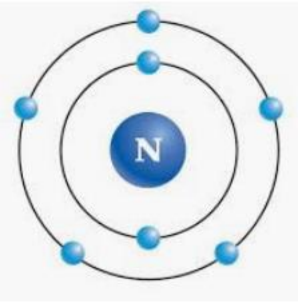
SOLID STATE

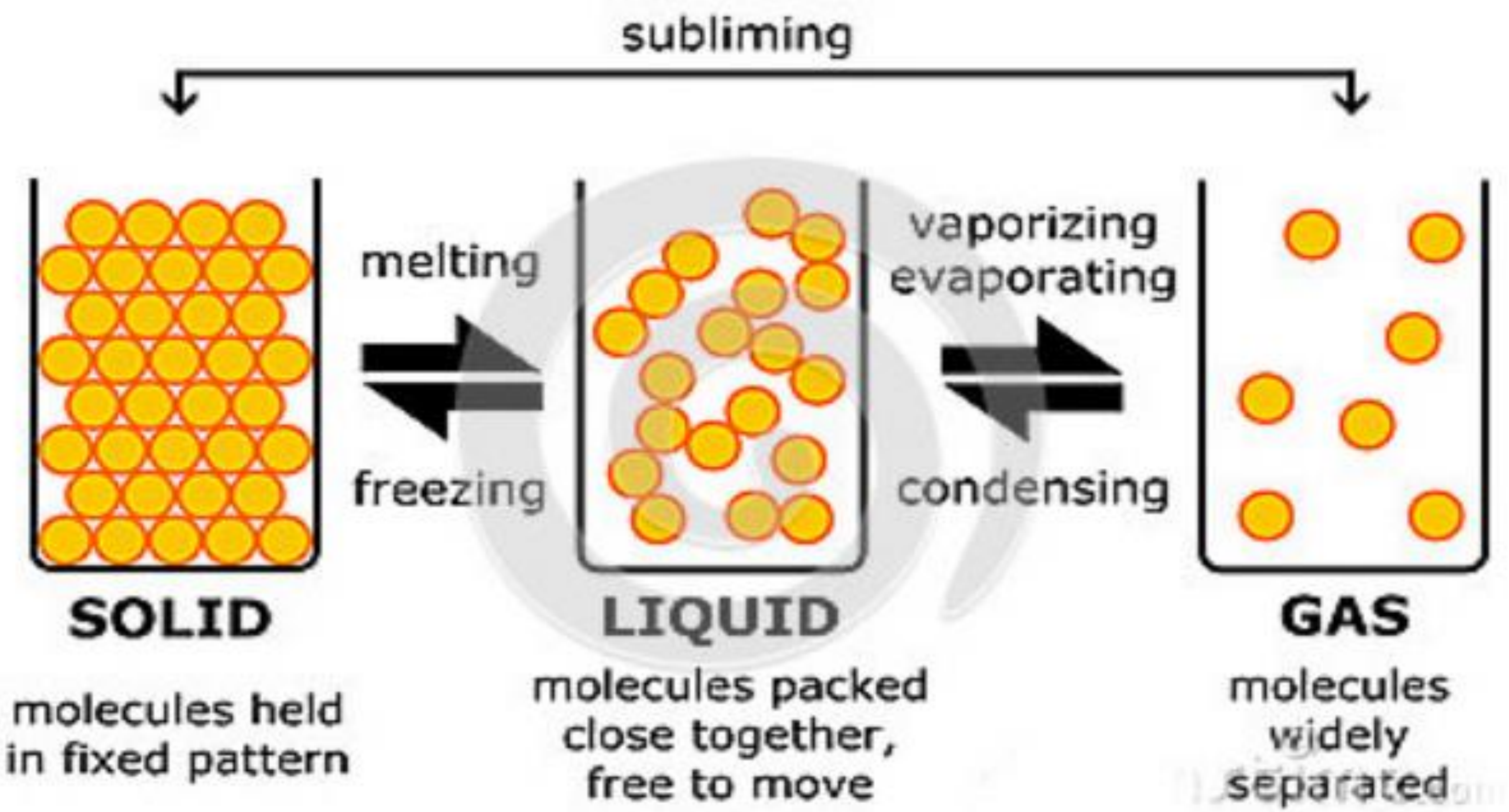
THREE STATES OF MATTER



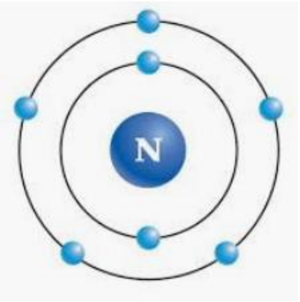


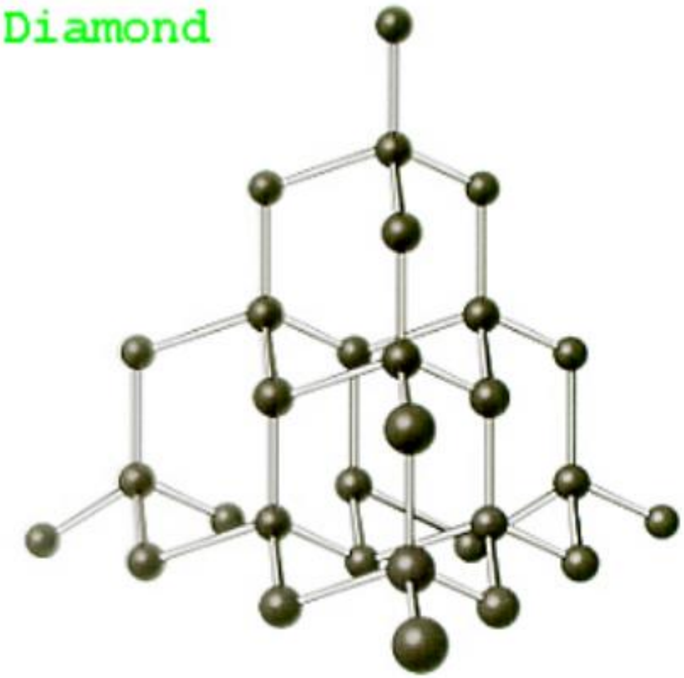
Change of States

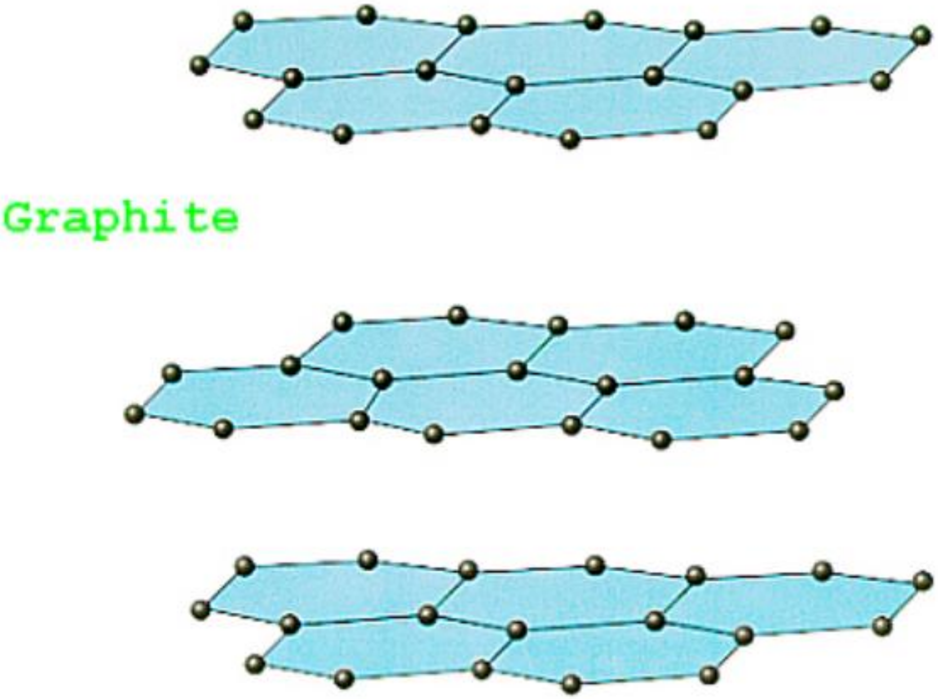




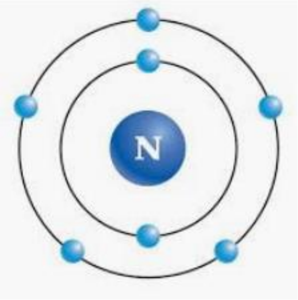
Allotropes of carbon

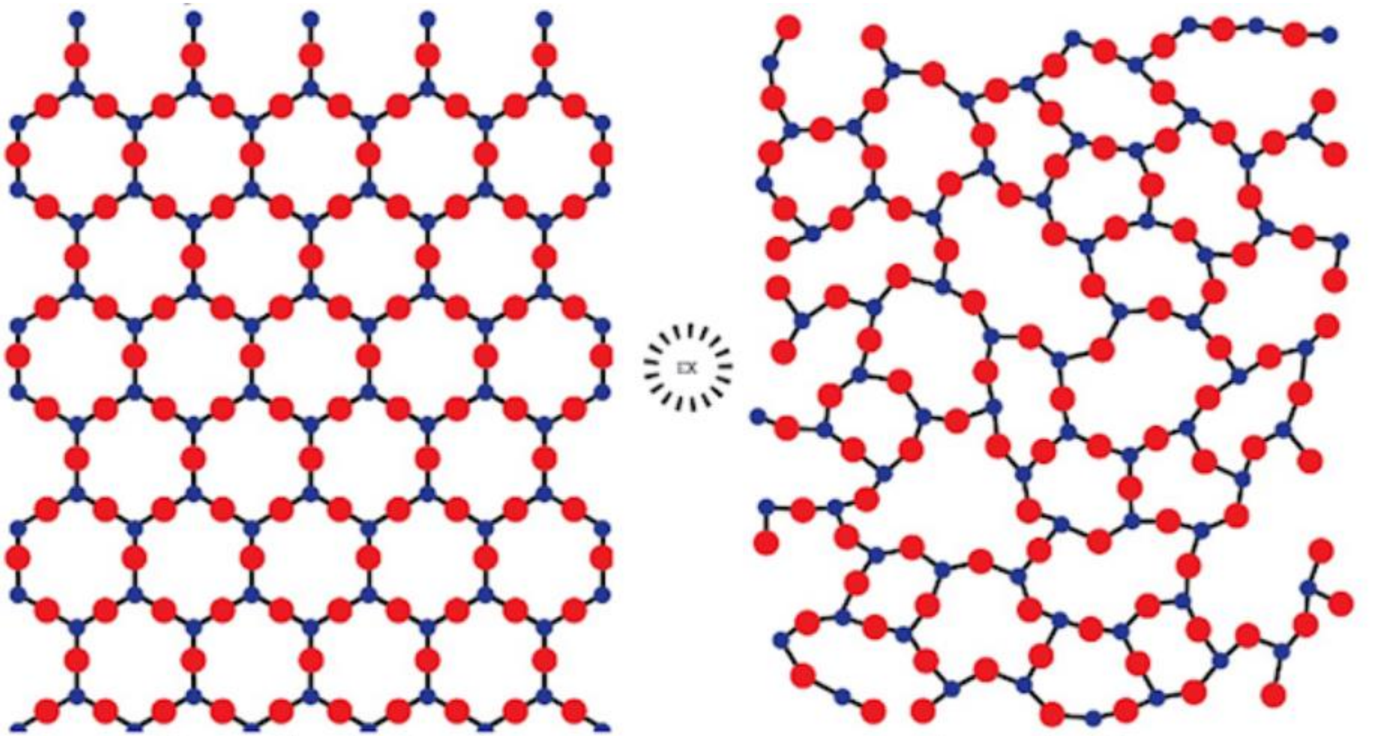






CRYST VS AMOR



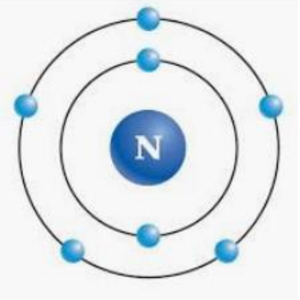


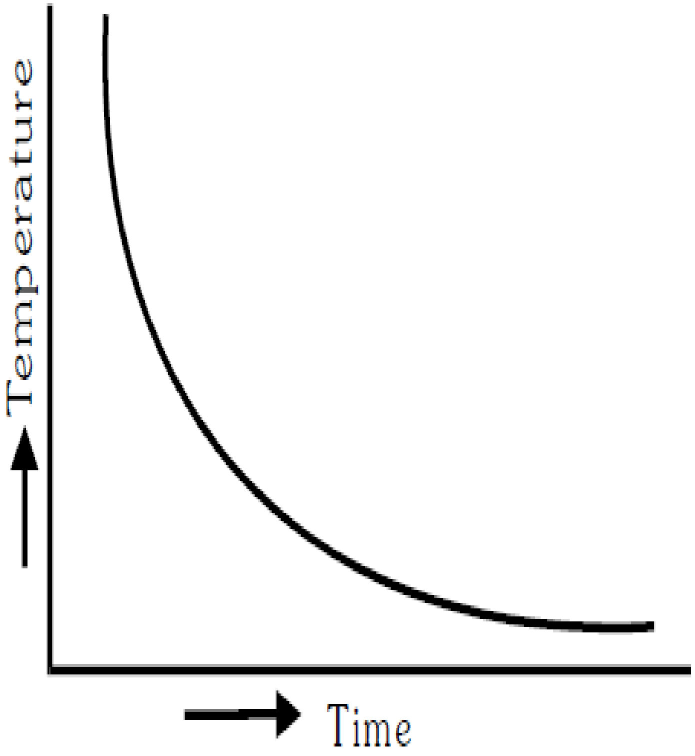
Example: Rock salt

Example: Glass

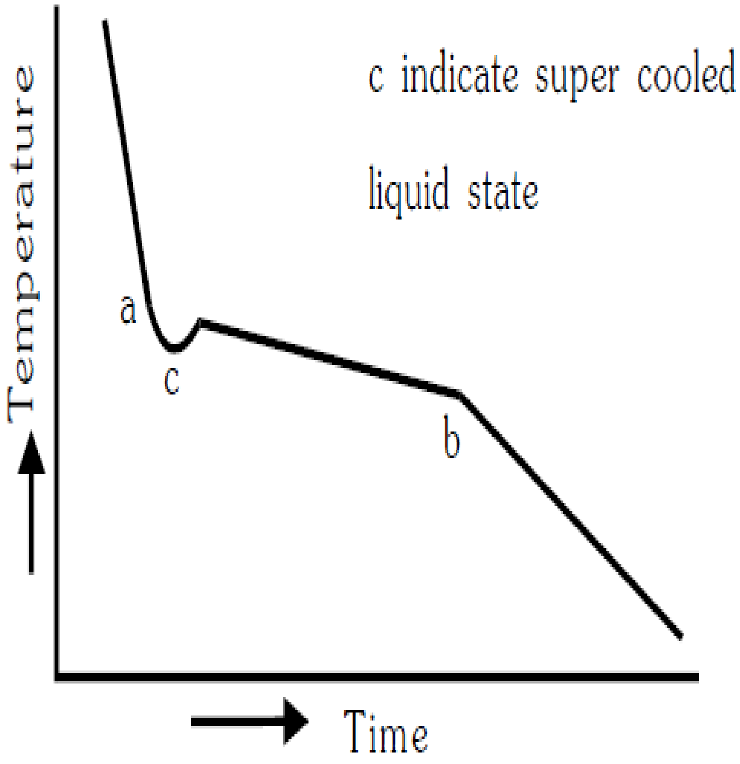
www.examplesof.net

Cooling curve



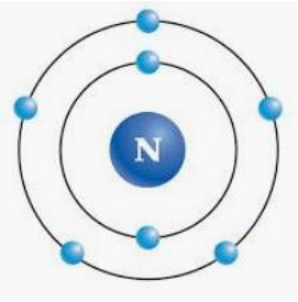


Cooling curve of an amorphous solid

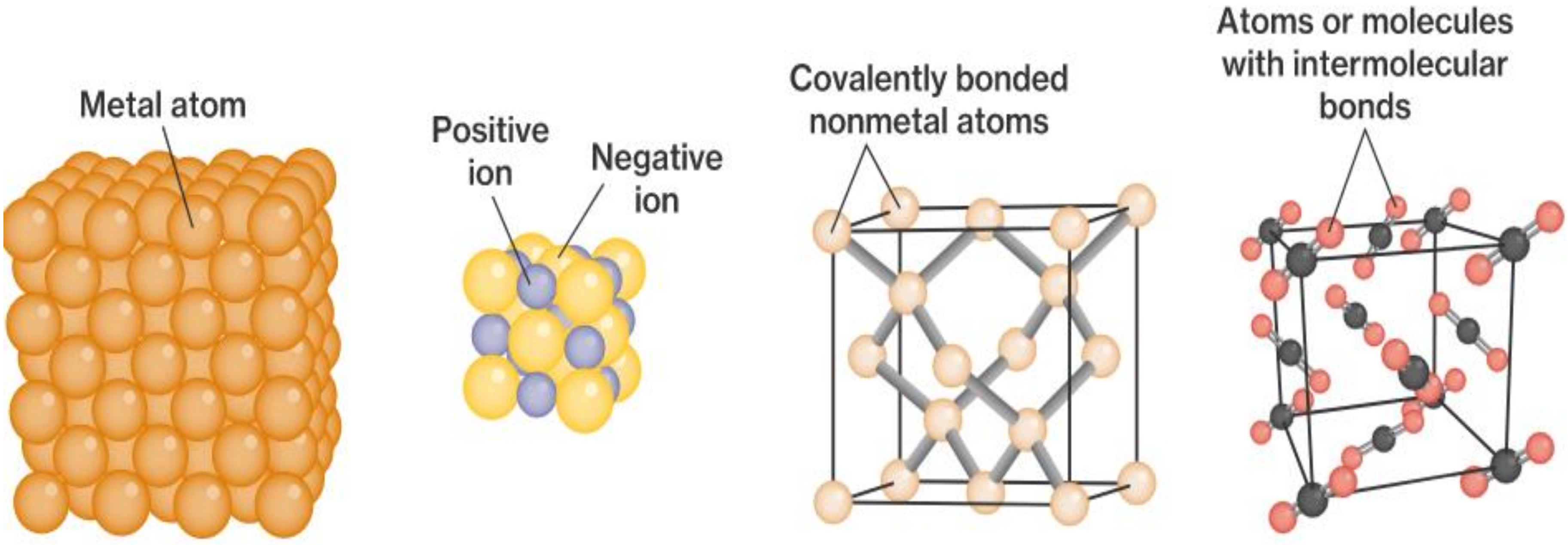


Cooling curve of crystalline solid

Crystalline Solids



Types of Crystalline Solids



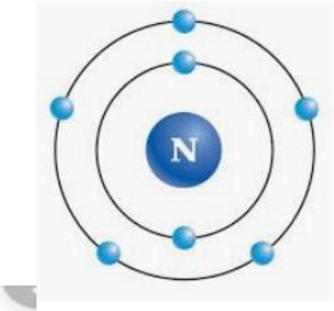
Metallic solid

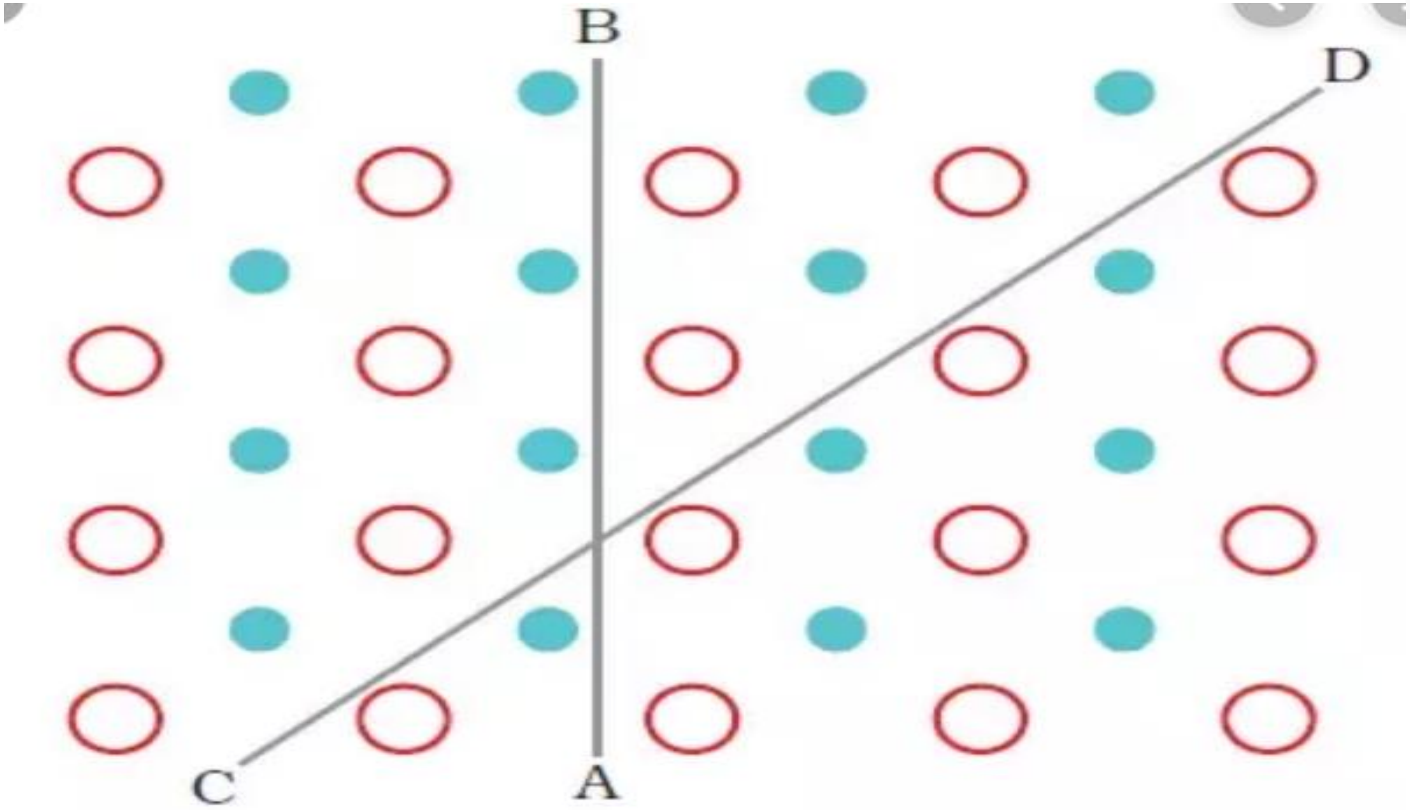
Ionic solid

Covalent solid

Molecular solid

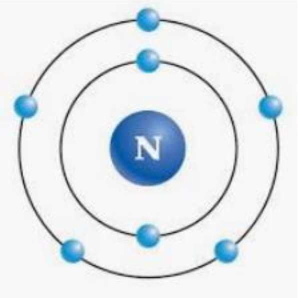
Anisotropy

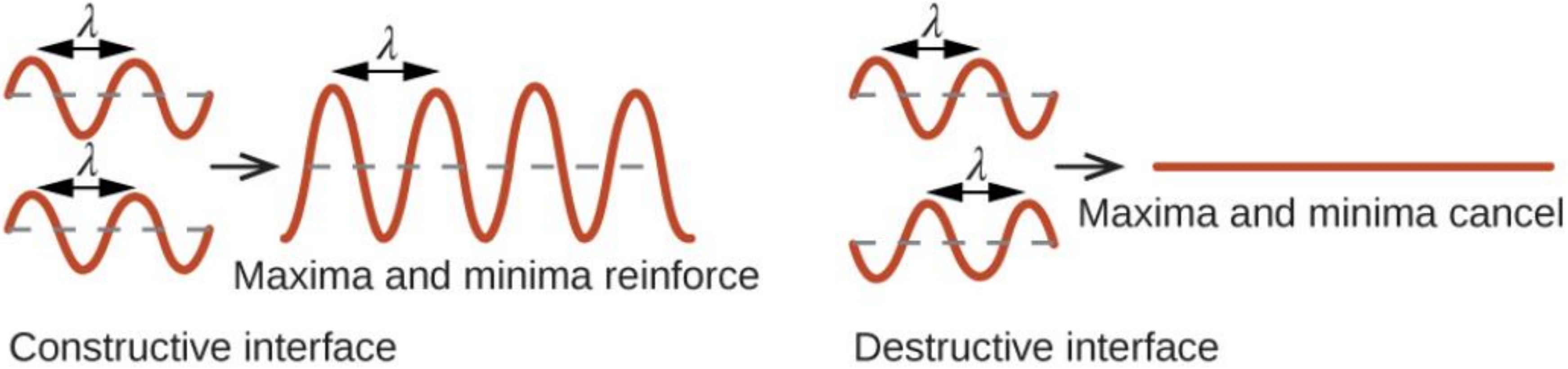




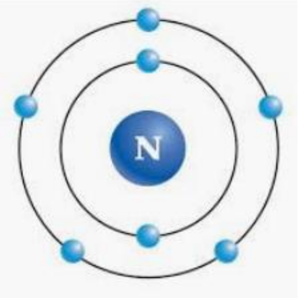
Anisotropy in crystals is due to different arrangement of particles along different directions.

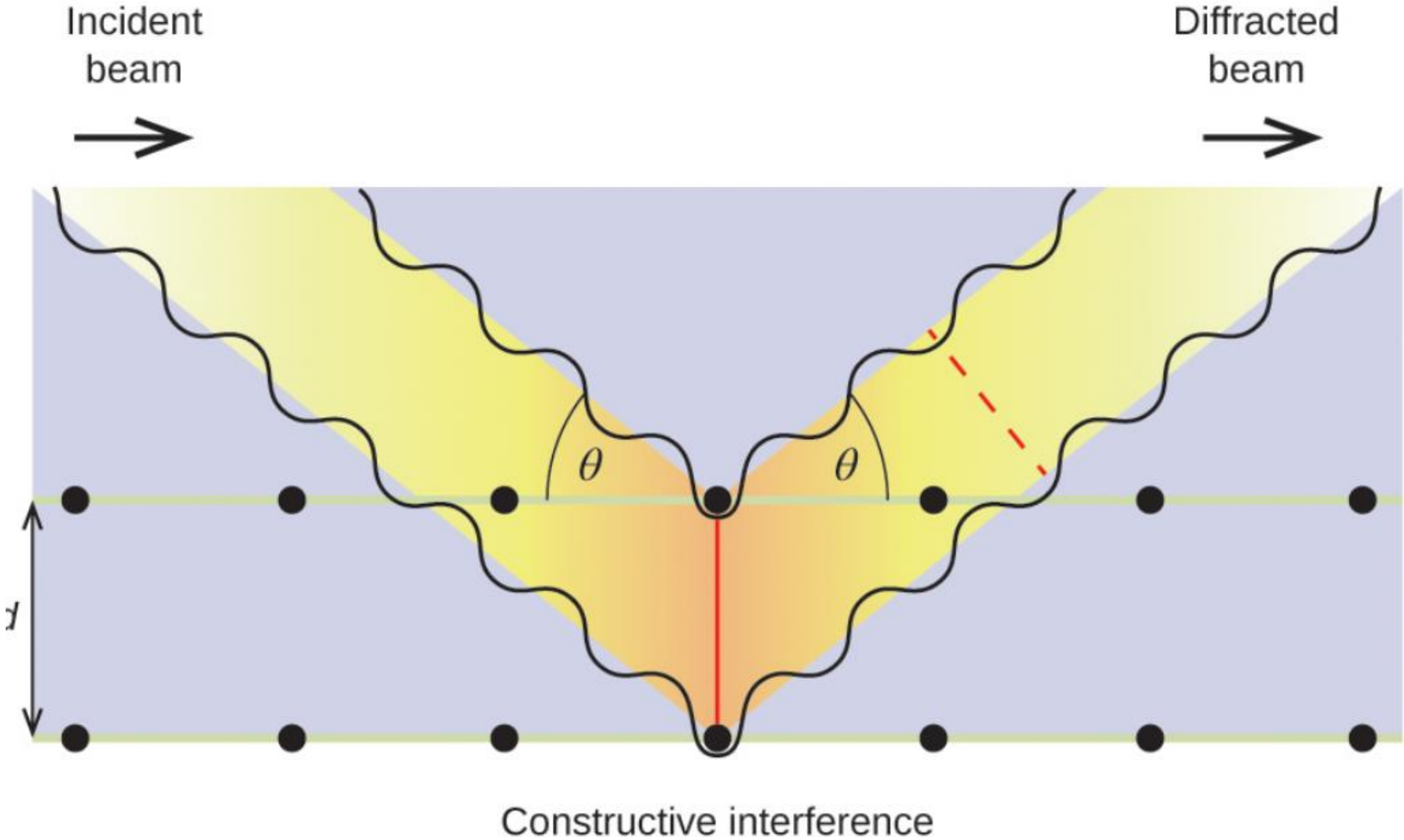
X-diffraction



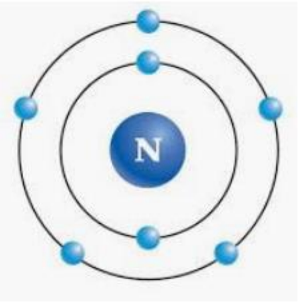


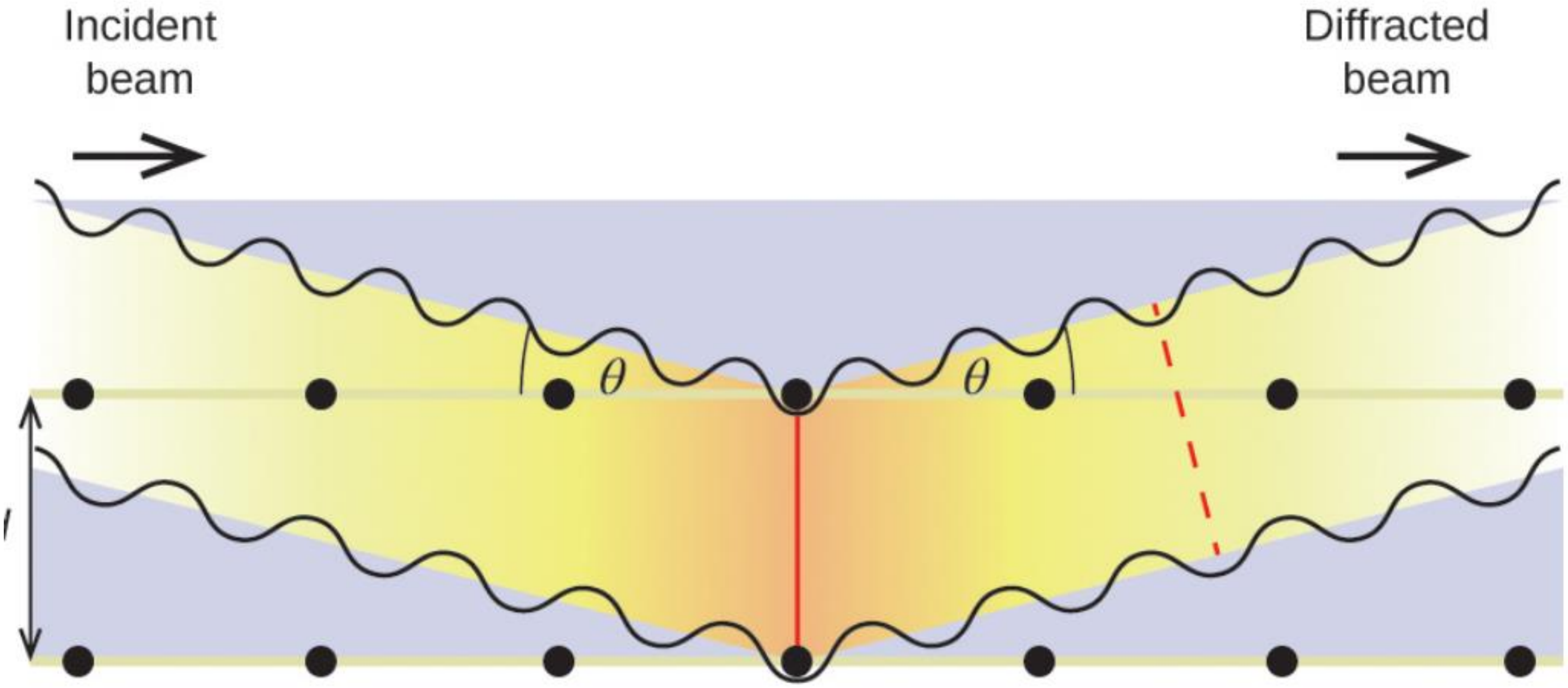
X-diffraction





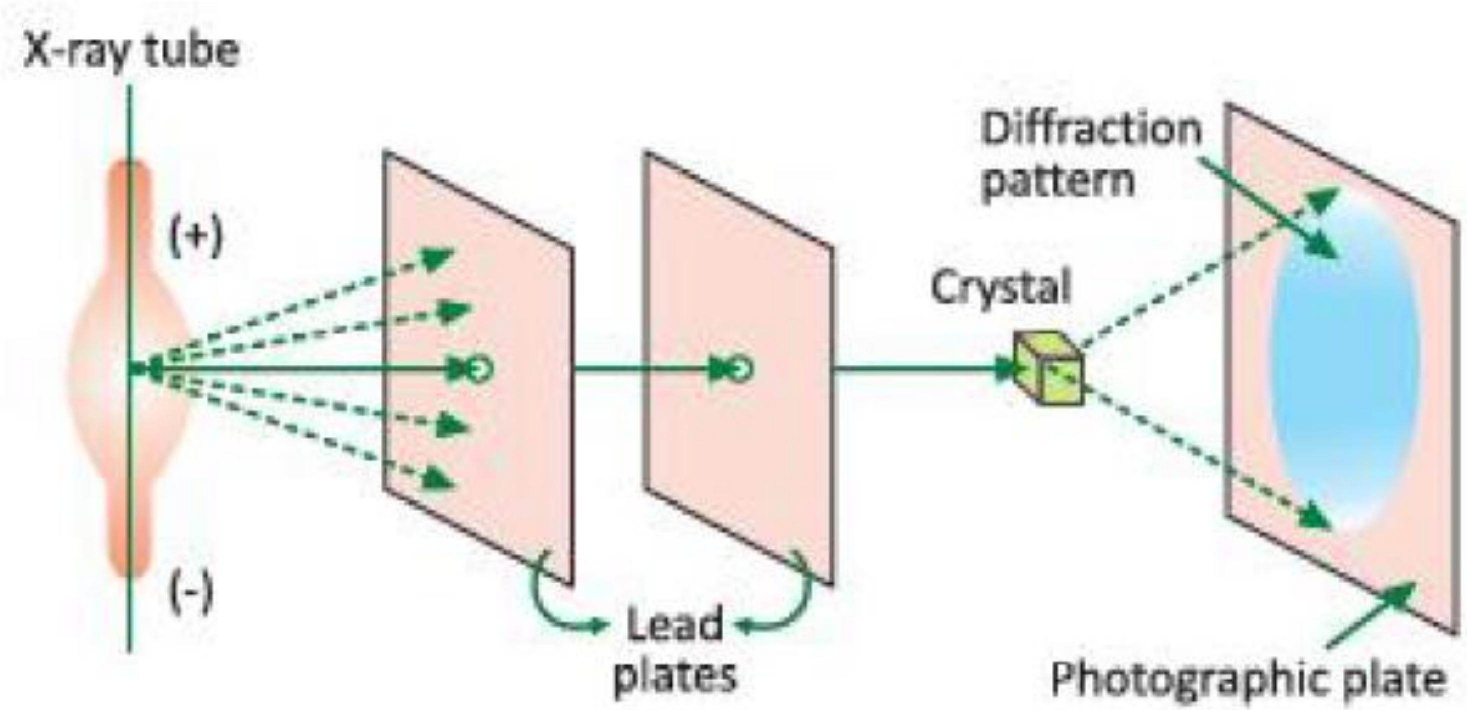
X-diffraction





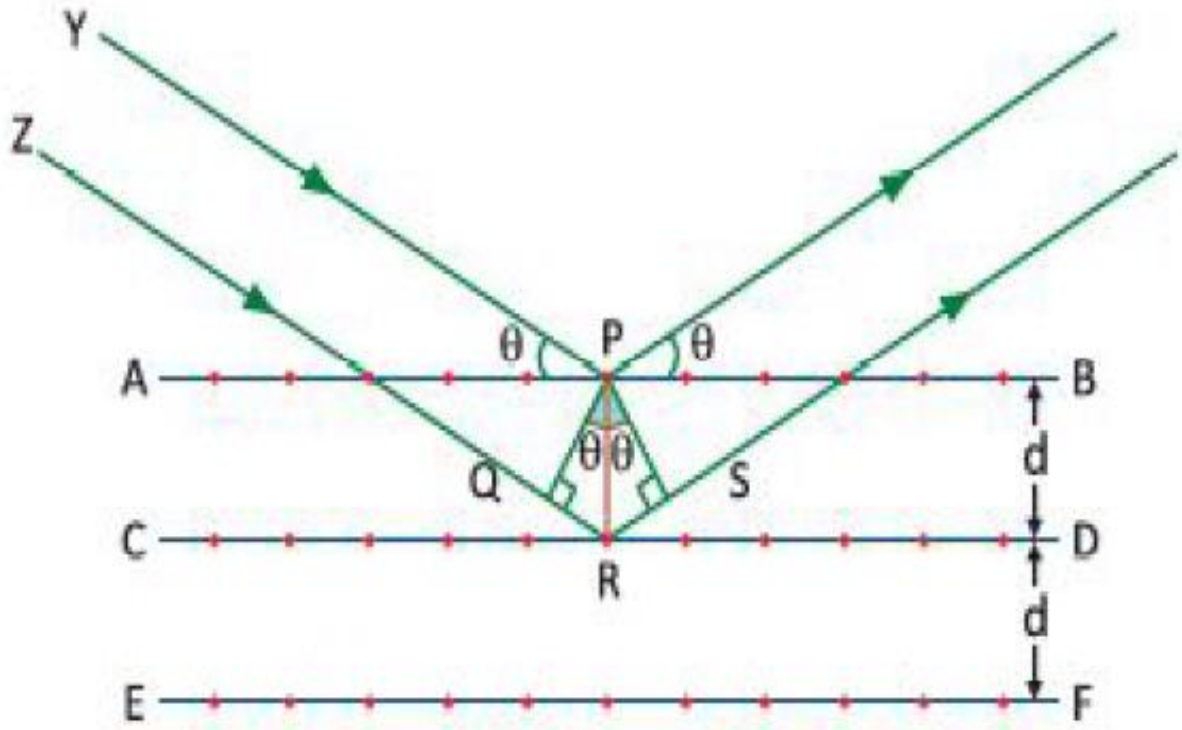
Destructive interference

X-diffraction



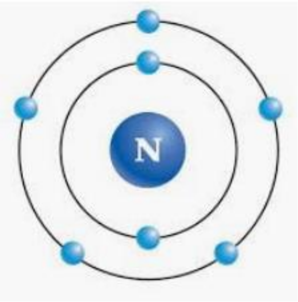
Study of the X-ray diffraction by crystal

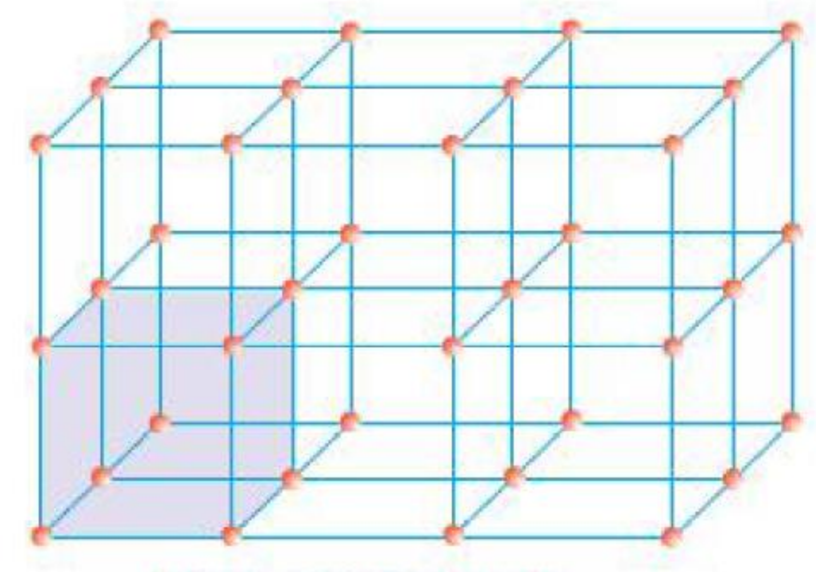
BRAGG´S LAW



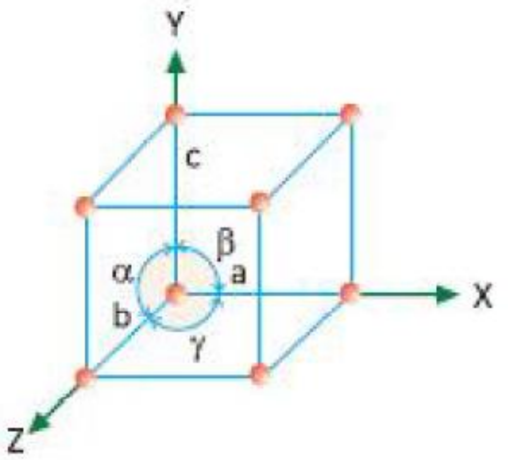
$$\lambda = 2d_{hkl} \sin\theta$$

Space lattice



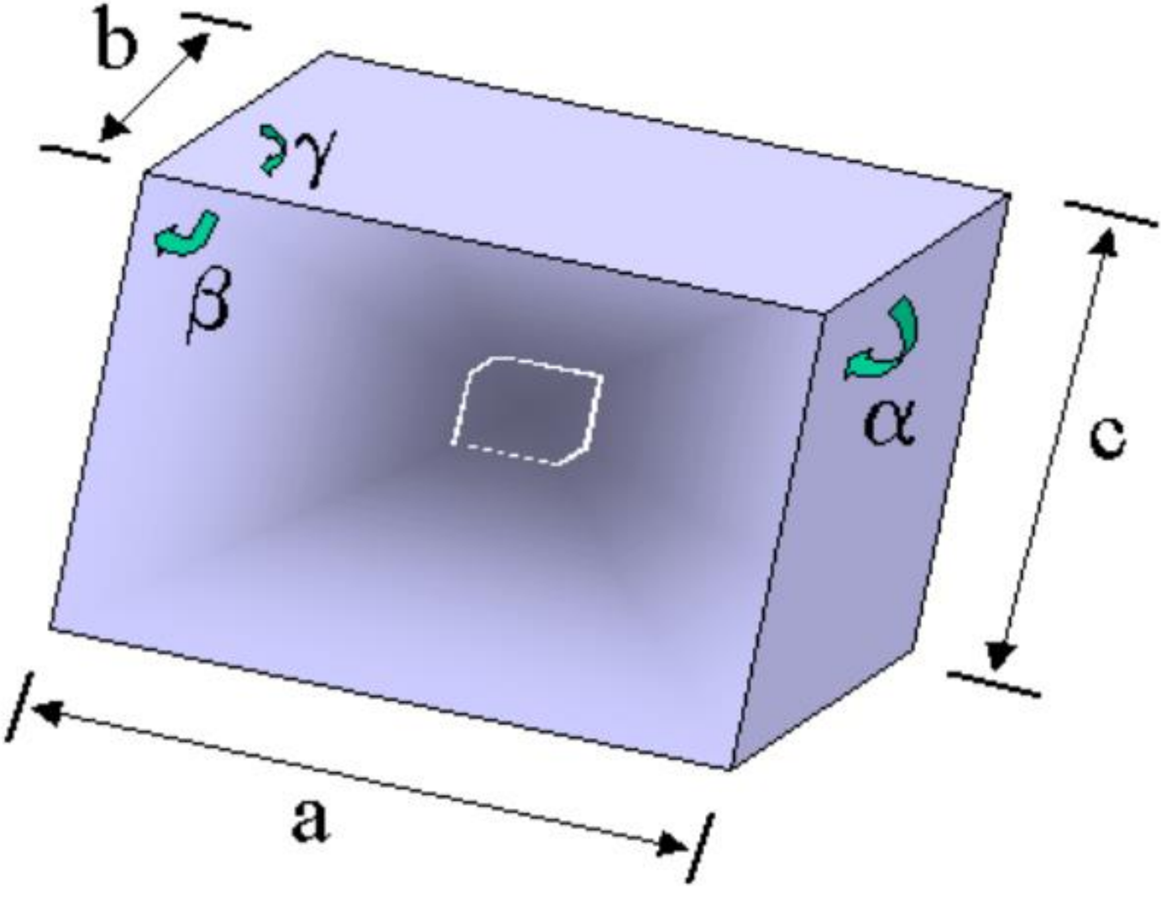


Representation of space lattice and unit cell

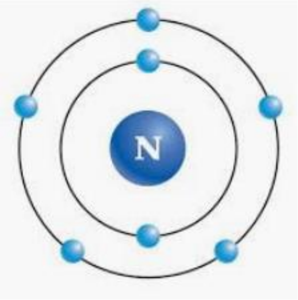


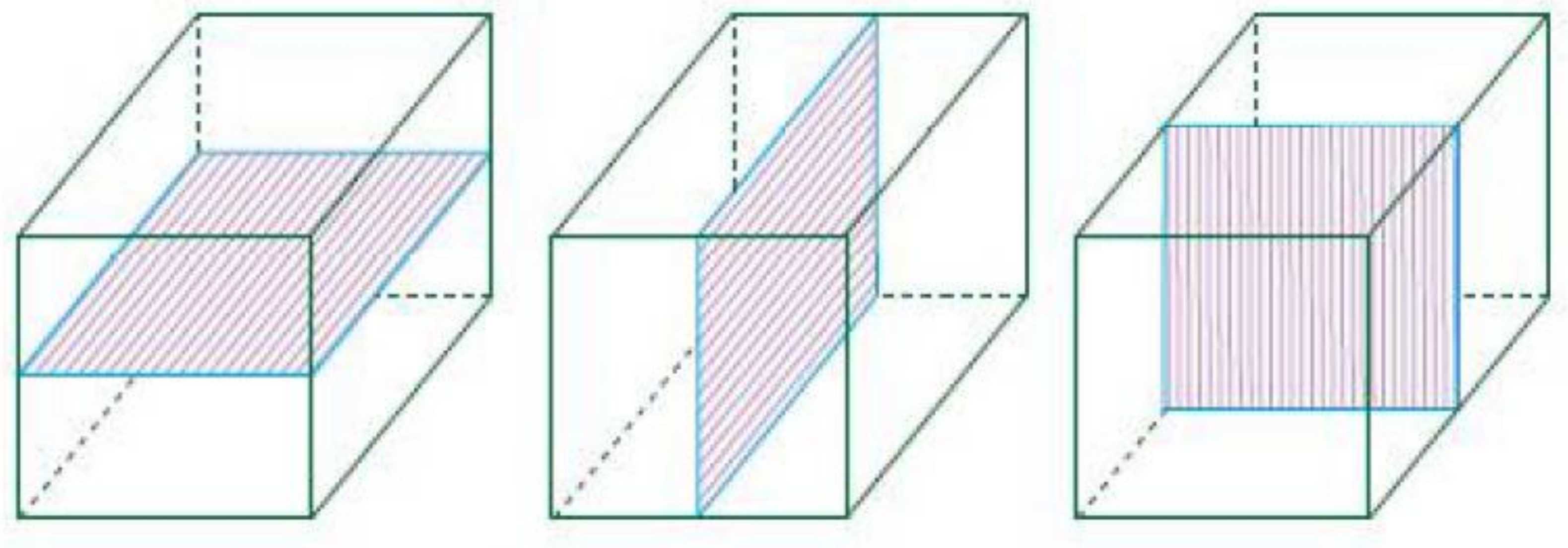
Representation of dimensions of a unit cell

Unit cell parameters



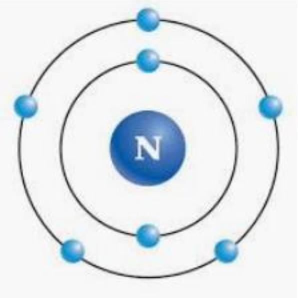
Rectangular-PS

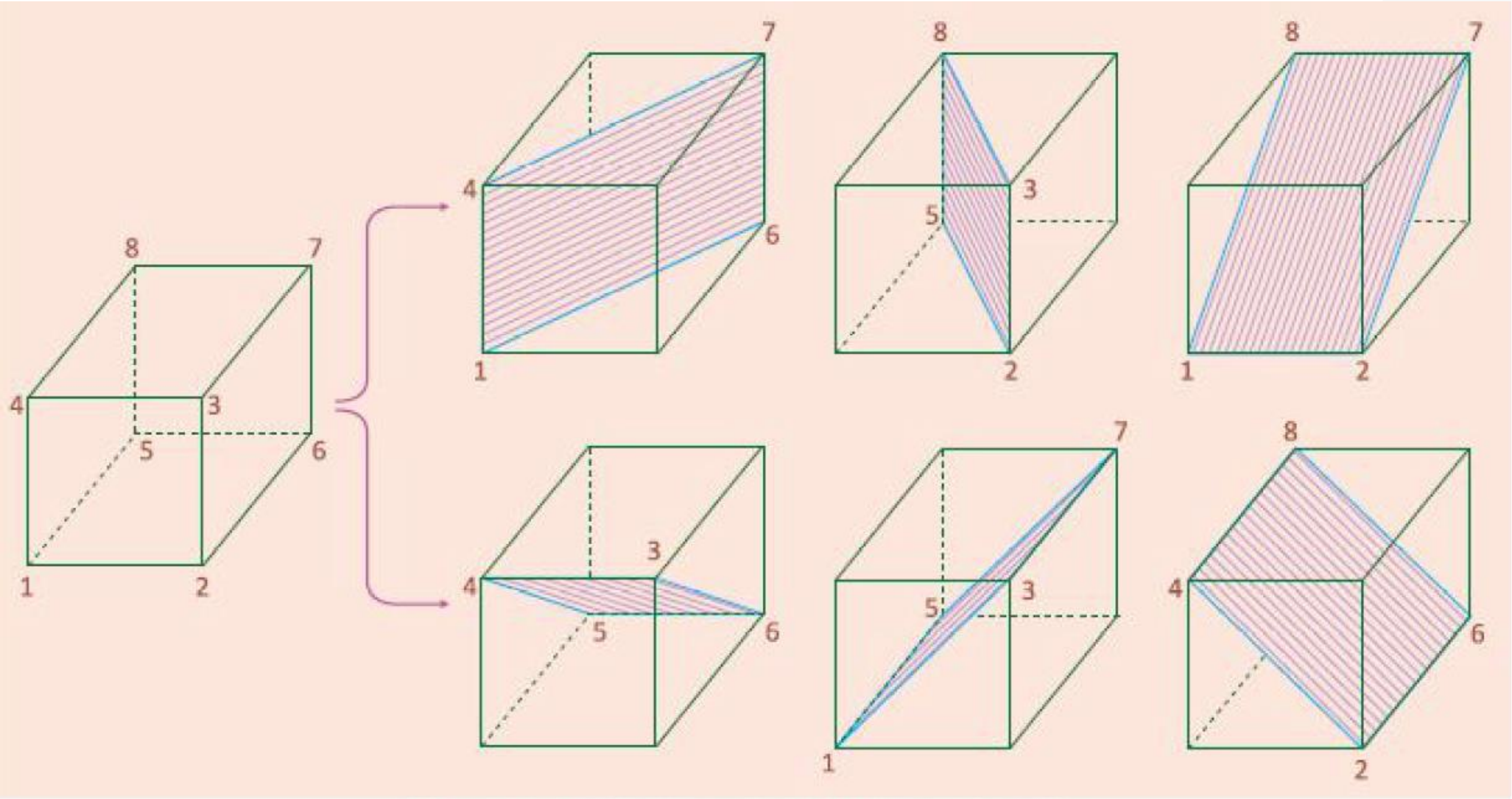




Rectangular planes of symmetry (there are 3 such planes)

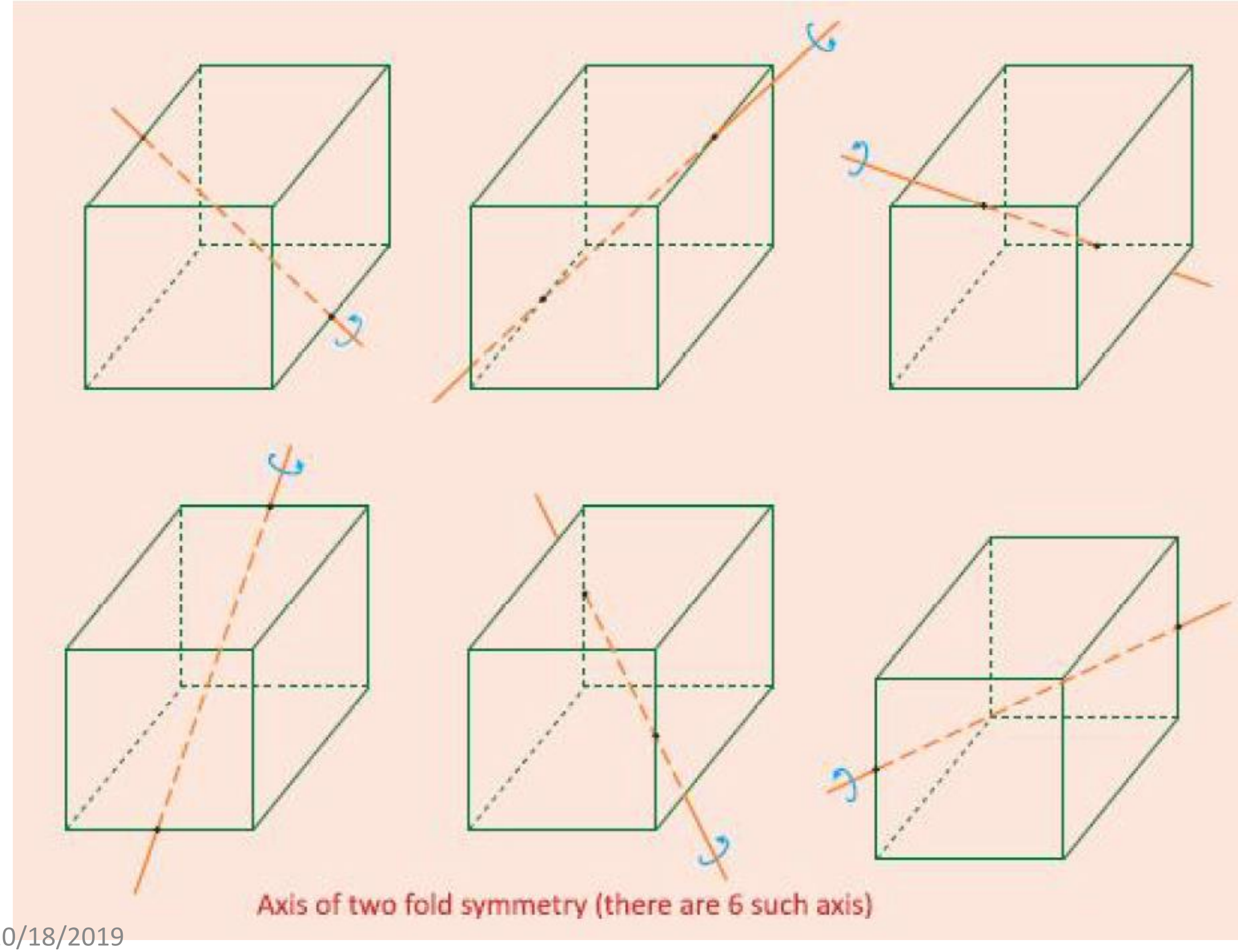
Diagonal-PS





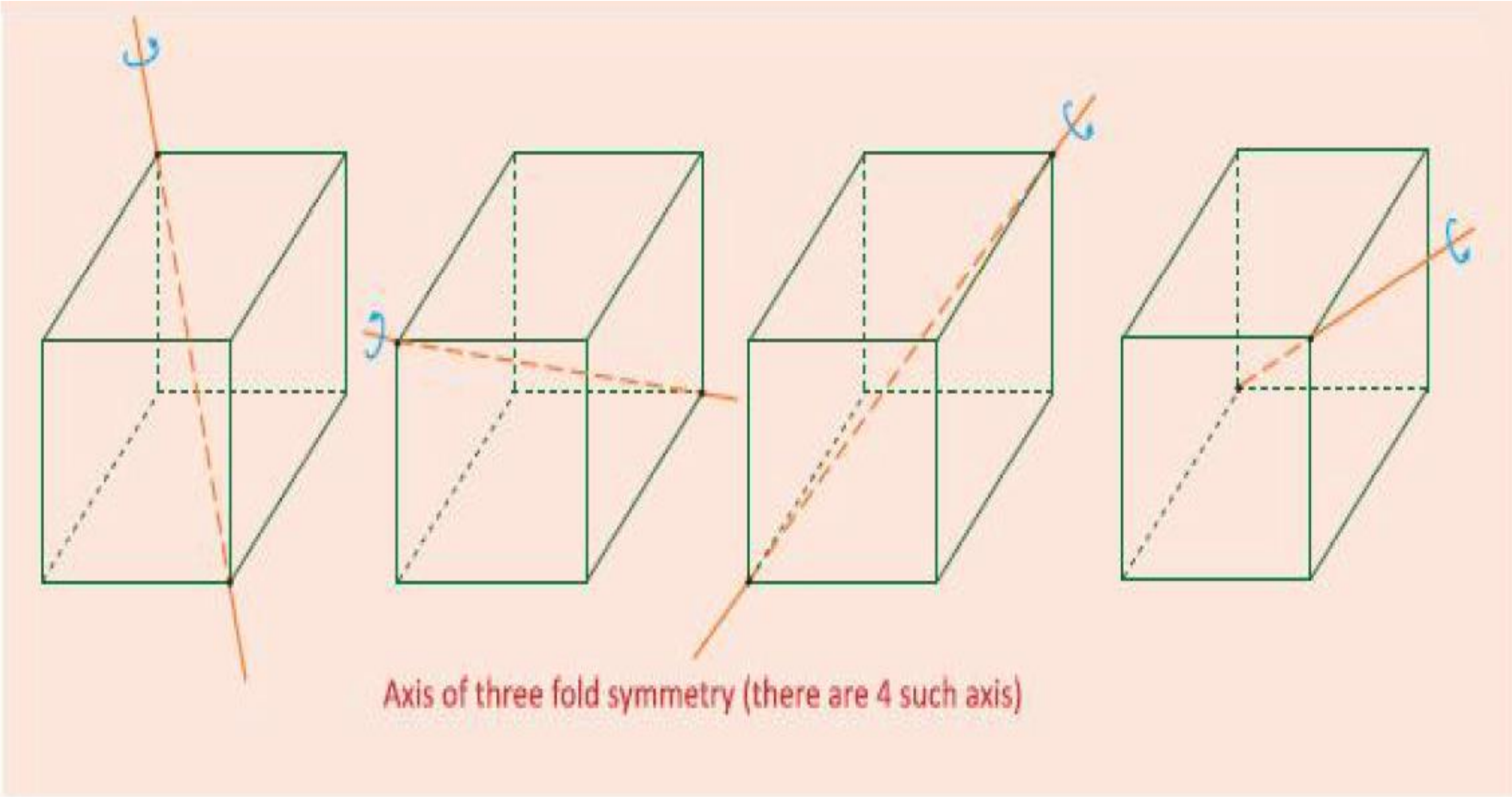
Diagonal planes of symmetry (there are 6 such planes)

2-FOLD symmetry



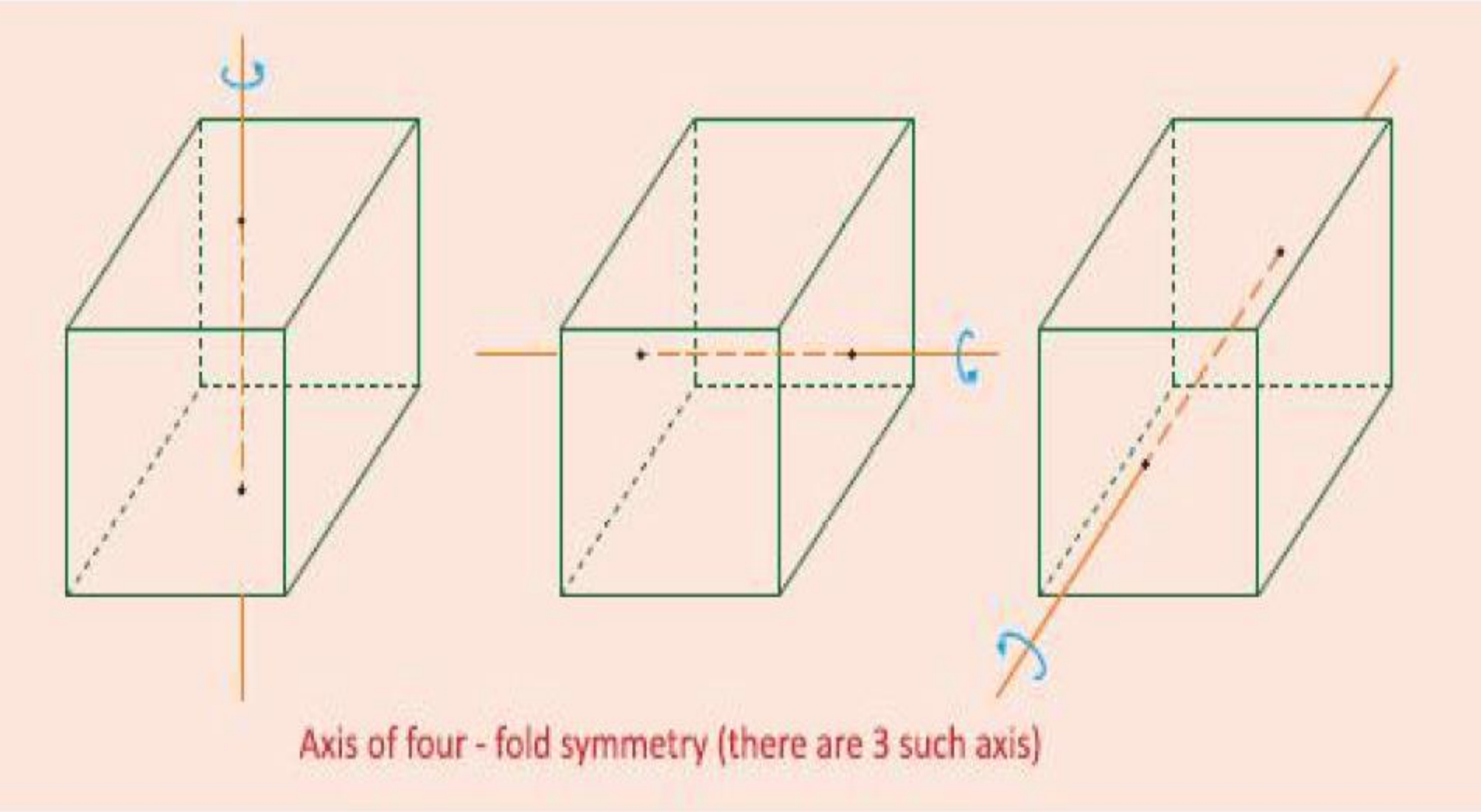
Axis of two fold symmetry (there are 6 such axis)

3-FOLD symmetry



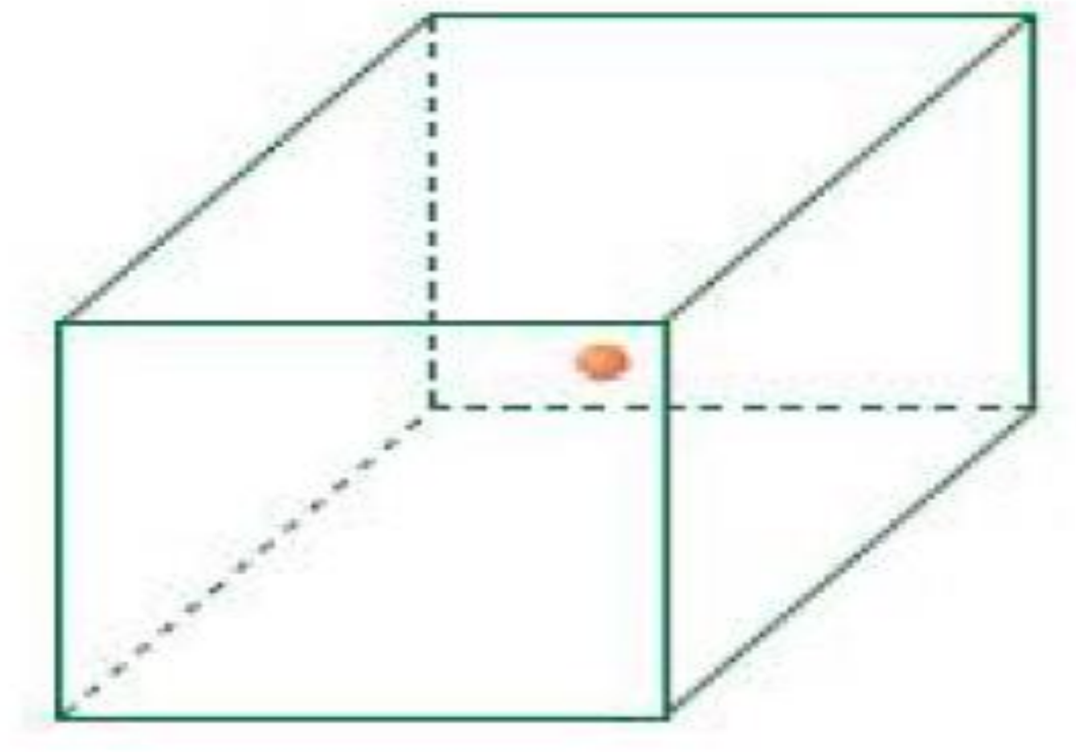
Axis of three fold symmetry (there are 4 such axis)

4-FOLD symmetry

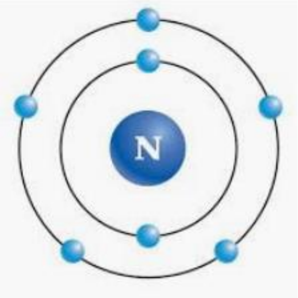


Axis of four - fold symmetry (there are 3 such axis)

CENTER OF SYM



SYMMETRY



Elements of symmetry :

The total number of planes, axes and centre of symmetry possessed by a crystal are termed as elements of symmetry. A cubic crystal possesses a total of 23 elements of symmetry.

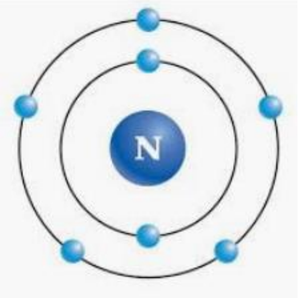
Planes of symmetry = (3 + 6) = 9

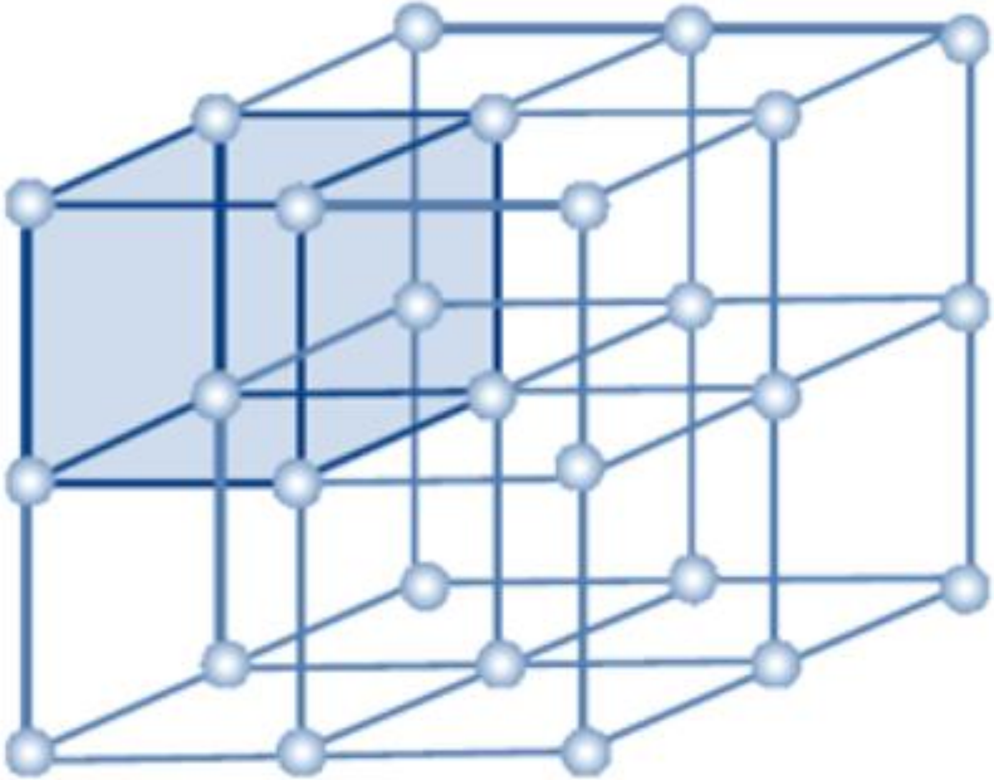
Axes of symmetry = (3 + 6 + 4) = 13

Centre of symmetry = 1

Total number of symmetry elements = 23

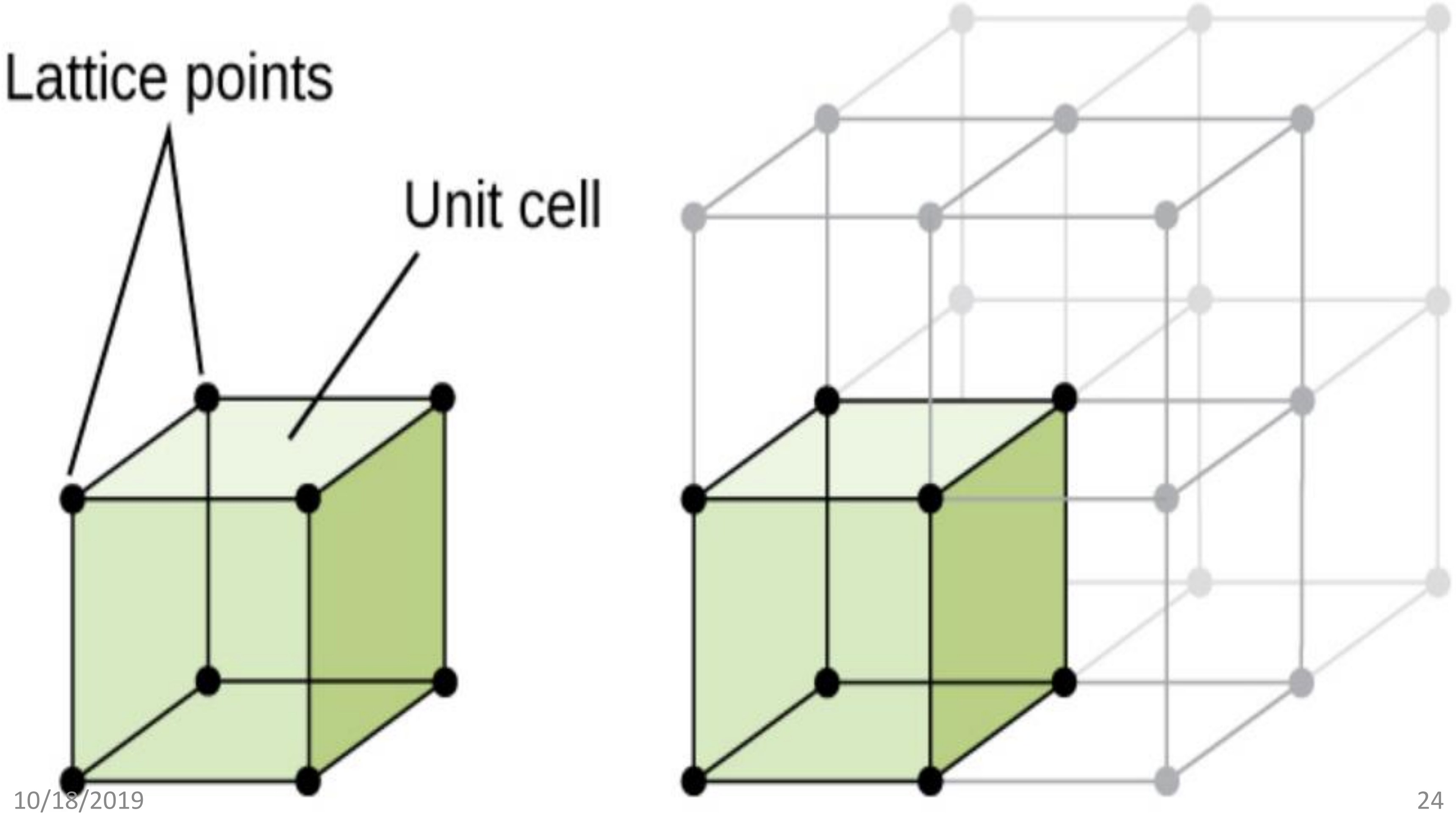
Unit cell and Lattice



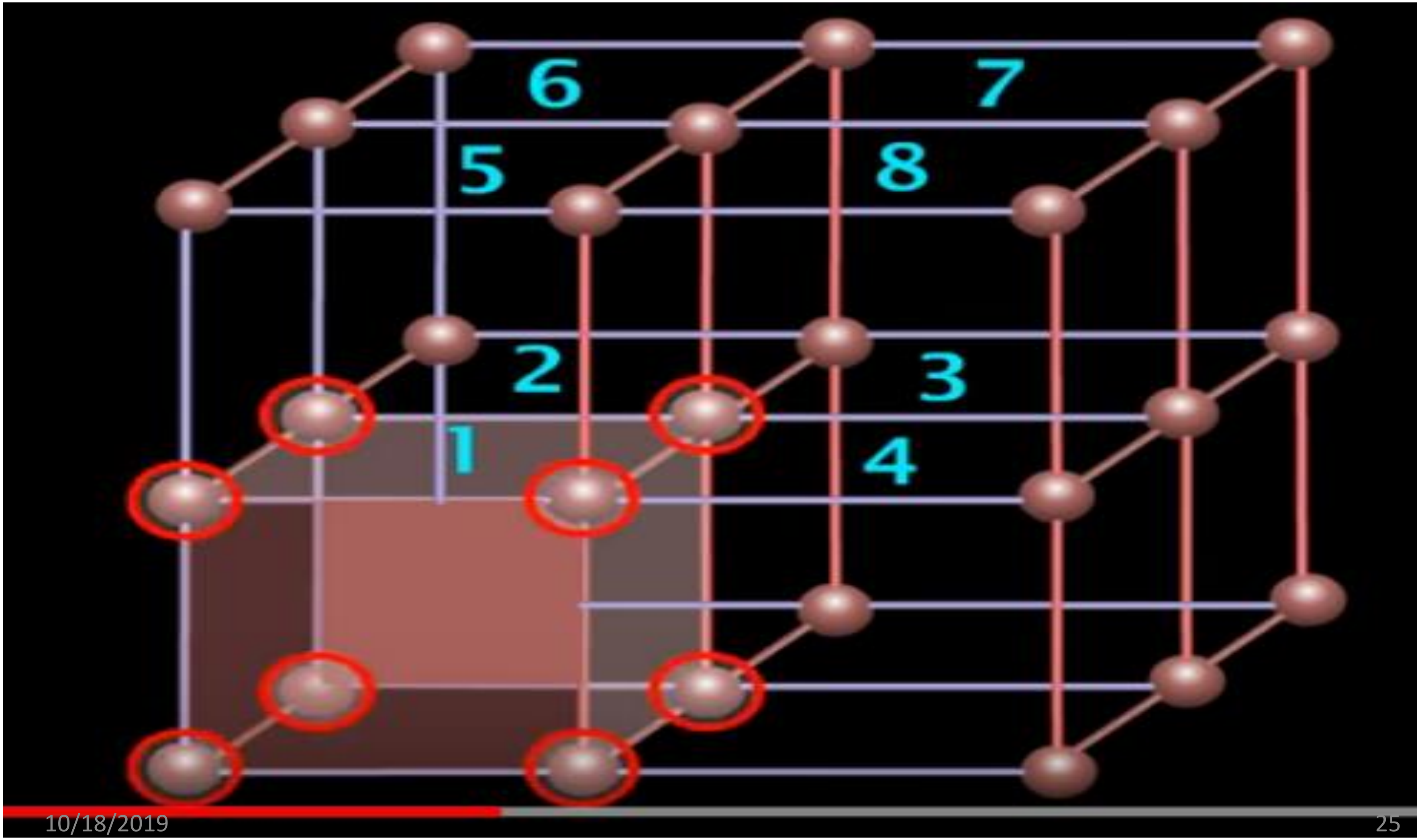


Representation of unit cell in cristal lattice

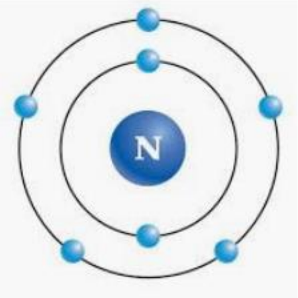
Unit cell in a lattice



Unit cell and Lattice



Unitcell GEOMETRY



GEOMETRY OF A CUBE

Number of corners = 8

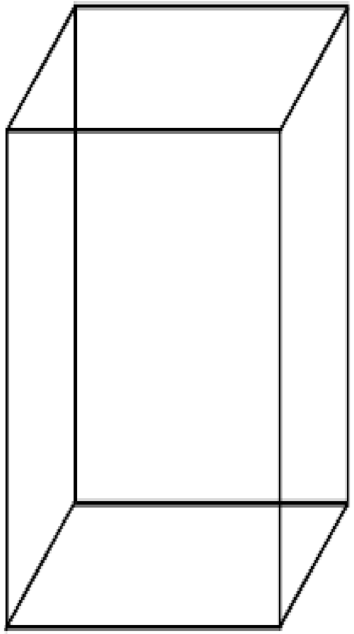
Number of faces = 6

Number of edges = 12

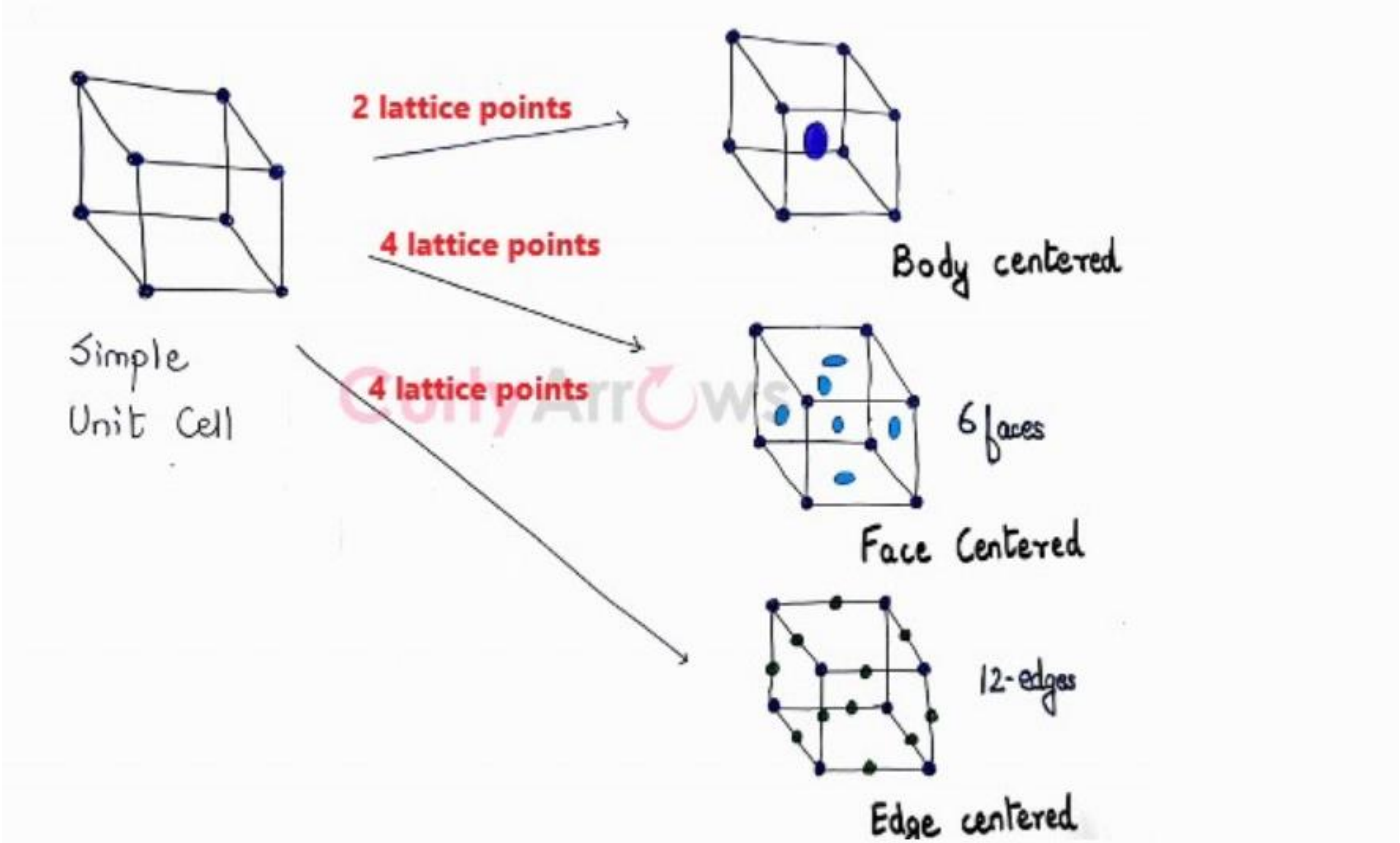
Number of cube centre = 1

Number of cube diagonals = 4

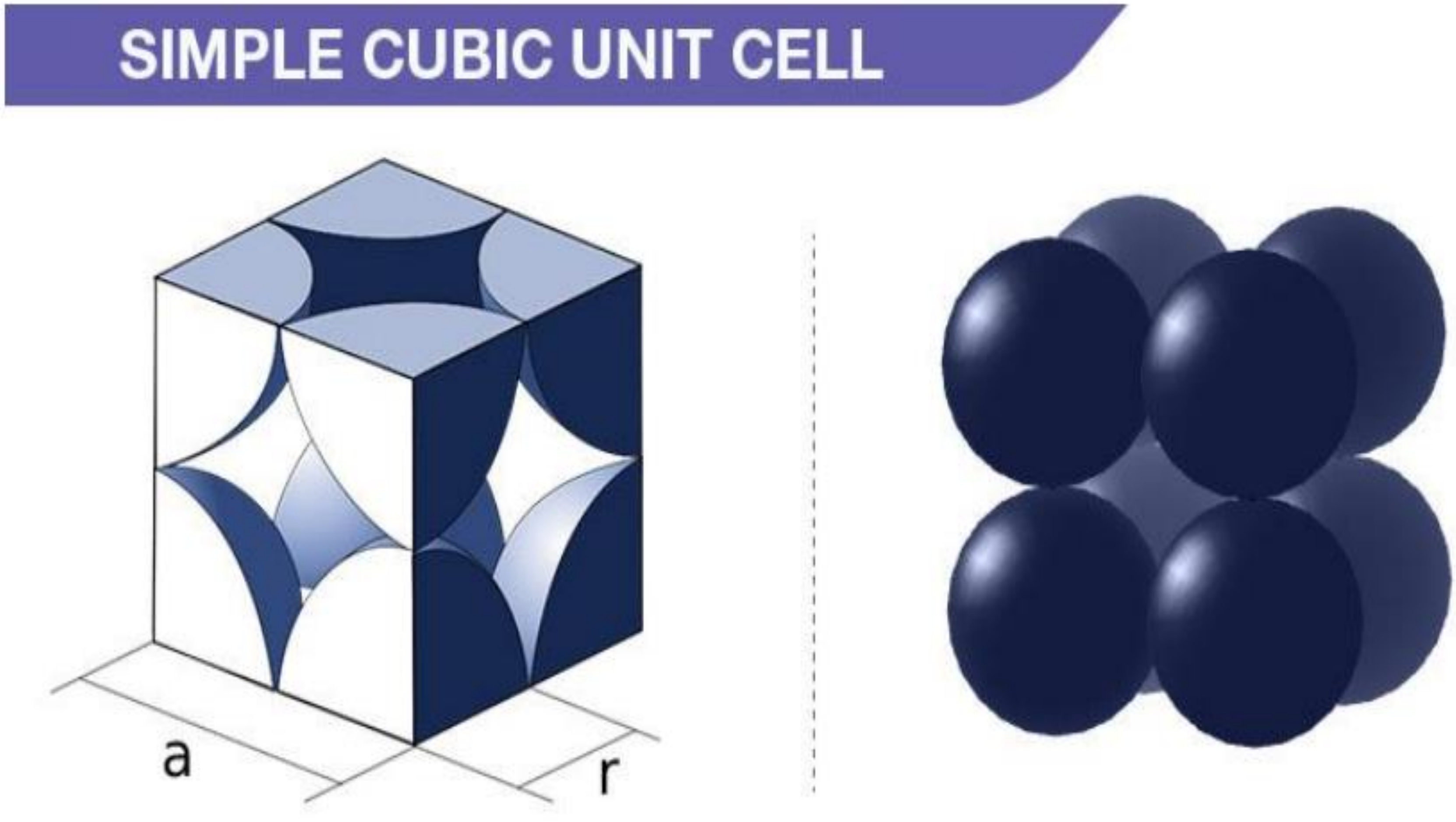
Number of face diagonals = 12



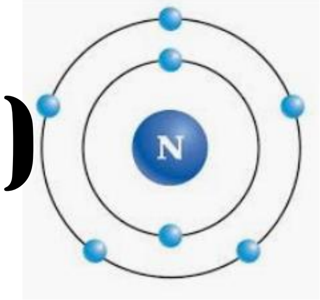
Unit cell types

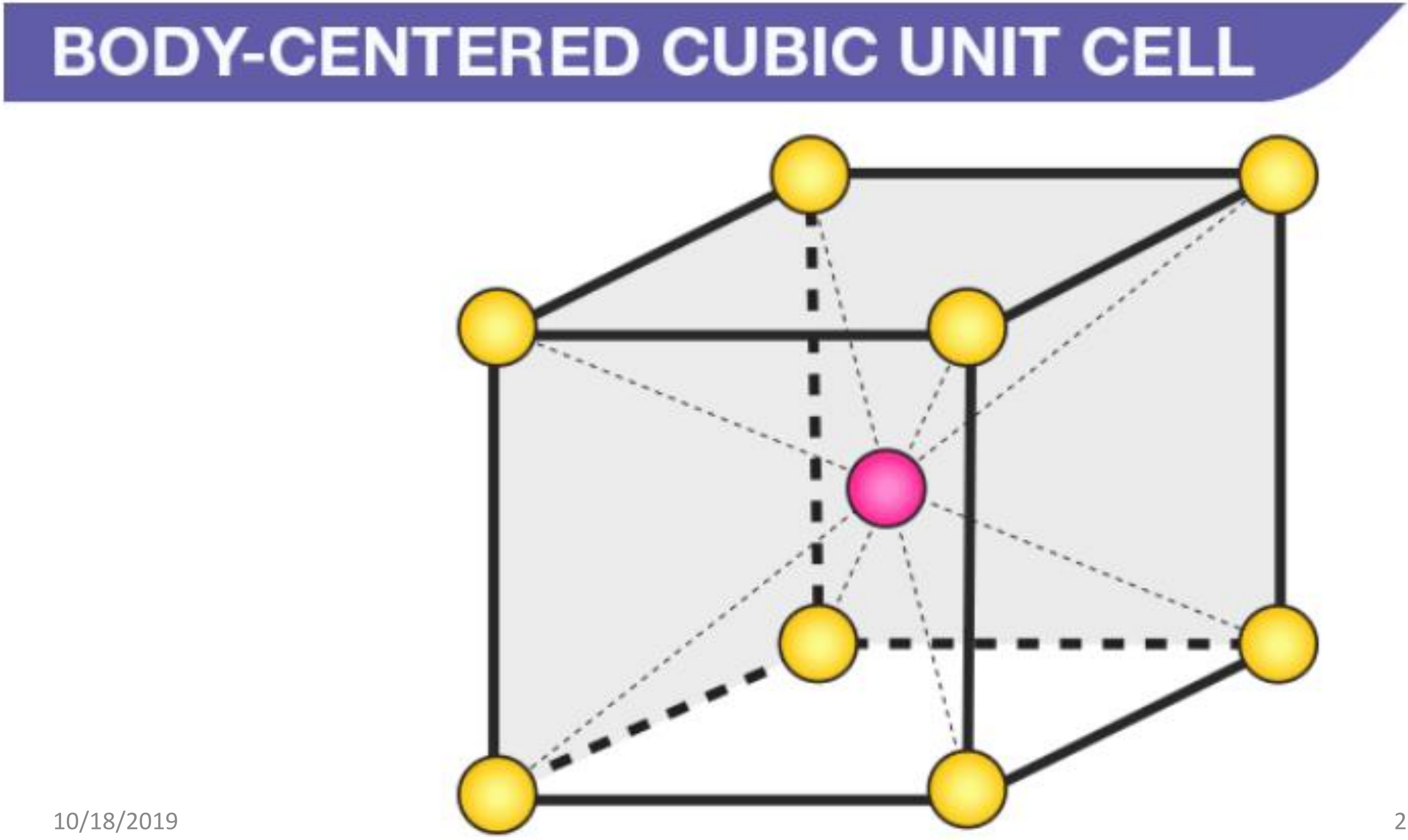


Simple cubic(SC)

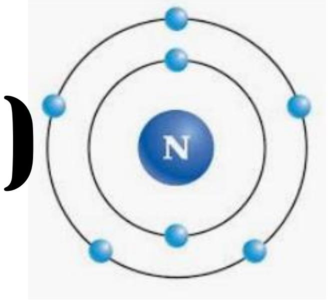


Body centered cubic(BCC)

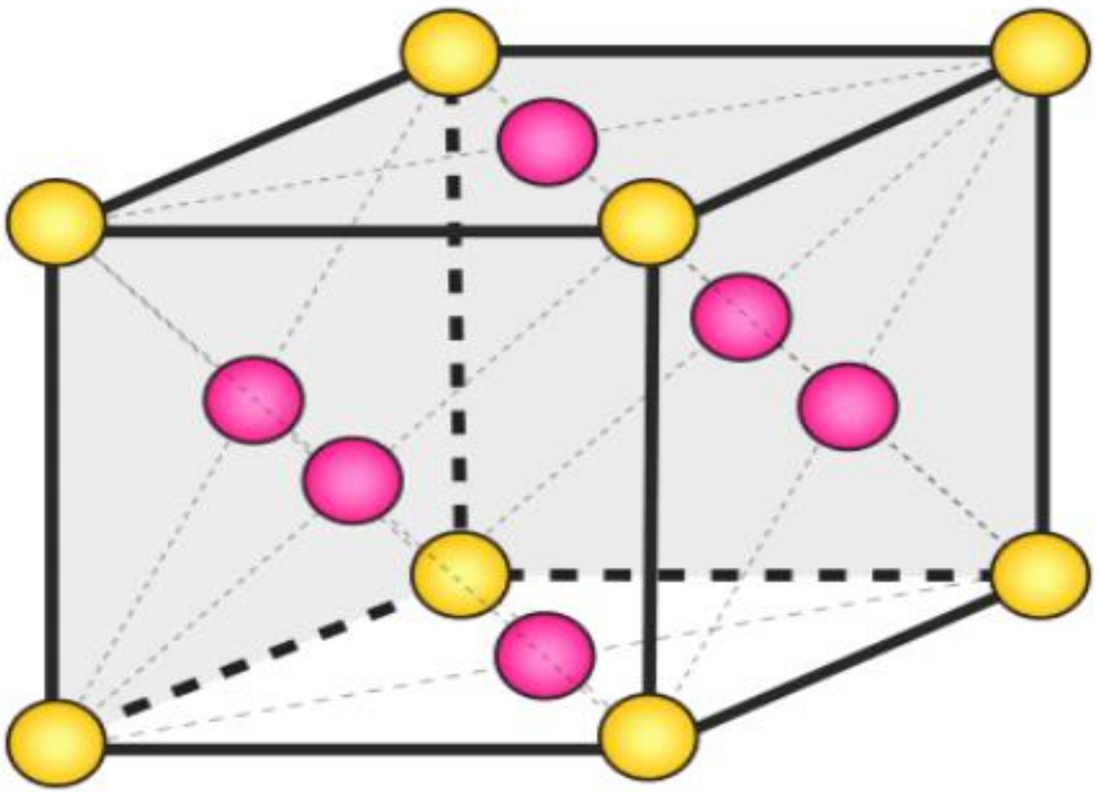



BODY-CENTERED CUBIC UNIT CELL

Face centered cubic(FCC)

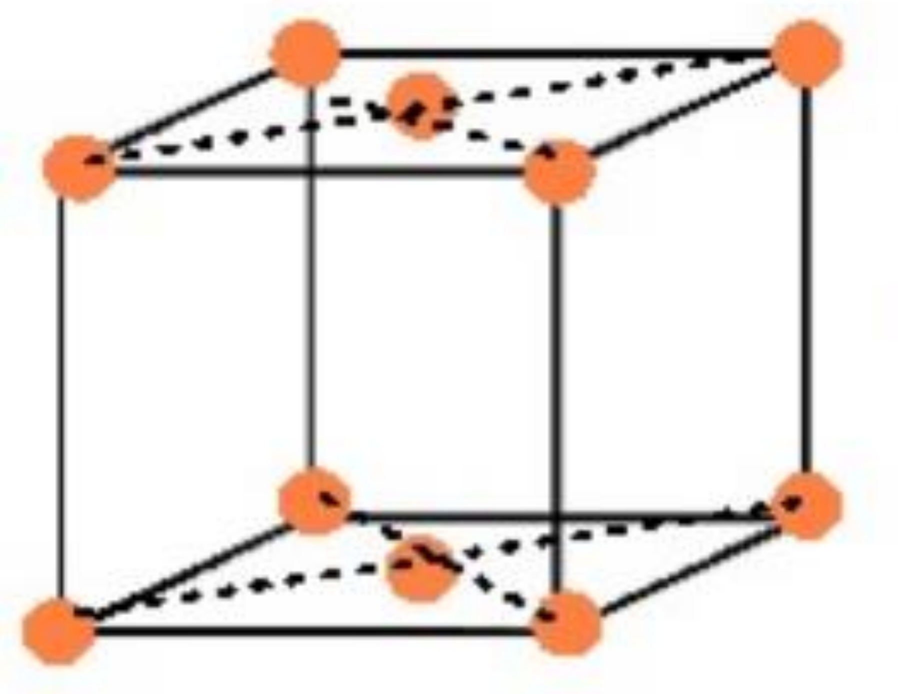


FACE-CENTERED CUBIC UNIT CELL



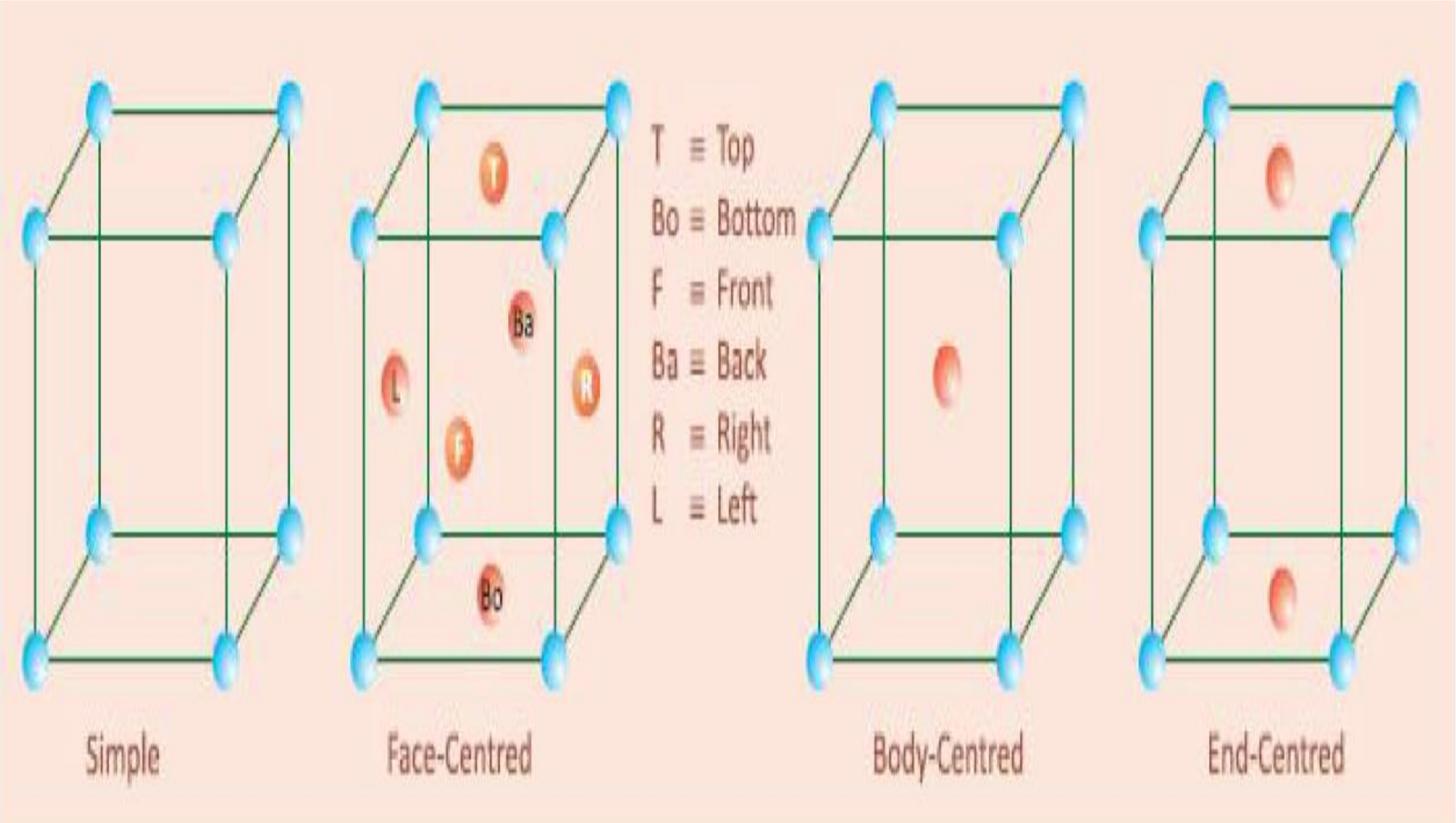
End face centered(EFC)

- ***End-Centred Unit Cells:***

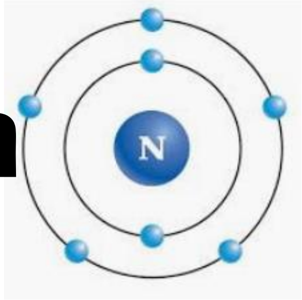


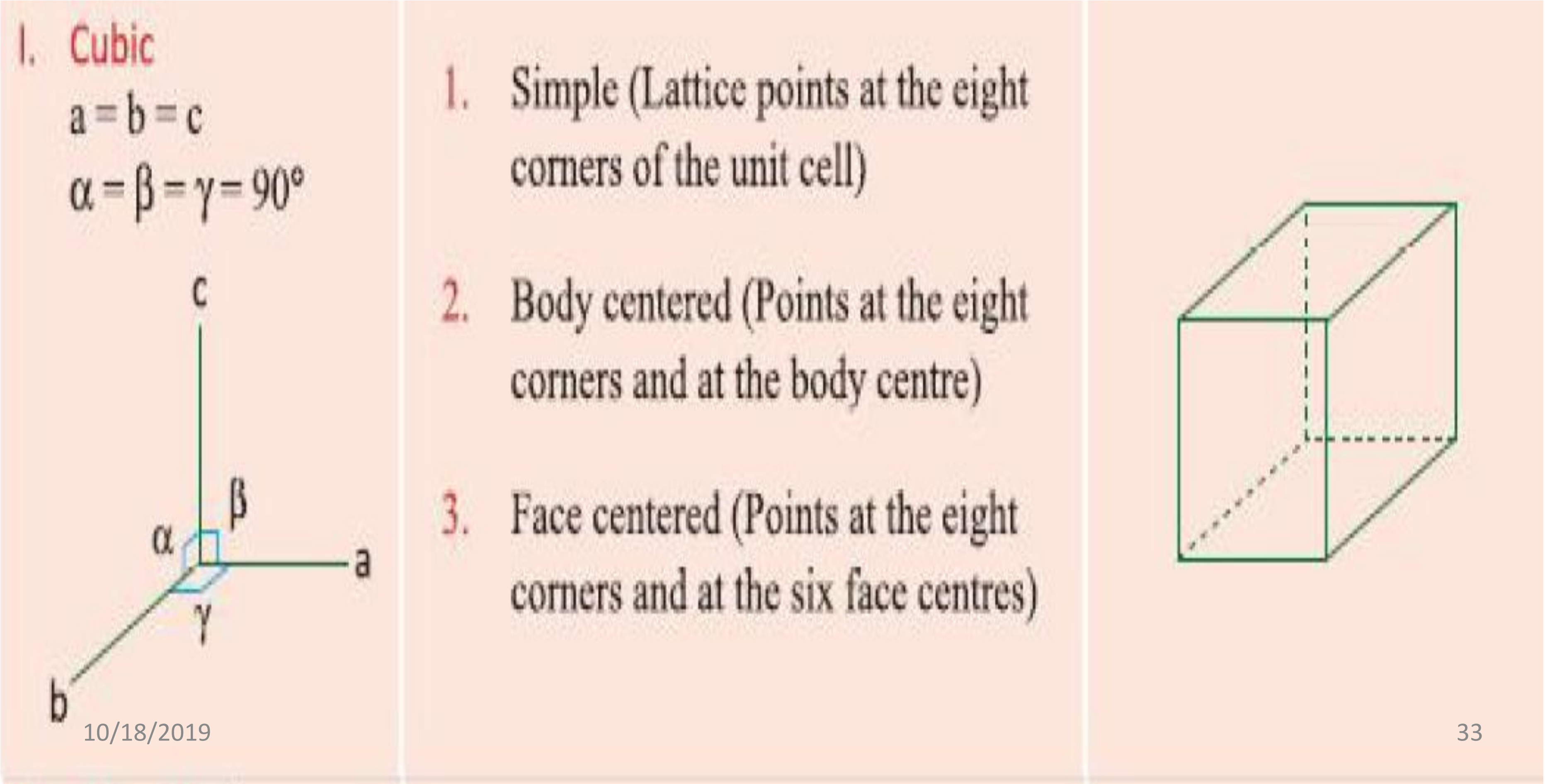
End Centered Unit Cell

UNIT CELLS


T ≡ Top
Bo ≡ Bottom
F ≡ Front
Ba ≡ Back
R ≡ Right
L ≡ Left
T
Ba
L
R
F
Bo
Simple
Face-Centred
Body-Centred
End-Centred

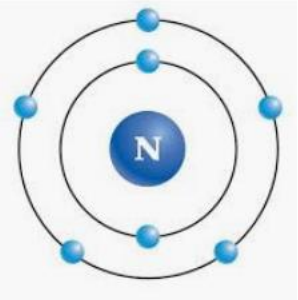
Cubic crystal SYStem

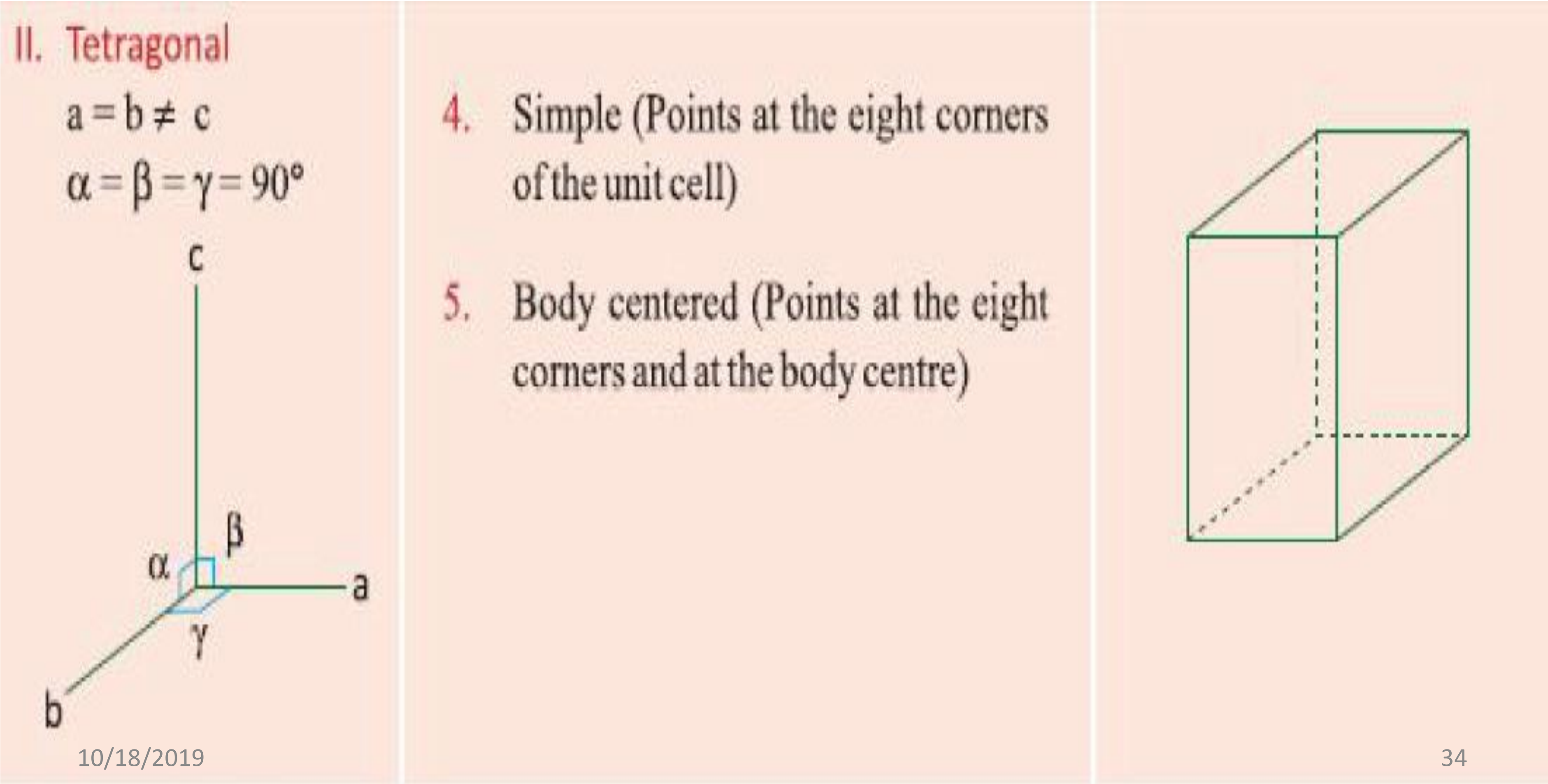




I. Cubic $a = b = c$ $\alpha = \beta = \gamma = 90°$	1. Simple (Lattice points at the eight corners of the unit cell) 2. Body centered (Points at the eight corners and at the body centre) 3. Face centered (Points at the eight corners and at the six face centres)

Tetragonal crystal SYS





II. Tetragonal

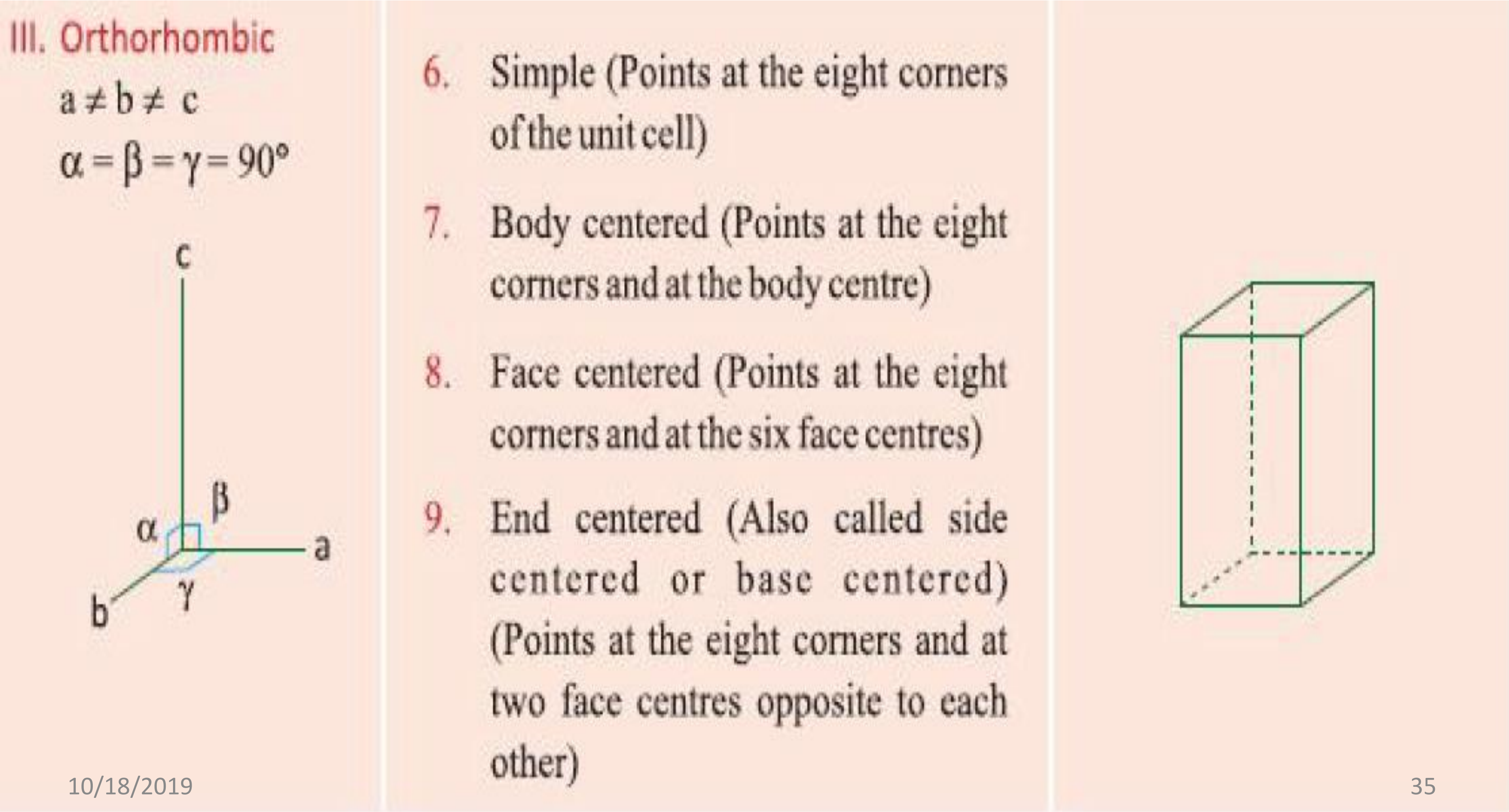
$a = b \neq c$

$\alpha = \beta = \gamma = 90°$

4. Simple (Points at the eight corners of the unit cell)

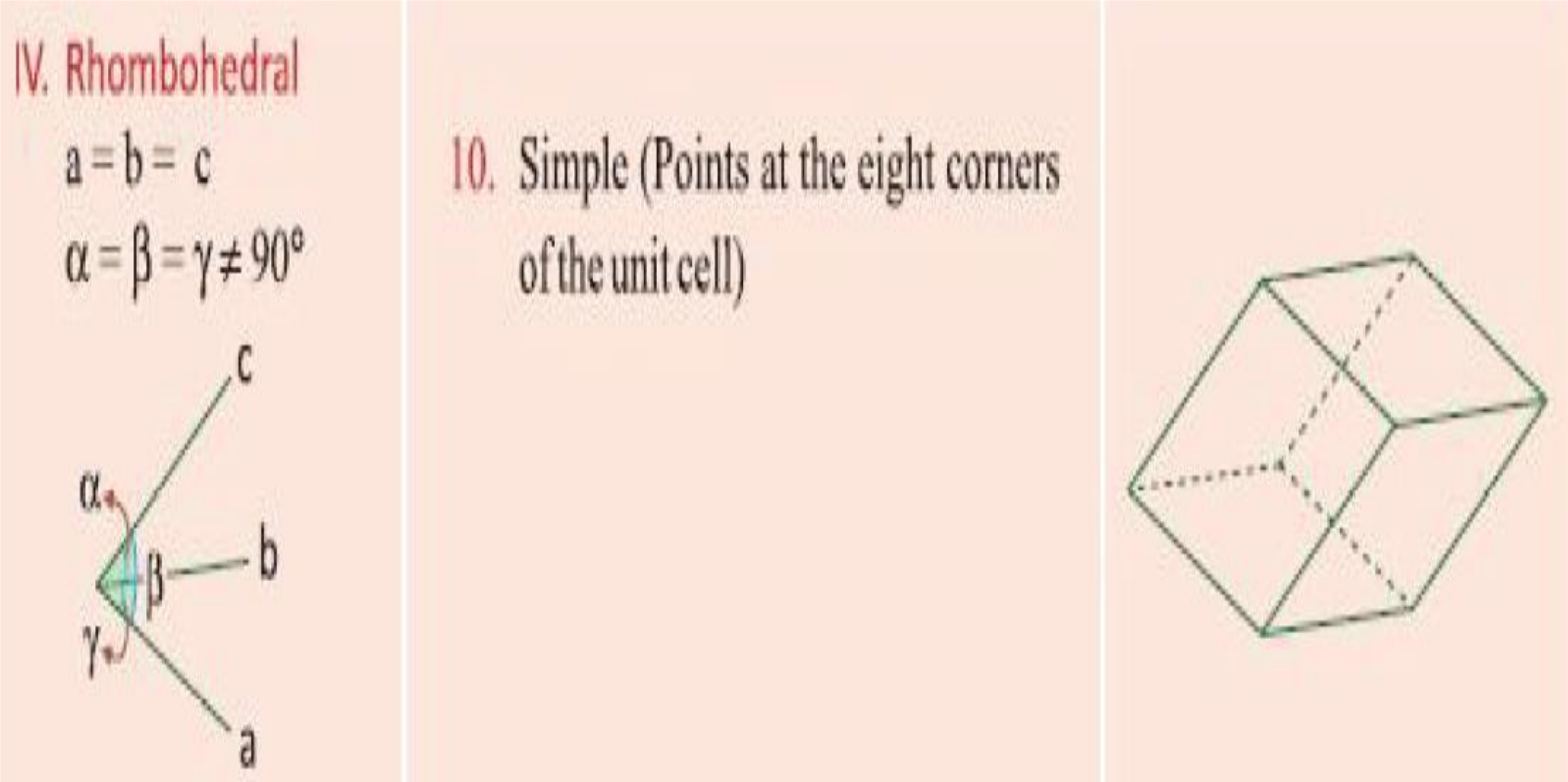
5. Body centered (Points at the eight corners and at the body centre)

Orthorhombic CRY SYS



III. Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	6. Simple (Points at the eight corners of the unit cell) 7. Body centered (Points at the eight corners and at the body centre) 8. Face centered (Points at the eight corners and at the six face centres) 9. End centered (Also called side centered or base centered) (Points at the eight corners and at two face centres opposite to each other)	

Rhombohedral CRY SYS



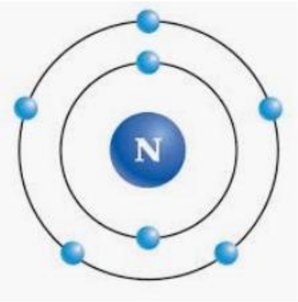
IV. Rhombohedral

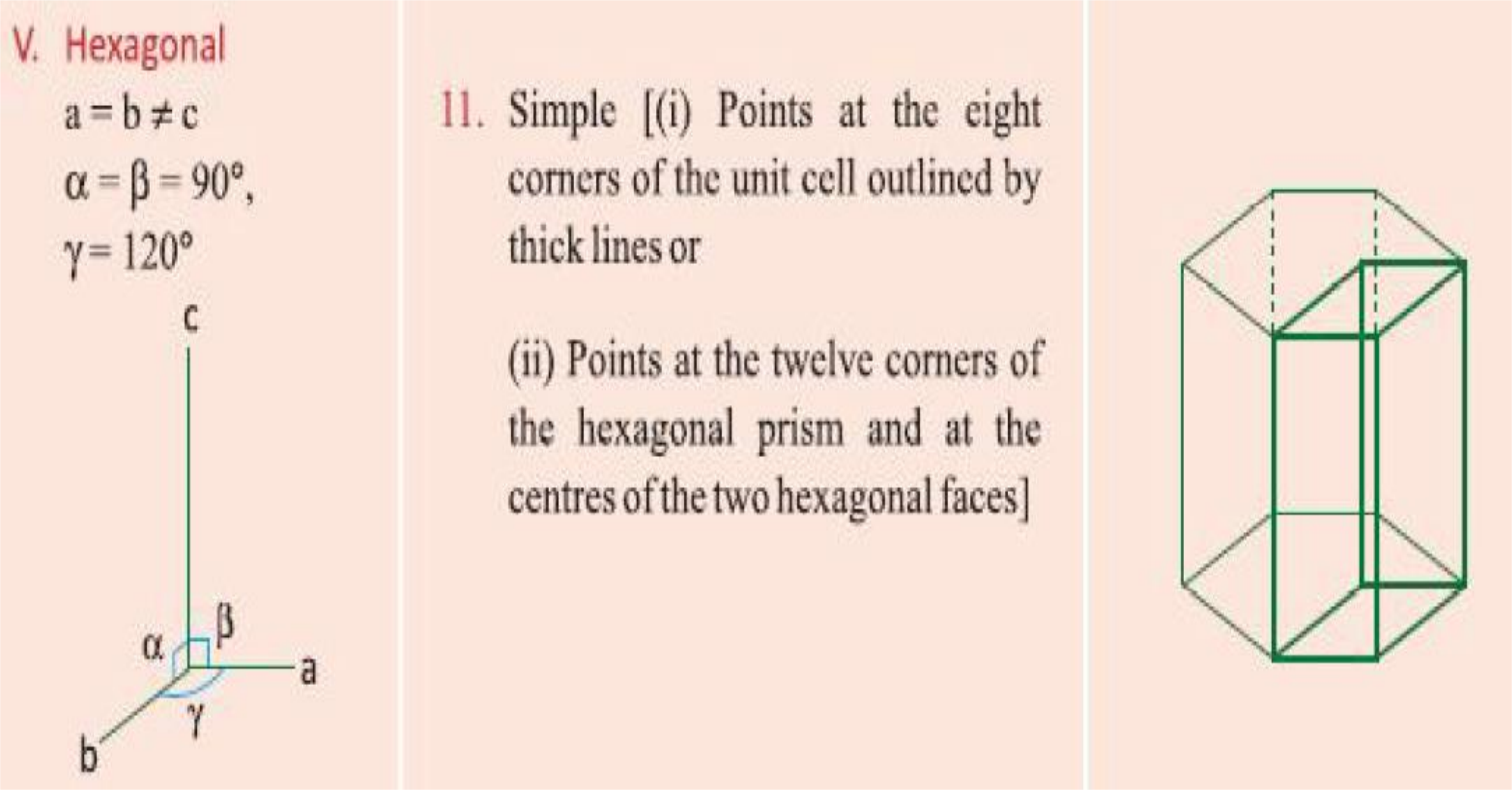
$a = b = c$

$\alpha = \beta = \gamma \neq 90°$

10. Simple (Points at the eight corners of the unit cell)

Hexagonal CRY SYS





V. Hexagonal

$a = b \neq c$

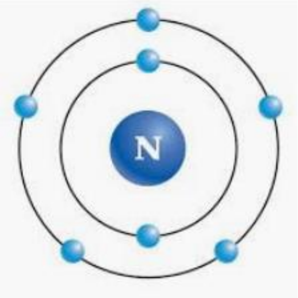
$\alpha = \beta = 90°$,

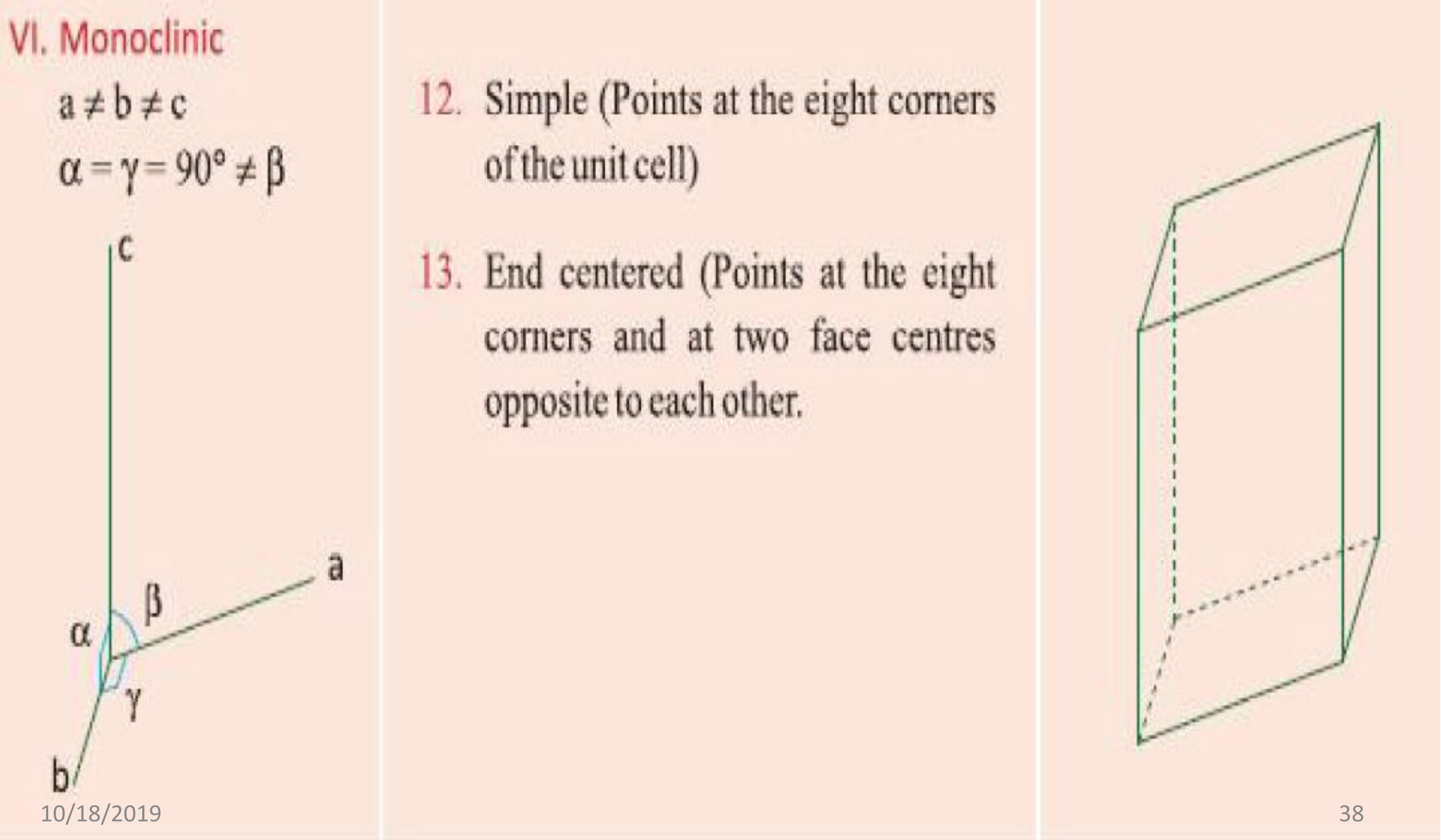
$\gamma = 120°$

11. Simple [(i) Points at the eight corners of the unit cell outlined by thick lines or

(ii) Points at the twelve corners of the hexagonal prism and at the centres of the two hexagonal faces]

Monoclinic CRY SYS





VI. Monoclinic

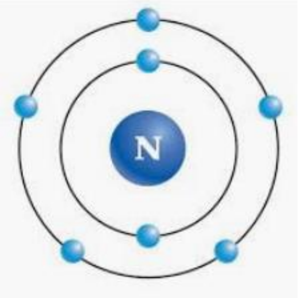
$a \neq b \neq c$

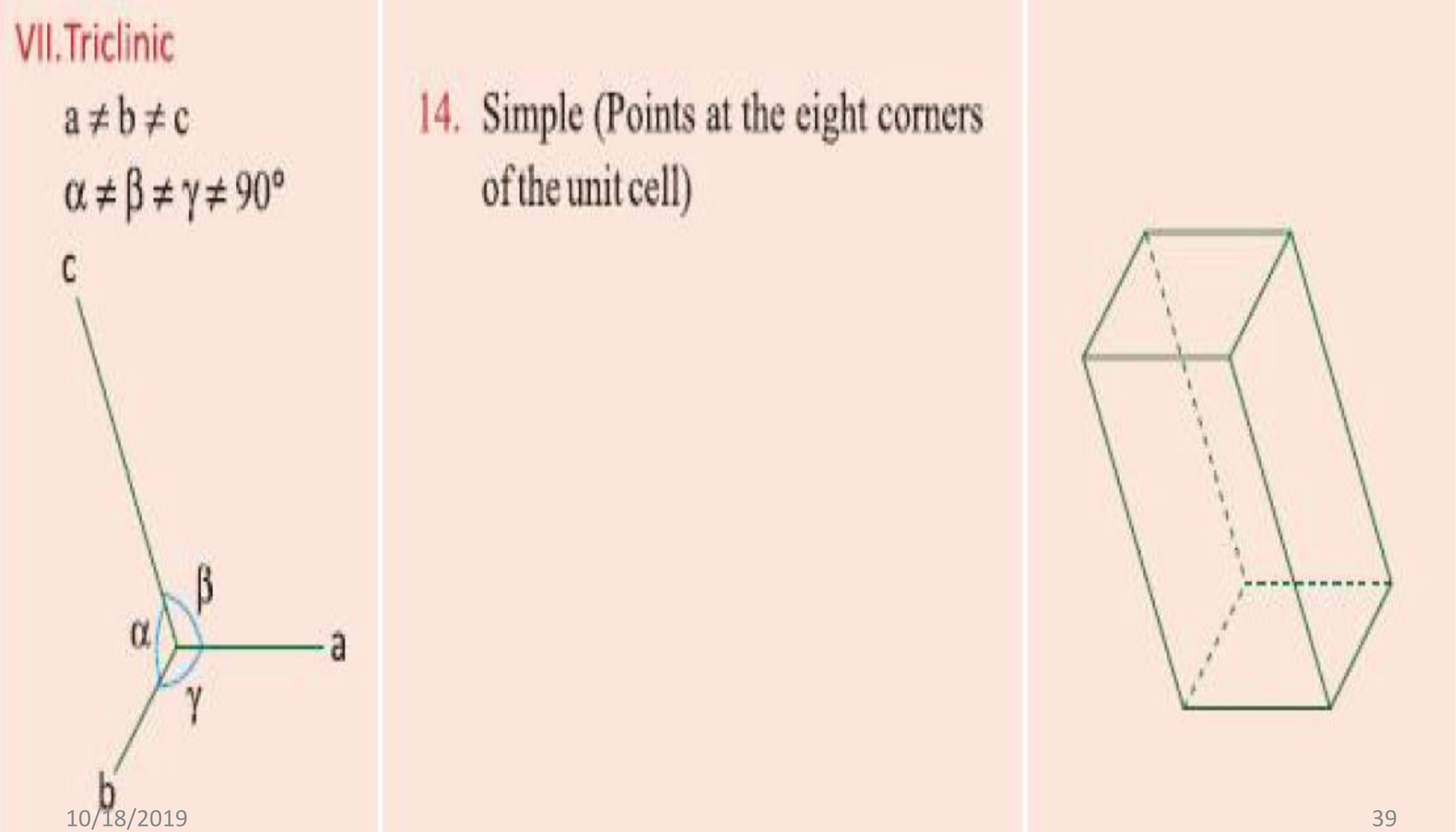
$\alpha = \gamma = 90° \neq \beta$

12. Simple (Points at the eight corners of the unit cell)

13. End centered (Points at the eight corners and at two face centres opposite to each other.

Triclinic CRY SYS





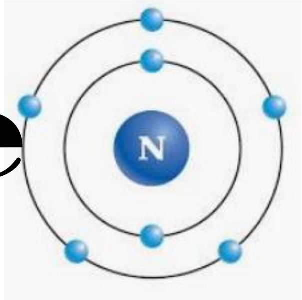
VII.Triclinic

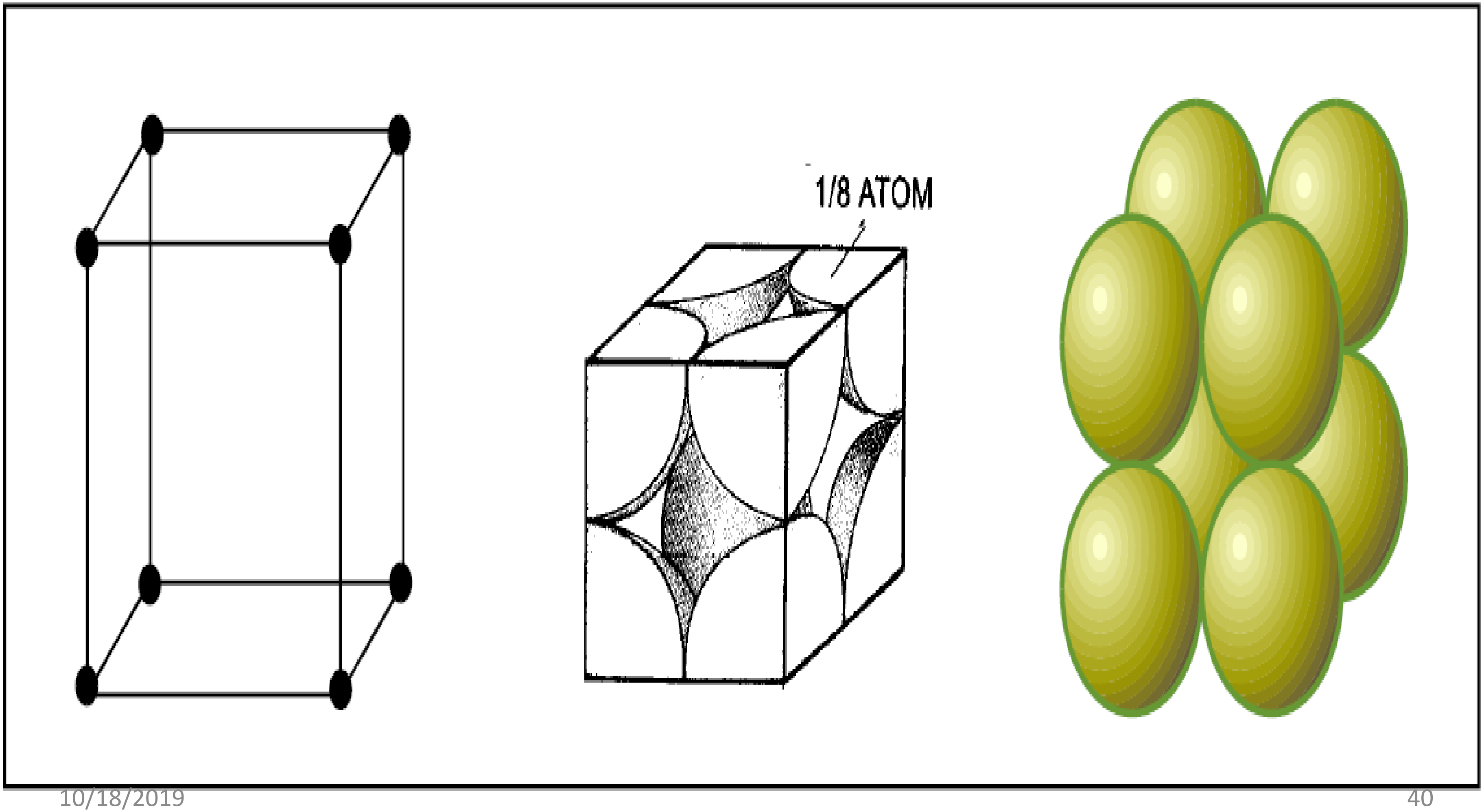
$a \neq b \neq c$

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

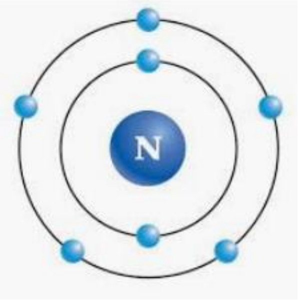
14. Simple (Points at the eight corners of the unit cell)

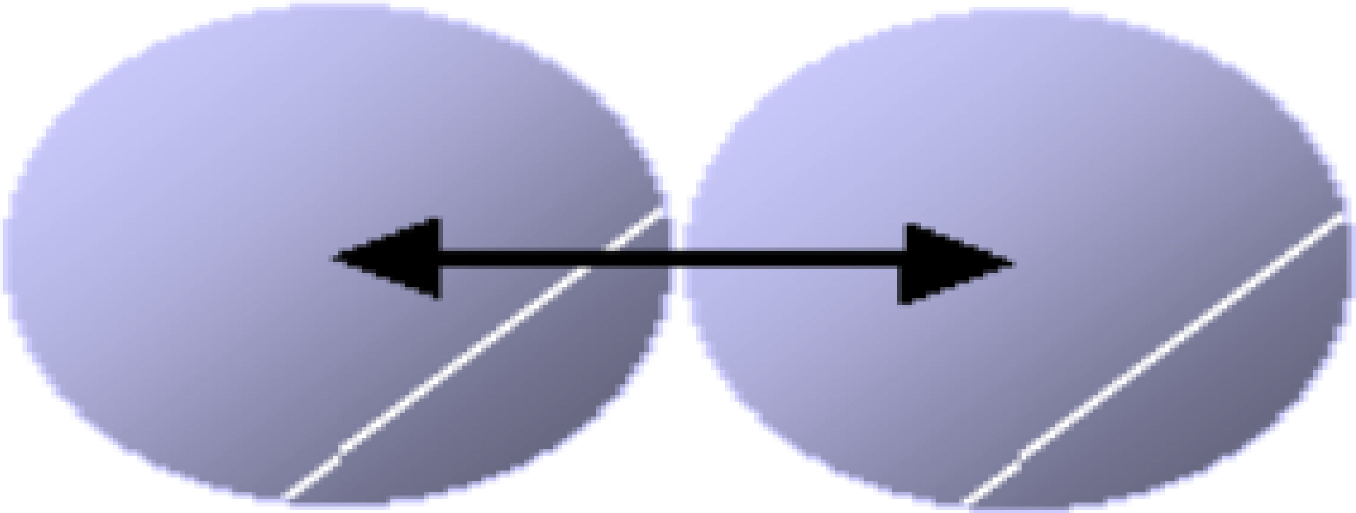
Simple cubic/primitive





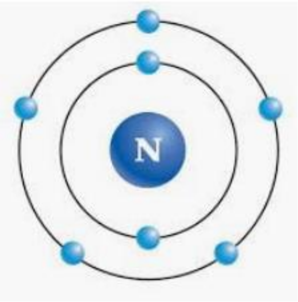
Radius of primitive

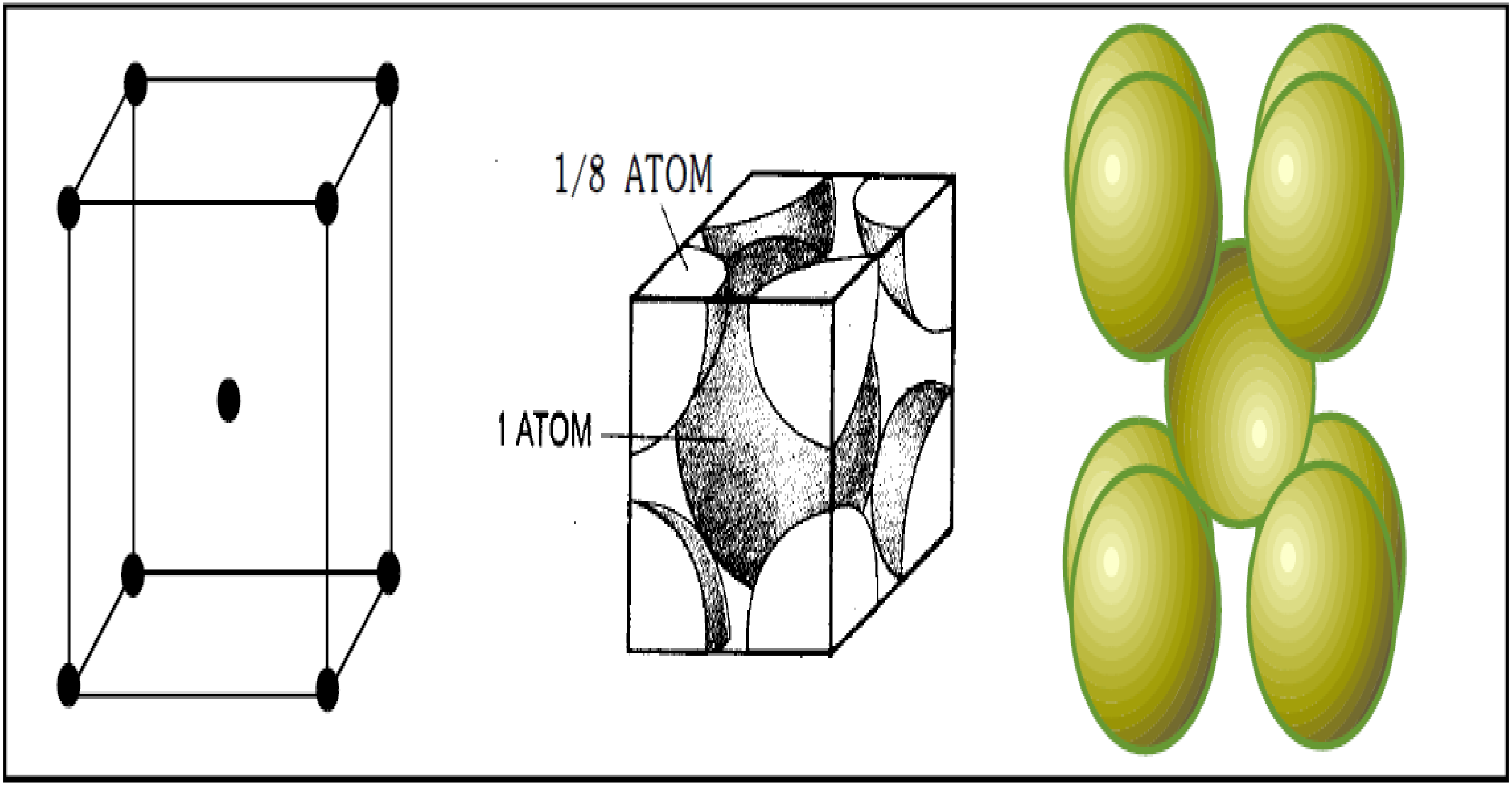




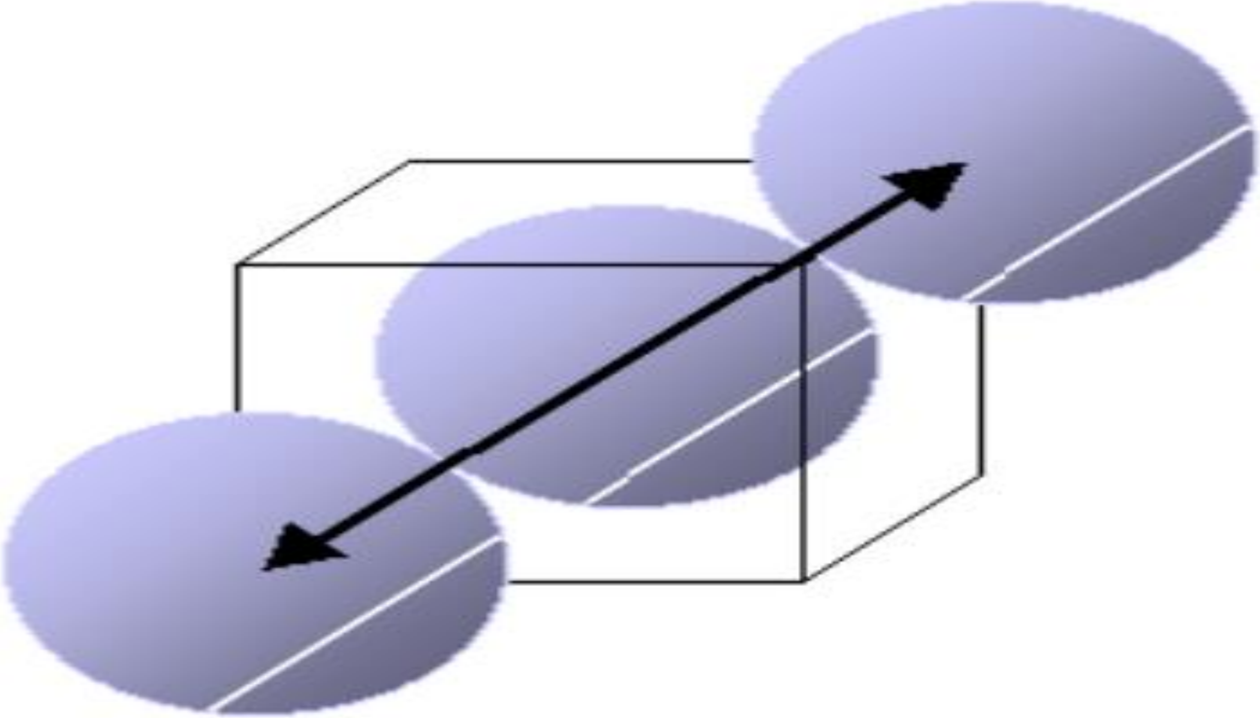
$$a = 2r$$

Body centered cubic



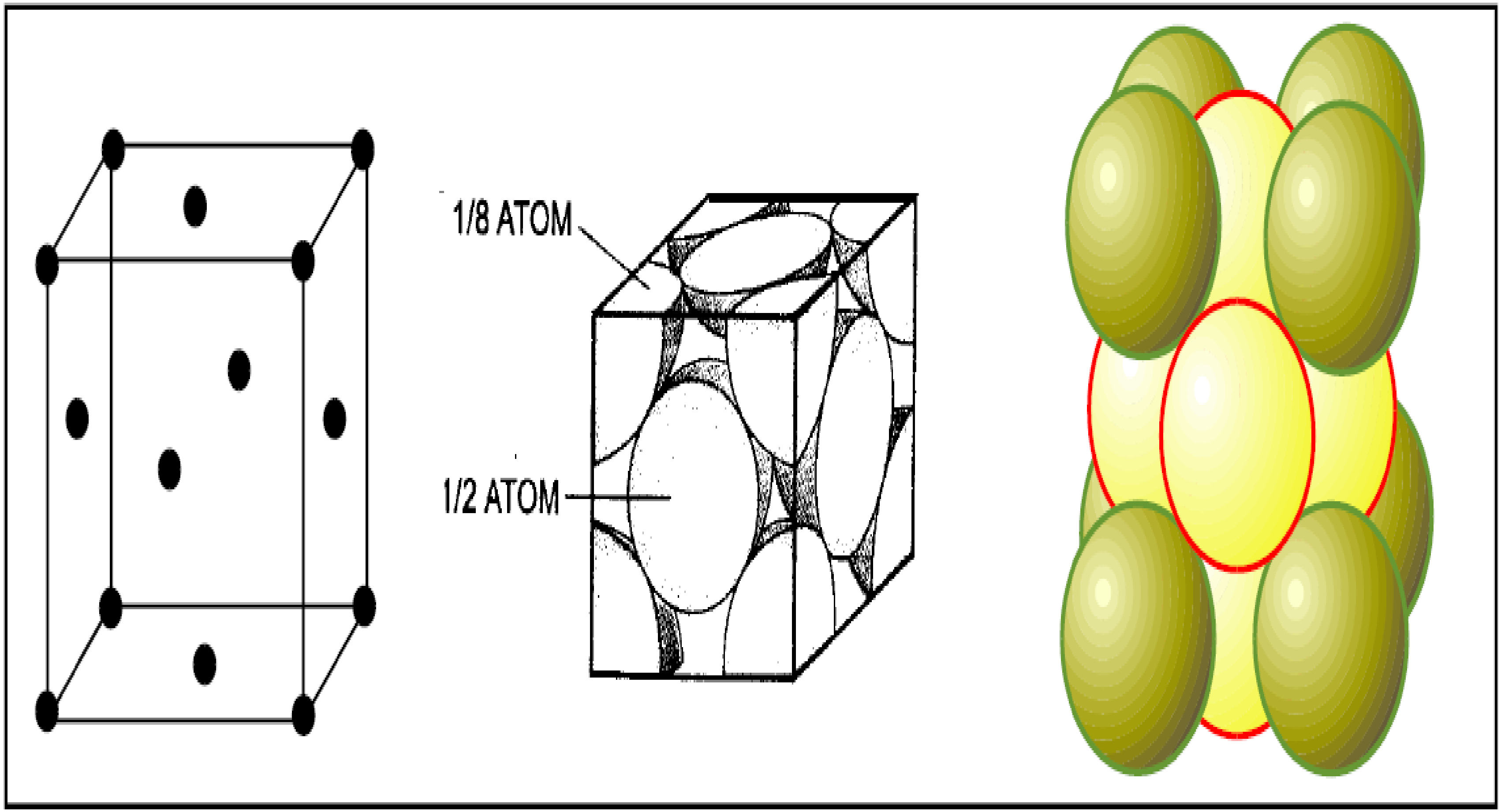


BCC radius

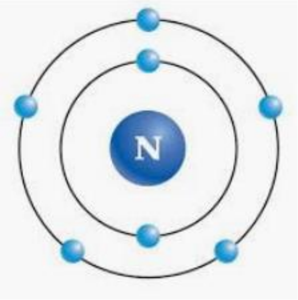


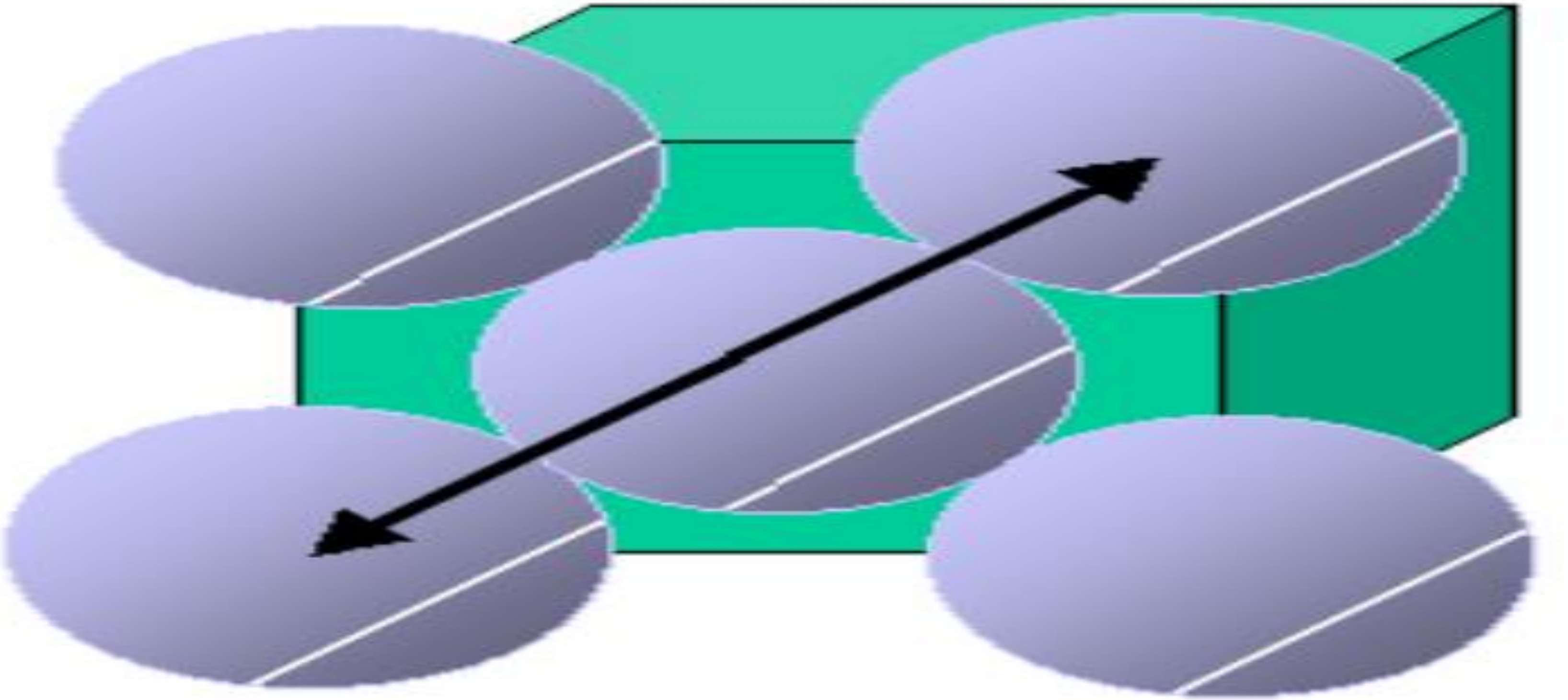
$$4r = (3)^{1/2}\ a$$

FCC



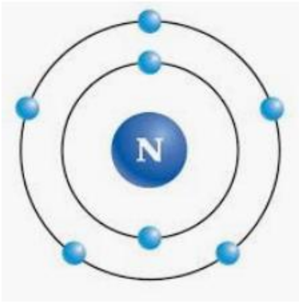
FCC radius



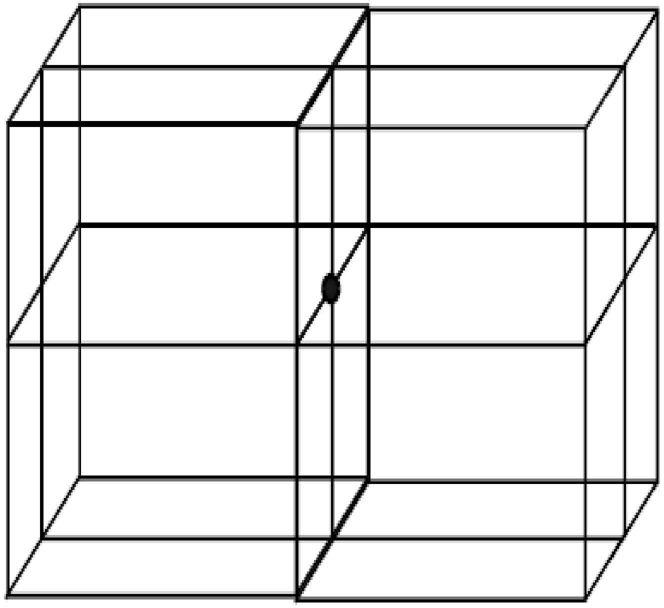


$$4r = (2)^{1/2}\ a$$

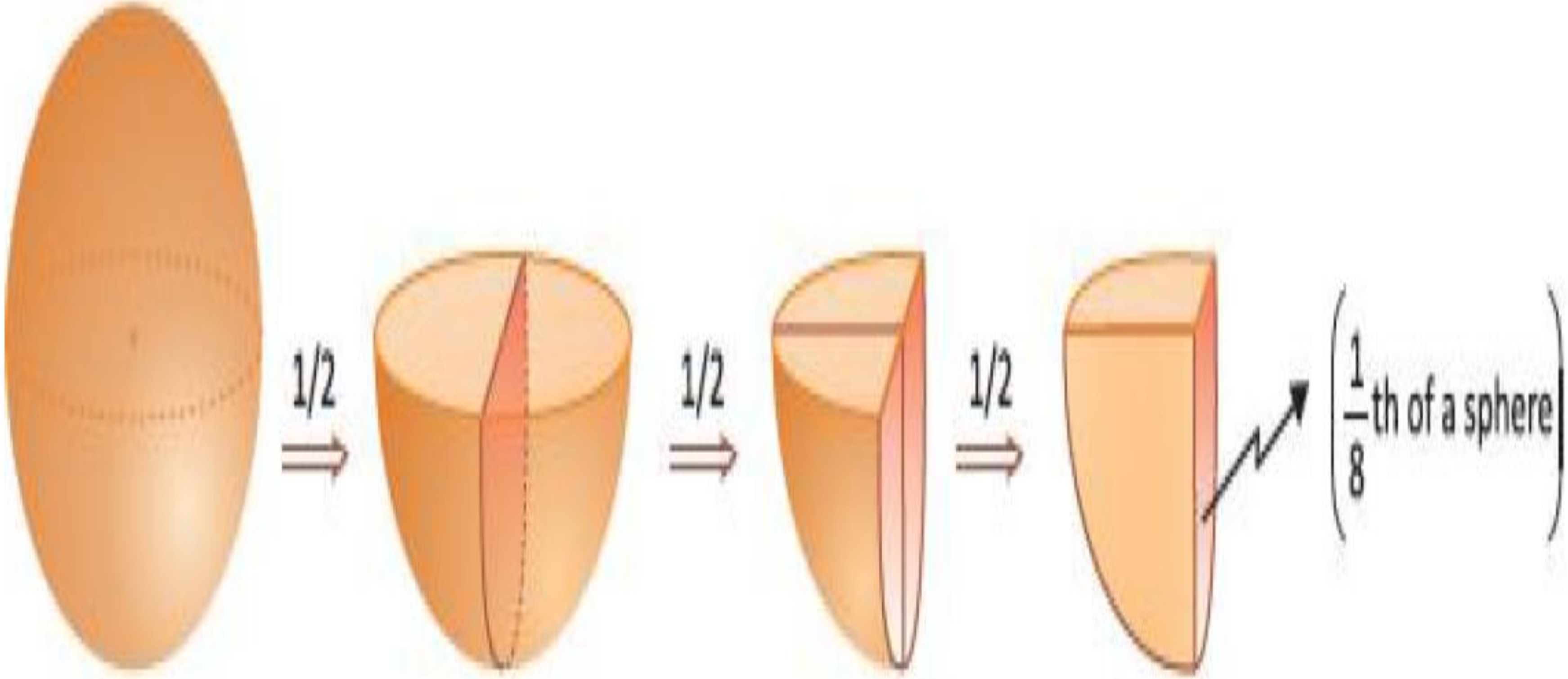
CORNER CONTRI



A corner of a cube is common in 8 cubes. So $\frac{1}{8}$ th part of an atom is present at this corner of cube.

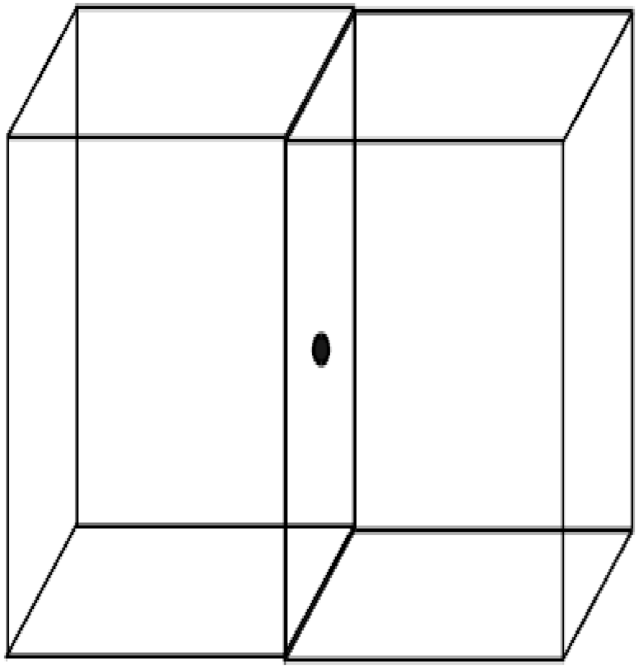


Corner contribution

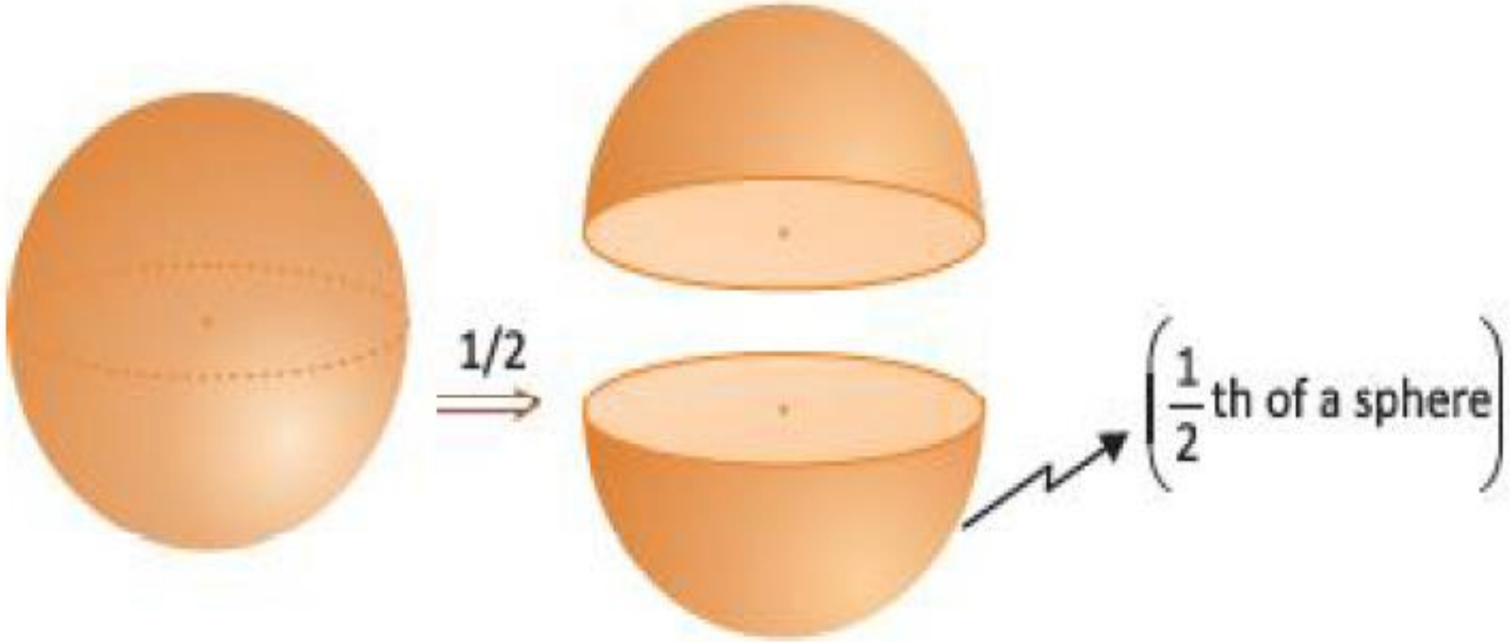


Face contribution

A face of a cube is common is 2 cubes. So $\frac{1}{2}$ th part of of an atom is present at the face of a cube.

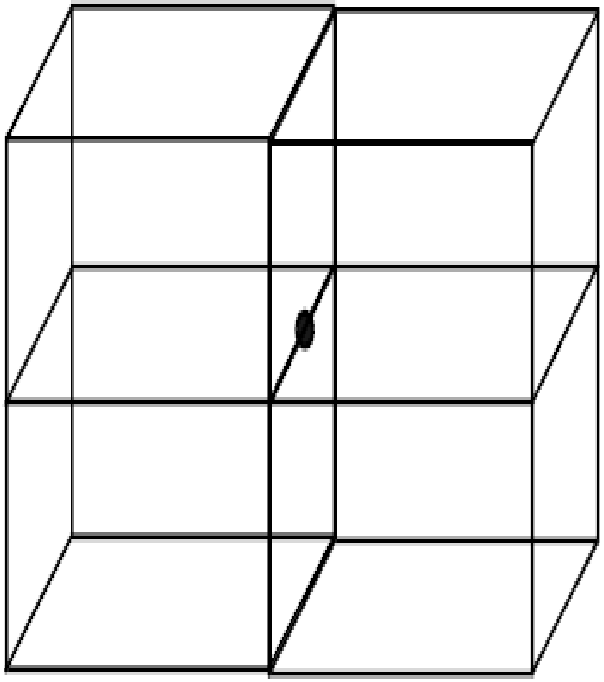


Face contribution

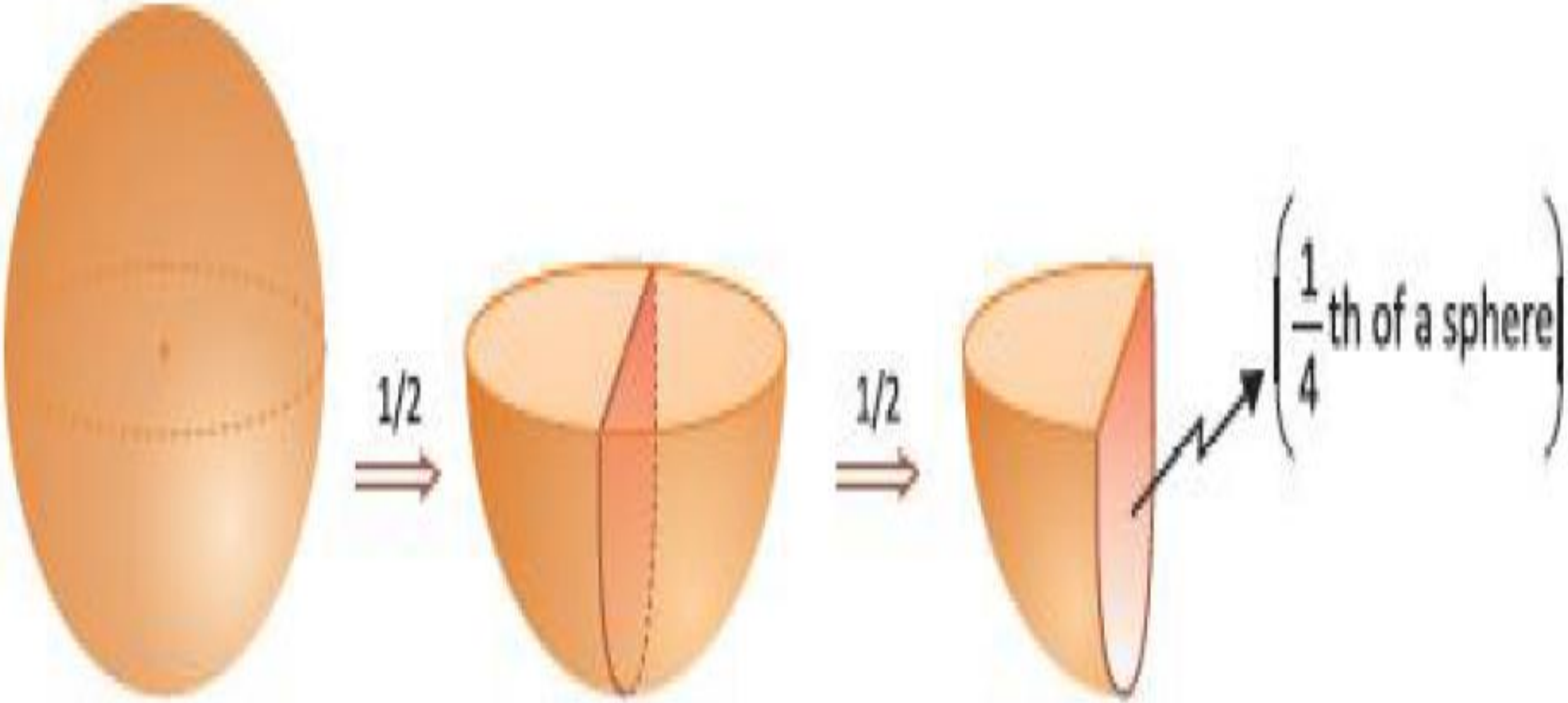


Edge contribution

An edge of a cube is common in four cubes, so $\frac{1}{4}$th part of the atom is present at the edge of a cube

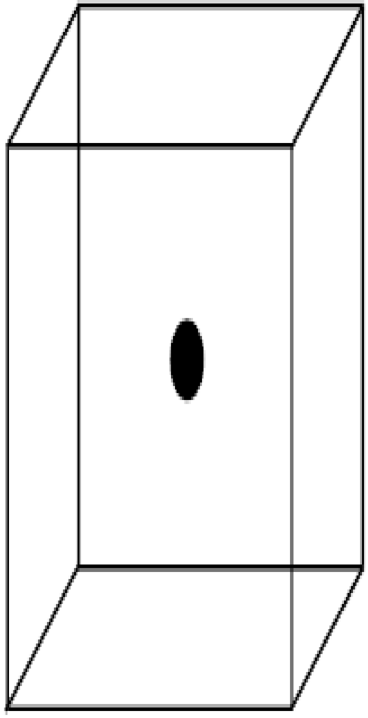


EDGE CONTRI

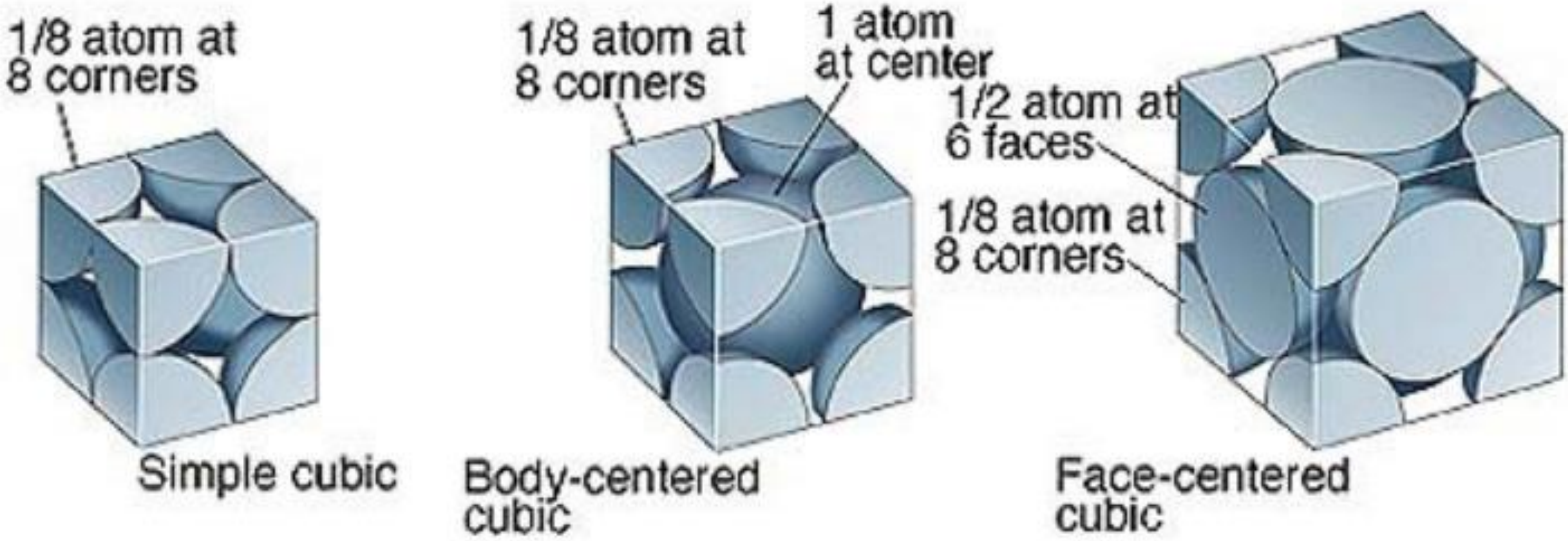


Center contribution

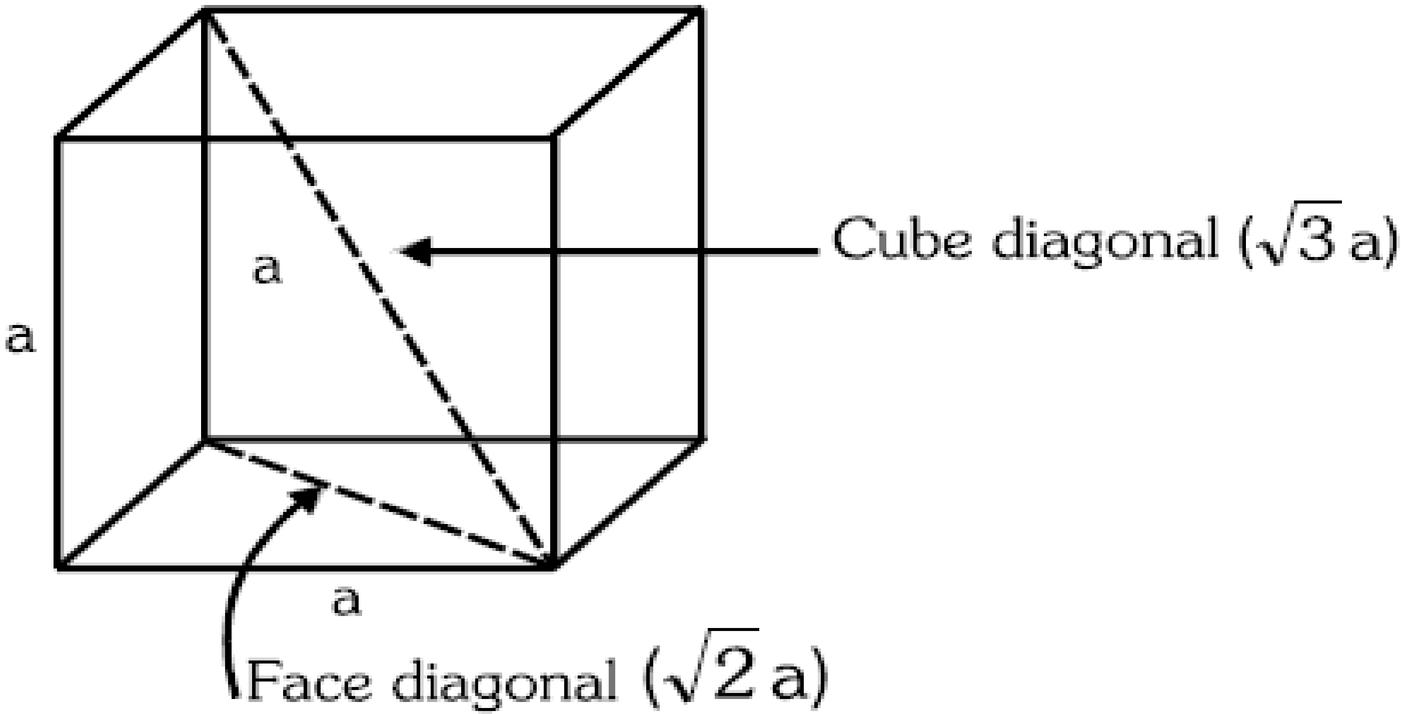
A cube centre is not common in any another cube, so one complete atom is present at the cube centre.



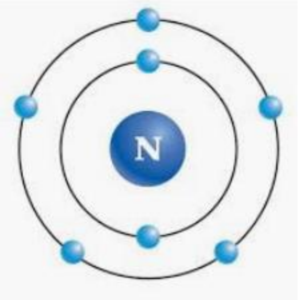
Contribution



body VS face diagonal



EFFECTIVE NUMBER



$$\text{Total number of atoms in unit cell} = \frac{n_e}{8} + \frac{n_f}{2} + \frac{n_i}{1} + \frac{n_e}{4}$$

When n_c : Number of atom at the corners of the unit cell

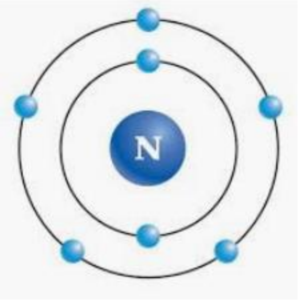
n_f : Number of atoms at six faces of the unit cell

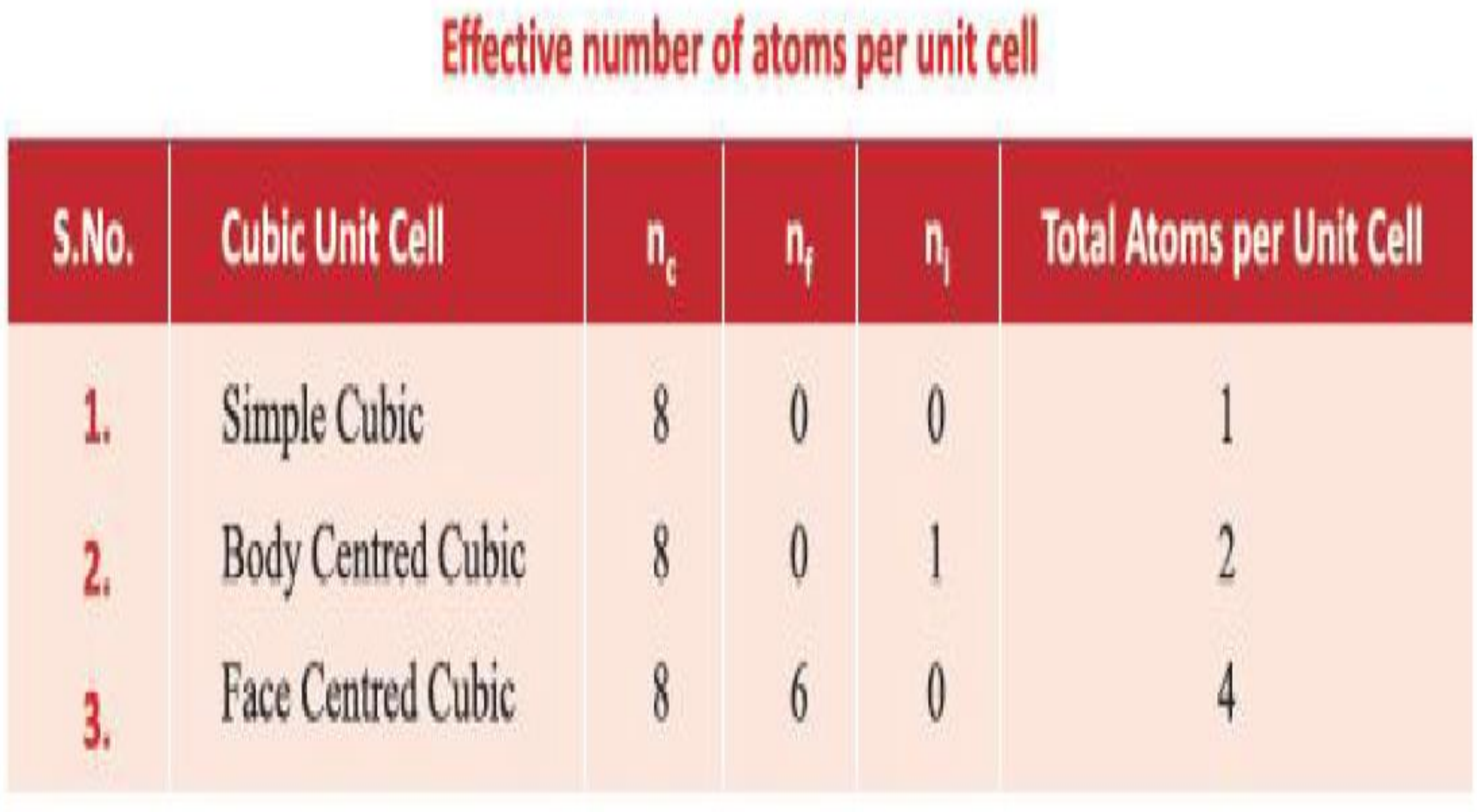
n_i : Number of atoms completely inside the unit cell

n_e : Number of atoms at the edge centres of the unit cell

Effective number of atoms per unit cell

EFFECTIVE NUMBER

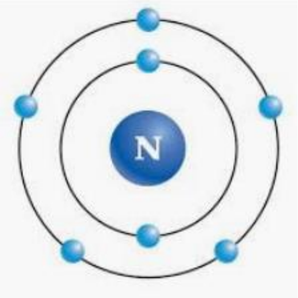




Effective number of atoms per unit cell

S.No.	Cubic Unit Cell	n_c	n_f	n_i	Total Atoms per Unit Cell
1.	Simple Cubic	8	0	0	1
2.	Body Centred Cubic	8	0	1	2
3.	Face Centred Cubic	8	6	0	4

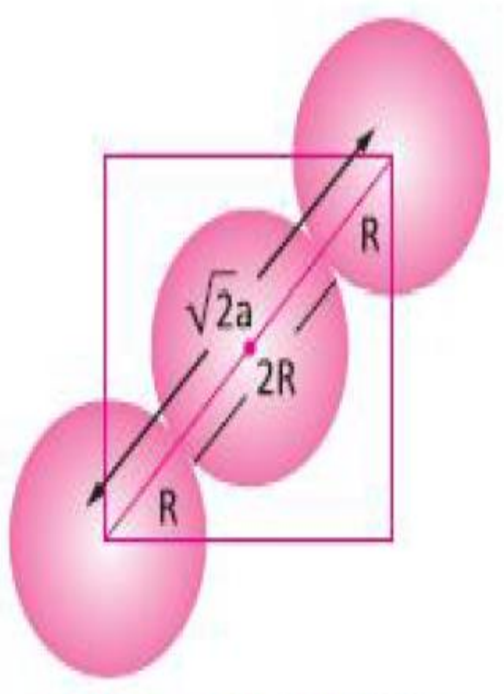
RADIUS OF FCC



Relation between radius of constituent particles and edge length of unit cell

Closest contact is along face diagonal of cube. Each corner of a particular face centre atom touches the face centre atom such that :

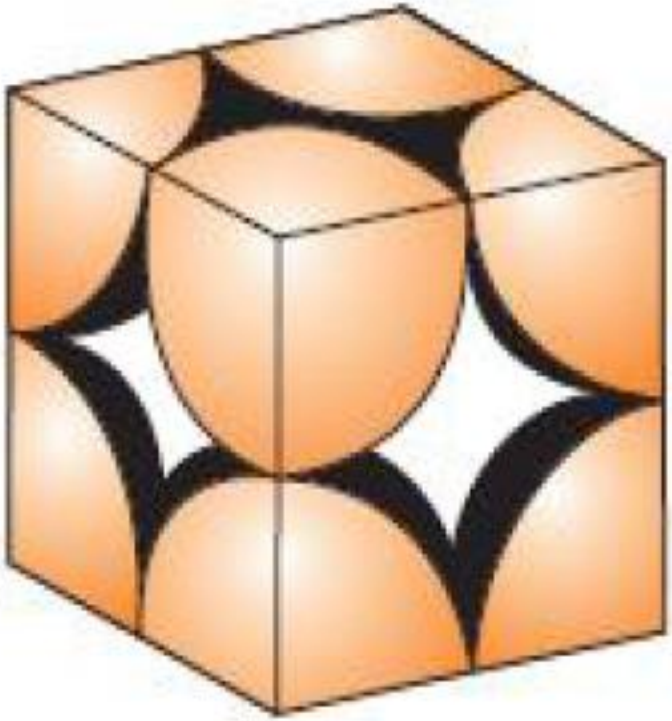
$$2R = \frac{a}{\sqrt{2}} \Rightarrow R = \frac{a}{2\sqrt{2}} \text{ or } \sqrt{2}a = 4R$$



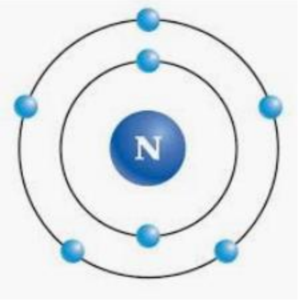
Closest contact is along face diagonal of cube

SCC

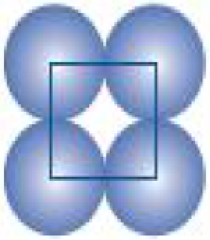
Arrangement of constituent particles in simple cubic.



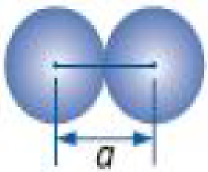
Radius of SCC



Top View of Unit Cell :



Relation between edge length of unit cell and radius of constituent particles.



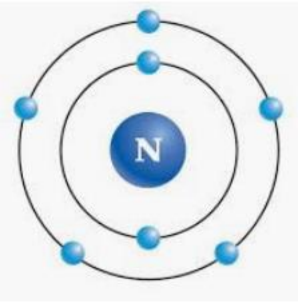
Each corner atom is in contact with its adjacent corner atom such that

$$2R = a \Rightarrow R = \frac{a}{2}$$

Rank of the unit cell (z) : Effective number of constituent particles per unit cell.

$$z = n_c \times \frac{1}{8} = 8 \times \frac{1}{8} = 1$$

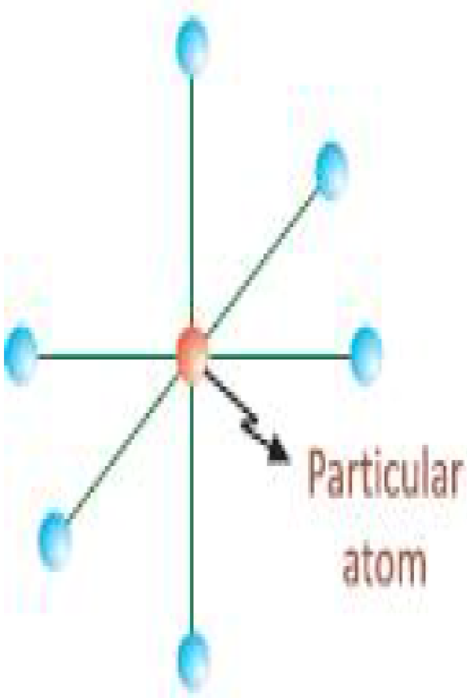
SC coordination no



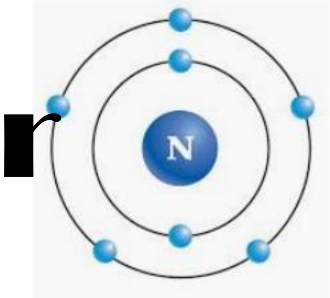
Simple Cubic (SC)

No. of atoms surrounding the (touching) the body centre atom = 6

Hence, Co-ordination No. = 6



SC nearest neighbour

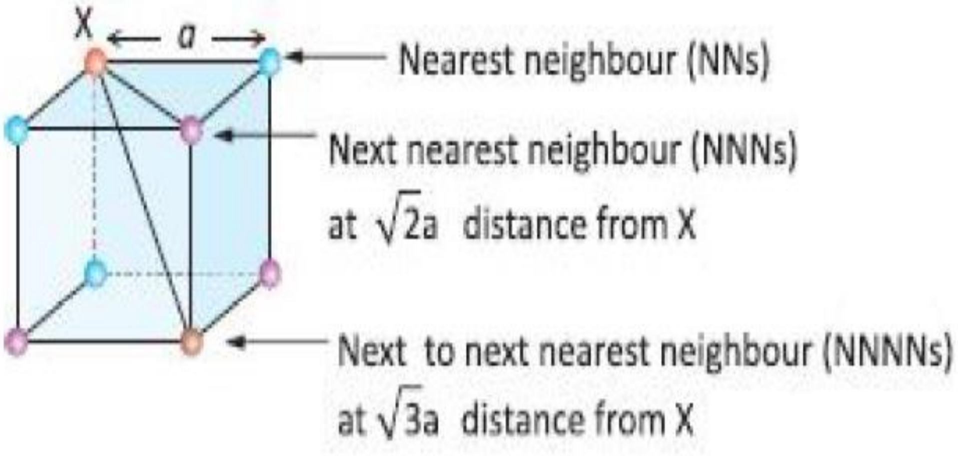


NNs is at ‘a’ distance from ‘X’ (NNs = 3)

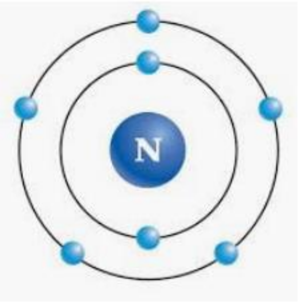
NNNs is at $\sqrt{2}$ a distance from ‘X’ (NNNs = 3)

NNNNs is at $\sqrt{3}$ a distance from X (NNNNs = 1)

In a simple cubic system for particle ‘X’



SCC PE



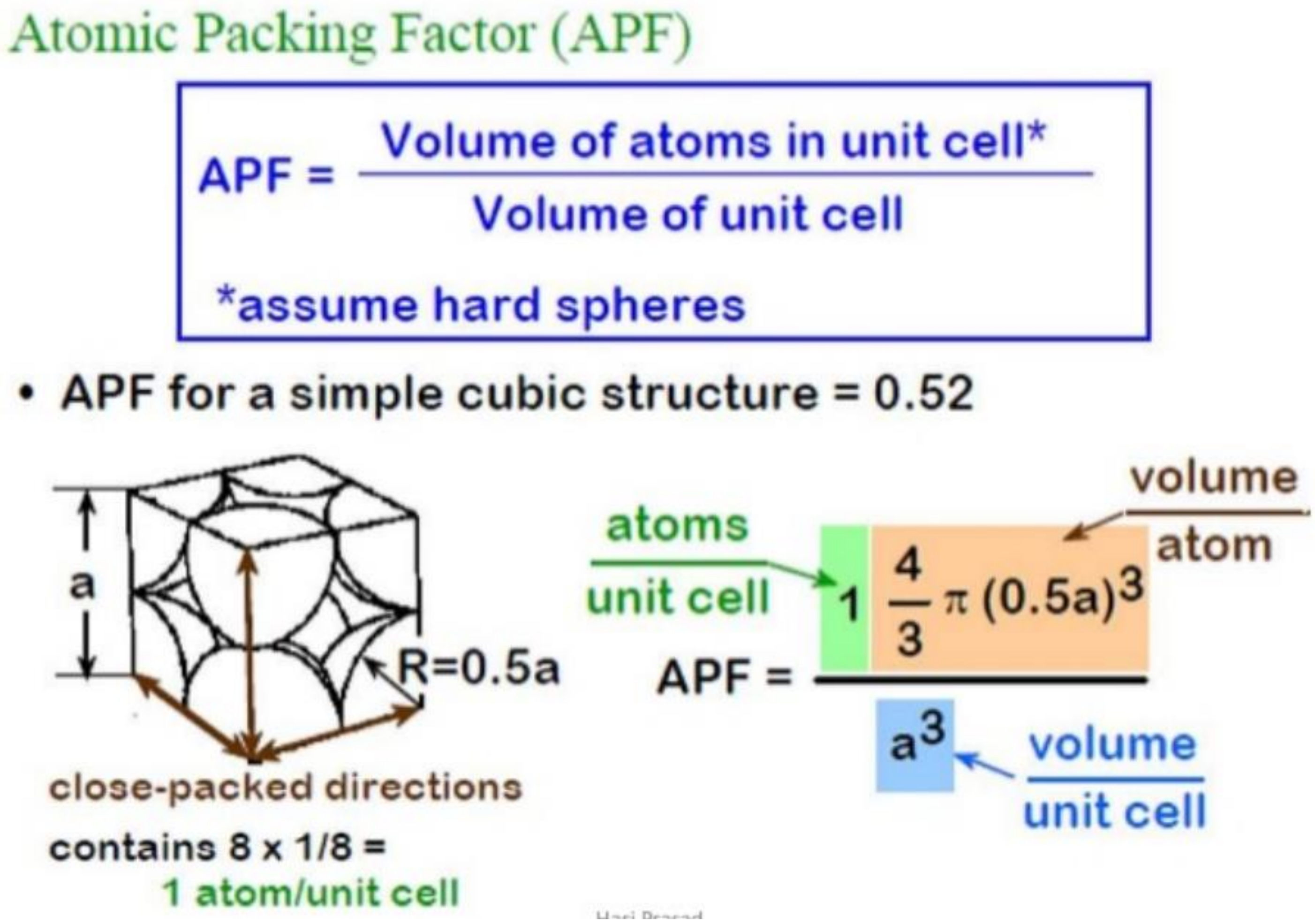
Packing Efficiency :

$$\text{Packing efficiencey} = \frac{\text{volume occupied by all constituent}}{\text{Volume of unit cell}}$$

For cubic unit cell

$$\text{Packing efficiency} = \frac{z \times \frac{4}{3}\pi r^3}{a^3} = \frac{1 \times \frac{4}{3}\pi r^3}{a^3} = \frac{1 \times \frac{4}{3}\pi r^3}{(2r)^3} = 0.52$$

APF of SC



Atomic Packing Factor (APF)

$$APF = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}}$$

*assume hard spheres

- APF for a simple cubic structure = 0.52

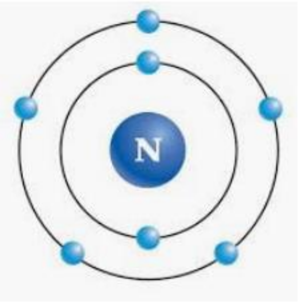
close-packed directions

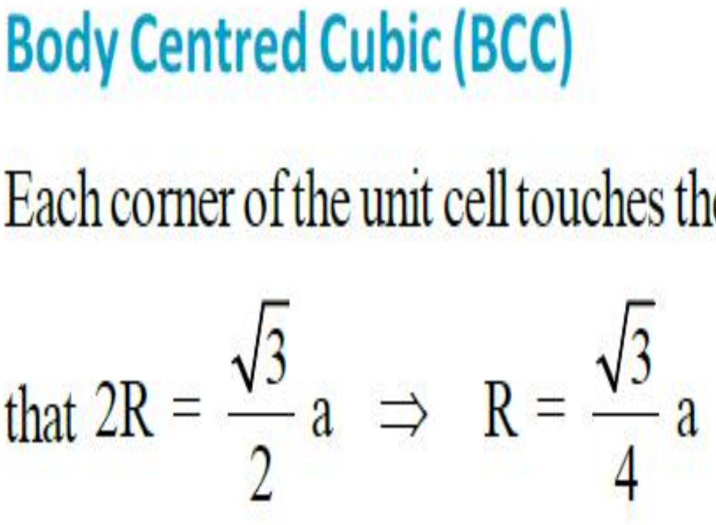
contains 8 x 1/8 =
1 atom/unit cell

$$APF = \frac{\overset{\frac{\text{atoms}}{\text{unit cell}}}{1}\ \overset{\frac{\text{volume}}{\text{atom}}}{\frac{4}{3}\pi(0.5a)^3}}{\underset{\frac{\text{volume}}{\text{unit cell}}}{a^3}}$$

Hari Prasad

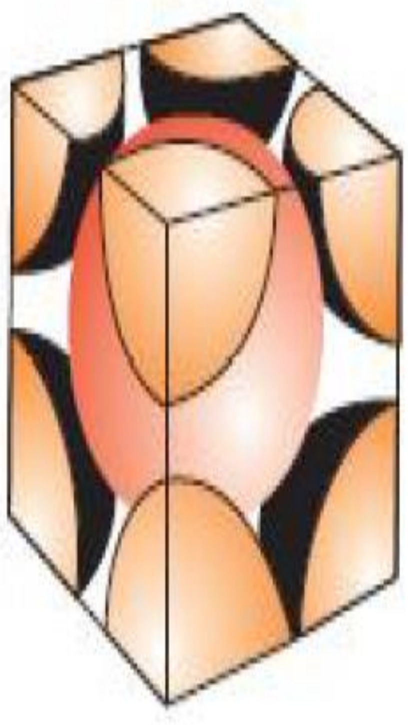
BCC radius



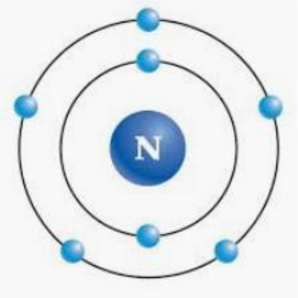


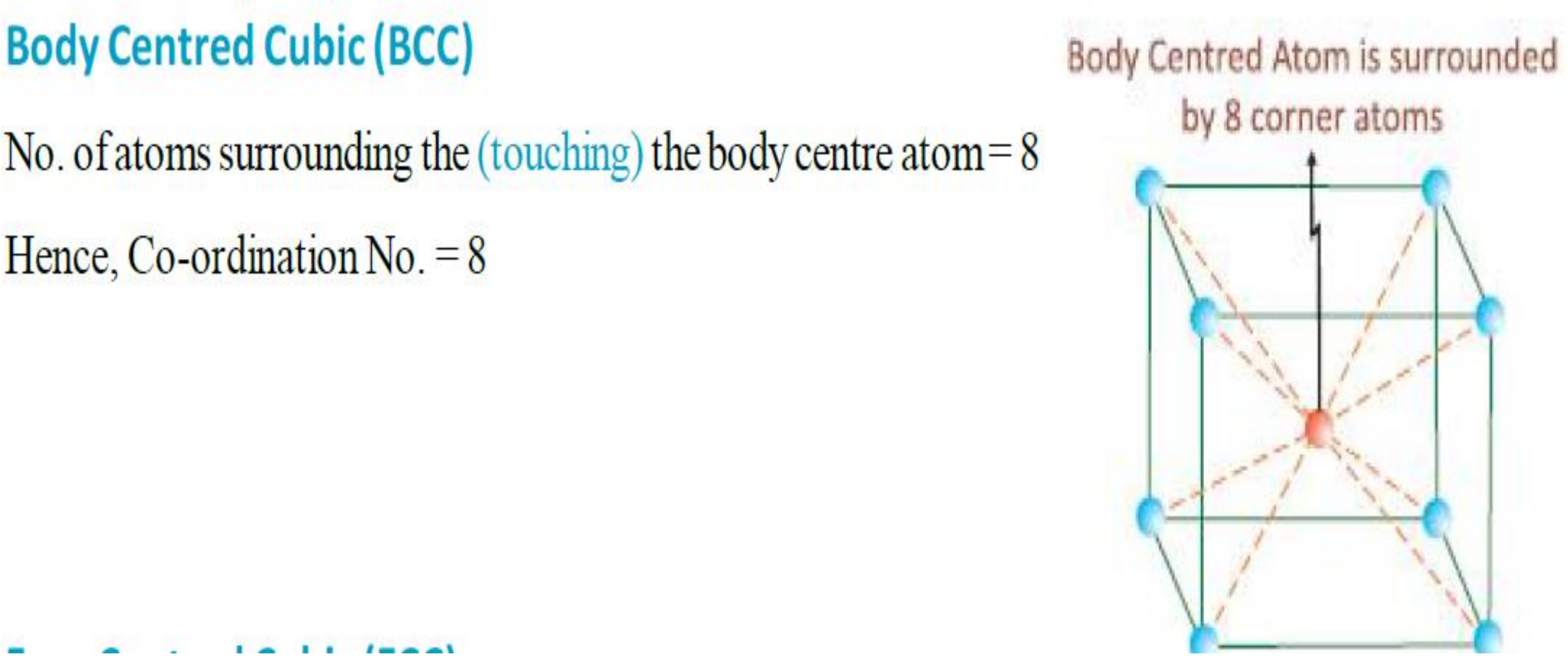
Body Centred Cubic (BCC)

Each corner of the unit cell touches the body centre atom such that $2R = \frac{\sqrt{3}}{2}a \Rightarrow R = \frac{\sqrt{3}}{4}a$



BCC coordination no





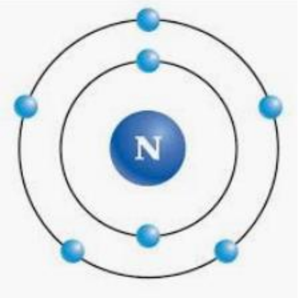
Body Centred Cubic (BCC)

No. of atoms surrounding the (touching) the body centre atom = 8

Hence, Co-ordination No. = 8

Body Centred Atom is surrounded by 8 corner atoms

PE BCC/ SCC



$$\text{Packing Efficiency} = \frac{(\text{No. of atoms per unit cell}) \times (\text{volume of one atom})}{\text{volume of unit cell}} \times 100$$

(i) Simple Cubic (SC)

$$\text{P.E.} = \frac{(1) \times \frac{4}{3}\pi r^3}{a^3} \times 100$$

Where $2r = a$ [a ≡ length of unit cell]

$$\text{P.E.} = \frac{4}{3}\pi\left(\frac{1}{2}\right)^3 \times 100 = \frac{\pi}{6} \times 100 = 52\%$$

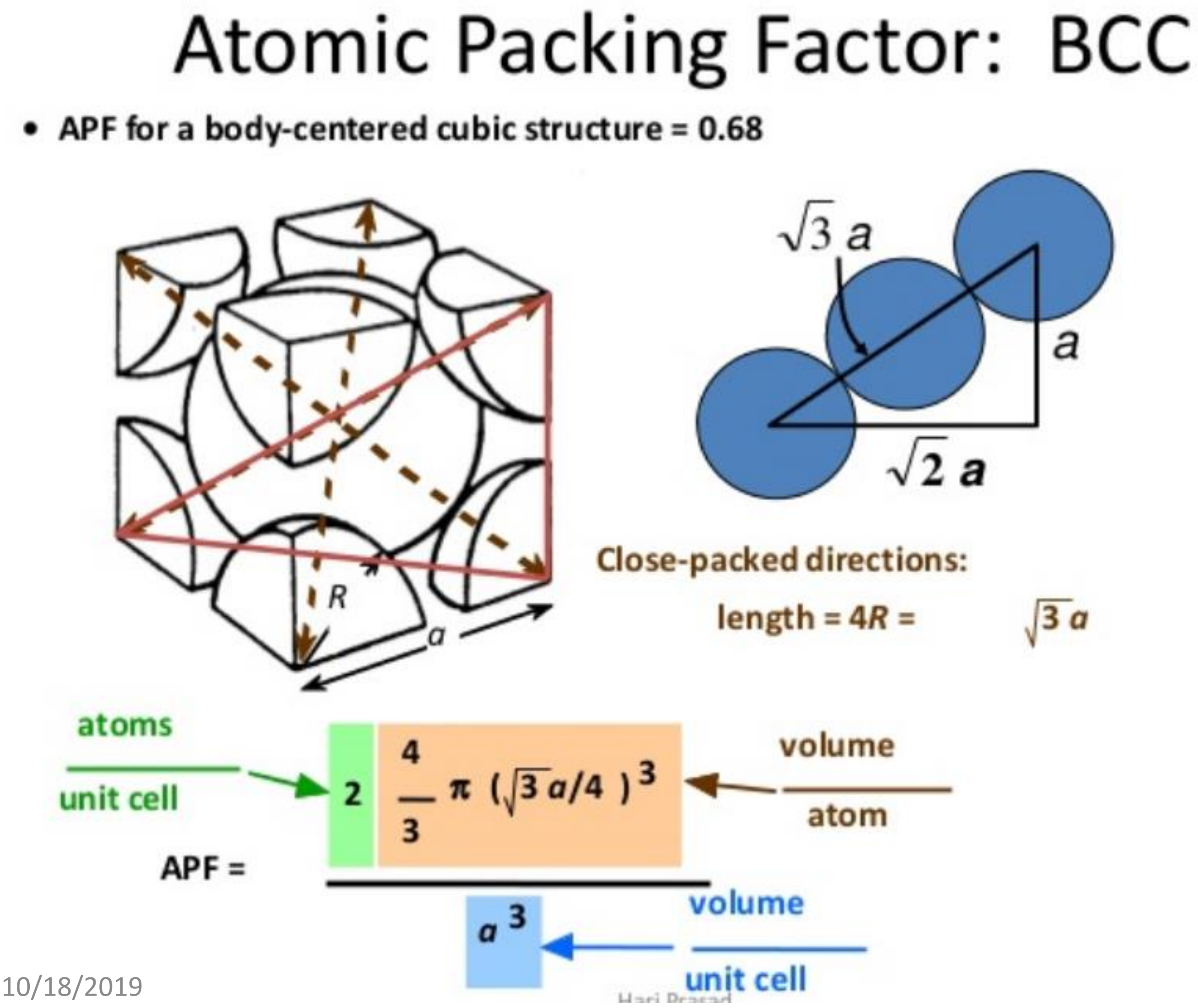
(ii) Body Centred cubic (BCC)

$$\text{P.E.} = \frac{(2) \times \frac{4}{3}\pi r^3}{a^3} \times 100$$

Where $2r = \frac{\sqrt{3}a}{2}$ [a ≡ length of unit cell]

$$\text{P.E.} = \frac{8}{3}\pi\left(\frac{\sqrt{3}}{4}\right)^3 \times 100 = \frac{\sqrt{3}\pi}{8} \times 100 = 68\%$$

APF of BCC



Atomic Packing Factor: BCC

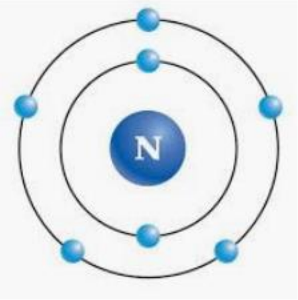
- **APF for a body-centered cubic structure = 0.68**

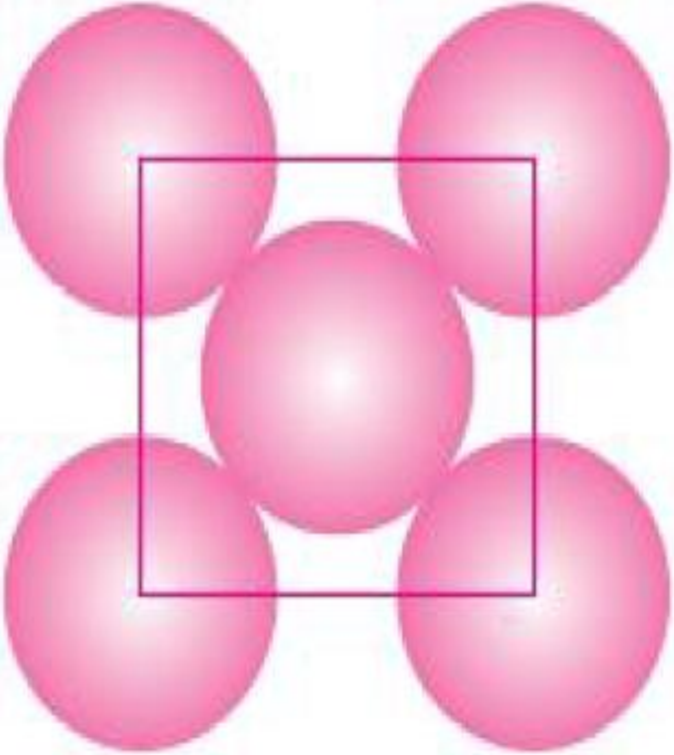
Close-packed directions:

length = 4R = $\sqrt{3}\,a$

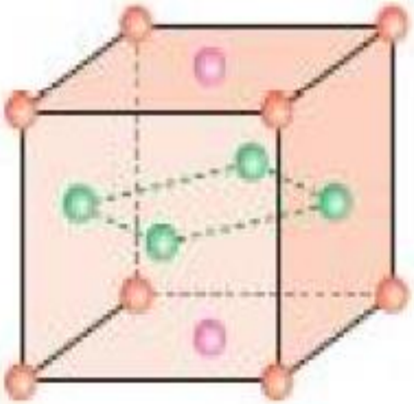
$$\text{APF} = \frac{\overset{\frac{\text{atoms}}{\text{unit cell}}}{2}\;\overset{\frac{\text{volume}}{\text{atom}}}{\frac{4}{3}\pi\left(\sqrt{3}\,a/4\right)^3}}{\underset{\frac{\text{volume}}{\text{unit cell}}}{a^3}}$$

FCC TOP VIEW



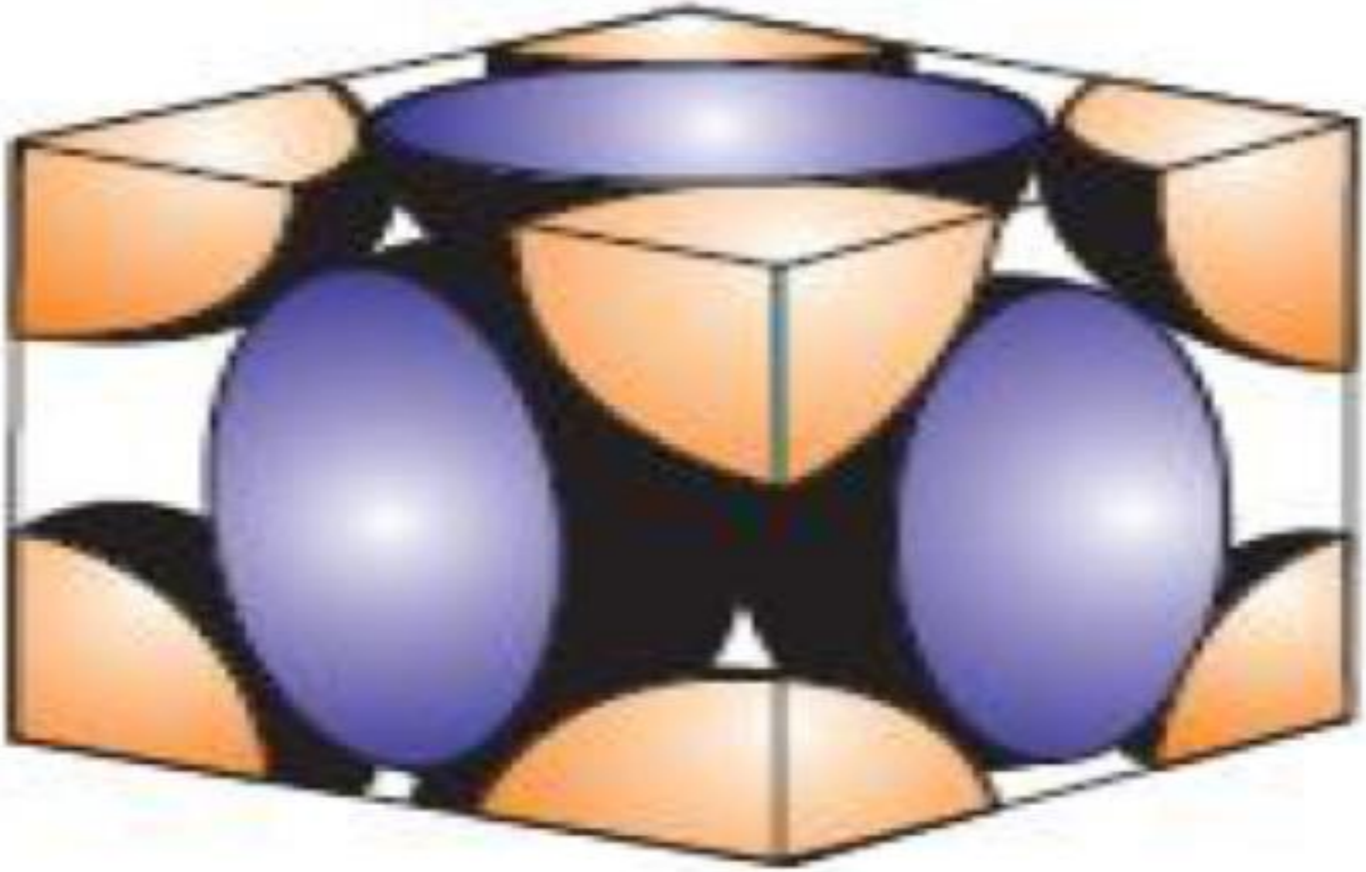


Top view of FCC unit cell

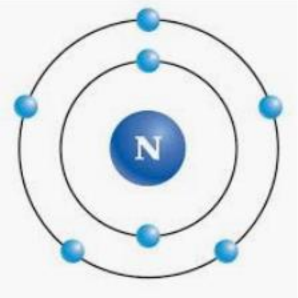


Face centre constituents of adjacent faces are in contact with each other

FCC



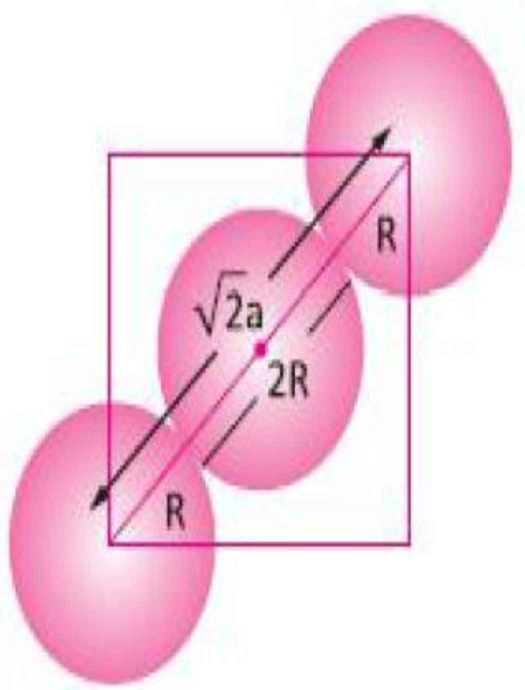
RADIUS FCC



Relation between radius of constituent particles and edge length of unit cell

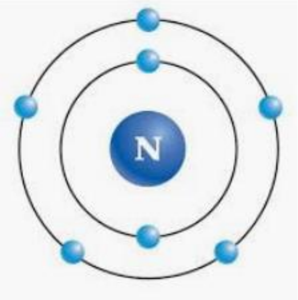
Closest contact is along face diagonal of cube. Each corner of a particular face centre atom touches the face centre atom such that :

$$2R = \frac{a}{\sqrt{2}} \Rightarrow R = \frac{a}{2\sqrt{2}} \text{ or } \sqrt{2}a = 4R$$



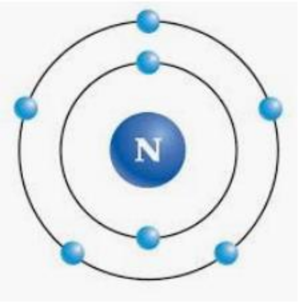
Closest contact is along face diagonal of cube

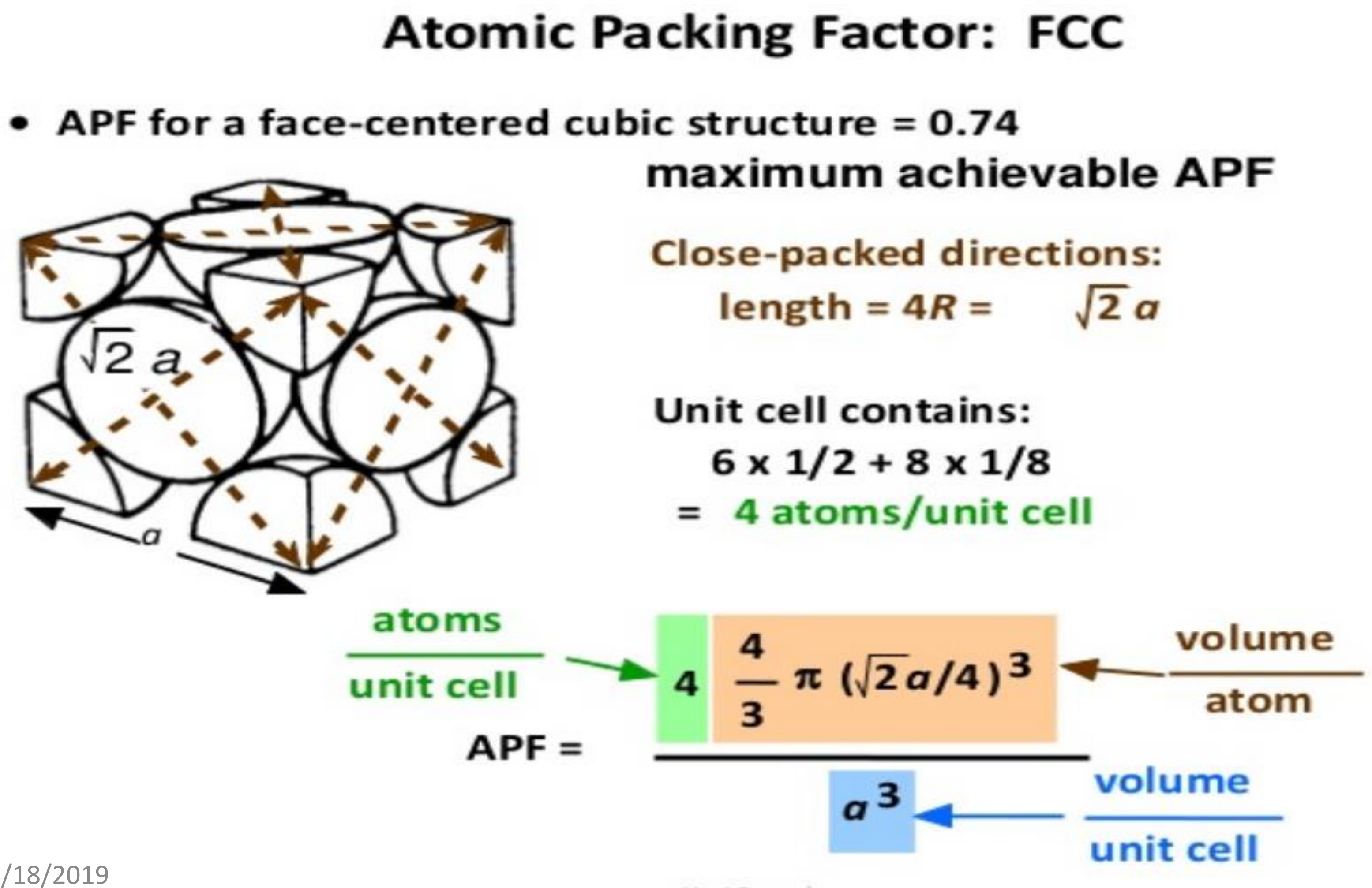
PE FCC



$$\text{Packing efficiency} = \frac{Z \times \frac{4}{3}\pi r^3}{a^3} = \frac{4 \times \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} = 0.74$$

APF of FCC





Atomic Packing Factor: FCC

- APF for a face-centered cubic structure = 0.74

maximum achievable APF

Close-packed directions:
length = 4R = $\sqrt{2}\,a$

Unit cell contains:
6 x 1/2 + 8 x 1/8
= 4 atoms/unit cell

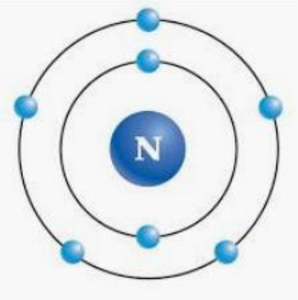
$$\text{APF} = \frac{\overset{\text{atoms/unit cell}}{4}\;\overset{\text{volume/atom}}{\frac{4}{3}\pi(\sqrt{2}a/4)^3}}{\underset{\text{volume/unit cell}}{a^3}}$$

atoms / unit cell → 4

volume / atom → $\frac{4}{3}\pi(\sqrt{2}a/4)^3$

volume / unit cell → a^3

PE FCC DC



(iii) Face centred Cubic (FCC)

$$\text{P.E.} = \frac{(4) \times \frac{4}{3}\pi r^3}{a^3} \times 100$$

where $2r = \frac{a}{\sqrt{2}}$ [a ≡ length of unit cell]

$$\text{P.E.} = \frac{16}{3}\pi\left(\frac{1}{2\sqrt{2}}\right)^3 \times 100 = \frac{\pi}{3\sqrt{2}} \times 100 = 74\%$$

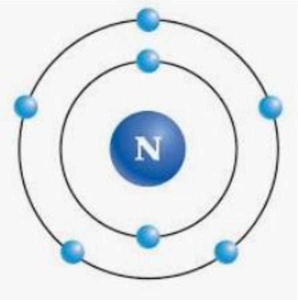
(iv) Diamond Cubic (DC)

$$\text{P.E.} = \frac{(8) \times \frac{4}{3}\pi r^3}{a^3} \times 100$$

where $2r = \frac{\sqrt{3}a}{4}$ [a ≡ length of unit cell]

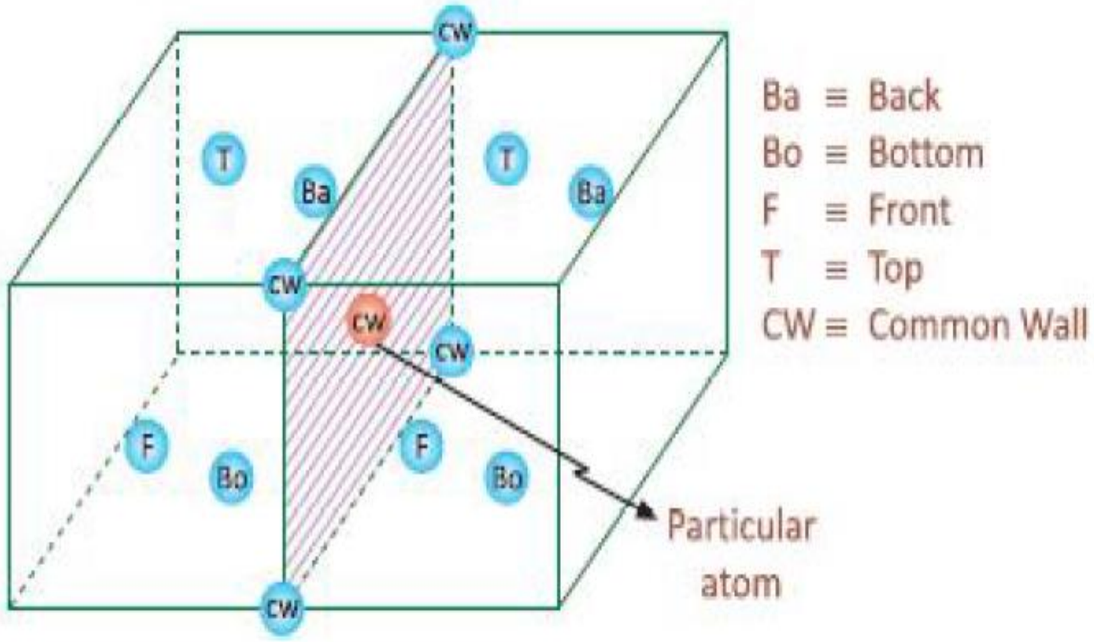
$$= \frac{32}{3}\pi\left(\frac{\sqrt{3}}{8}\right)^3 \times 100 = \frac{\sqrt{3}\pi}{16} \times 100 = 34\%$$

FCC CN

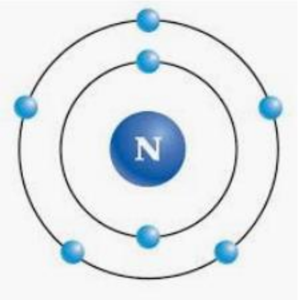


No. of atoms surrounding (touching) the face centre of any face = 12

Hence, co-ordination No. = 12.



Z OF FCC

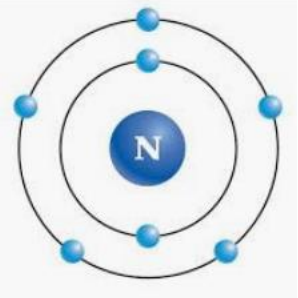


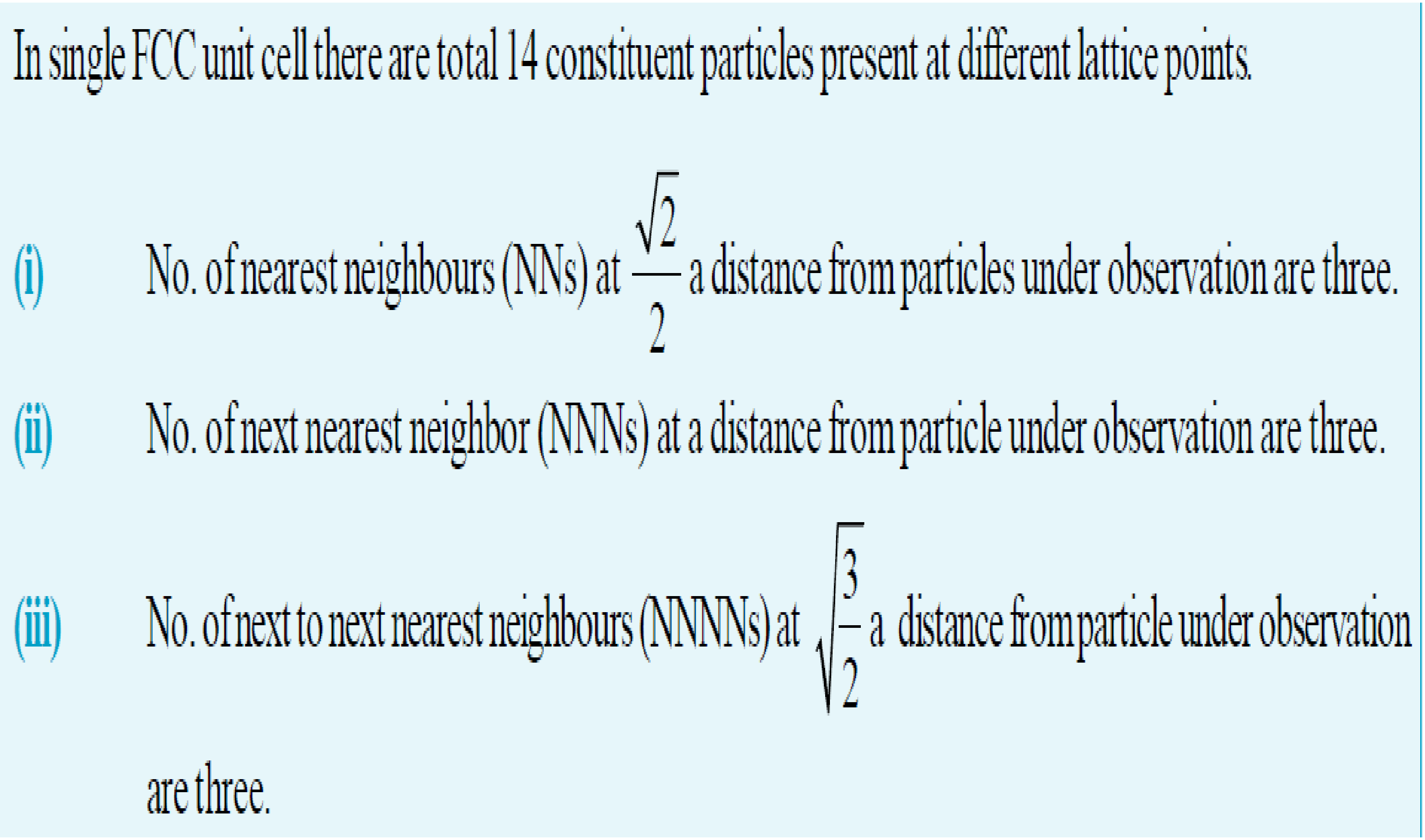
Rank of the unit cell (z) : Effective number of constituent particles per unit cell.

$$Z = \frac{1}{8} \times (\text{No. of corner}) + \frac{1}{2} \times (\text{No. of face centres})$$

$$= \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 1 + 3 = 4$$

FCC NNS



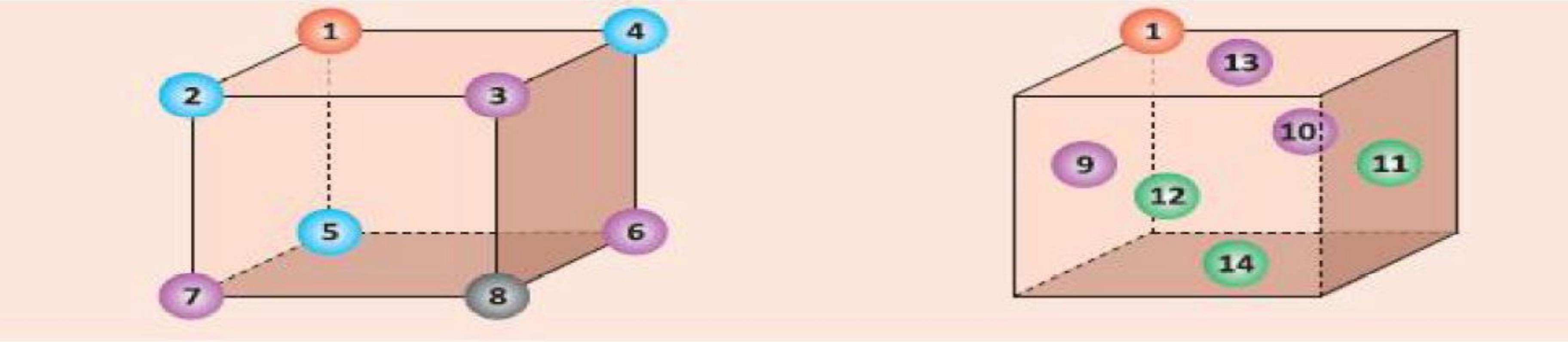

In single FCC unit cell there are total 14 constituent particles present at different lattice points.

(i) No. of nearest neighbours (NNs) at $\frac{\sqrt{2}}{2}$ a distance from particles under observation are three.

(ii) No. of next nearest neighbor (NNNs) at a distance from particle under observation are three.

(iii) No. of next to next nearest neighbours (NNNNs) at $\sqrt{\frac{3}{2}}$ a distance from particle under observation are three.

FCC NNS

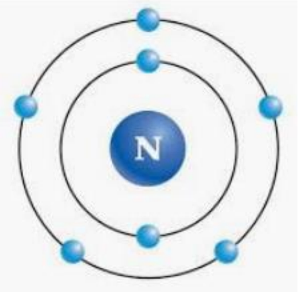


Reference Atom/Constituent Particle is 1.

- No of atoms at distance $\frac{\sqrt{2}\,a}{2}$ (NNs) are 3. [9, 10, 13]
- No. of atoms at distance a (NNNs) are 3 [2, 4, 5]
- No. of atoms at distance $\sqrt{\frac{3}{2}}$ a (NNNNs) are 3 [11, 12, 14]
- No. of atom at distance $\sqrt{2}$ a are 3 [3, 6, 7]
- No. of atoms at distance $\sqrt{3}$ a is 1 [8]

Total No. of atoms for reference atom = 3 + 3 + 3 + 3 + 1 = 13

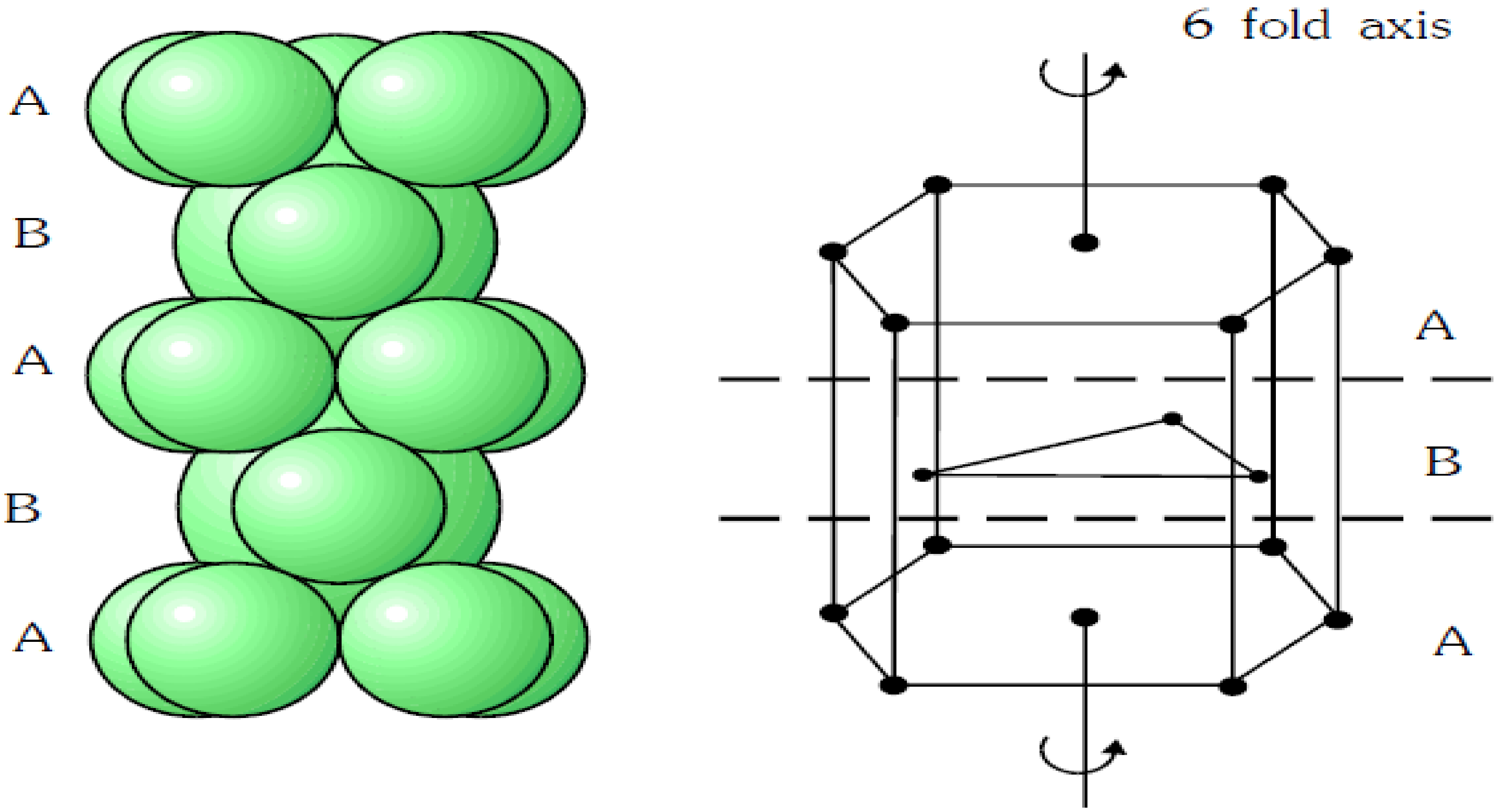
Summary



Contents	BCC	CCP/FCC	HCP
Type of packing packing but not close packing	ABAB....... close packing	ABCABC ...... close packing	ABAB ......
No. of atoms	2	4	6
Co-ordination no.	8	12	12
Packing efficiency	68%	74%	74%
Examples V & Cr group Fe	IA, Ba Co group, Ni group, Copper group, all inert gases except helium	Ca, Sr, Al d-block elements Be & Mg	Remaining

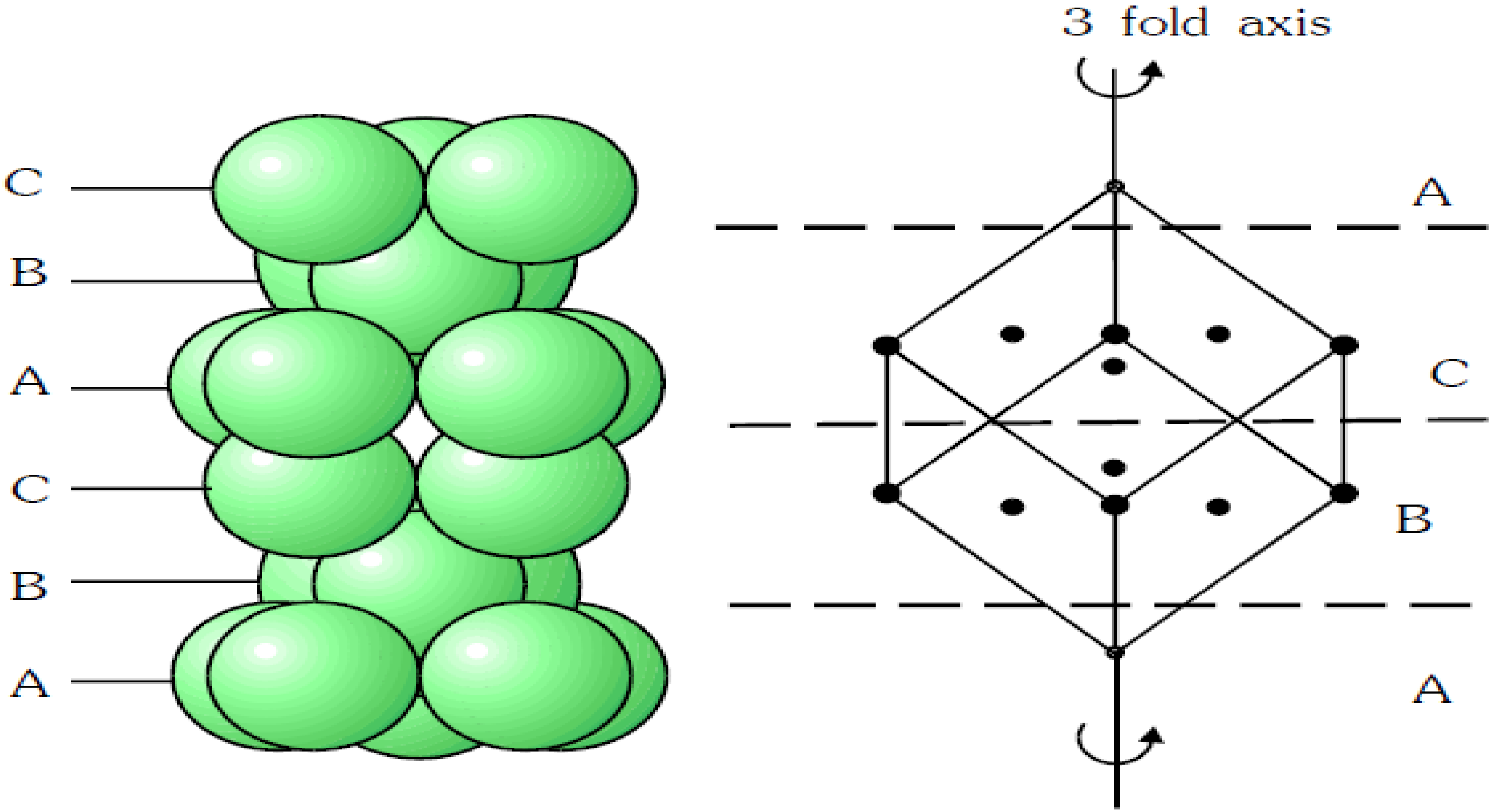
Note :- Only Mn crystallizes in S.C.C.

HCP



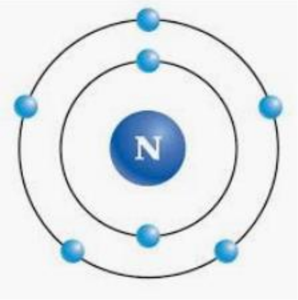
ABABAB... or hexagonal close packing (hcp) of spheres

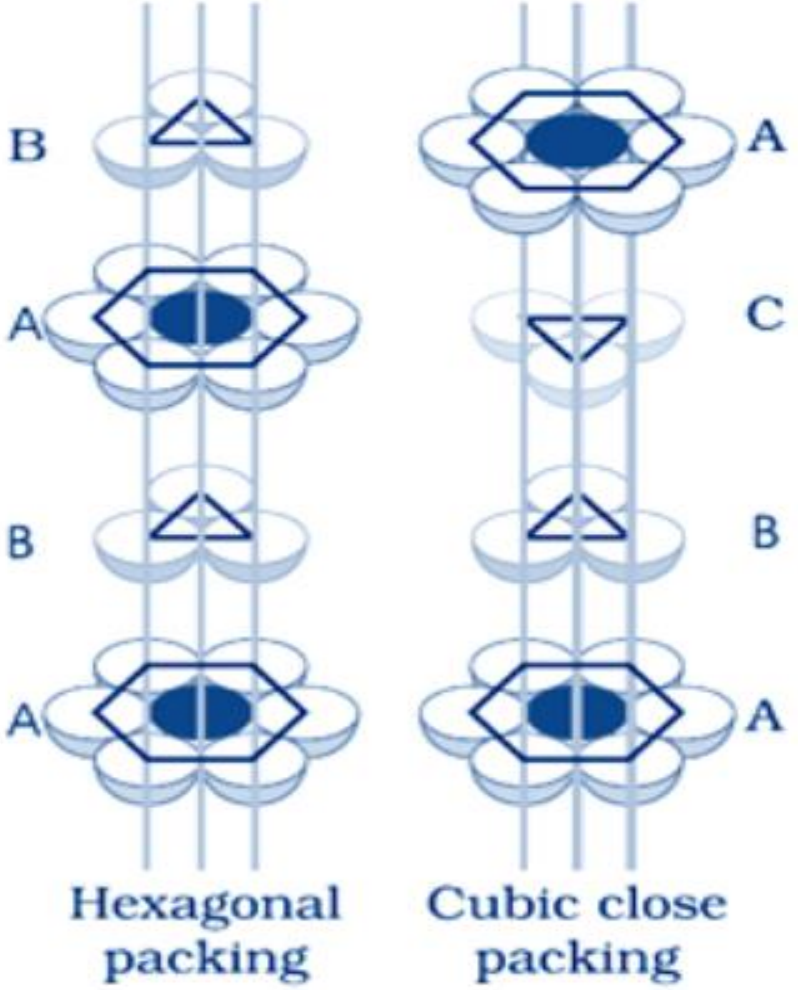
CCP

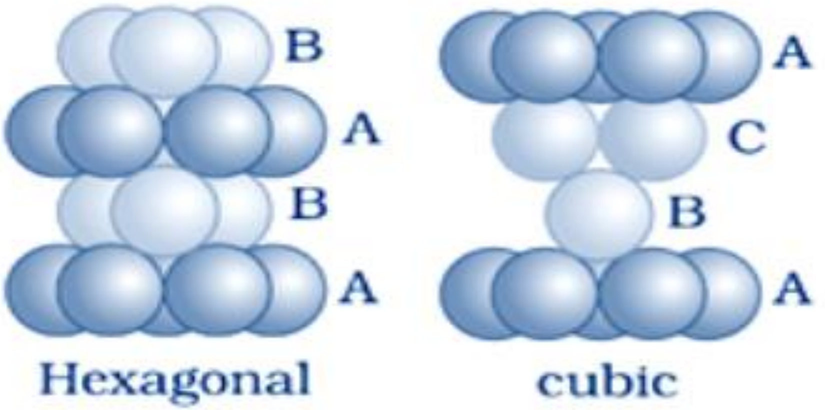


ABCABCA... or cubic close packing (ccp) of spheres

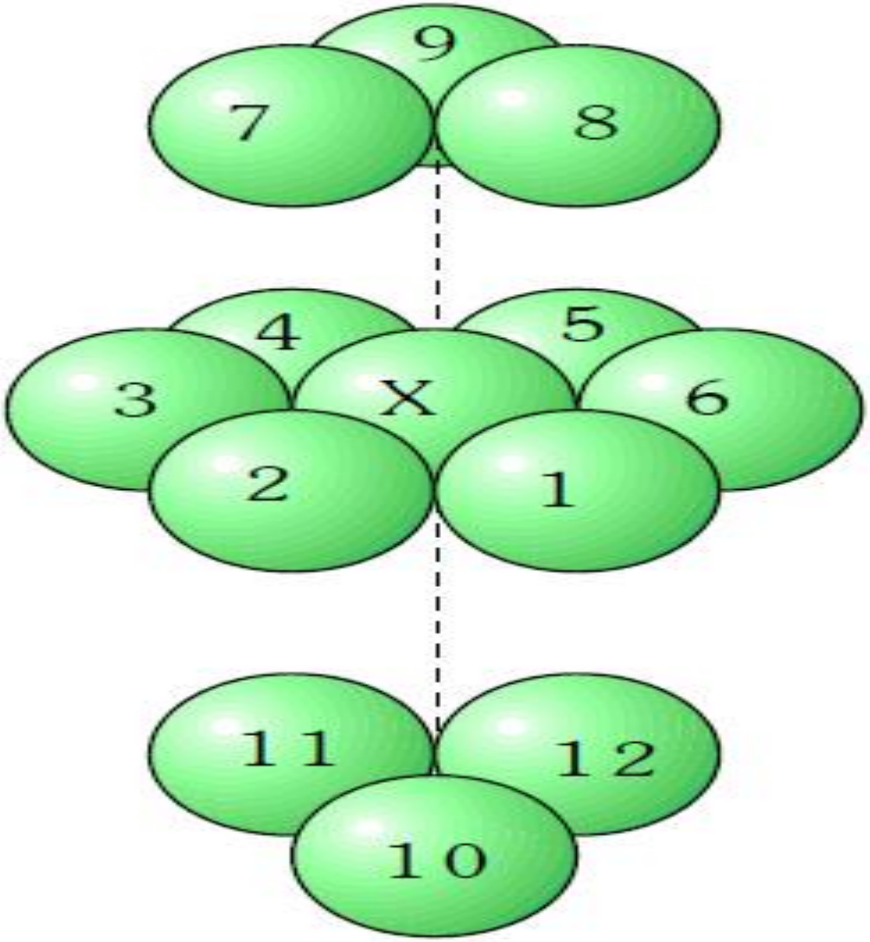
HCP and CCP




B
A
B
A
Hexagonal packing
A
C
B
A
Cubic close packing

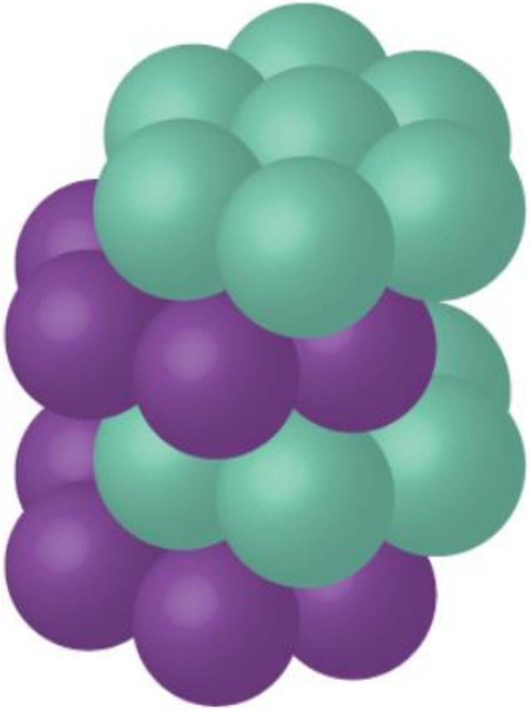

B
A
B
A
Hexagonal
A
C
B
A
cubic

CCP HCP CN

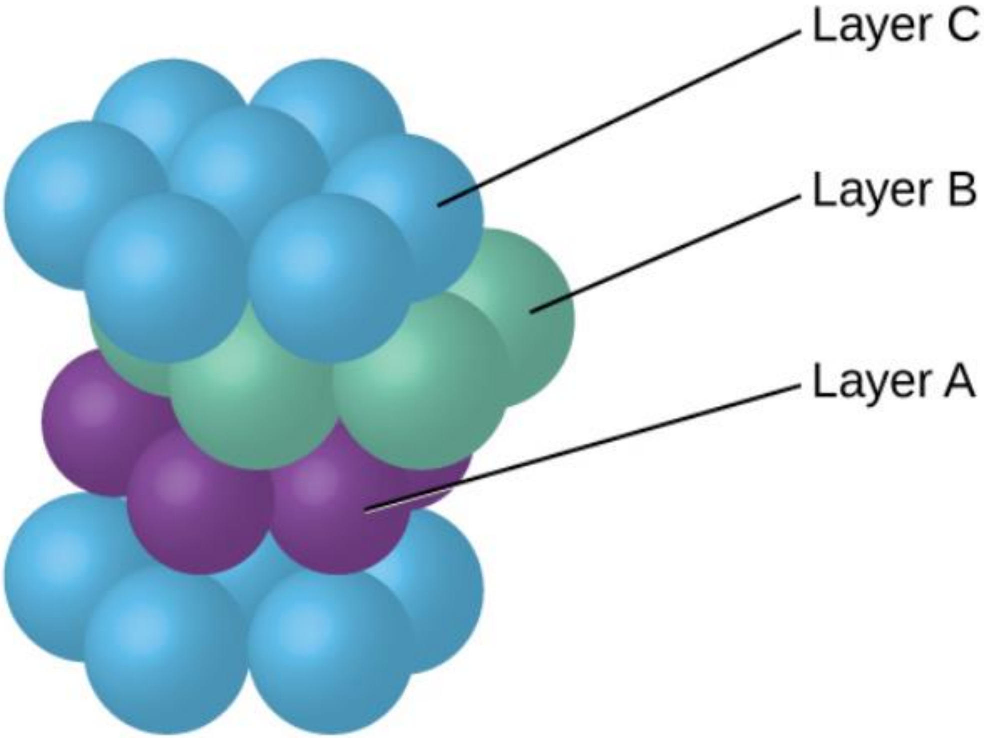


Coordination number of hcp and ccp structure

HCP Vs CCP

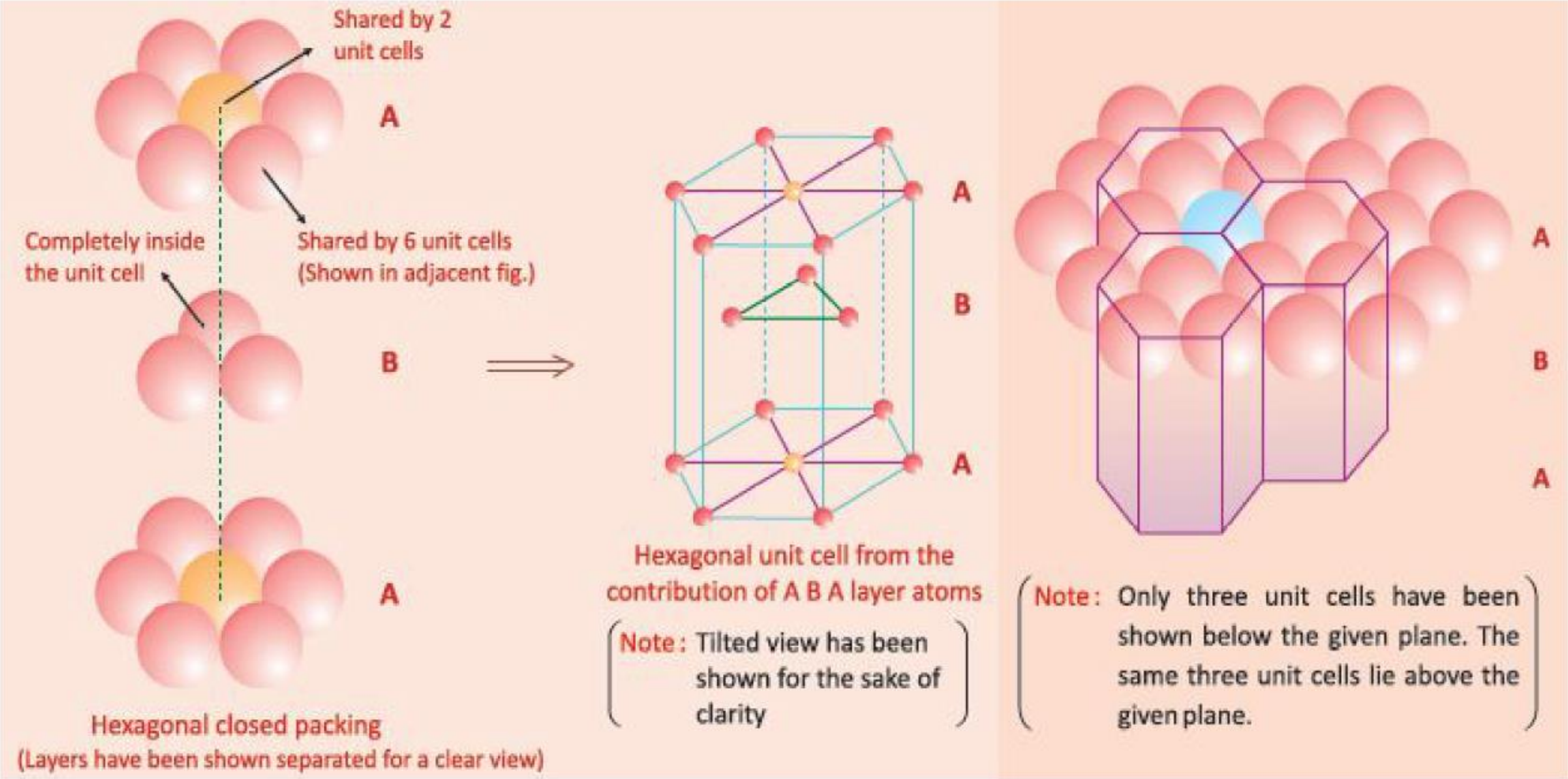


Hexagonal closest packed



Cubic closest packed

Z OF HCP



Hexagonal closed packing (Layers have been shown separated for a clear view)

Hexagonal unit cell from the contribution of A B A layer atoms

(Note: Tilted view has been shown for the sake of clarity)

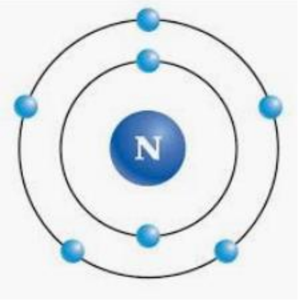
(Note: Only three unit cells have been shown below the given plane. The same three unit cells lie above the given plane.)

Figure shows Hexagonal Closed Packing

Figure shows '*e*' is shared by sic unit cells

$$\text{Effective number of atoms per HCP unit cell} = \left(\frac{1}{6}\times 12\right) + \left(\frac{1}{2}\times 2\right) + (1\times 3) = 6$$

PE HCP



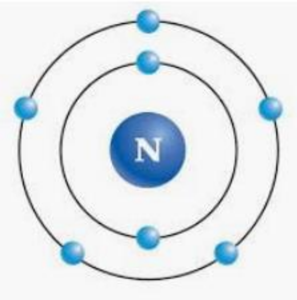
Hexagonal Crystal Closed Packed (HCP)

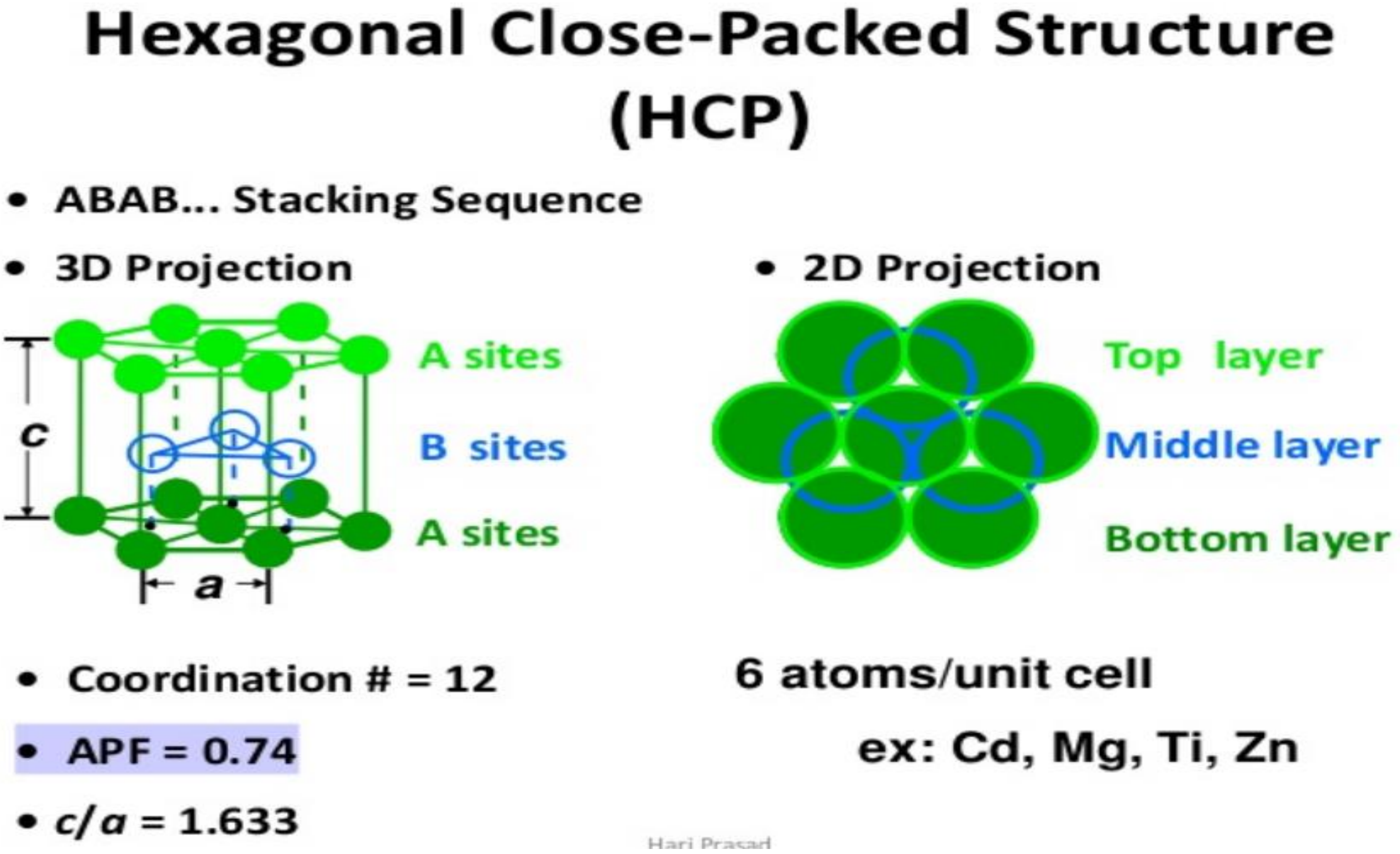
$$\text{P.E.} = \frac{(6) \times \frac{4}{3}\pi r^3}{6 \times \frac{\sqrt{3}}{4} a^2 \times c} \times 100$$

where $c = \frac{2\sqrt{2}}{\sqrt{3}} a$ and $2r = a$ $[a \equiv \text{length of unit cell}]$

$$\text{P.E.} = \frac{\pi}{3\sqrt{2}} \times 100 = 74\%$$

APF of HCP





Hexagonal Close-Packed Structure (HCP)

- ABAB... Stacking Sequence
- 3D Projection
- 2D Projection

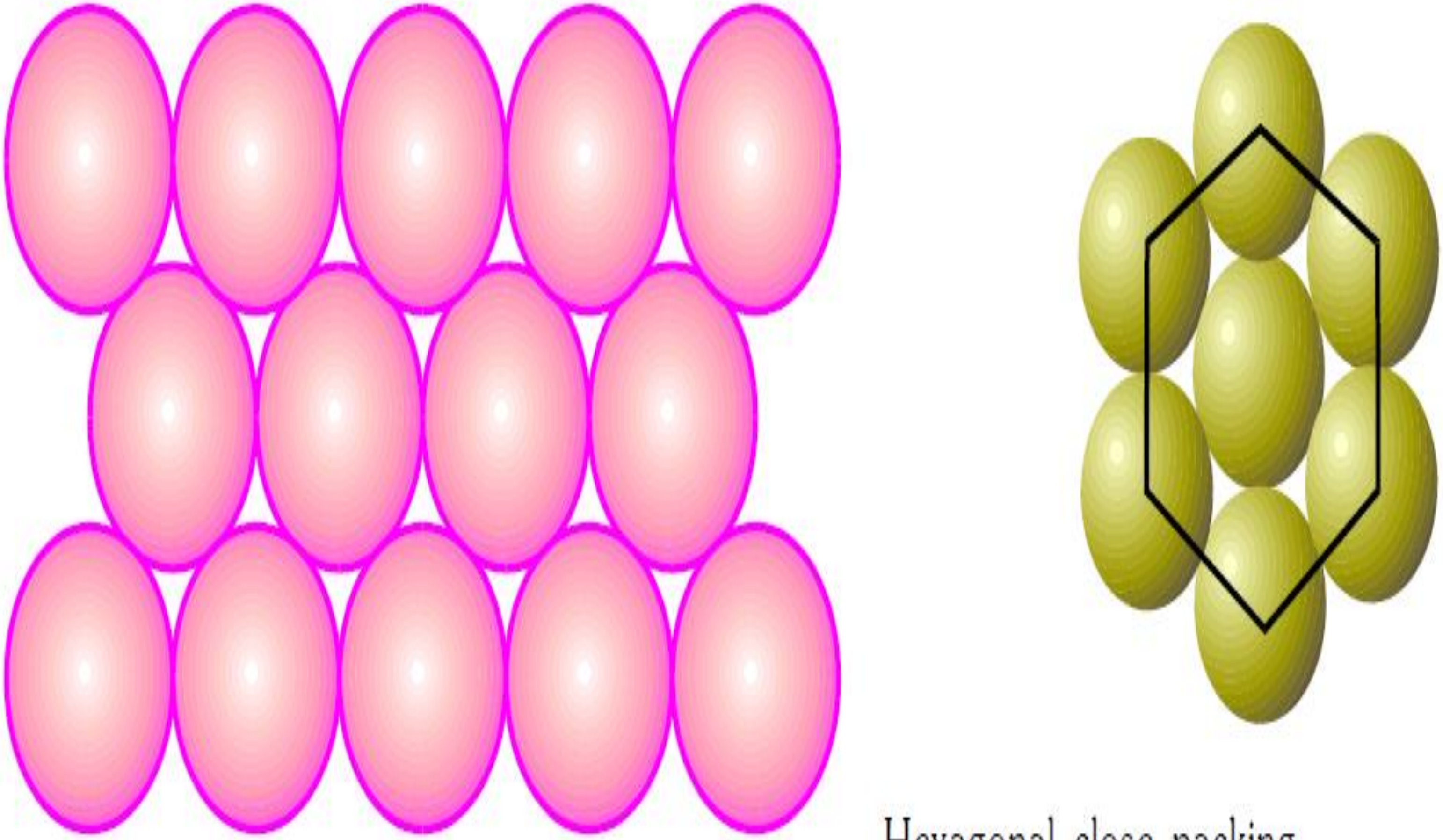
- Coordination # = 12
- APF = 0.74
- *c*/*a* = 1.633

6 atoms/unit cell

ex: Cd, Mg, Ti, Zn

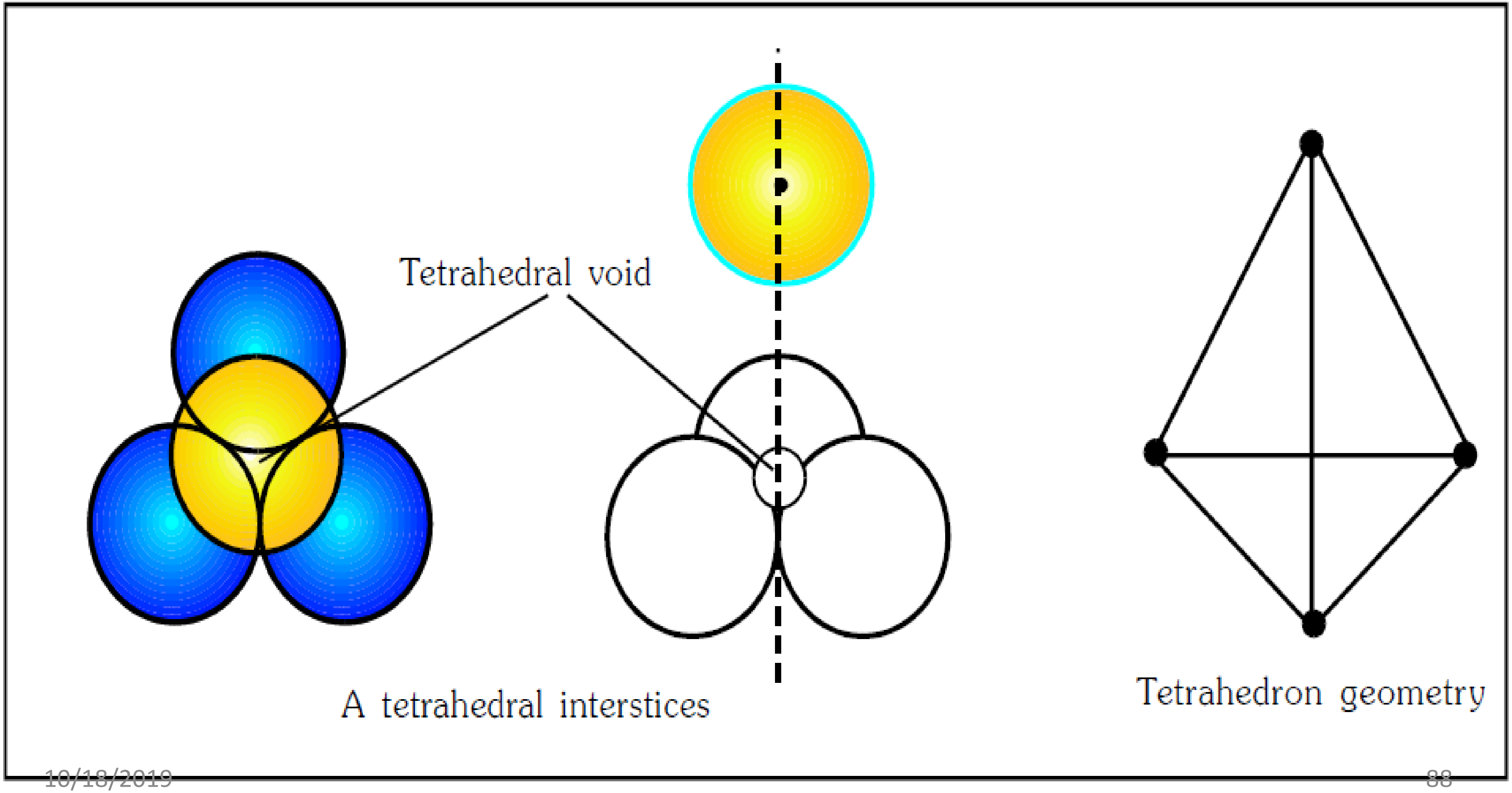
Hari Prasad

HCP



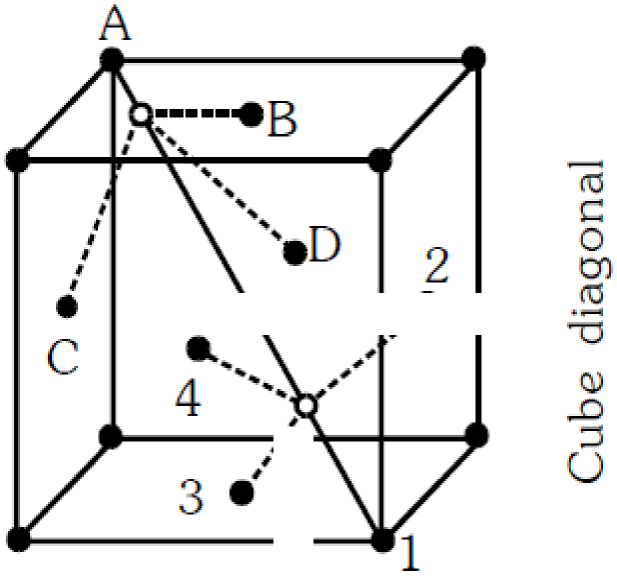
Hexagonal close packing

TH VOID


Tetrahedral void
A tetrahedral interstices
Tetrahedron geometry

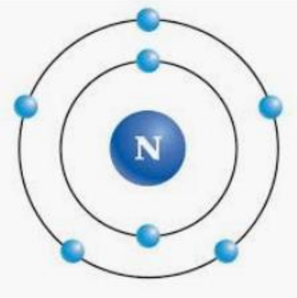
TH VOID

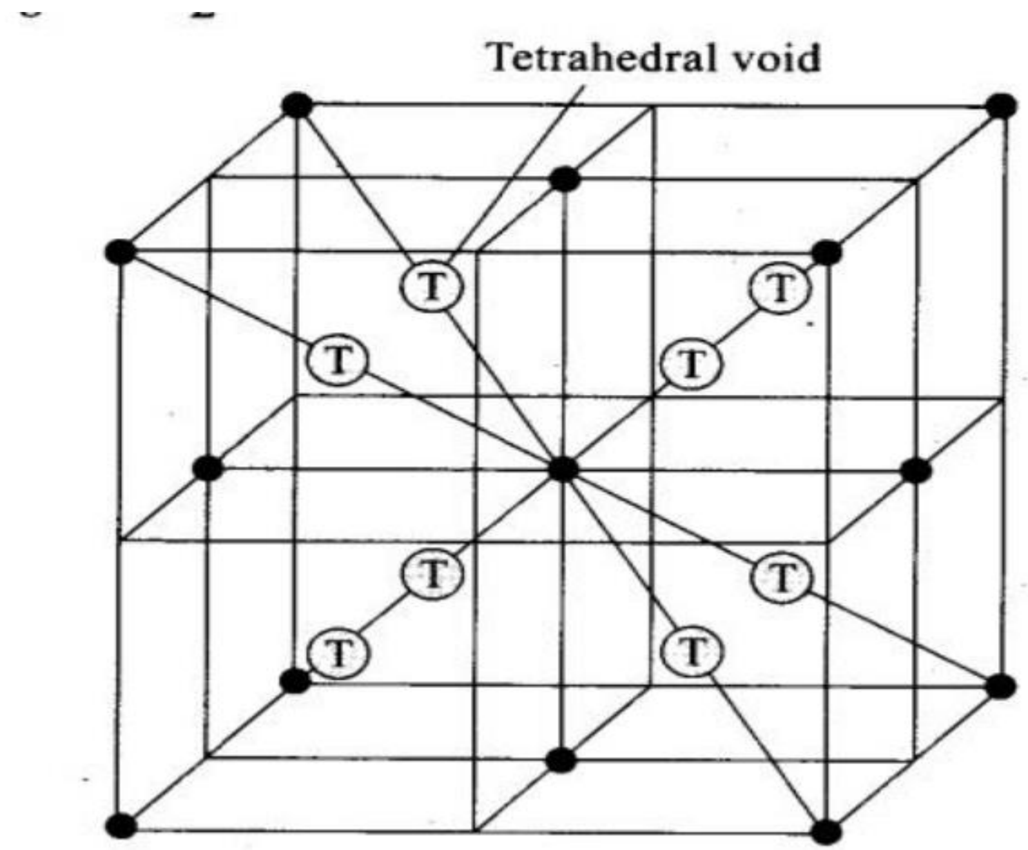
we can say that, in 3D close packing 2 tetrahedral voids are attached with one atom.



Tetrahedral void

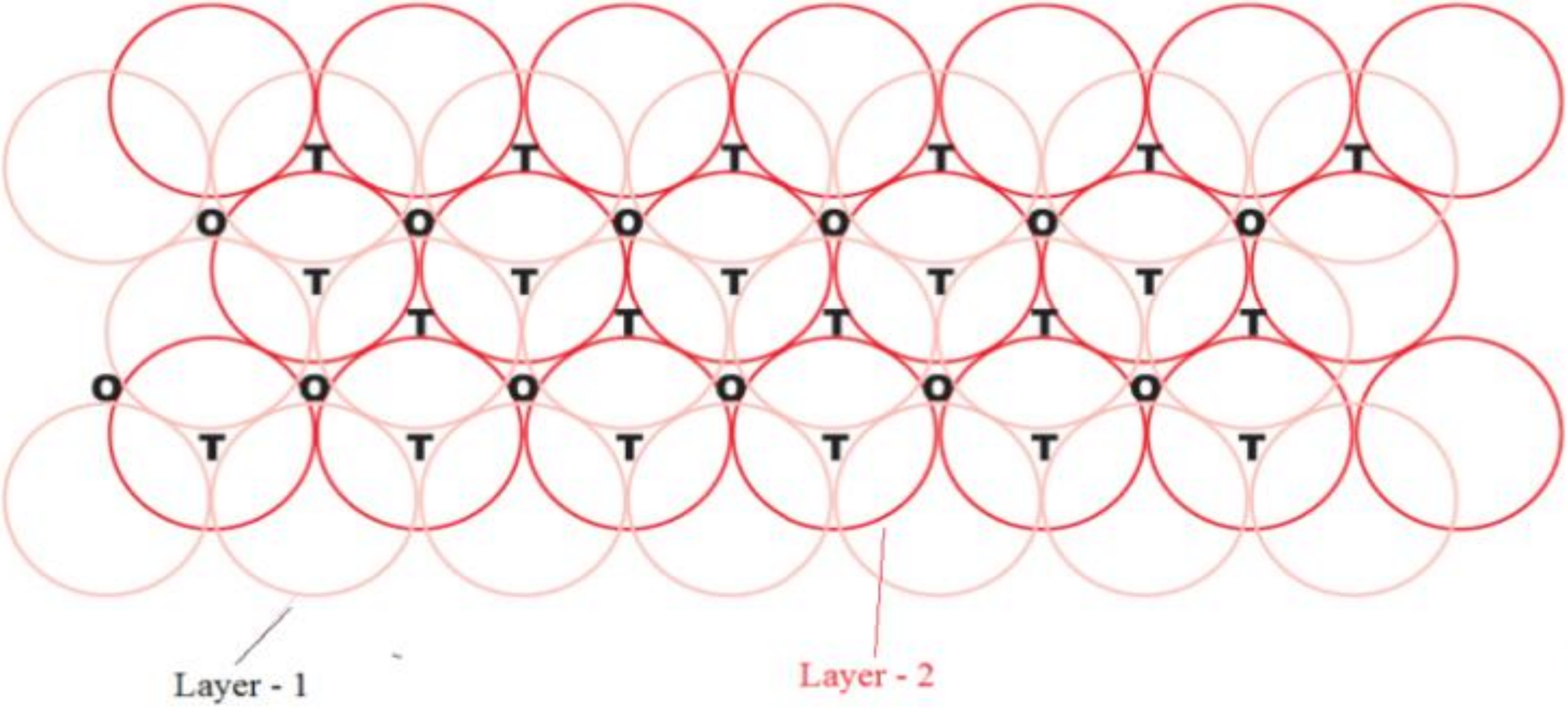
Th void





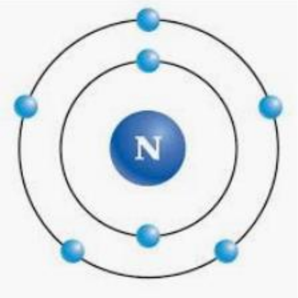
Position of tetrahedral Voids = At the centre of each cubic component Number of tetrahedral voids per unit cell in cubic close packing = 8×1=8 Number of tetrahedral Voids = 8.

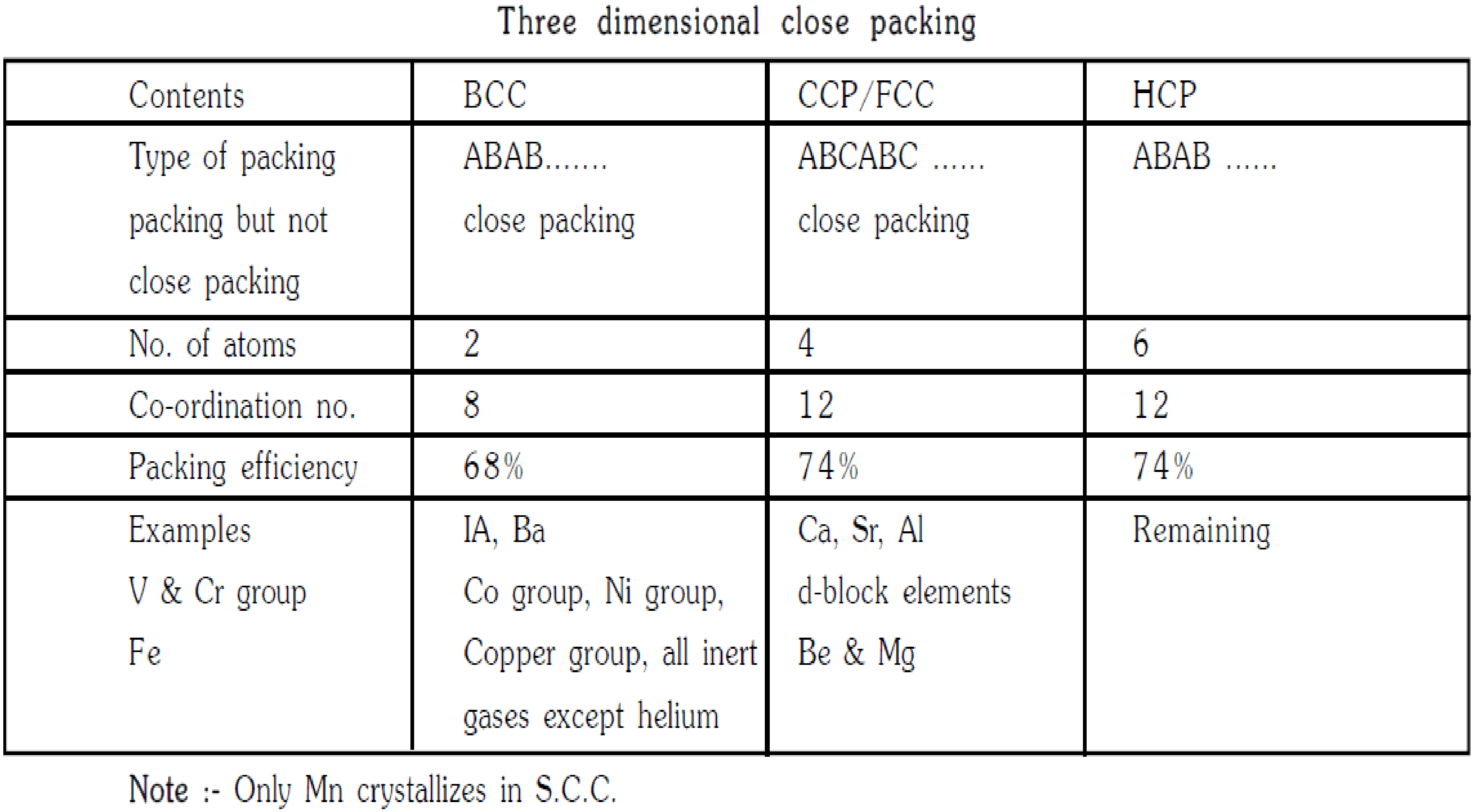
T/O void



T = Tetrahedral void and O = Octahedral void

SUMMARY



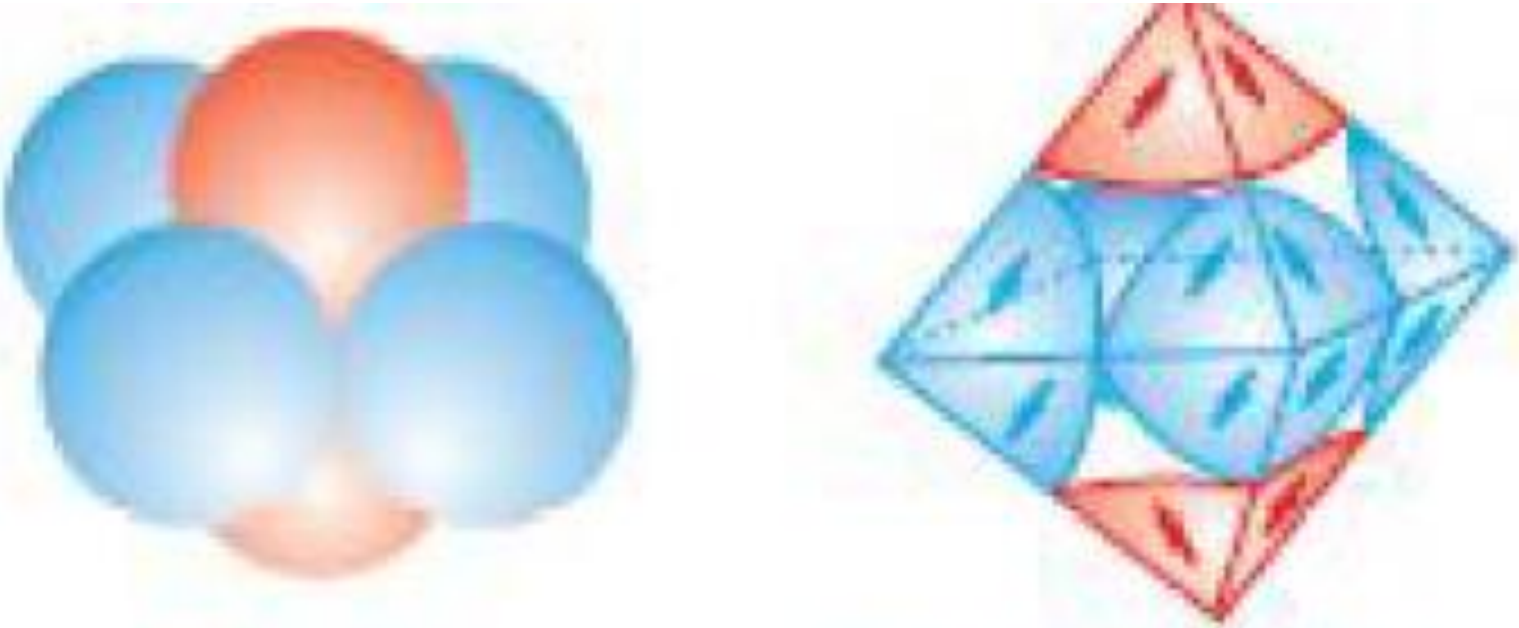


Three dimensional close packing

Contents	BCC	CCP/FCC	HCP
Type of packing packing but not close packing	ABAB....... close packing	ABCABC ...... close packing	ABAB ......
No. of atoms	2	4	6
Co-ordination no.	8	12	12
Packing efficiency	68%	74%	74%
Examples V & Cr group Fe	IA, Ba Co group, Ni group, Copper group, all inert gases except helium	Ca, Sr, Al d-block elements Be & Mg	Remaining

Note :- Only Mn crystallizes in S.C.C.

OH VOID

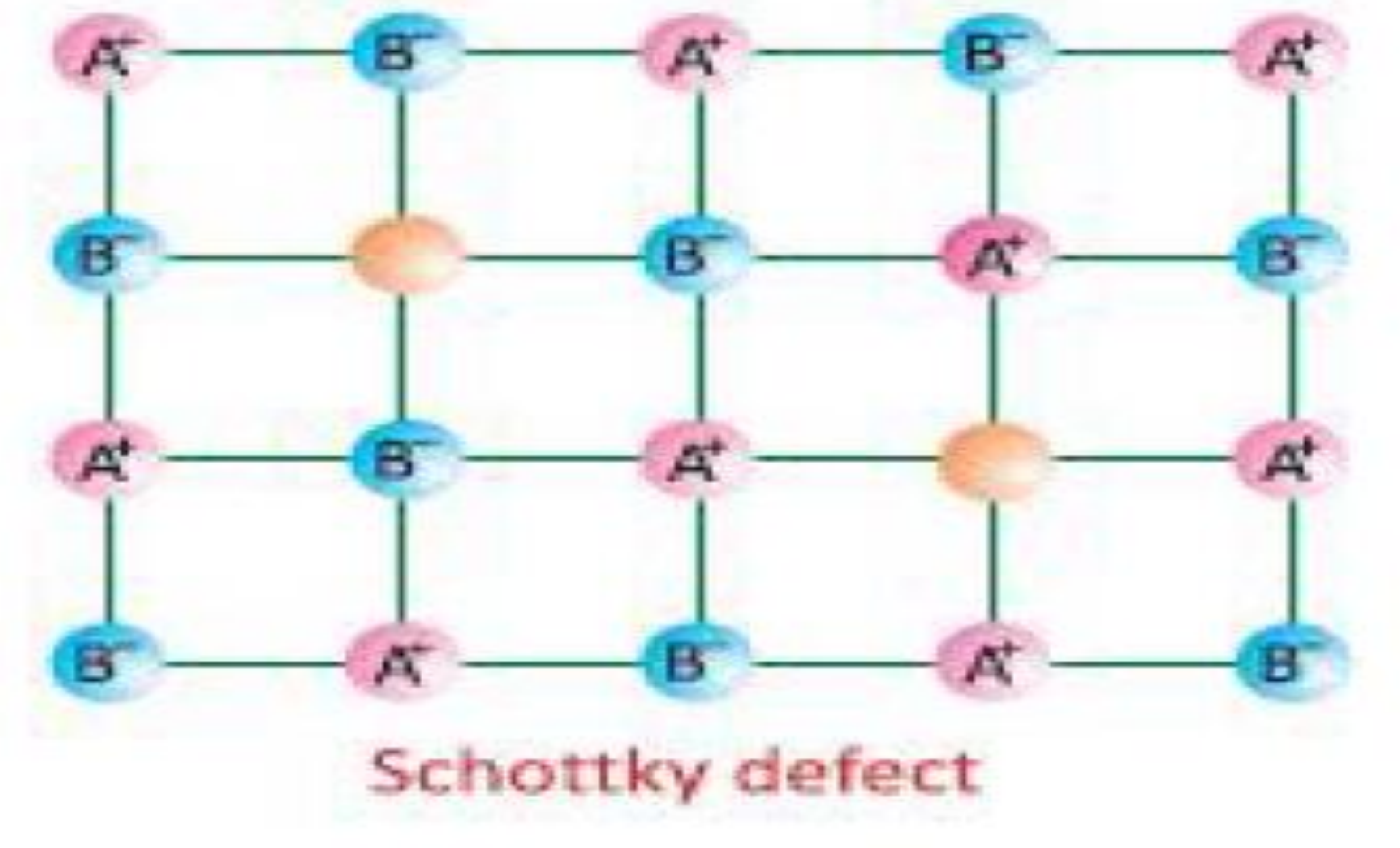


3-D view

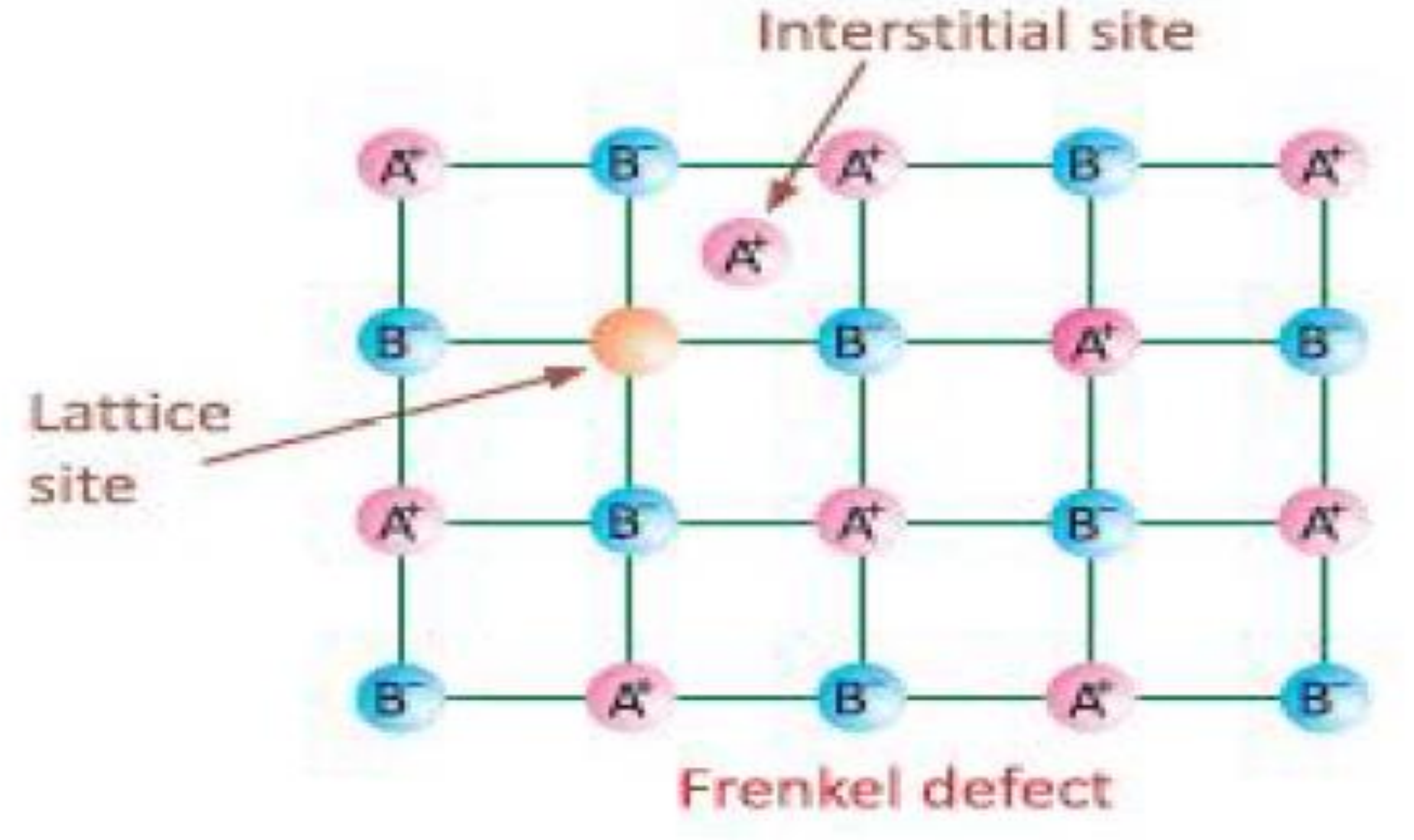
Octahedral view

Geometry of octahedral voids in closed packed structures

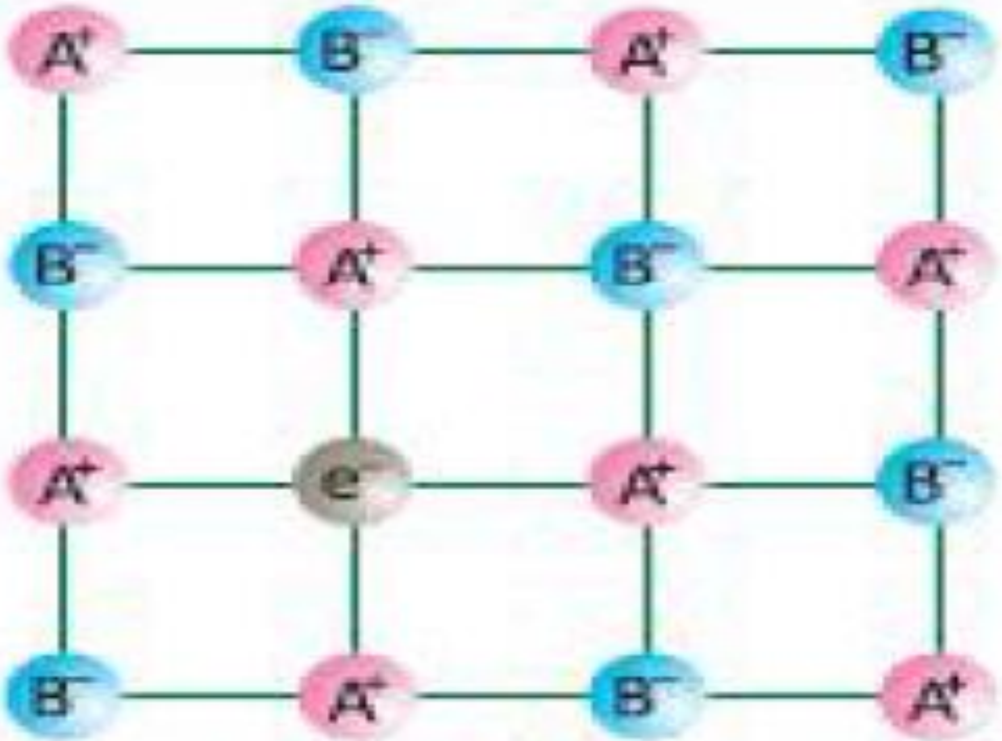
Schottky defect



Frenkel defect

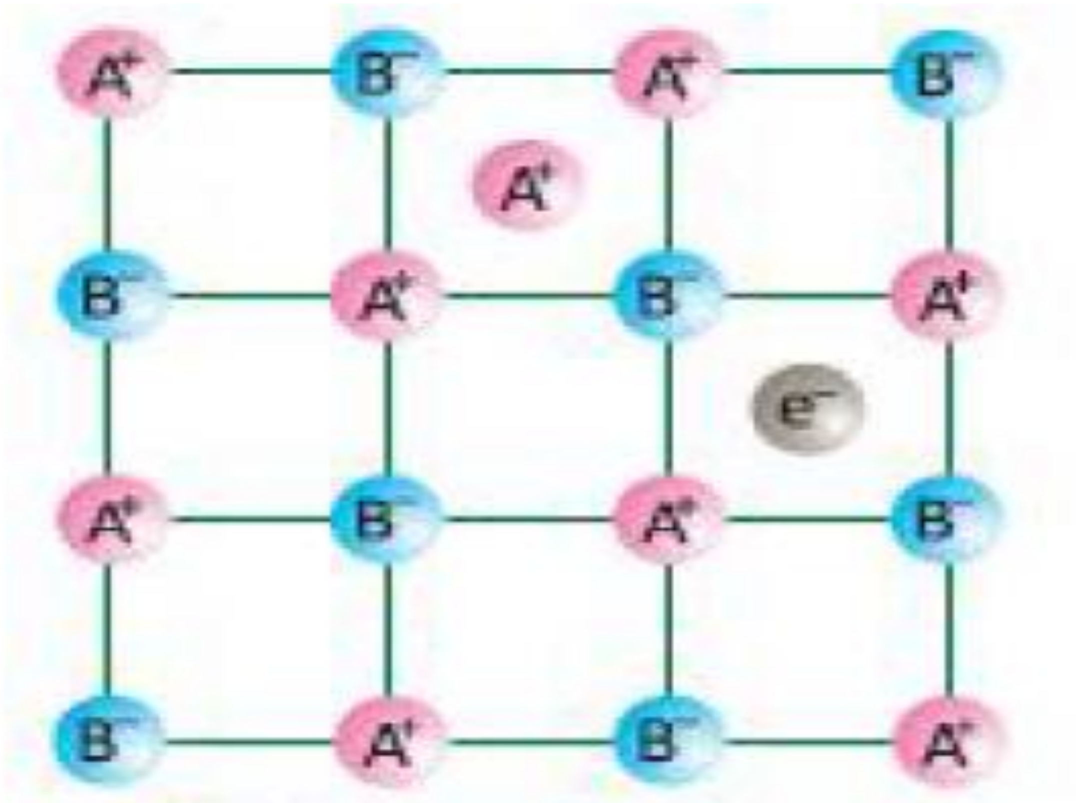


Metal excess



Metal excess defect due to anion vacancy

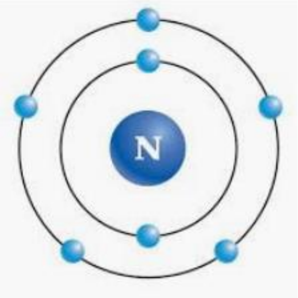
Metal excess

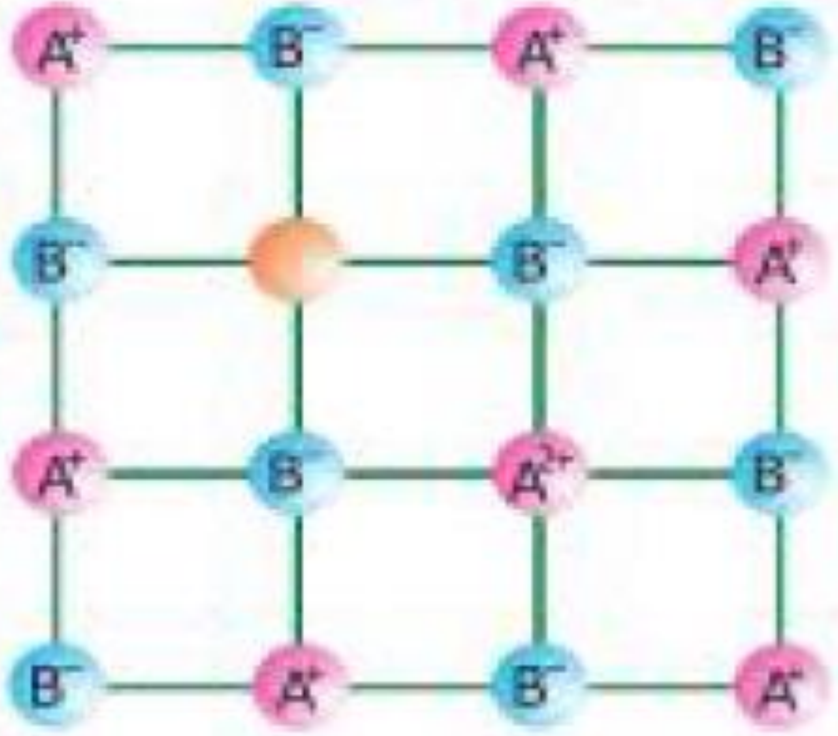


Metal excess defect

caused by extra cation in interstitial position

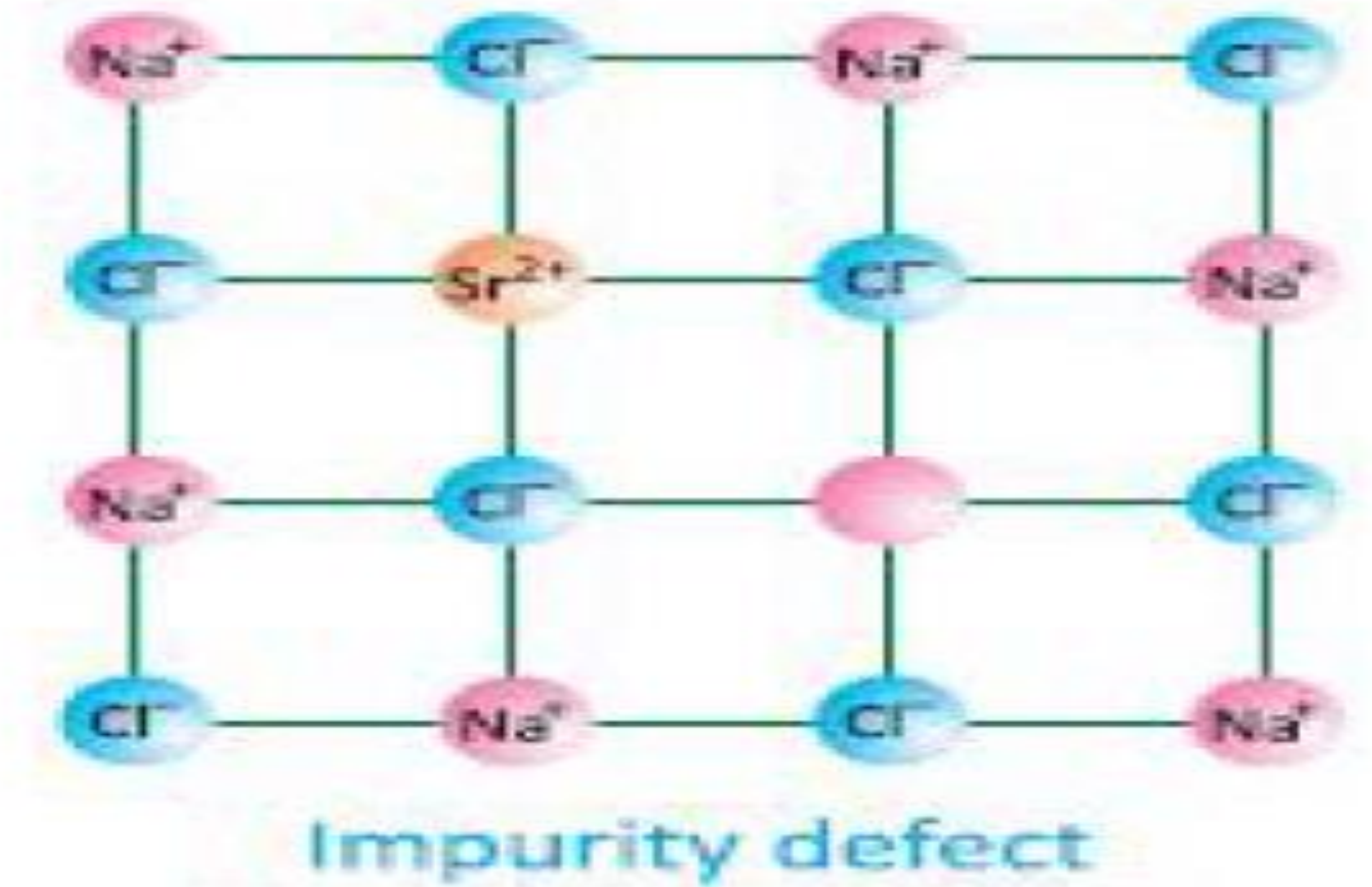
Metal deficiency





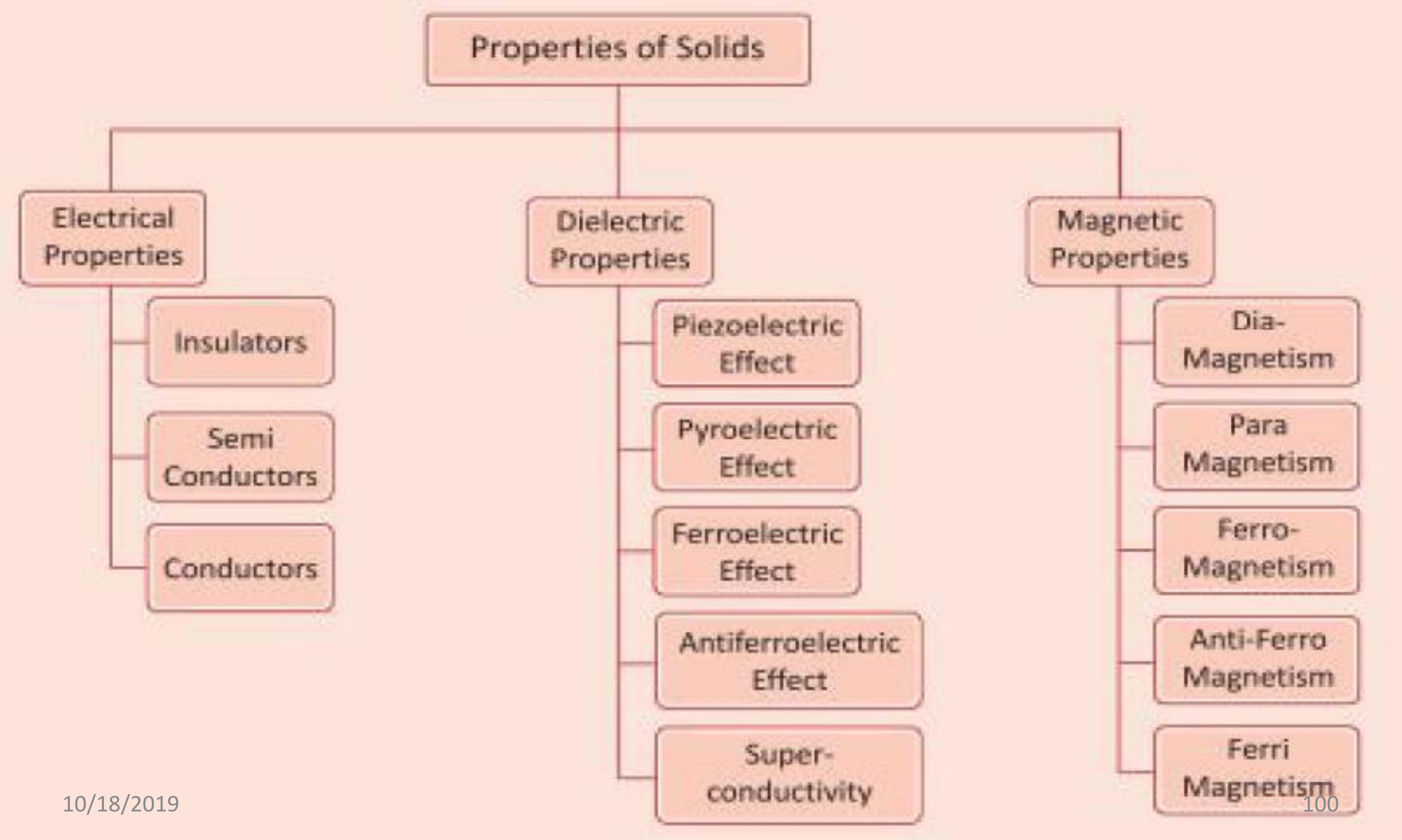
Metal deficiency due to missing of a cation of lower valency and presence of a cation of higher valency

Impurity defect



Impurity defect

Properties



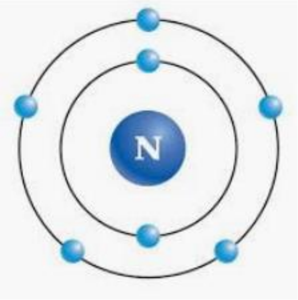
Properties of Solids

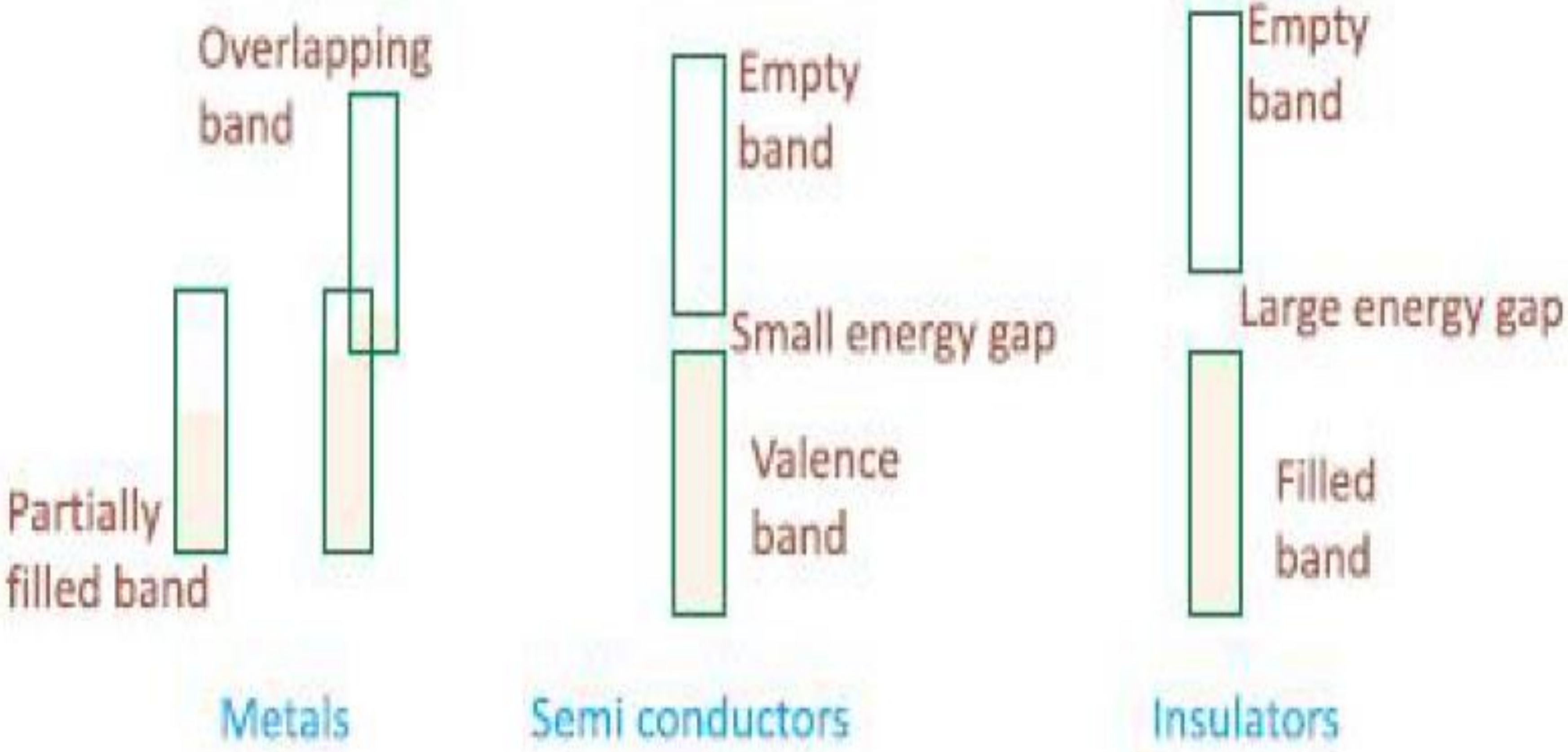
Electrical Properties
- Insulators
- Semi Conductors
- Conductors

Dielectric Properties
- Piezoelectric Effect
- Pyroelectric Effect
- Ferroelectric Effect
- Antiferroelectric Effect
- Super-conductivity

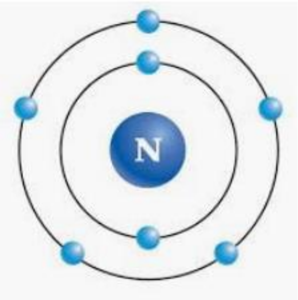
Magnetic Properties
- Dia-Magnetism
- Para Magnetism
- Ferro-Magnetism
- Anti-Ferro Magnetism
- Ferri Magnetism

Electrical properties

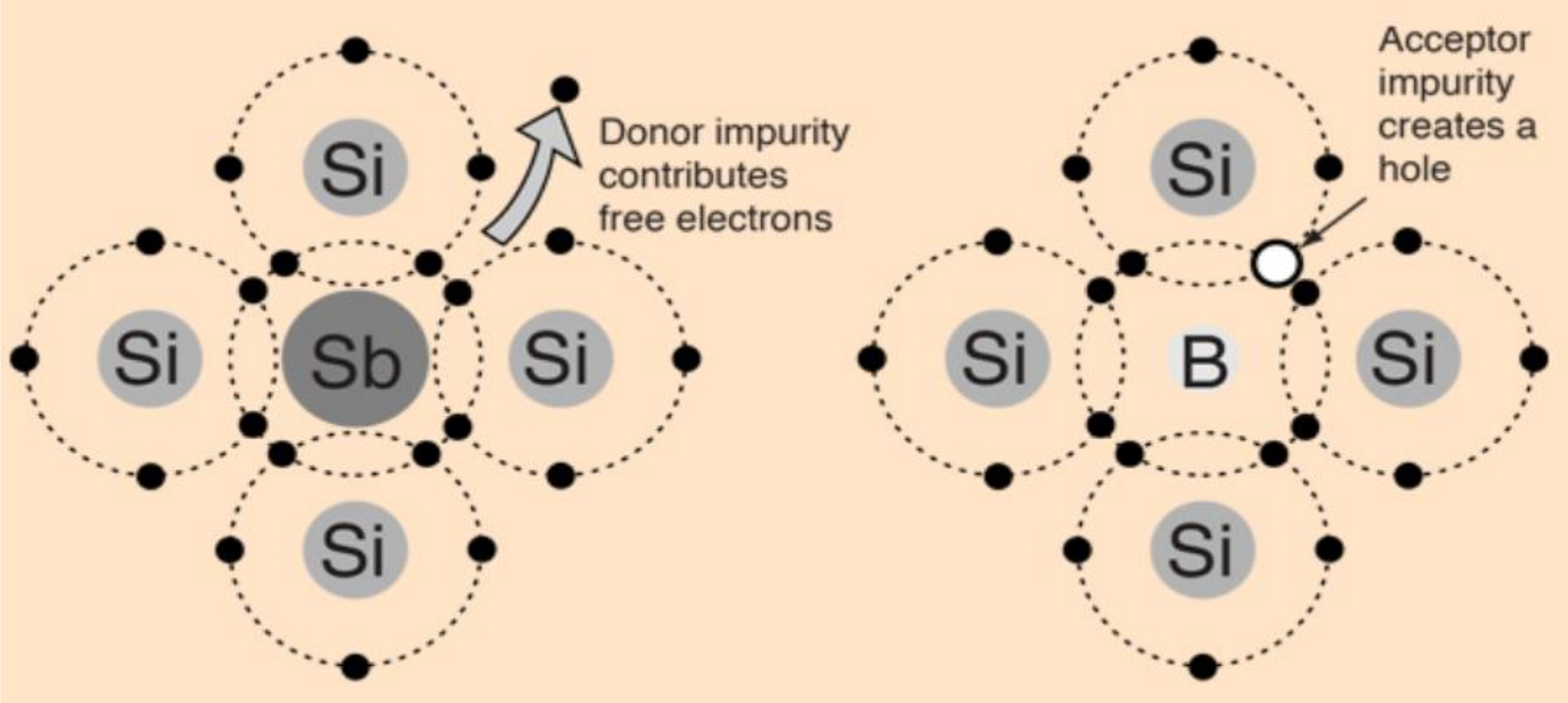




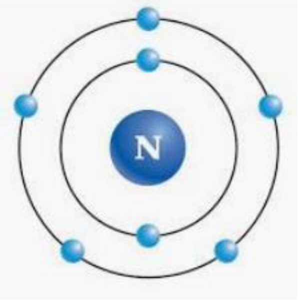
Semi conductors

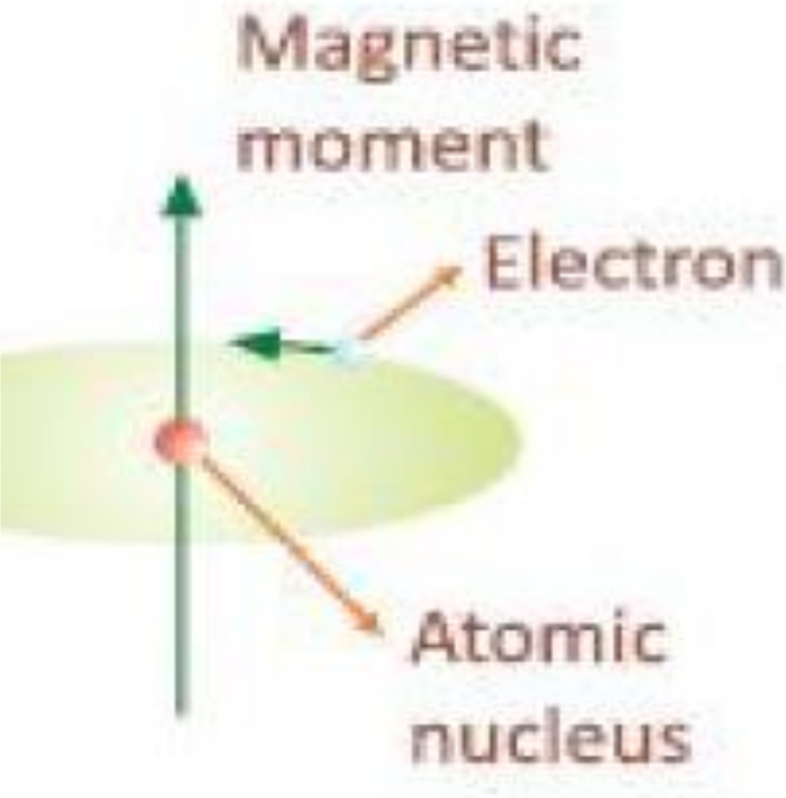


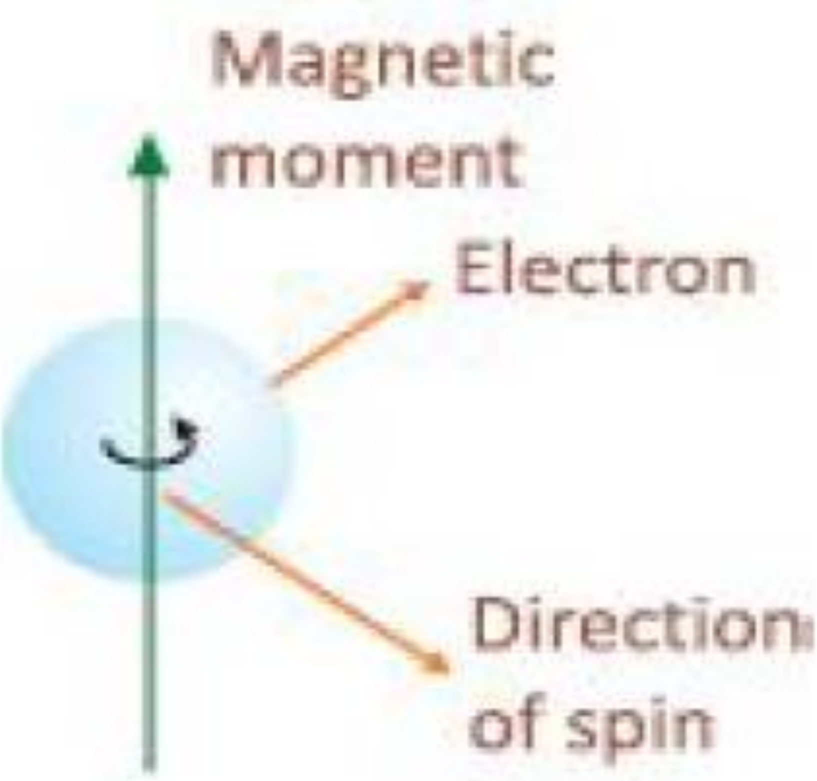
P- and N- Type Semiconductors



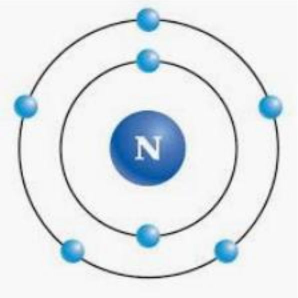
Magnetic properties



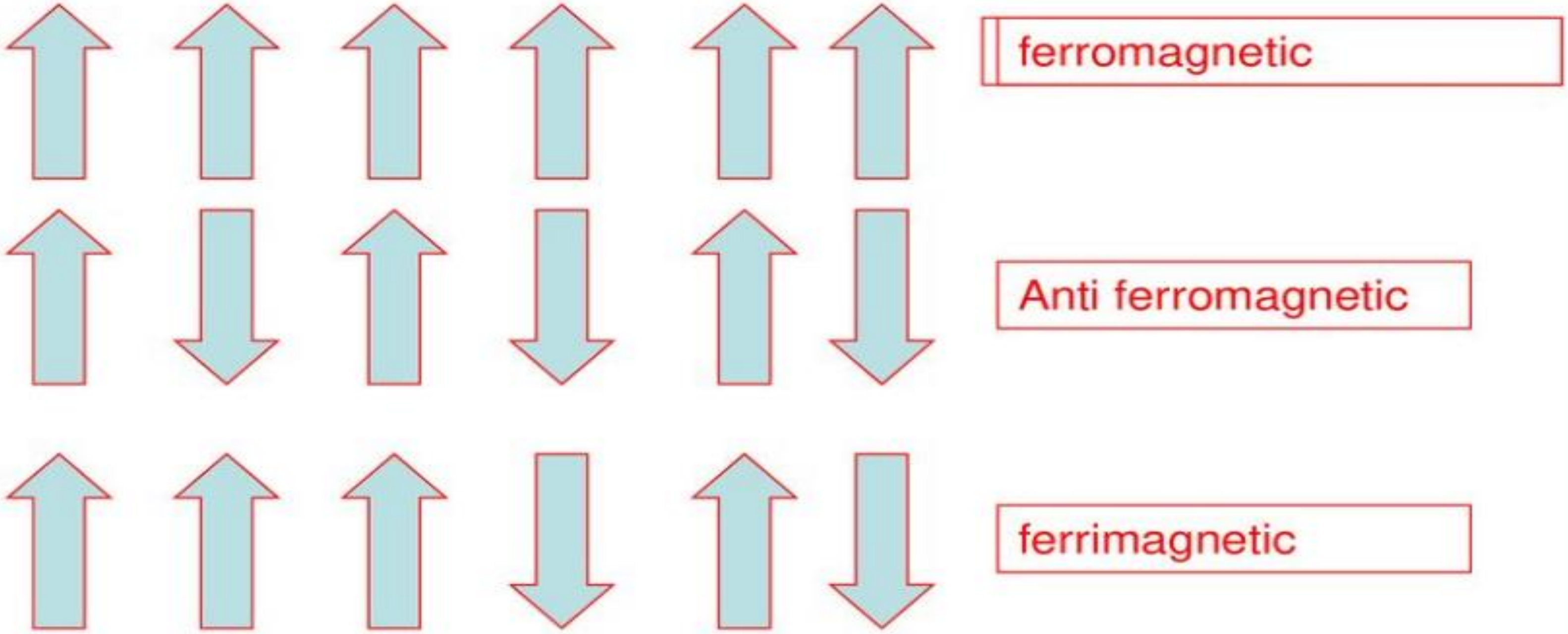




Magnetism



Schematic alignment of magnetic moments in
(a) ferromagnetic
(b) antiferromagnetic and (c) ferrimagnetic.

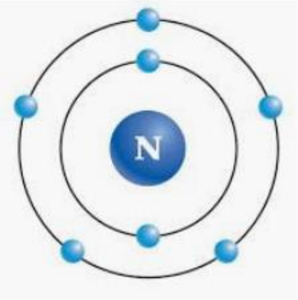


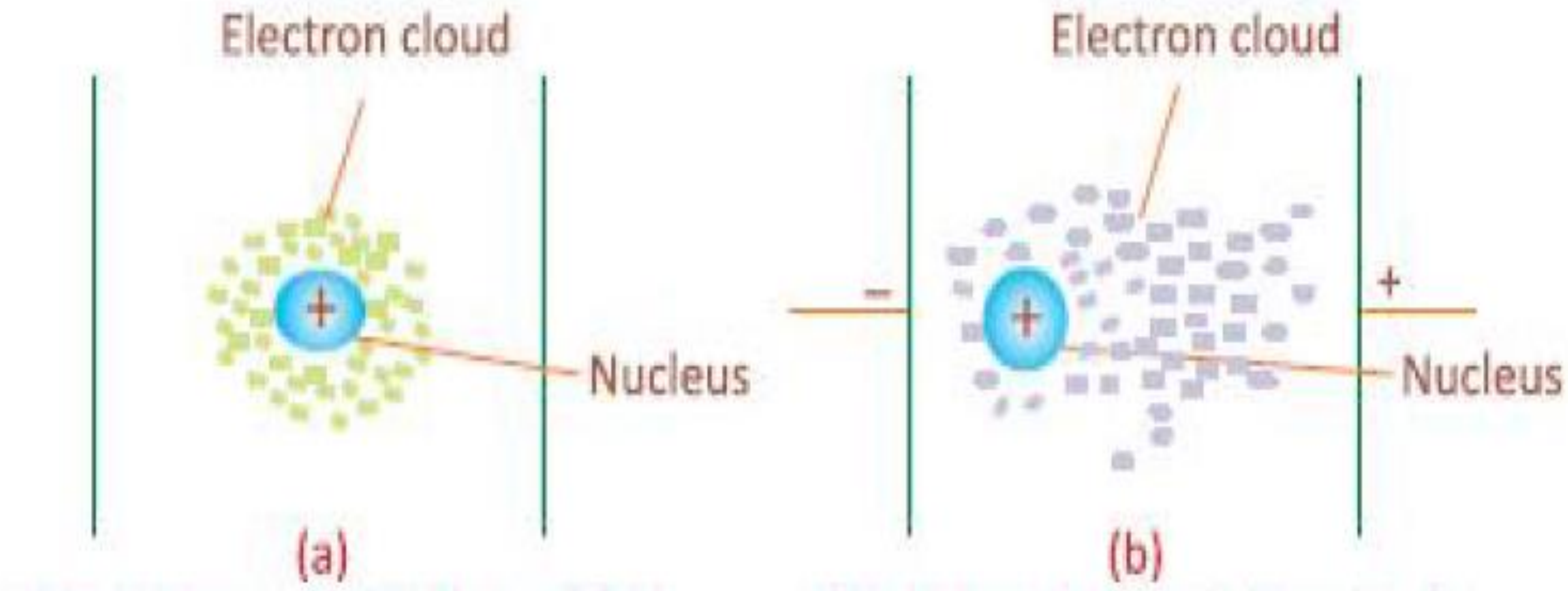
ferromagnetic

Anti ferromagnetic

ferrimagnetic

Dielectric properties





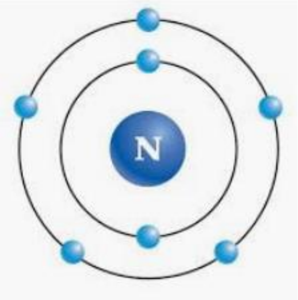
Before electrical field is applied

After electrical field is applied

These formed dipoles may align themselves in an ordered manner.

So that the crystal has net dipole moment.

NH of Primitive(SC)

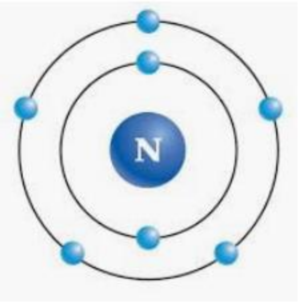


NEIGHBOUR HOOD OF A PARTICLE :

Simple Cubic (SC) Structure :

Type of neighbour	Distance	no.of neighbours
nearest	a	6 (shared by 4 cubes)
(next)^1	$a\sqrt{2}$	12 (shared by 2 cubes)
(next)^2	$a\sqrt{3}$	8 (unshared)

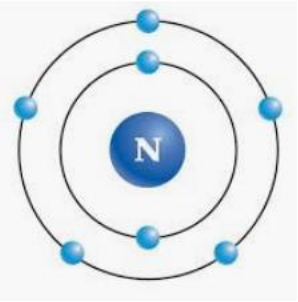
NH of BCC



Body Centered Cubic (BCC) Structure :

Type of neighbour	Distance	no.of neighbours
nearest	$2r = a\frac{\sqrt{3}}{2}$	8
$(\text{next})^1$	$= a$	6
$(\text{next})^2$	$= a\sqrt{2}$	12
$(\text{next})^3$	$= a\frac{\sqrt{11}}{2}$	24
$(\text{next})^4$	$= a\sqrt{3}$	8

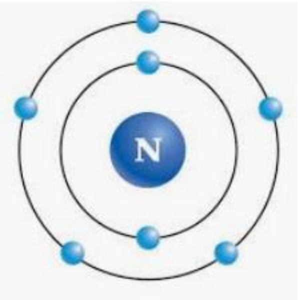
NH of FCC



Face Centered Cubic (FCC) Structure :

Type of neighbour	Distance	no. of neighbours
nearest	$\frac{a}{\sqrt{2}}$	$12 = \left(\frac{3\times 8}{2}\right)$
$(\text{next})^1$	a	$6 = \left(\frac{3\times 8}{4}\right)$
$(\text{next})^2$	$a\sqrt{\frac{3}{2}}$	24
$(\text{next})^3$	$a\sqrt{2}$	12
$(\text{next})^4$	$a\sqrt{\frac{5}{2}}$	24

NaCL



No. of NaCl formula units per FCC unit cell = 4

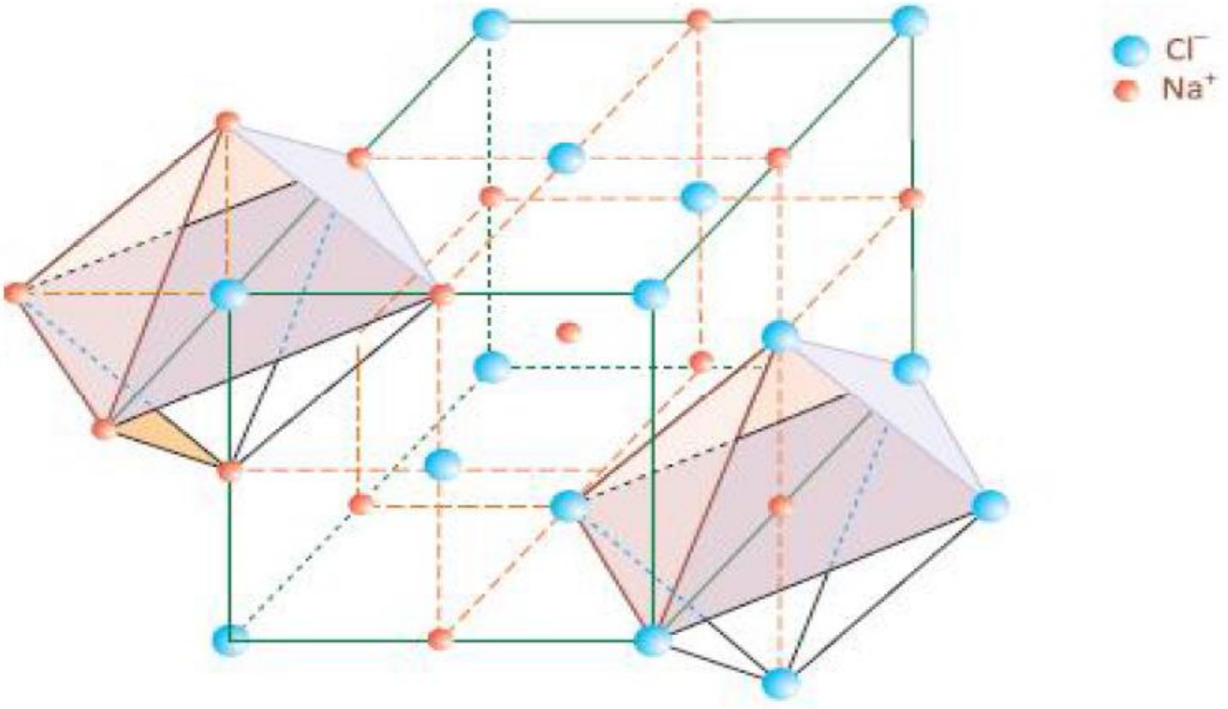


Figure shows the concept of reversibility in the case of NaCl crystal

Co-ordination no. of $Na^+ = 6$ [Na^+ is present in octahedral void formed by six Cl^- ions]

Co-ordination no. of $Cl^- = 6$ [Cl^- is present is octahedral void formed by six Na^+ ions using reversibility principle]

CsCL

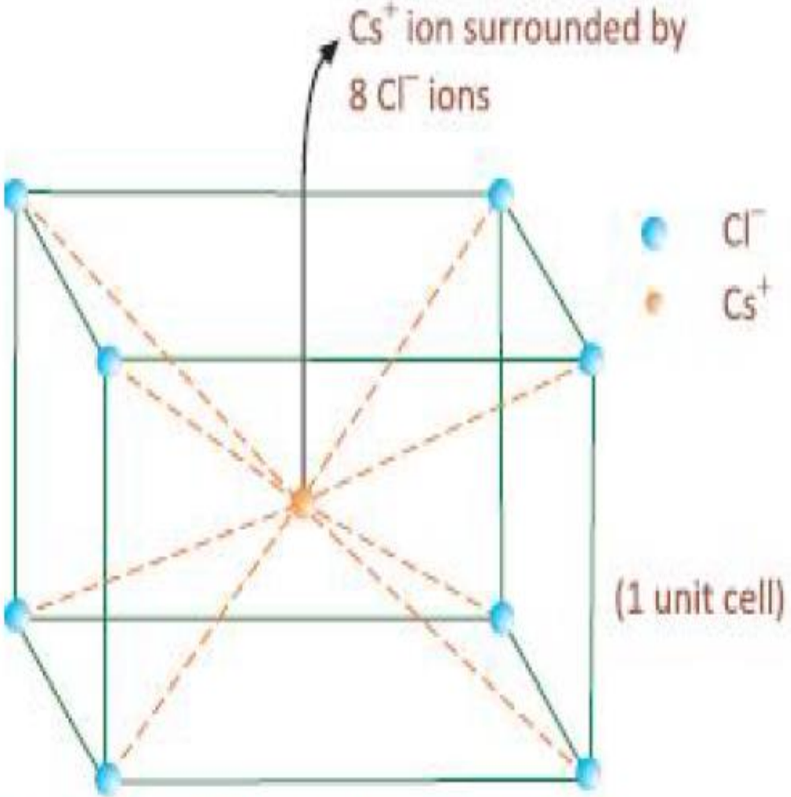


Figure shows Cs^+ at body centre of CsCl unit cell is surrounded by 8 Cl^-

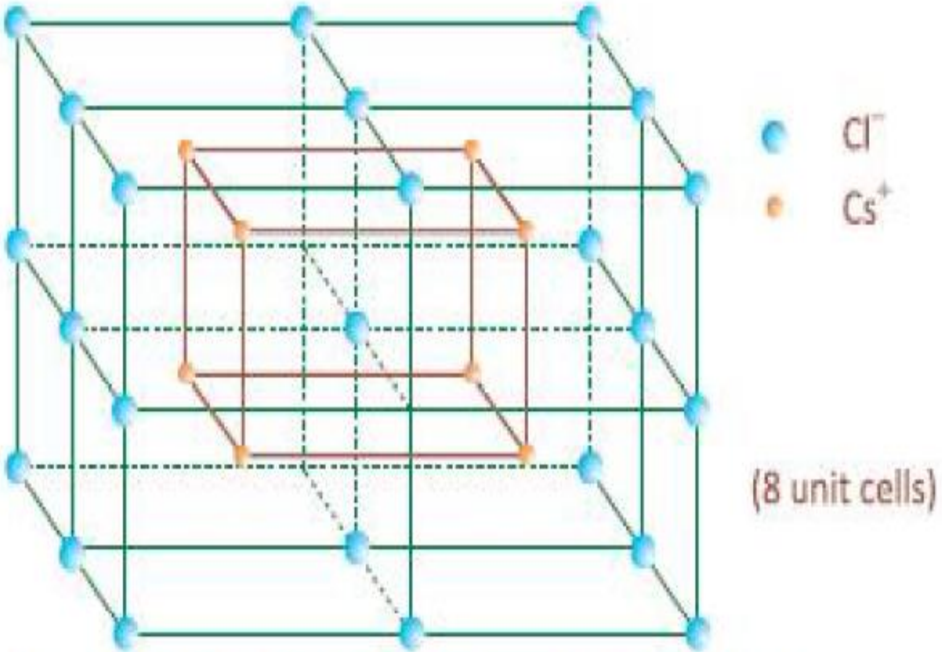
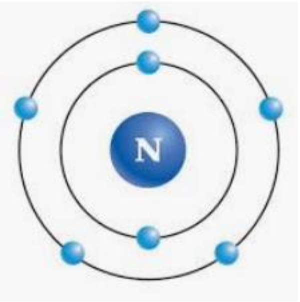


Figure shows the concept of reversibility in the case of CsCl crystal such Cl^- lies in the simple cubic of Cs^+

(Note : Some Cl^- have not been shown for the sake of clarity)

ZnS



No. of ZnS formula units per FCC unit cell = 4

Co-ordination no. of Zn^{2+} = 4 [Zn^{2+} is present in the tetrahedral void formed by $4S^{2-}$ ions]

Co-ordination no. of S^{2-} = 4 [One S^{2-} supports 8 tetrahedrons out of which 4 are fillled with Zn^{2+}]

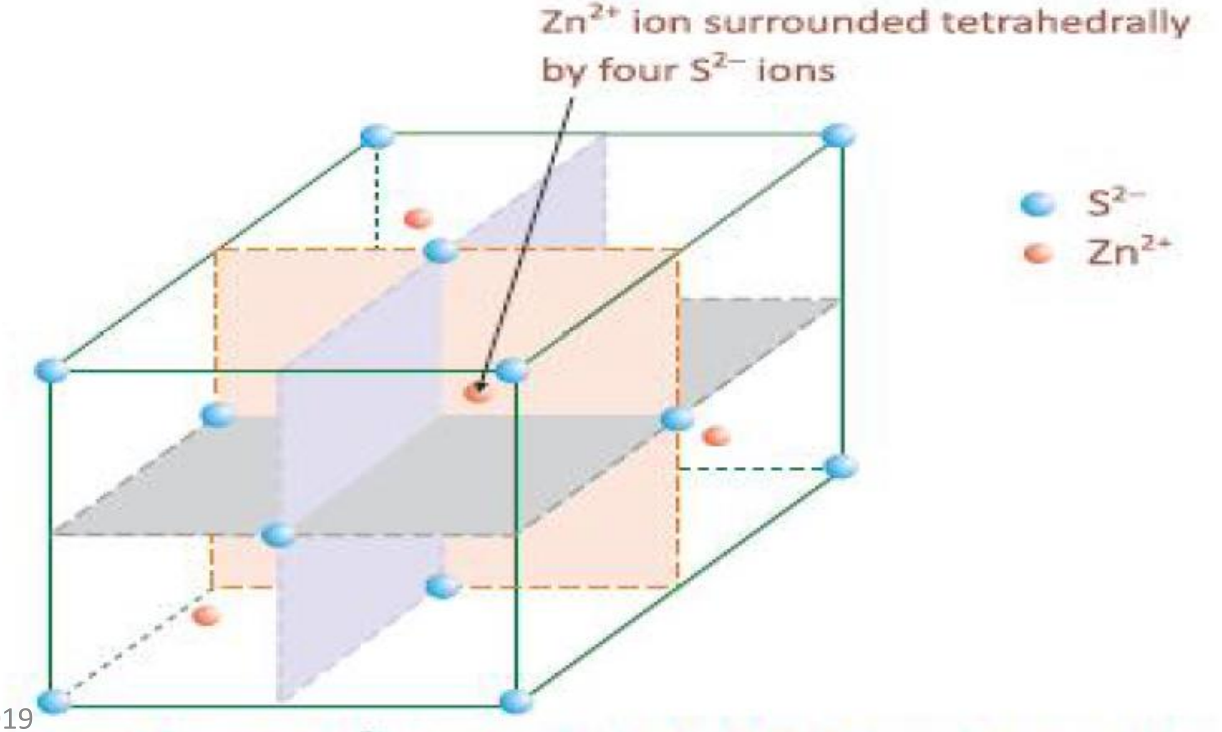
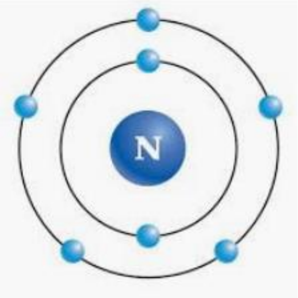


Figure shows 4 Zn^{2+} ions placed in alternate tetrahedral voids

CaF2



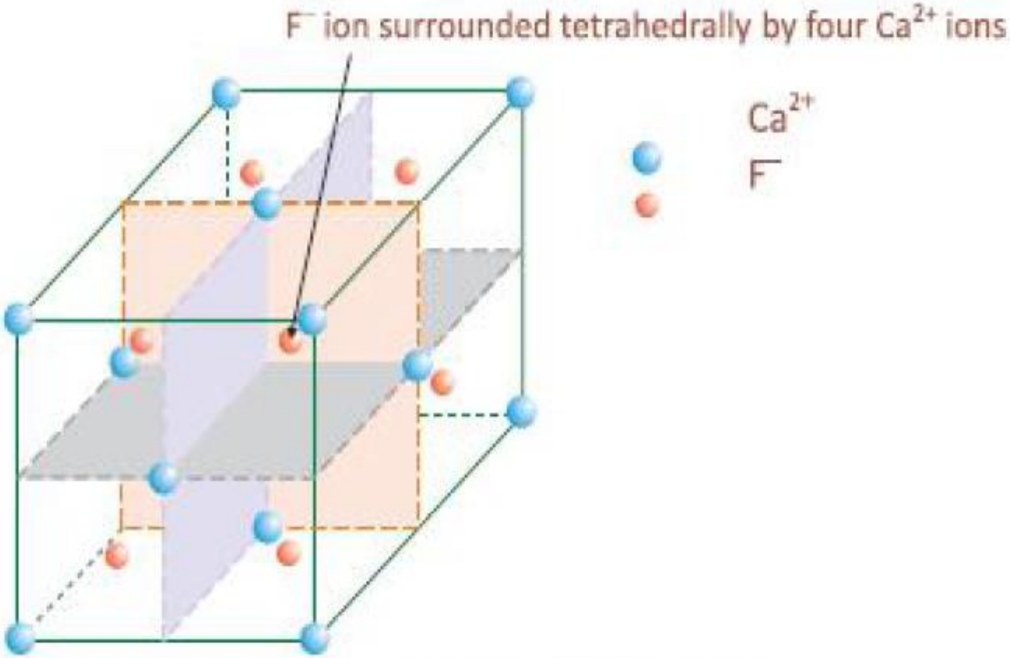
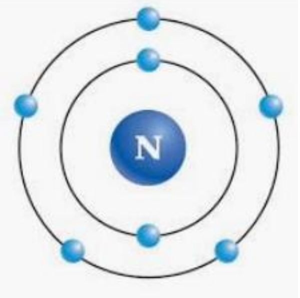


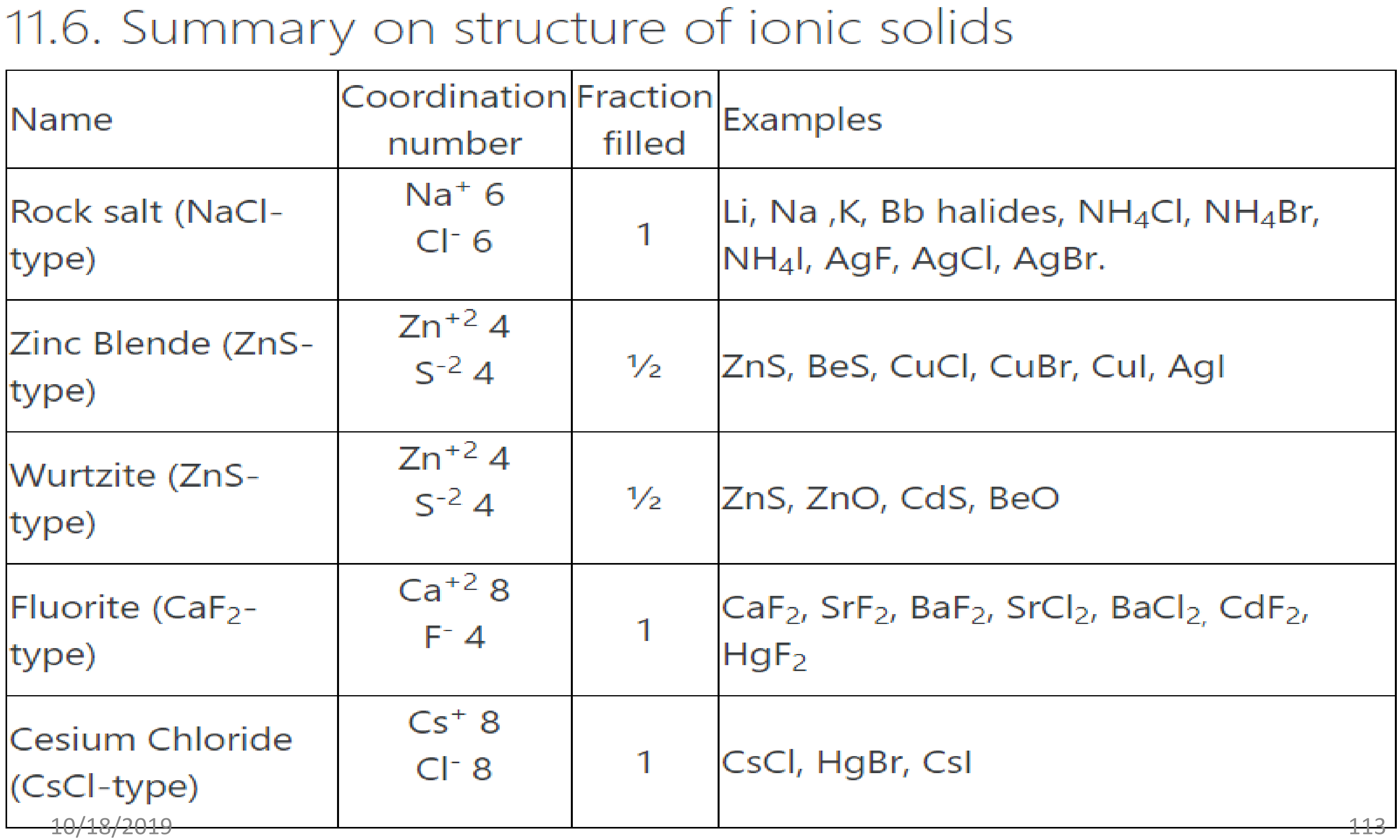
Figure shows 8 F⁻ ions placed in all the tetrahedral voids

Co-ordination no. of F^- = 4 [F^- is present in the tetrahedral void formed by 4 Ca^{2+} ions]

Co-ordination no. of Ca^{2+} = 8 [One Ca^{2+} supports 8 tetrahedral voids and all are filled with F^-]

Ionic Solids

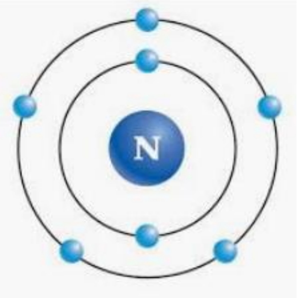




11.6. Summary on structure of ionic solids

Name	Coordination number	Fraction filled	Examples
Rock salt (NaCl-type)	Na^+ 6 Cl^- 6	1	Li, Na ,K, Bb halides, NH_4Cl, NH_4Br, NH_4I, AgF, AgCl, AgBr.
Zinc Blende (ZnS-type)	Zn^{+2} 4 S^{-2} 4	½	ZnS, BeS, CuCl, CuBr, CuI, AgI
Wurtzite (ZnS-type)	Zn^{+2} 4 S^{-2} 4	½	ZnS, ZnO, CdS, BeO
Fluorite (CaF_2-type)	Ca^{+2} 8 F^- 4	1	CaF_2, SrF_2, BaF_2, $SrCl_2$, $BaCl_2$, CdF_2, HgF_2
Cesium Chloride (CsCl-type)	Cs^+ 8 Cl^- 8	1	CsCl, HgBr, CsI

LRR for Triangular

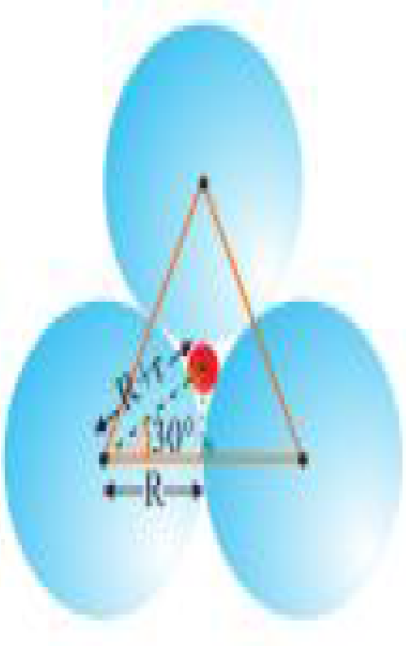


The critical condition for triangular coordination is shown in the adjacent figure.

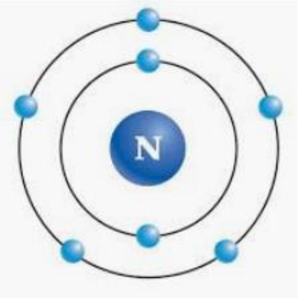
The three anions touch one another as well as the central cation. From the simple geometry, we can write :

$$(R+r)\cos 30^{\circ} = r \quad \Rightarrow \quad R + r = \frac{2}{\sqrt{3}}R$$

$$\frac{r}{R} = \frac{2}{\sqrt{3}} - 1 = 0.155$$



LRR for Tetrahedral



The critical condition for tetrahedral co-ordination is shown in the adjacent figure. Than anions touch one another as well as the central cation. From the simple geometry, we can write :

$$\ell = 2\text{ R} \quad \text{and} \quad \frac{3}{4}\text{h} = \text{R} + \text{r} \quad \text{where} \quad \text{h} = \frac{\sqrt{2}}{\sqrt{3}}\ell$$

$$\Rightarrow \quad \frac{3}{4} \times \frac{\sqrt{2}}{\sqrt{3}} \times 2\text{R} = \text{R} + \text{r}$$

$$\frac{\text{r}}{\text{R}} = \frac{\sqrt{3}}{\sqrt{2}} - 1 = 0.225$$

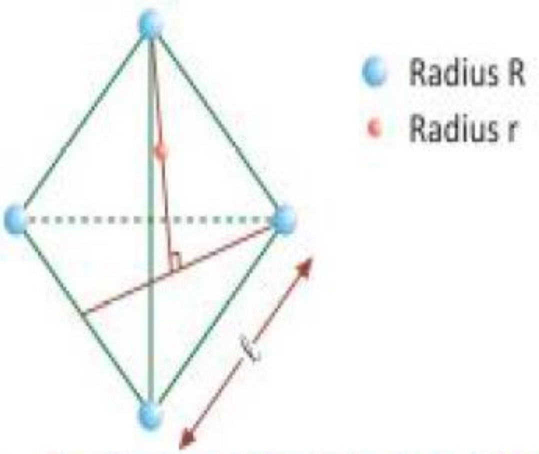
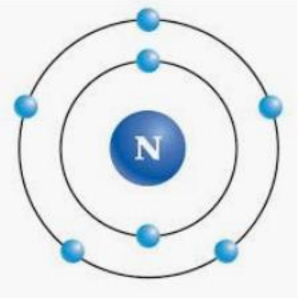


Figure shows ' ● ' is present in tetrahedral void ' ● ' atoms

(Note : Atoms have been shown separated for clarity)

LRR for Octahedral



The critical condition for octahedral co-ordination is shown in the adjacent figure. The anions touch one another as well as the central. From the simple geometry, we can write :

$$\left(2r + 2R\right)\cos 45^\circ = 2R$$

$$\Rightarrow \quad \frac{r}{R} = \sqrt{2} - 1 = 0.414$$

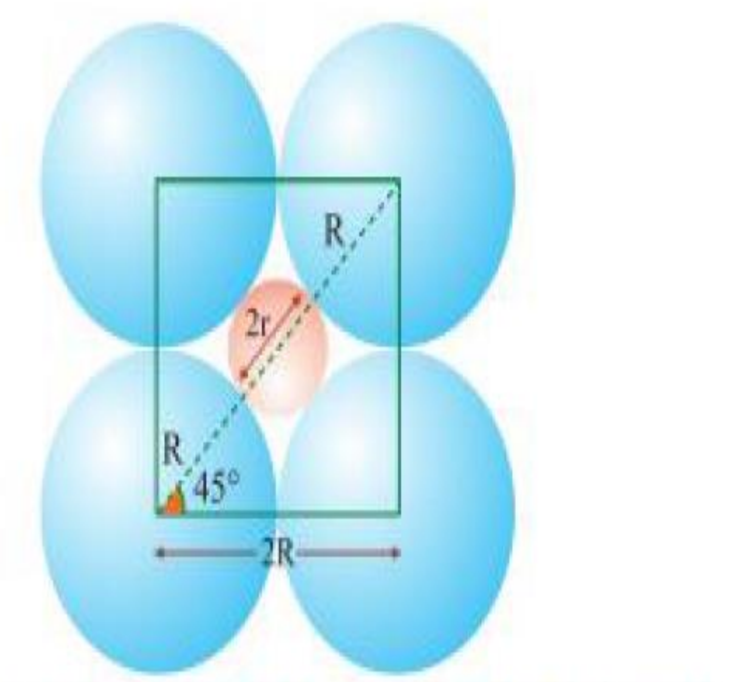


Figure shows '●' is present in octahedral void of '●' atoms

(Note : Only square plane has been shown)

LRR for cubic

The critical condition for cubic void shown in the adjacent figure. The anions touch one another as well as the central cation. From the simple geometry, we can write :

$$a = 2R \text{ and } \sqrt{3}a = 2R + 2r$$

$$\Rightarrow \quad \frac{r}{R} = \sqrt{3} - 1 = 0.732$$

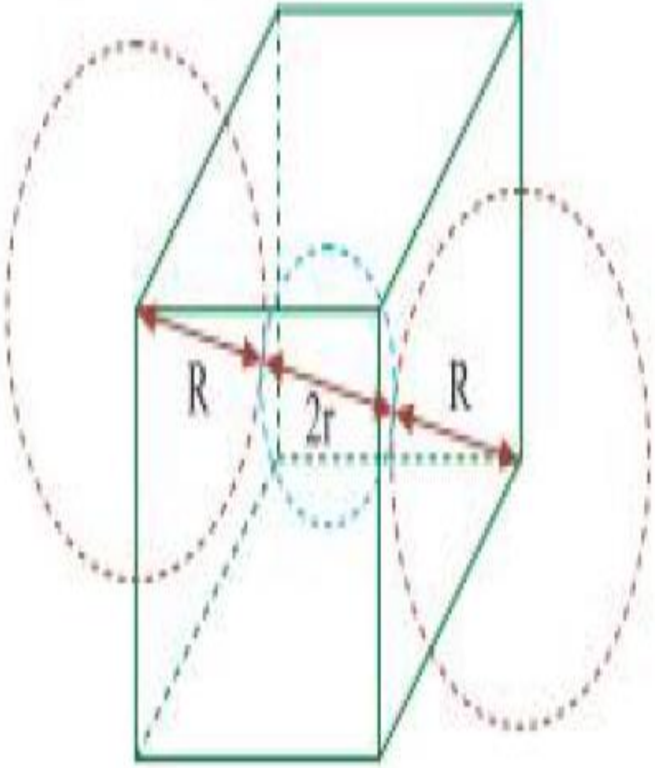
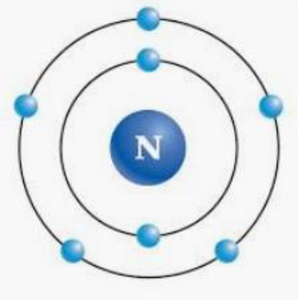
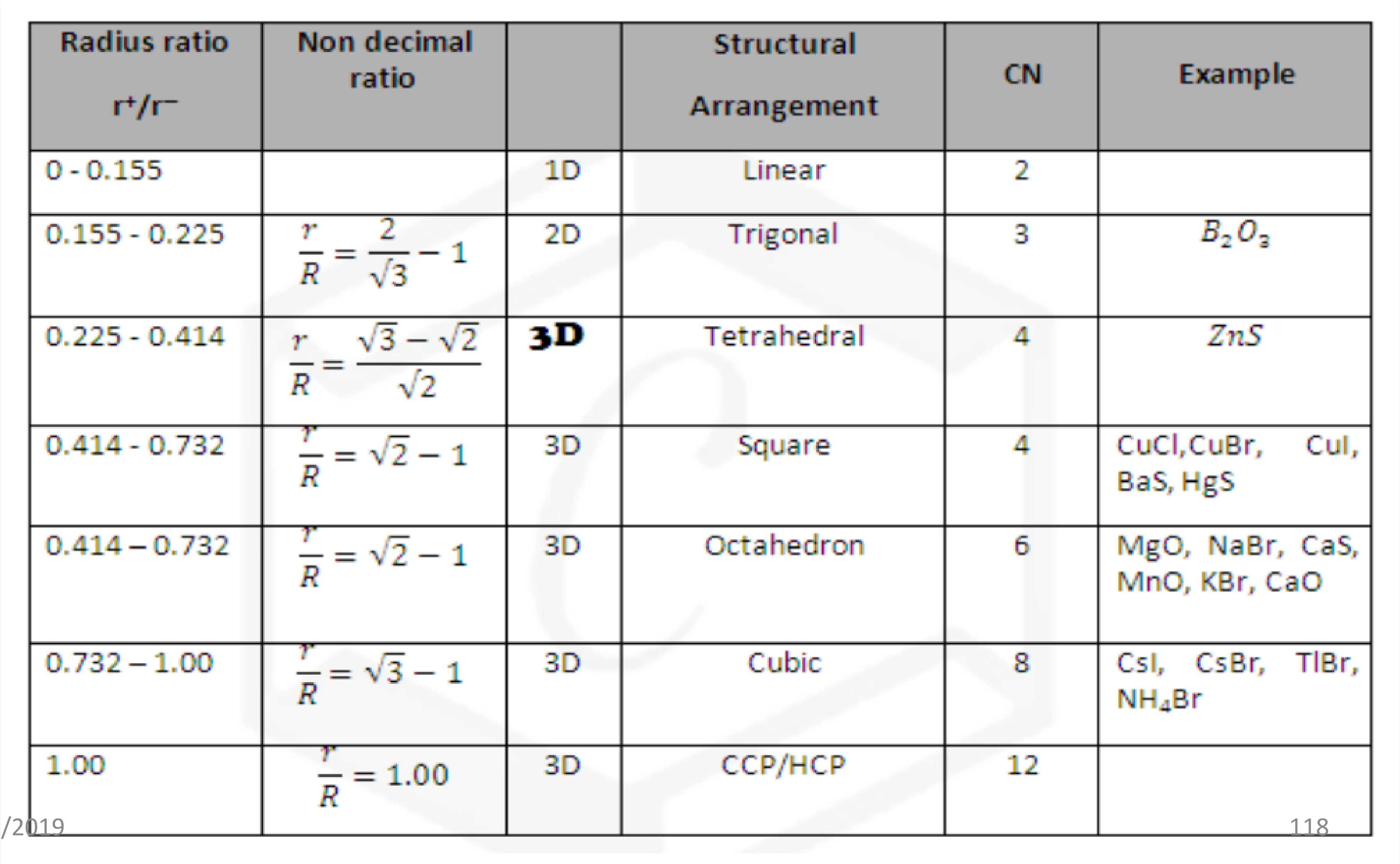


Figure shows '◌' is present in the cubic void of '◌' atoms

Radius ratio rule

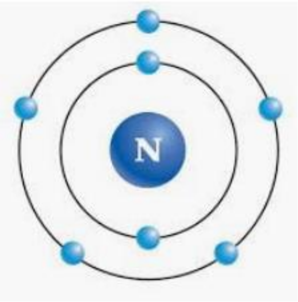


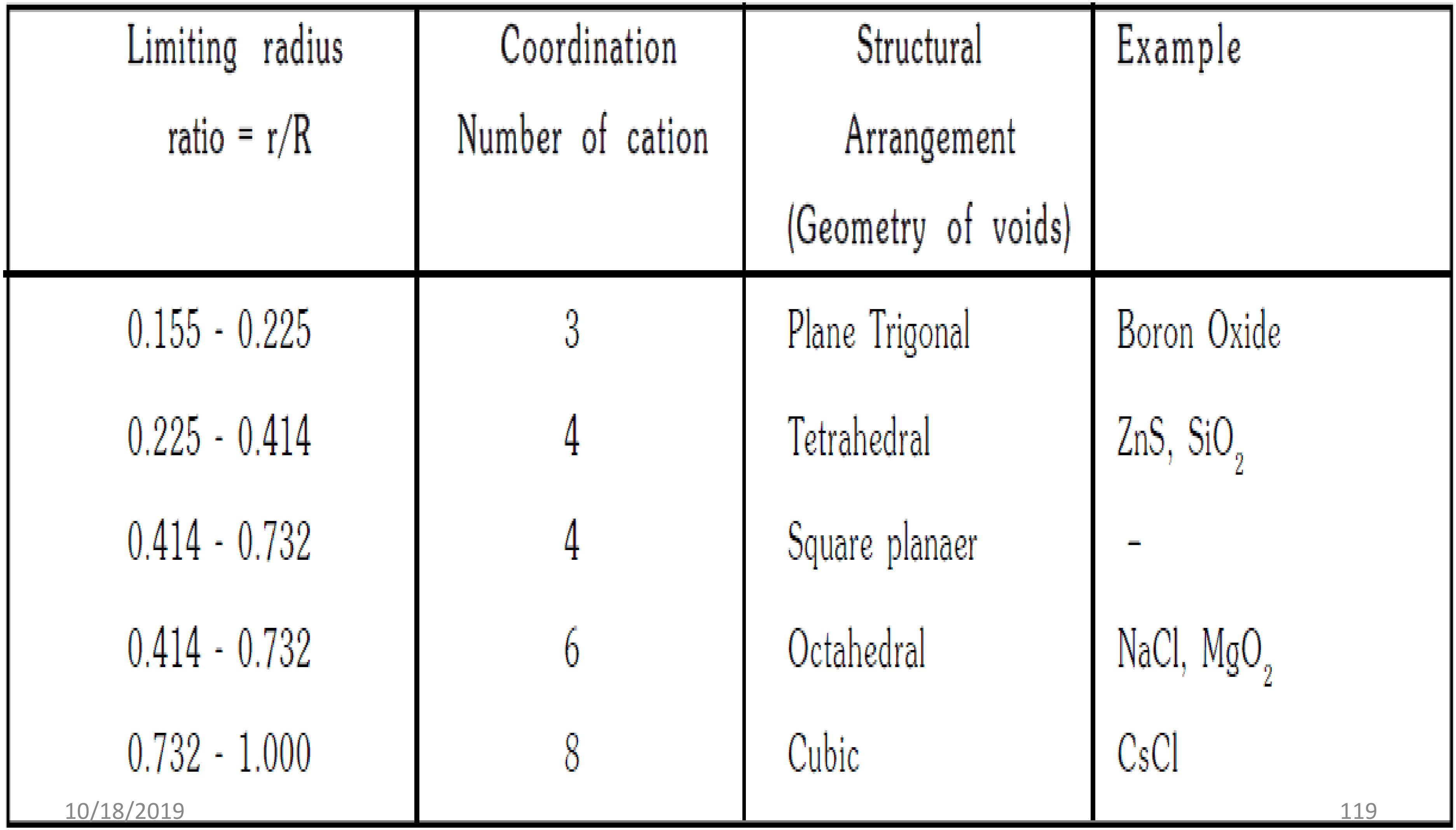
RADIUS RATIO AND COORDINATION NUMBER:



Radius ratio r^+/r^-	Non decimal ratio		Structural Arrangement	CN	Example
0 - 0.155		1D	Linear	2	
0.155 - 0.225	$\frac{r}{R}=\frac{2}{\sqrt{3}}-1$	2D	Trigonal	3	B_2O_3
0.225 - 0.414	$\frac{r}{R}=\frac{\sqrt{3}-\sqrt{2}}{\sqrt{2}}$	**3D**	Tetrahedral	4	ZnS
0.414 - 0.732	$\frac{r}{R}=\sqrt{2}-1$	3D	Square	4	CuCl, CuBr, CuI, BaS, HgS
0.414 – 0.732	$\frac{r}{R}=\sqrt{2}-1$	3D	Octahedron	6	MgO, NaBr, CaS, MnO, KBr, CaO
0.732 – 1.00	$\frac{r}{R}=\sqrt{3}-1$	3D	Cubic	8	CsI, CsBr, TlBr, NH_4Br
1.00	$\frac{r}{R}=1.00$	3D	CCP/HCP	12	

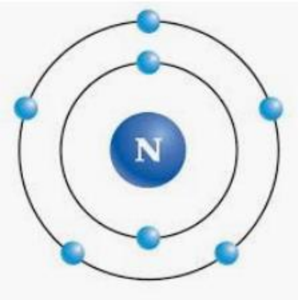
Limiting radius

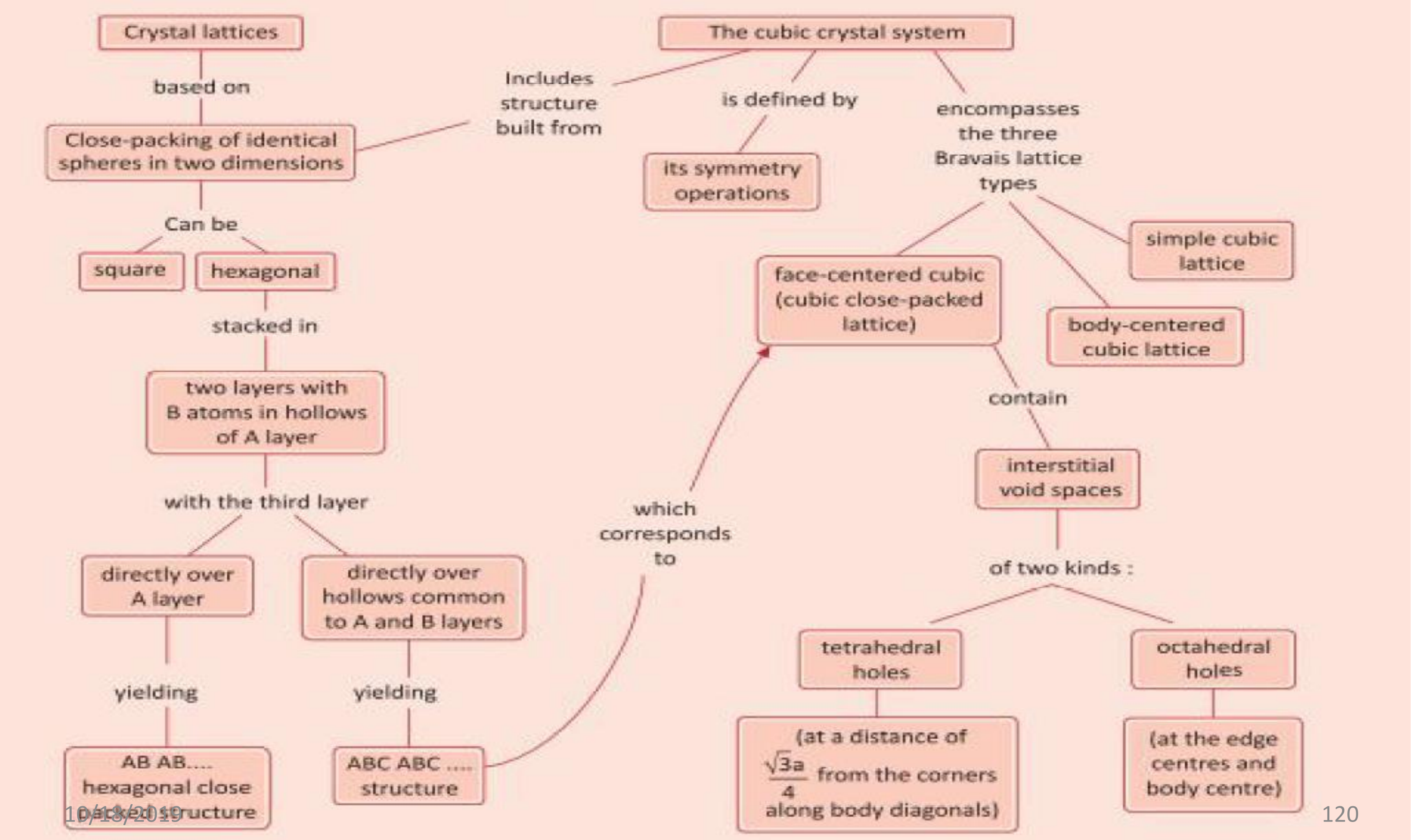




Limiting radius ratio = r/R	Coordination Number of cation	Structural Arrangement (Geometry of voids)	Example
0.155 - 0.225	3	Plane Trigonal	Boron Oxide
0.225 - 0.414	4	Tetrahedral	ZnS, SiO_2
0.414 - 0.732	4	Square planaer	–
0.414 - 0.732	6	Octahedral	NaCl, MgO_2
0.732 - 1.000	8	Cubic	CsCl

Concept map





Crystal lattices

based on

Close-packing of identical spheres in two dimensions

Includes structure built from

The cubic crystal system

is defined by

its symmetry operations

encompasses the three Bravais lattice types

Can be

square

hexagonal

stacked in

two layers with B atoms in hollows of A layer

with the third layer

directly over A layer

directly over hollows common to A and B layers

yielding

yielding

AB AB.... hexagonal close [illegible] structure

ABC ABC .... structure

which corresponds to

face-centered cubic (cubic close-packed lattice)

body-centered cubic lattice

simple cubic lattice

contain

interstitial void spaces

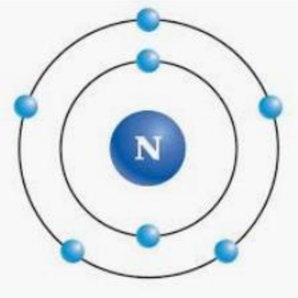
of two kinds :

tetrahedral holes

octahedral holes

(at a distance of $\frac{\sqrt{3}a}{4}$ from the corners along body diagonals)

(at the edge centres and body centre)



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PRESENTATION