THIRD YEAR T.D.C., SCIENCE

PAPER-III, Part C

Paper Code - 3163

SOLID STATE, NUCLEAR AND PARTICLE PHYSICS

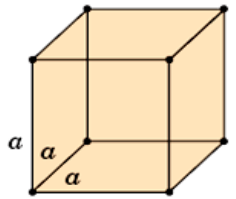
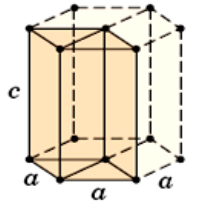
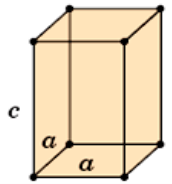
UNIT – 1 : CRYSTAL GEOMETRY

Typical Crystal Structures: Classification

- The axes labelled as a, b, c α, β, γ (angle between the axes)

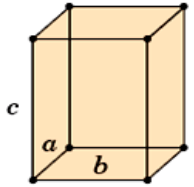
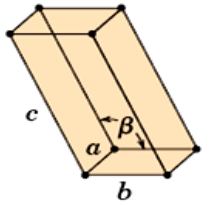
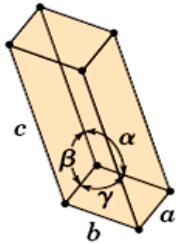
- There are seven different possible combinations of lattice parameters a, b, and c (axes), and α, β, γ (angle between the axes) the and each of this represents a distinct crystal system.

Relation ships between the lattice parameters and unit cell geometry for the seven crystal systems

Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	

UNIT – 1 : CRYSTAL GEOMETRY

Relation ships between the lattice parameters and unit cell geometry for the seven crystal systems

Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

Typical Crystal Structures: Classification

UNIT – 1 : CRYSTAL GEOMETRY

Typical Crystal Structures : Classification of lattice : The Seven Crystal Systems

CRYSTAL SYSTEM	CONVENTIONAL UNIT CELL
1. Cubic	$a=b=c$, $\alpha=\beta=\gamma=90°$
2. Tetragonal	$a=b\neq c$, $\alpha=\beta=\gamma=90°$
3. Orthorhombic	$a\neq b\neq c$, $\alpha=\beta=\gamma=90°$
4. Hexagonal	$a=b\neq c$, $\alpha=\beta= 90°$, $\gamma=120°$
5. Rhombohedral OR Trigonal	$a=b=c$, $\alpha=\beta=\gamma\neq90°$
6. Monoclinic	$a\neq b\neq c$, $\alpha=\beta=90°\neq\gamma$
7. Triclinic	$a\neq b\neq c$, $\alpha\neq\beta\neq\gamma$

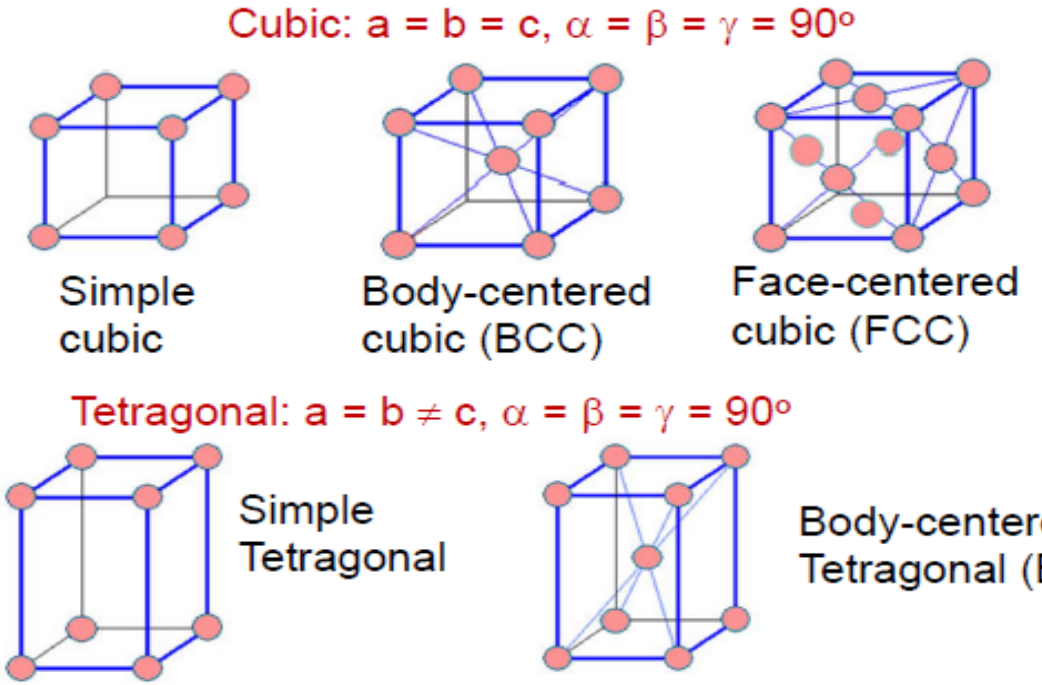
UNIT – 1 : CRYSTAL GEOMETRY

Typical Crystal Structures: Classification

In addition, with the centering (face, base and body centering) added to these, 14 kinds of 3D lattices, known as Bravais lattices, can be generated

- In the cubic system, we have simple cubic, Body centered cubic (BCC), Face Centered Cubic (FCC).
- As shown in the figure, this refers to where the basis (atoms/molecules) are placed in the structure.
- For example, when we say Body Centered Cubic (BCC), it means that in addition to the atoms at the corners of the cube, there is also one at the body centre.

CRYSTAL SYSTEMS



- In the tetragonal system, we have simple tetragonal and Body centered tetragonal (BCT

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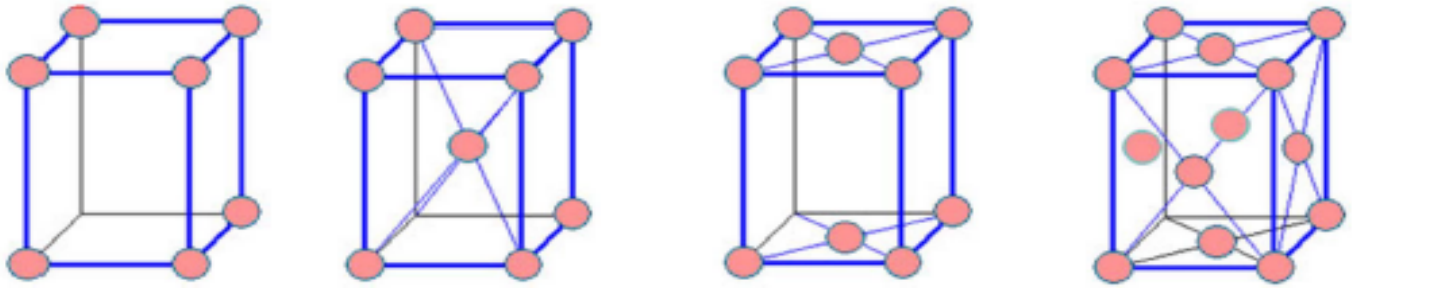
Typical Crystal Structures: Classification

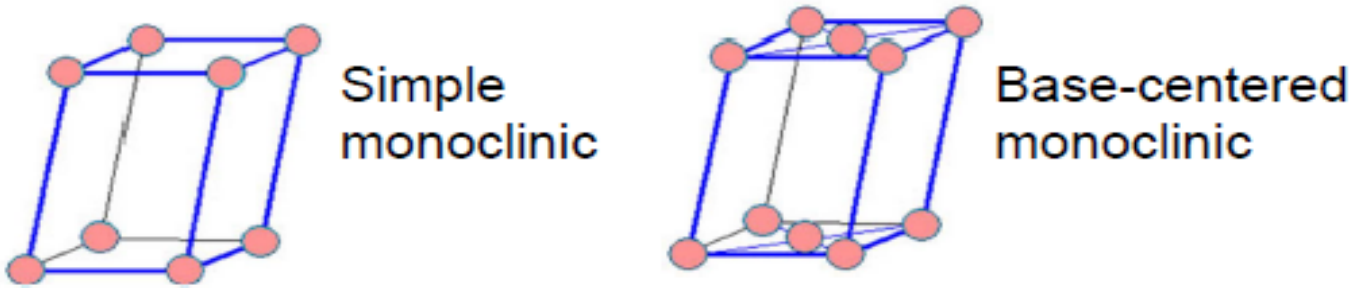
CRYSTAL SYSTEMS

Orthorhombic: $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^{o}$



Simple Body-centered Base-centered Face-centered

Monoclinic: $a \neq b \neq c$, $\alpha = \gamma = 90^{o} \neq \beta$



Simple monoclinic

Base-centered monoclinic

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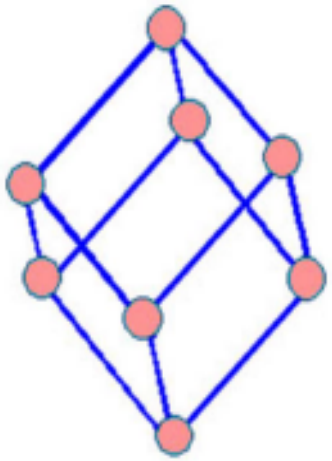
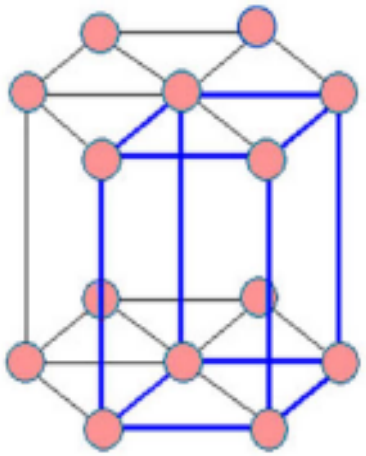
Typical Crystal Structures: Classification

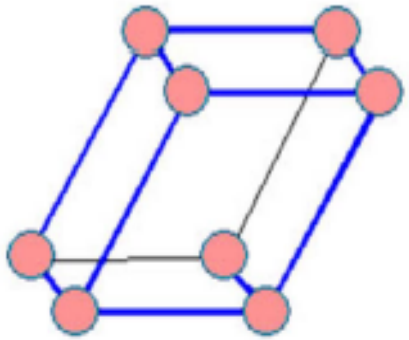
CRYSTAL SYSTEMS



Rhombohedral
a = b = c
α = β = γ ≠ 90°



Hexagonal
a = b ≠ c
α = β = 90° γ = 120°



Triclinic
a ≠ b ≠ c
α ≠ β ≠ γ ≠ 90°

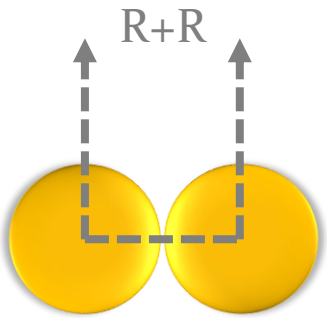
In summary :

- 3 for Cubic
- 2 for Tetragonal
- 4 for Orthorhombic
- 2 for Monoclinic
- 1 for Rhombohedral
- 1 for Hexagonal
- 1 for Triclinic

Adding up we have a total of 14 3D lattices, known as Bravais lattices

UNIT – 1 : CRYSTAL GEOMETRY

Coordination number and packing fraction : Definitions



To discuss crystalline structures it is useful to consider atoms as being hard spheres, with well-defined radii. Thus the shortest distance between two like atoms is one diameter.

A. Coordination Number (CN) : It is the number of nearest neighbours that an atom has in a crystal structure.

B. Nearest Neighbour distance : It is the distance between two nearest neighbours in a crystal

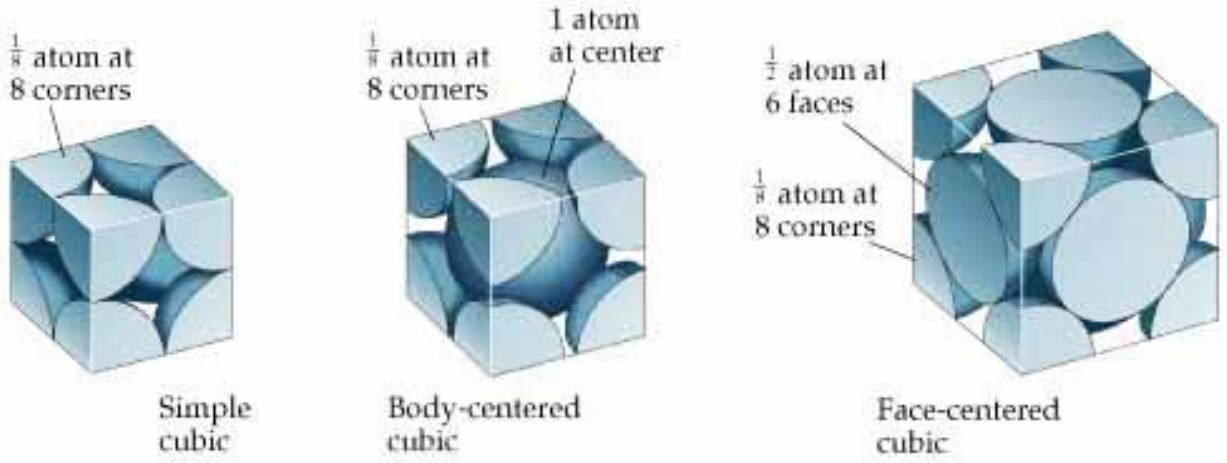
C. Atomic packing factor (APF) or Packing fraction : It is the fraction of space occupied by atoms in a unit cell and is defined as the ratio of volume occupied by atoms in a unit cell to the volume of the unit cell.

D. Thus, APF = Sum of atomic volumes/Volume of cell.

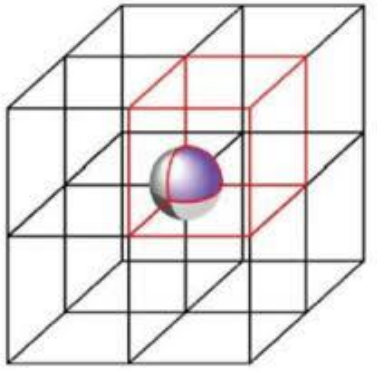
UNIT – 1 : CRYSTAL GEOMETRY

Coordination number and packing fraction : Definitions

Additional Important properties of the unit cells are



- The type of atoms and their radii R.
- Cell dimensions (side a in cubic cells, side of base a and height c in HCP) in terms of R.



- n, number of atoms per unit cell. For an atom that is shared with m adjacent unit cells, we only count a fraction of the atom, 1/m. For example, in the figure above, in a simple cubic cell, since each of the atoms at each corner is in touch with eight other atoms, effectively, it is as 1/8.
- Therefore, the total number of atoms/unit cell, n = (1/8)x8 = 1

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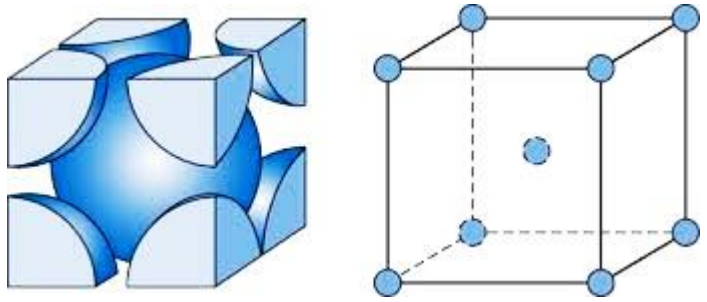
Coordination number and packing fraction

Unit Cell	n	CN	a/R	APF
SC	1	6	2	0.52
BCC	2	8	$4\sqrt{3}$	0.68
FCC	4	12	$2\sqrt{2}$	0.74
HCP	6	12		0.74



In the above figure, we can see that in a BCC structure, n=2 because each of the corner atoms in a unit cell are shared by 8 other cells, whereas the one in the middle is not shared. Thus, n=(1/8) x 8 + 1 = 2

- The direction of closest packing also varies
- For example, The closest packed direction in a BCC cell is along the diagonal of the cube; in a FCC cell is along the diagonal of a face of the cube.