



SNS College of Engineering Coimbatore – 641 107



Crystal Physics



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- Parameters Determining Structure

Introduction

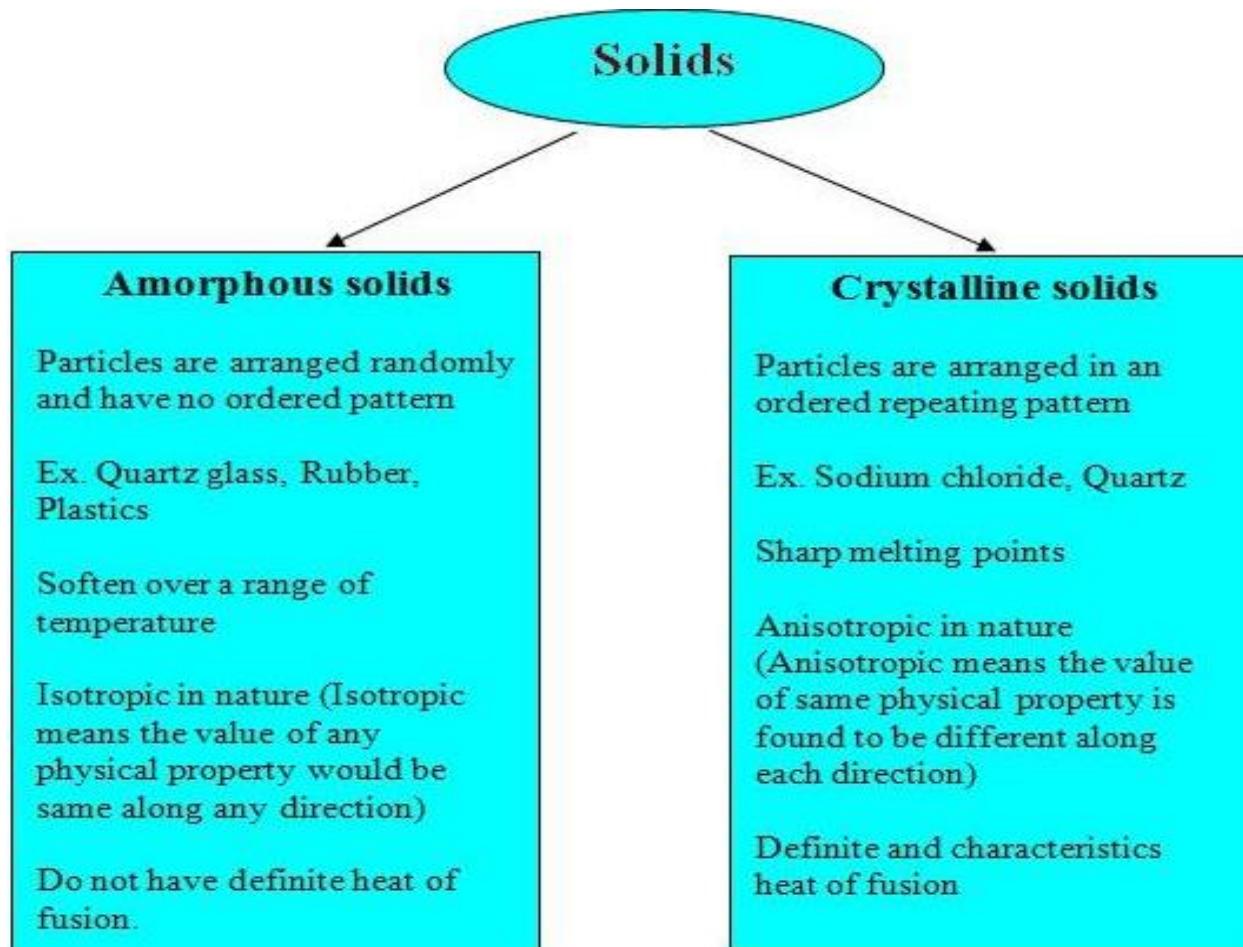
A. States of matter

- ④ **States of matter**- The physical forms in which a substance exist.
- ④ -Solids, Liquids, Gases.



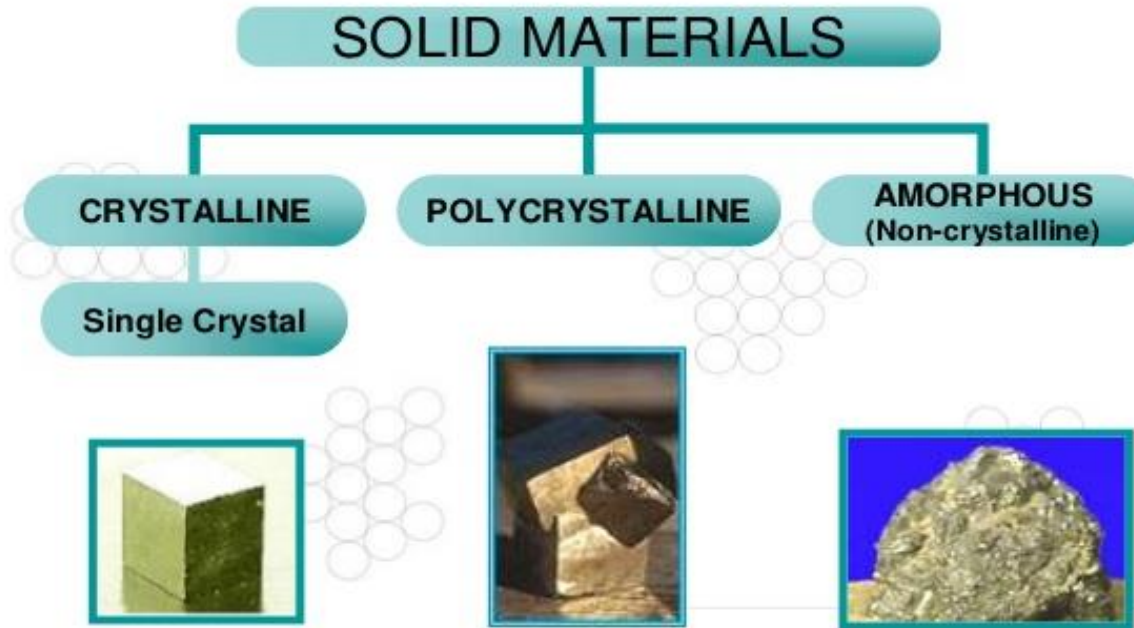


Classification of Solids





Classification of Crystalline Material



Eg : Gold, Al, Diamond ect.,



Fundamentals of Crystal Physics



- Lattice
- Space Lattice
- Lattice Points
- Lattice Lines
- Lattice Planes
- Basis/Motif
- Crystal Structure
- Unit Cell
- Primitive Cell
- Non Primitive Cell

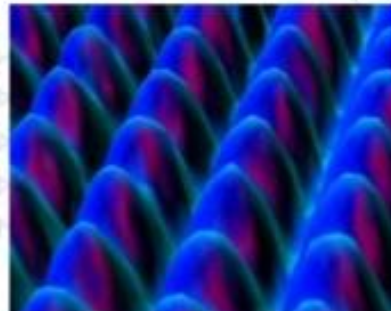
CRYSTAL LATTICE

What is a crystal lattice?

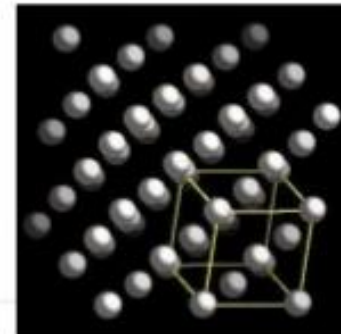
In crystallography, only the geometrical properties of the crystal are of interest, therefore one replaces each atom by a geometrical point located at the equilibrium position of that atom.



Platinum



Platinum surface
(scanning tunneling microscope)



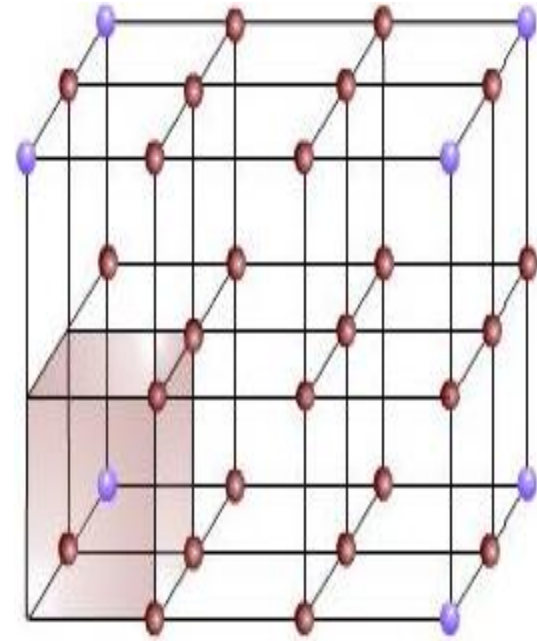
Crystal lattice and
structure of Platinum

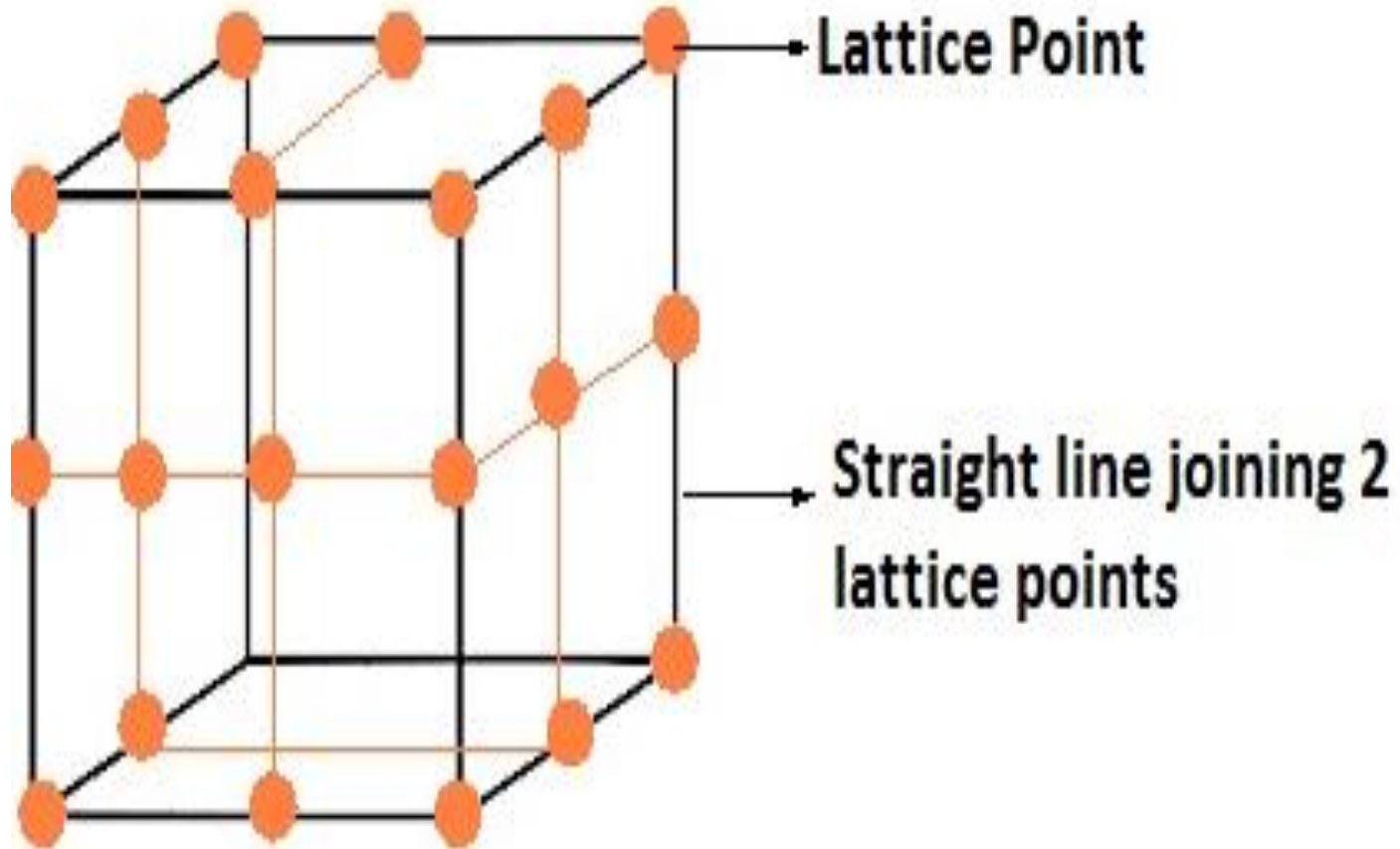
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SPACE LATTICE

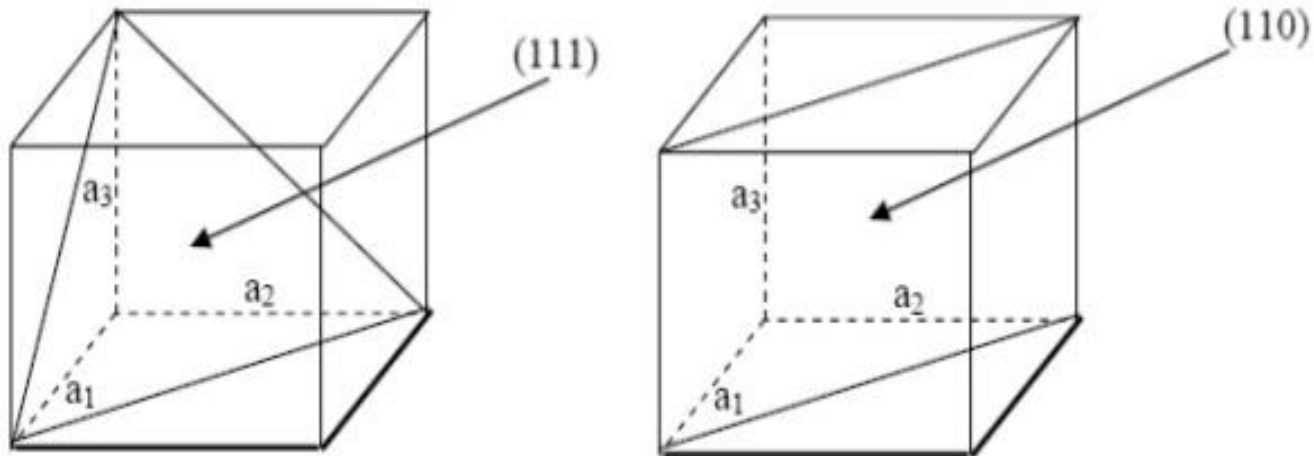
It is defined as an **infinite array** of points in **three dimension** in which every point has surroundings identical to that of every other point in the array.





Lattice planes

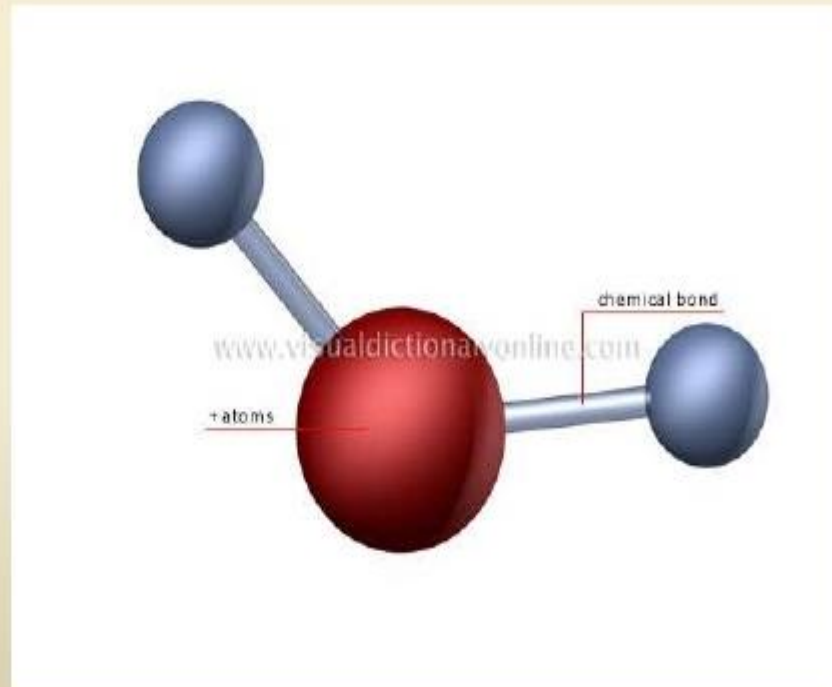
- Lattice planes are flat parallel planes separated by equal distance. All the lattice points lie on these lattice planes





Basis

- Group of atom is called as basis

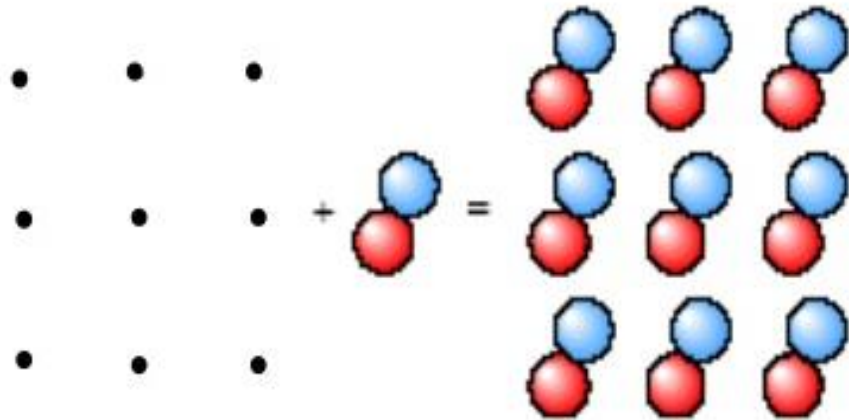




Crystal Structure

- Crystal structures can be obtained by attaching atoms, groups of atoms or molecules which are called basis (motif) to the lattice sites of the lattice point.

Crystal Structure = Crystal Lattice • + Basis 

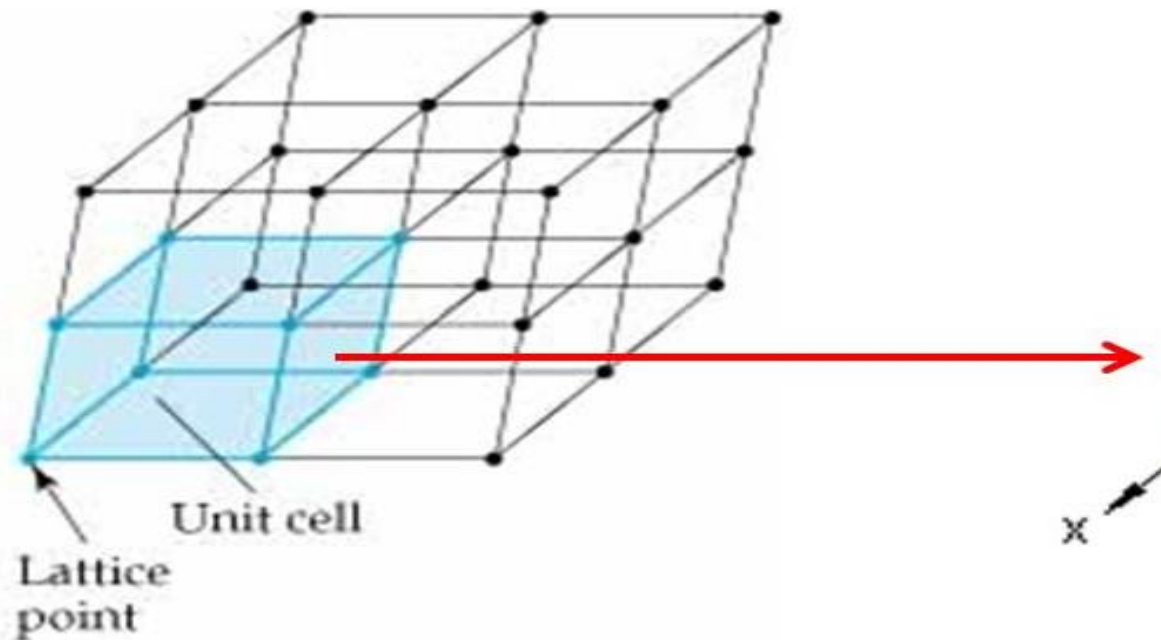




Unit Cell

➤ Crystal Structure: Unit Cell

The smallest structural unit of a crystal that has all its symmetry and by repetition in three dimensions makes up its full lattice.





Unit Cell is of two types

- **Primitive Unit Cell**
- **Non-Primitive Unit Cell**

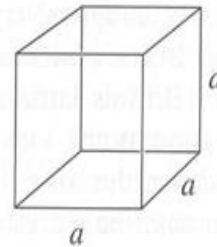
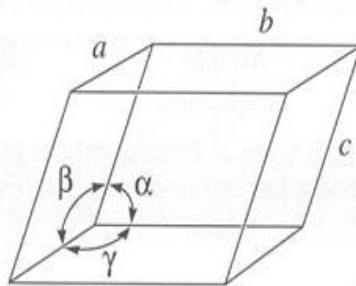
Primitive Unit cell has one lattice point

Non Primitive Unit cell has more than one

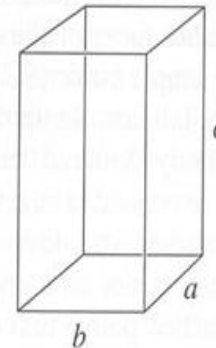


Lattice Parameters

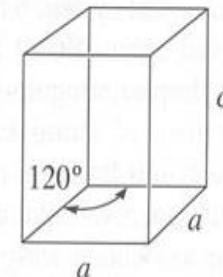
- The lattice parameters describe the size and shape of the unit cell.
- There are **three lengths**, a , b , and c that describe the cell's edges.
- There are **three angles**, α , β , and γ , that describe the three angles between the adjacent cell axes.



Cubic

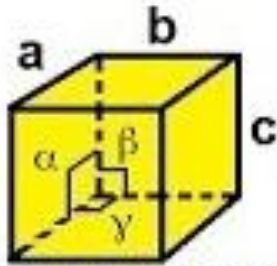


Orthorhombic

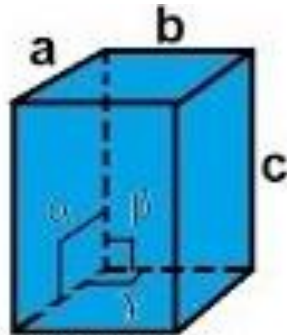


Hexagonal

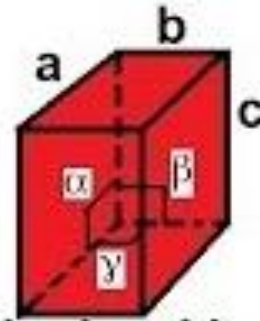
THE 7 CRYSTAL SYSTEMS



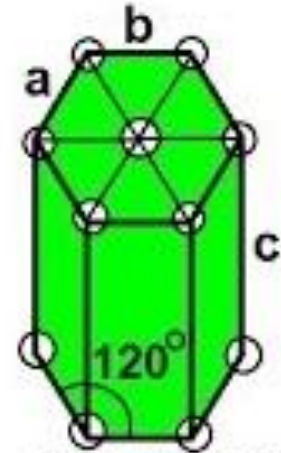
simple cubic
 $a = b = c$
 $\alpha = \beta = \gamma = 90^\circ$



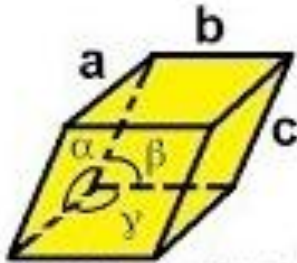
tetragonal
 $a = b \neq c$
 $\alpha = \beta = \gamma = 90^\circ$



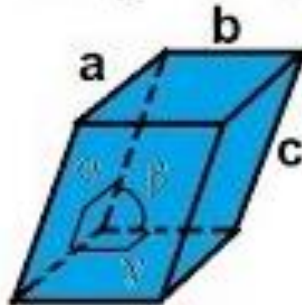
orthorhombic
 $a \neq b \neq c$
 $\alpha = \beta = \gamma = 90^\circ$



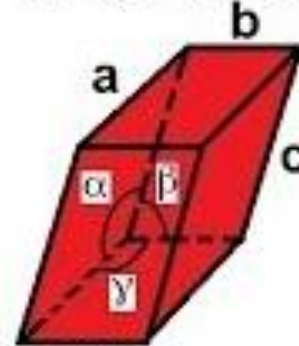
hexagonal
 $a = b \neq c$
 $\alpha = \beta = 90^\circ$
 $\gamma = 120^\circ$



rhombohedral
 $a = b = c$
 $\alpha = \beta = \gamma \neq 90^\circ$



monoclinic
 $a = b \neq c$
 $\alpha = \gamma = 90^\circ \neq \beta \neq 90^\circ$



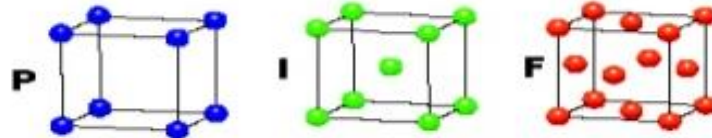
triclinic
 $a \neq b \neq c$
 $\alpha \neq \beta \neq \gamma \neq 90^\circ$

14 Bravais lattices

CUBIC

$$a = b = c$$

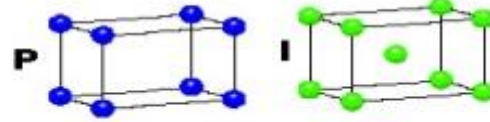
$$\alpha = \beta = \gamma = 90^\circ$$



TETRAGONAL

$$a = b \neq c$$

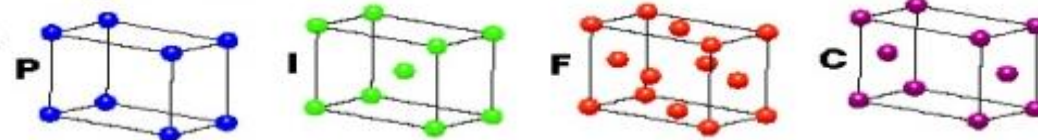
$$\alpha = \beta = \gamma = 90^\circ$$



ORTHORHOMBIC

$$a \neq b \neq c$$

$$\alpha = \beta = \gamma = 90^\circ$$

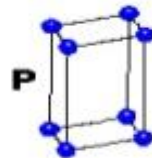


HEXAGONAL

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ$$

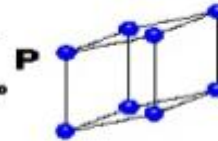
$$\gamma = 120^\circ$$



TRIGONAL

$$a = b = c$$

$$\alpha = \beta = \gamma \neq 90^\circ$$

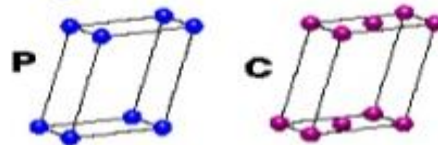


MONOCLINIC

$$a \neq b \neq c$$

$$\alpha = \gamma = 90^\circ$$

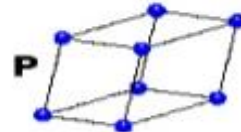
$$\beta \neq 120^\circ$$



TRICLINIC

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$

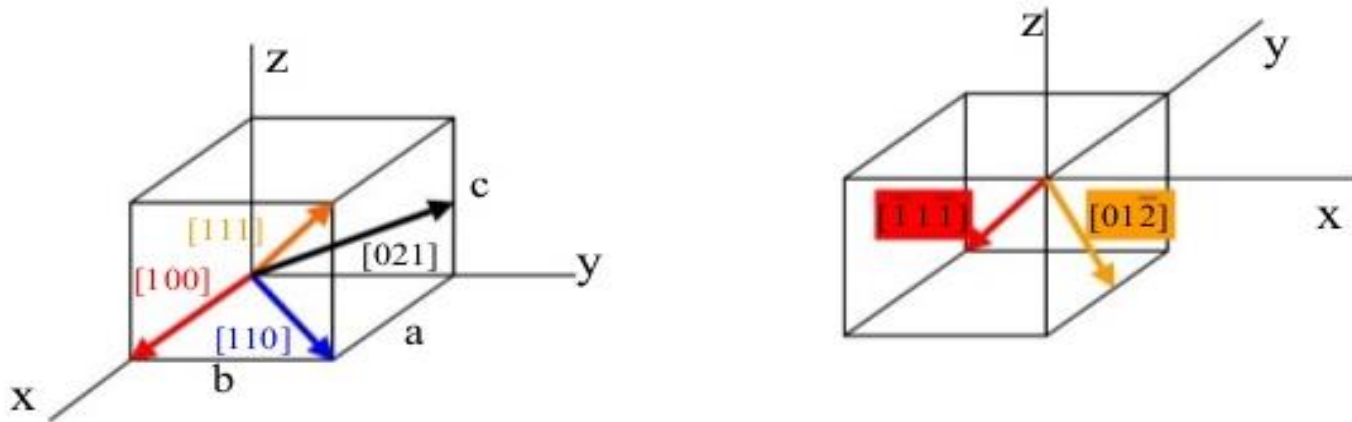


4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
 +
7 Crystal Classes
 → **14 Bravais Lattices**



Miller Indices

- Miller Indices are used to represent the directions and the planes in a crystal
- Miller Indices is a group of smallest integers which represent a direction or a plane





Worked Example:

✓ Calculate the miller indices for the plane with intercepts $2a$, $-3b$ and $4c$ the along the crystallographic axes.

▪ The intercepts are 2, -3 and 4

✓ Step 1: The intercepts are 2, -3 and 4 along the 3 axes

✓ Step 2: The reciprocals are

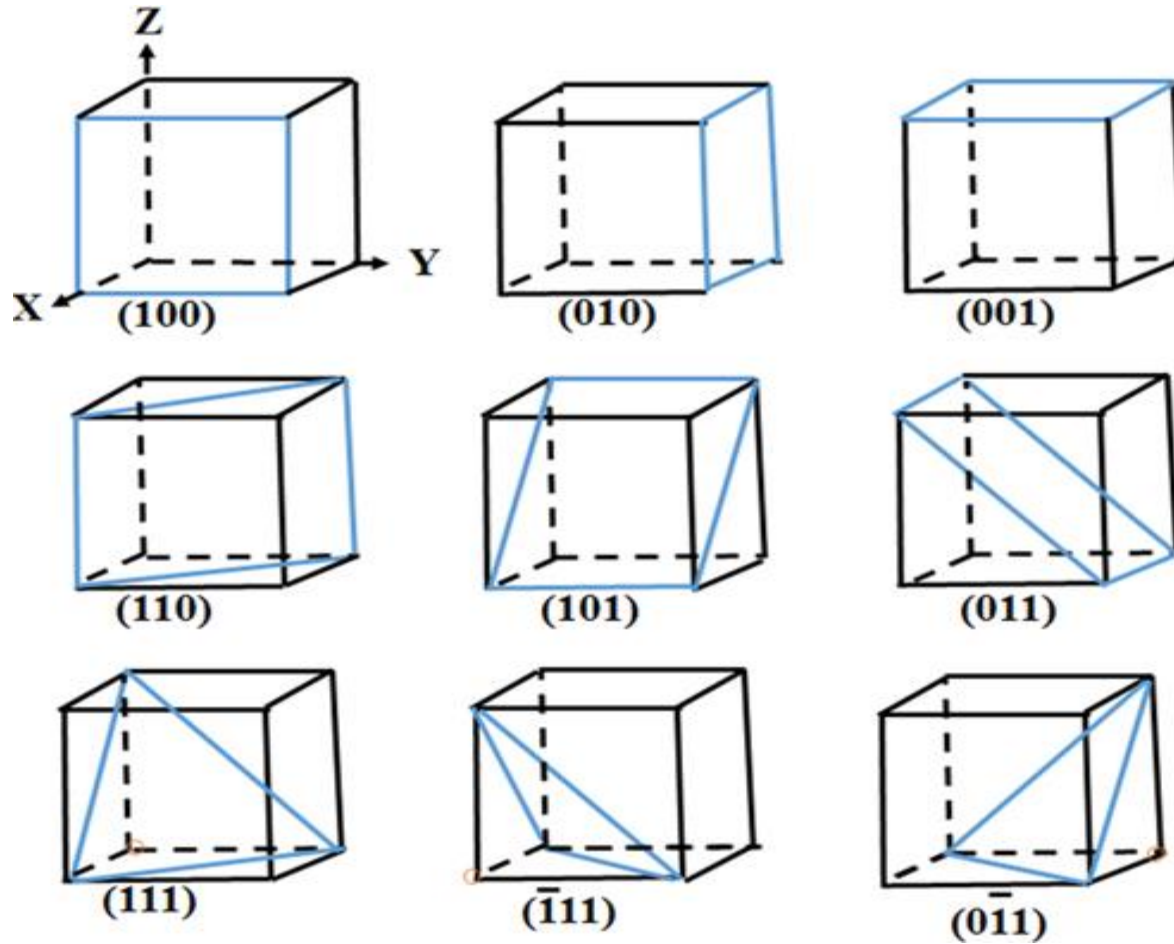
✓ Step 3: The least common denominator is 12.

Multiplying each reciprocal by lcd, we get 6 -4 and 3

Step 4: Hence the Miller indices for the plane is $(6 \bar{4} 3)$



Crystal Planes





Crystal Parameters - Determination



Number Of Atoms/Unit Cell

- A specific number of lattice points define each of the unit cells.

Atomic Radius : Half the distance
between two nearest neighbors



Crystal Parameters - Determination



Coordination Number

This is the number of atoms touching a particular atom or the number of nearest neighbors for that particular atom.

$$\text{Atomic Packing Factor} = \frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}}$$



Thank You