Crystal Structure

Subject: Solid State Physics
Subject Code: MDSE(P)-202A

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Class Objectives

From this class you will learn:

- ❑ To Classify the Solid state materials.
- ❑ To Differentiate between amorphous and crystalline nature of materials.
- ❑ To understand the structure of the crystals in 2D and 1D.
- ❑ To understand various types of crystal symmetry .

What is solid state physics?

Explains the properties of solid materials.

Explains the properties of a collection of atomic nuclei and electrons interacting with electrostatic forces.

Formulates fundamental laws that govern the behaviour of solids.

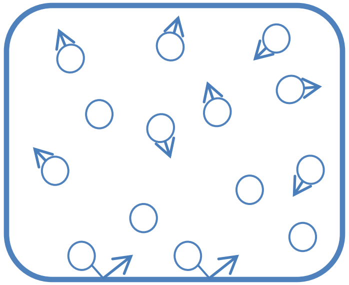
Forms of matter

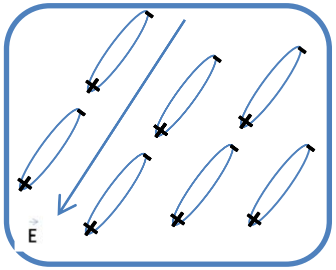
MATTER

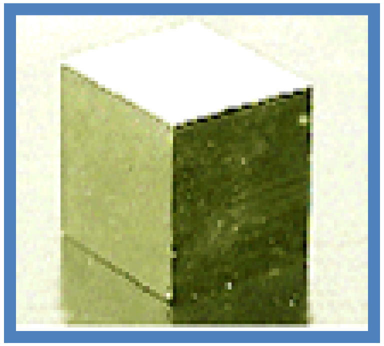
GASES

LIQUIDS AND LIQUID CRYSTALS

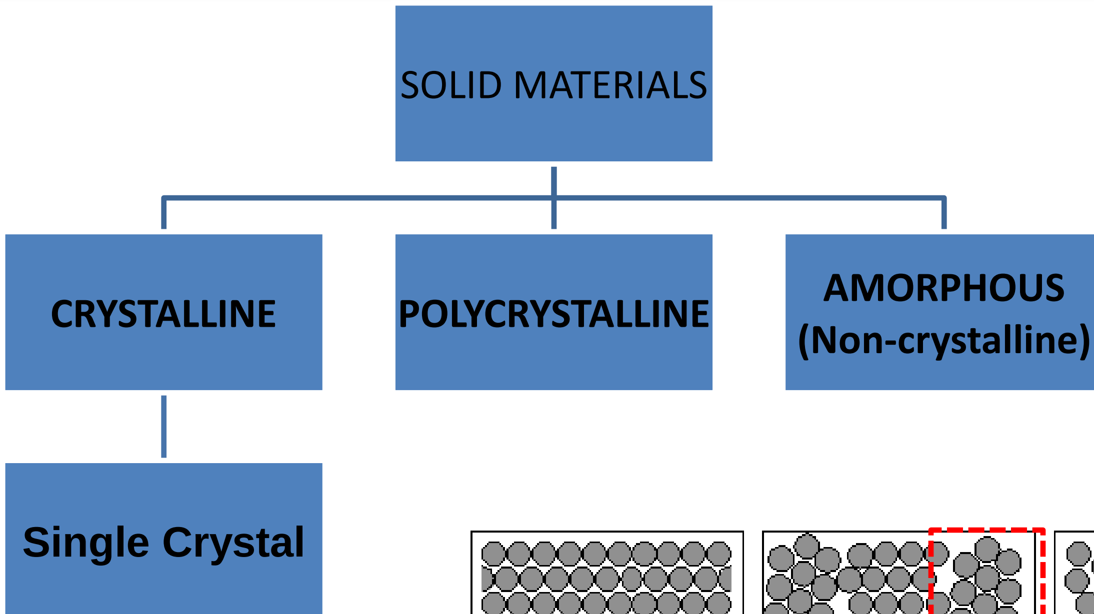
SOLIDS





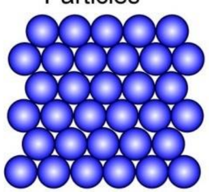


Classification of Solids

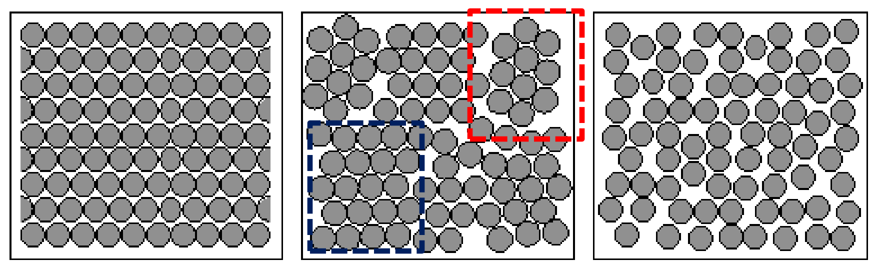


Crystalline Solid

Particles



Example: Table Salt



Single crystal

Periodic across the whole volume.

Polycrystal

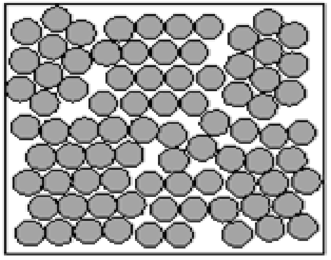
Periodic across each grain.

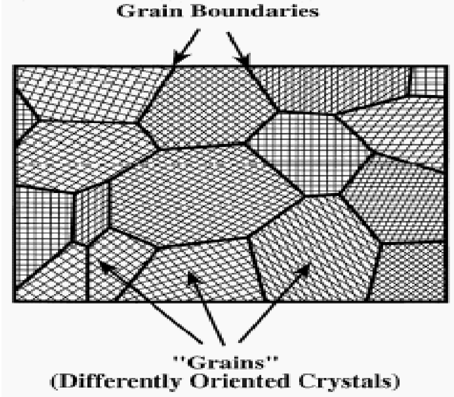
Amorphous solid

Not periodic.

Polycrystalline Solids

- **Polycrystalline materials** are made up of an aggregate of ***many small single crystals*** (also called crystallites or grains).
- **Polycrystalline materials** have a high degree of order over many atomic or molecular dimensions.
- ***Grains (domains)*** are separated by ***grain boundaries.*** *The atomic order can vary from one domain to the next.*
- Grains size: ***100 nm - 100 microns in diameter***.
- Polycrystals with grains less than 10 nm in diameter are ***nano-crystalline***





Amorphous Solids

Amorphous (Non-crystalline) Solids are made up of *randomly orientated atoms , ions, or molecules* that do not form defined patterns or lattice structures.

How to Study geometric structure of solids?

✓Amorphous materials have order only within a few atomic or molecular dimensions.

✓Amorphous materials do not have any long-range order, but they have varying degrees of short-range order.

✓Examples to amorphous materials include amorphous silicon, plastics, and glasses.

✓Amorphous silicon can be used in solar cells and thin film transistors.

CRYSTALLOGRAPHY

Crystallography deals with geometric description of crystals and their internal atomic arrangement.

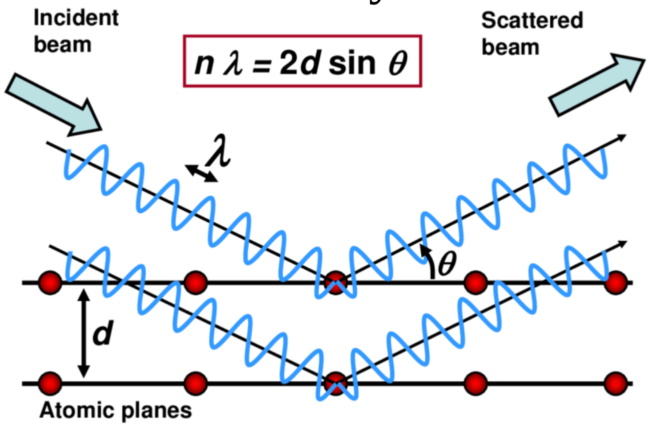
It's important to know symmetry of a crystal because it has a profound influence on its properties.

Structures should be classified into different types according to the symmetries they possess.

Energy bands can be calculated for known structure(s).

CRYSTALLOGRAPHY

Modern crystallography is largely based on the analysis of the X-ray diffraction by the crystals which help in understanding the geometric structure of crystal lattices.



Crystallographic Axes: (ox, oy, oz)

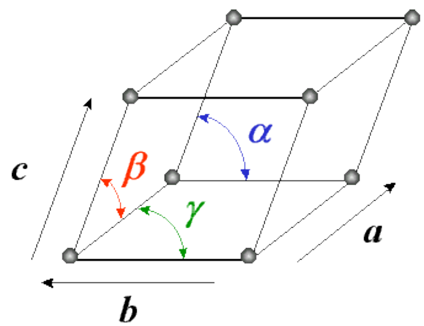
The lines drawn parallel to the lines of intersection of any three faces of a unit cell, which do not lie in the same plane.

Interfacial Angles: (α, β, γ)

The angles between three crystallographic axis

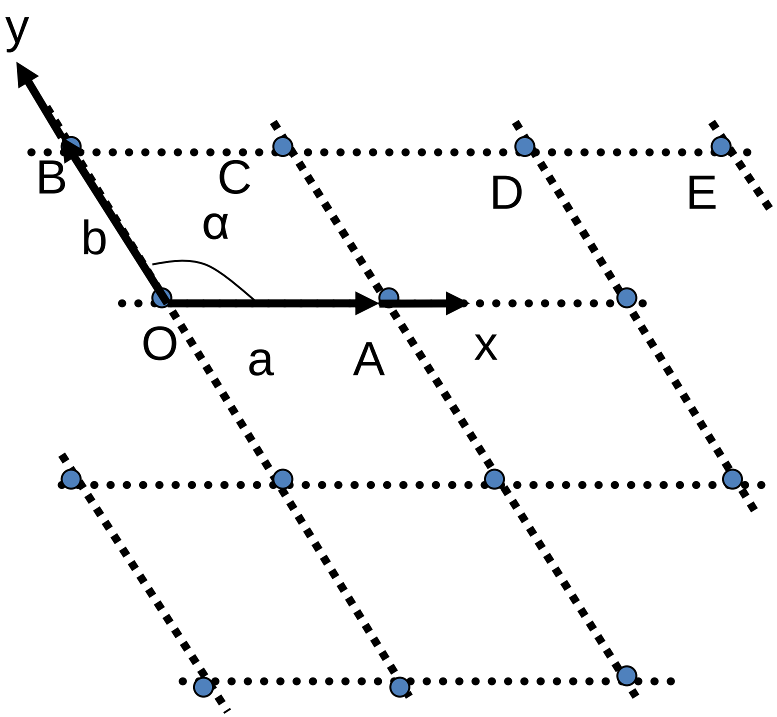
Primitives: (a, b, c)

The three sides of the unit cell



What is a Crystal Lattice ?

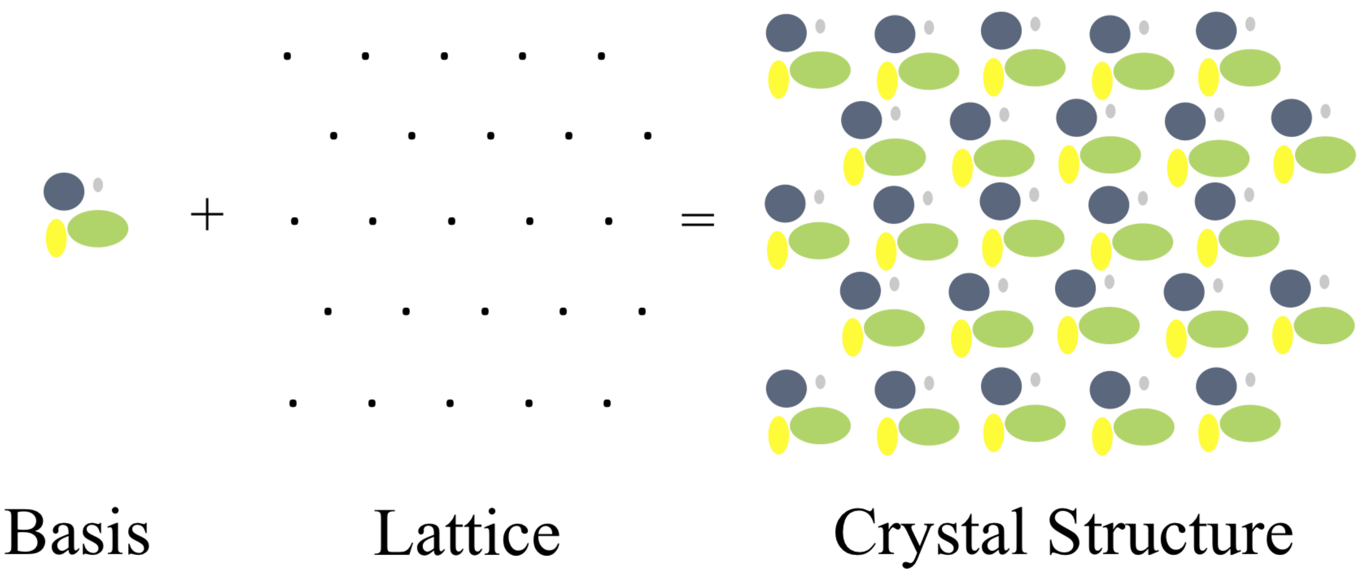
In crystallography, only the geometrical properties of the crystal are of interest, therefore one replaces each atom by a geometrical point located at the equilibrium position of that atom.



- ✓An infinite array of points in space,
- ✓Each point has identical surroundings to all others.
- ✓Arrays are arranged in a periodic manner.

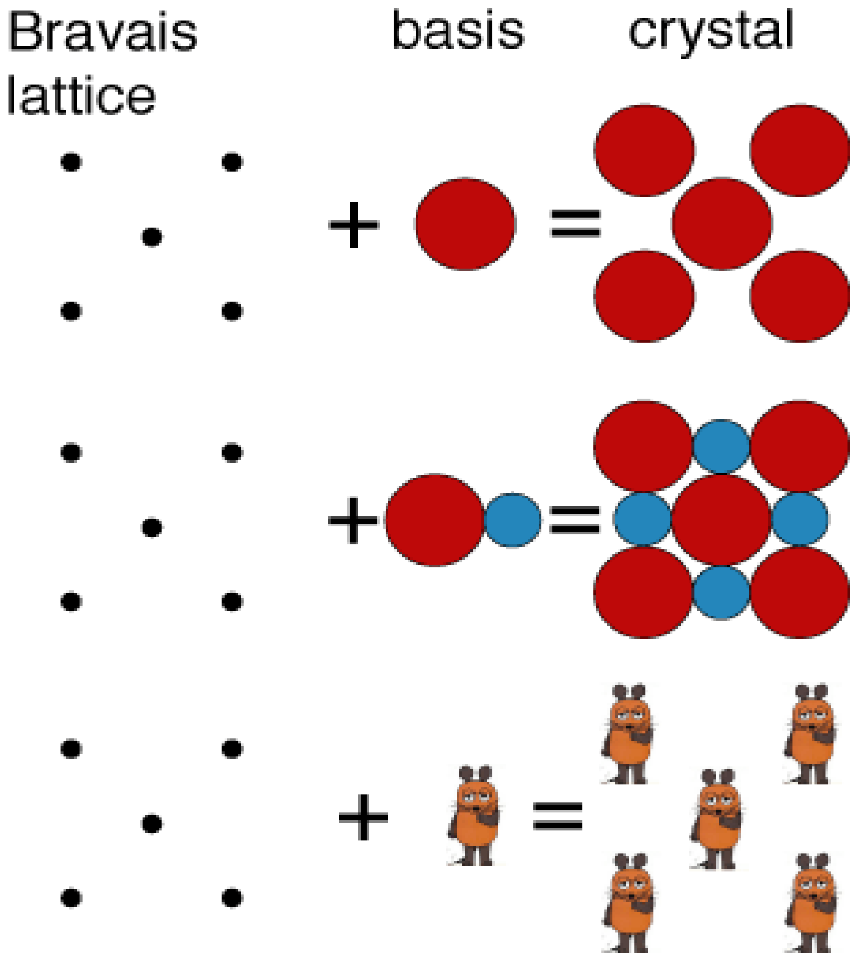
Crystal Structure

Crystals are a repeating unit in space.
Crystal structures can be obtained by attaching atoms, groups of atoms or molecules which are called basis (motif) to the lattice sides of the lattice point.



There are several ways to describe a lattice. The most fundamental description is known as the ***Bravais lattice***.

Choice of basis

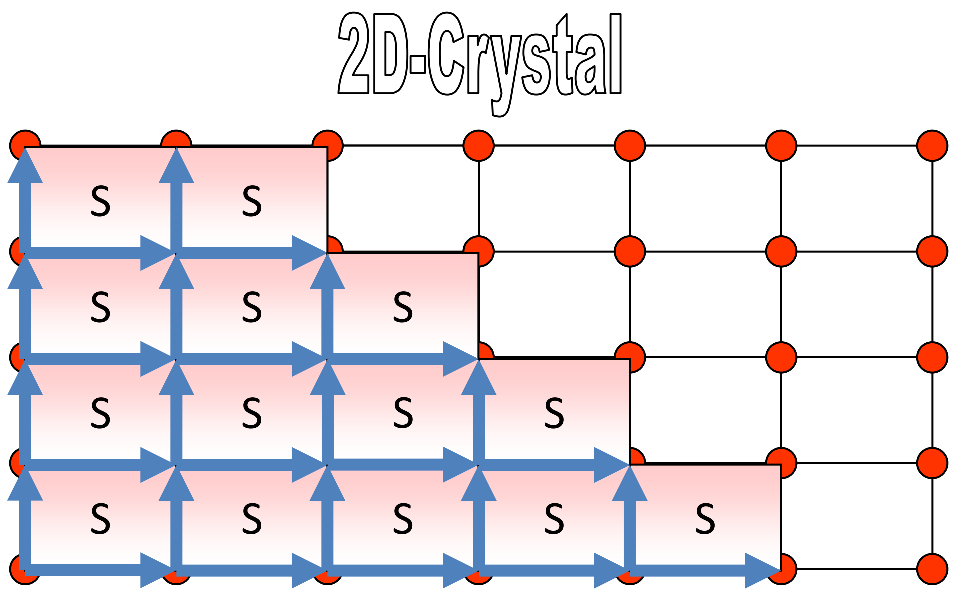


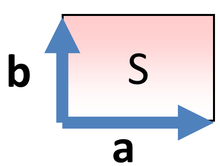
Unit Cell in 2D

The smallest component of the crystal (group of atoms, ions or molecules), which when stacked together with pure translational repetition reproduces the whole crystal.

A ***unit cell*** is the smallest area which produces this coverage

In rectangular 2D lattice unit cell is the rectangle, whose sides are the vectors **a** and **b**





Unit cell vs primitive cell

A **unit cell** is the smallest group of atoms which has the overall symmetry of a crystal, and from which the entire lattice can be built up by repetition in three dimensions.

A **primitive cell** is the smallest possible unit cell of a lattice, having lattice points at each of its eight vertices only.

A primitive cell is the smallest possible unit cell of a lattice.

Geometry

Unit cell has parallelepiped geometry.

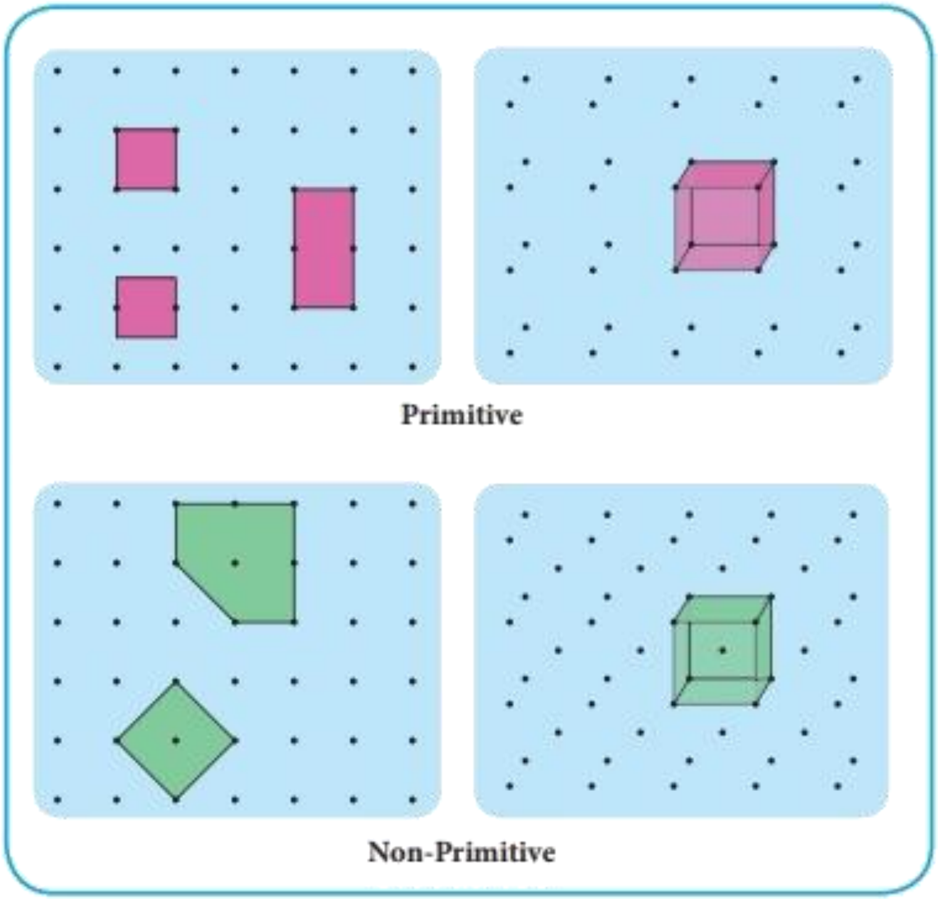
2D primitive cell has parallelogram geometry whereas 3D primitive cell has parallelepiped geometry

Shape

Unit cell is a three-dimensional structure.

Primitive cell can be given as a 2D or 3D structure

Primitive cell vs Non-primitive unit cell



Primitive or P-cell:

- All fundamental unit cells associated with a single lattice point
- lattice points are present at the edges of unit cell only

Non- primitive cell:

- unit cells with more than one lattice points are non primitive
- Lattice points are present in the unit cell and at edges

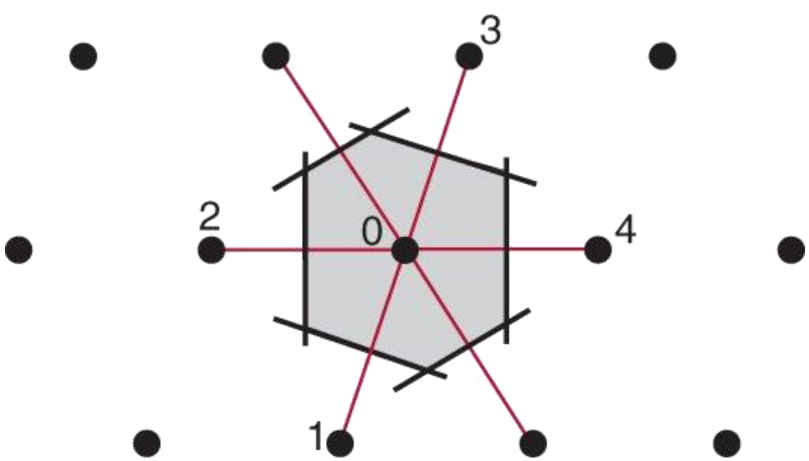
Wigner-Seitz Cell

There is a special type of primitive-cells known as *Wigner-Seitz cell*.

Wigner-Seitz unit cell can be constructed as

(i) Draw lines to connect a given lattice point to all nearby lattice points.

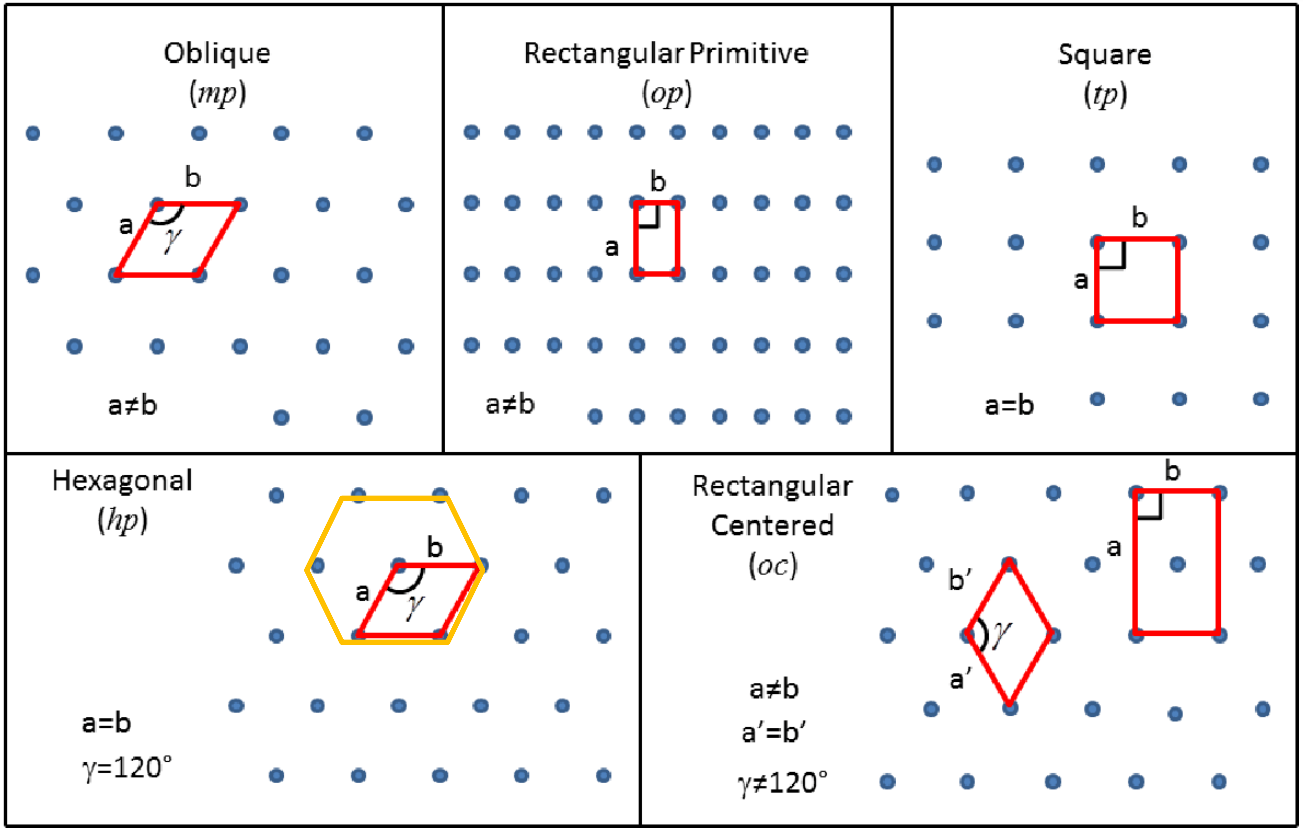
(ii) At the midpoint and normal to these lines, draw new lines (planes in 3D).



The *smallest volume enclosed* is the *Wigner Seitz primitive cell*.

All the space of the crystal may be filled by these primitive cells, by translating the unit cell by the lattice vectors.

Types of Lattices (2D)



letters **a, b,** and **c** denotes the ***dimensions of the unit cells***

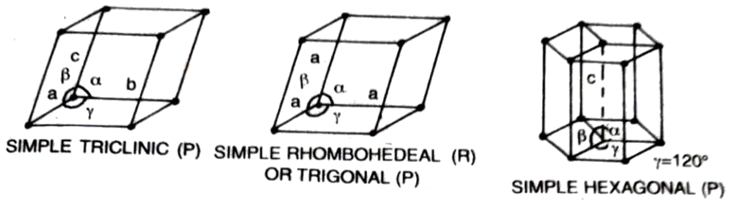
letters ***α, β, and γ*** denote the corresponding **angles** in the unit cells.

Bravais in 1848 introduced the concept of space lattice to describe structure of crystals.

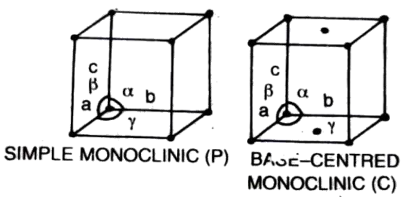
Types of the Lattices (3D)

System	Axial lengths and angles	Bravais Lattice	Lattice Symbol
Cubic	Three equal axes at right angles $a = b = c;\ \alpha = \beta = \gamma = 90°$	Simple Body-centered Face-centered	P I F
Tetragonal	Three axes at right angles, two equal $a = b \neq c;\ \alpha = \beta = \gamma = 90°$	Simple Body-centered	P I
Orthorhombic	Three unequal axes at right angles $a \neq b \neq c;\ \alpha = \beta = \gamma = 90°$	Simple Body-centered Base-centered Face-centered	P I C F
Rhombohedral (trigonal)	Three equal axes, equally inclined $a = b = c;\ \alpha = \beta = \gamma \neq 90°$	Simple	R
Hexagonal	Three equal coplanar axes at 120°, third axis at right angles $a = b \neq c;\ \alpha = \beta = 90°;\ \gamma = 120°$	Simple	P
Monoclinic	Three unequal axes, one pair not at right angles $a \neq b \neq c;\ \alpha = \gamma = 90° \neq \beta$	Simple Base-centered	P C
Triclinic	Three unequal axes, unequally inclined and none at right angles $a \neq b \neq c;\ \alpha \neq \beta \neq \gamma \neq 90°$	Simple	P

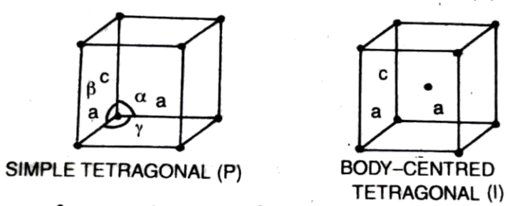
Crystal Structure (3D)

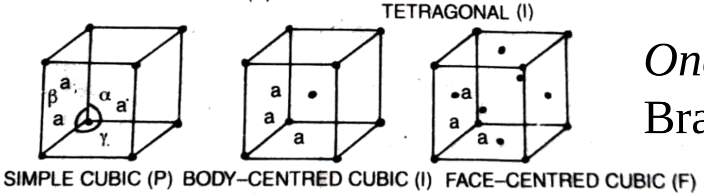


Three Crystal systems (Triclinic, Trigonal, Hexagonal)
Bravais Lattices = 1

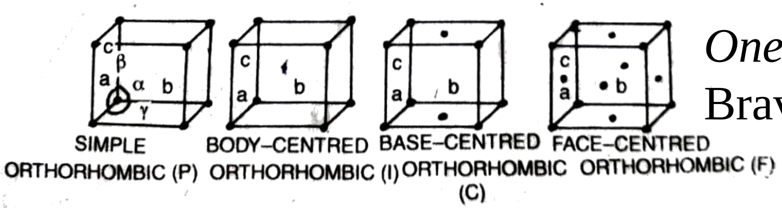


Two Crystal systems (Monoclinic and Tetragonal)
Bravais lattices = 2





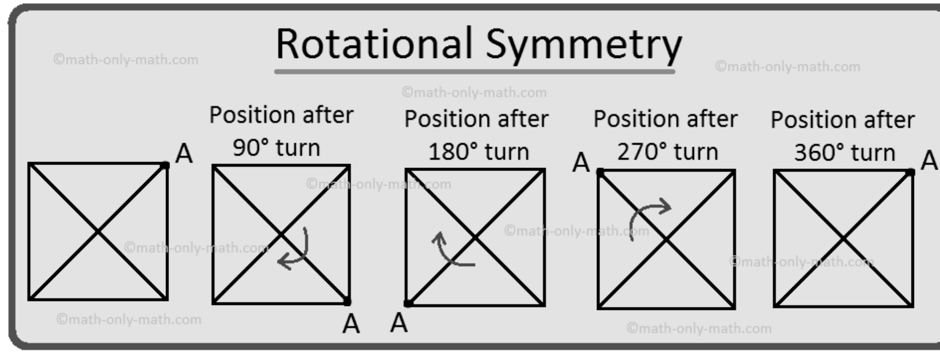
One Crystal systems (Cubic)
Bravais Lattices = 3



One Crystal systems (Cubic)
Bravais Lattices = 3

Crystal Symmetry

An object is described as *symmetric* with respect to a *transformation* if the object appears to be in a state that is identical to its initial state, after the transformation.

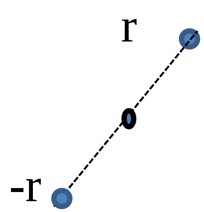


Rotation Axes of symmetry:

If Body remain invariant after a rotation through an angle

Inversion Centre:

If for every lattice point at position r, another lattice point at position –r is also present



Reflection Symmetry:

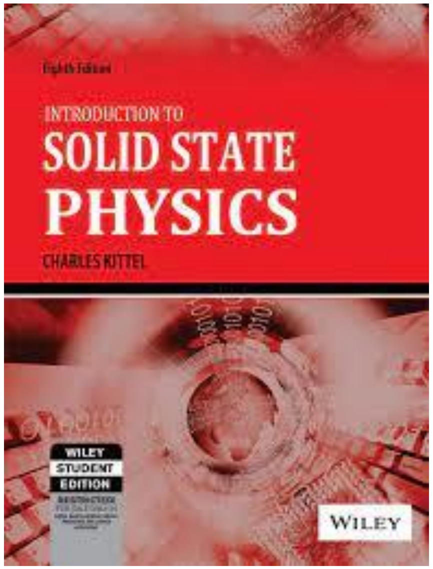
If there exist a line or plane which divides the crystal into two identical half which are mirror image to each other.

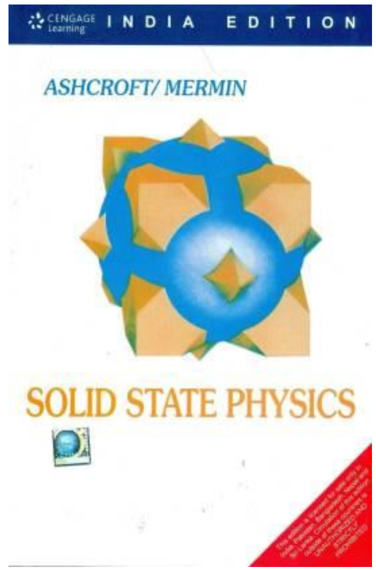
Summary

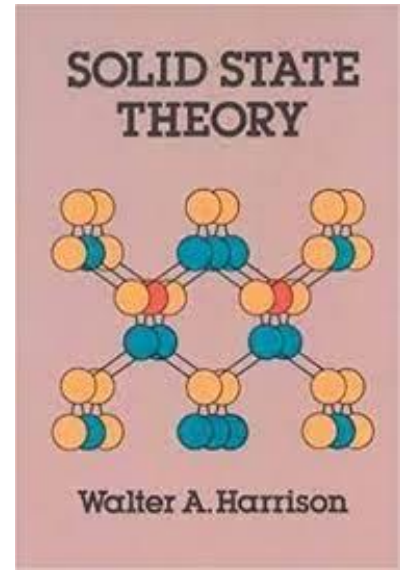
In this lecture, we learnt about

- Classification of Solids: *Crystalline and Amorphous*
- how points periodically arrange themselves in space giving rise to the formation of **point lattice** .
- When points in the **unit-cells** are replaced by motif which is defined as an atom or group of atoms, they give rise to what we call as crystal structures.
- Further these **seven crystal systems can be divided into 14 Bravais lattices** consisting of primitive as well as non-primitive cells.
- The existence of each system is defined by **symmetry considerations** (other than translation) which consist of rotational, mirror and inversion symmetry.

Useful Books







C. Kittel, *Introduction to Solid State Physics* (Wiley, New York) 8^{th} edition (2005)

N.W. Ashcroft , N.D. Mermin, *Solid State Physics (Saunders College Publishing, USA) (1976)*

W. A. Harrison, *Solid State Theory* (Tata McGraw-Hill, New Delhi) 1^{st} edition (1980)