

## Chapter-1 Crystal Structure of Metals

Crystal :- A crystal is a solid whose constituent atoms or molecules are arranged in a systematic geometric pattern.

Crystallography :- It is a branch of science in which the internal structure of crystals, their properties, external or internal symmetries of crystals are studied.

Crystal Structure :- A metal is composed of several atoms which are arranged in a regular repeated three dimensional pattern. This arrangement is known as "Crystal Structure."

Lattice :- Three-dimensional regular arrangement of points in space is called lattice.

Space Lattice :- Three dimensional periodic or regular arrangement of infinite number of points in space, is called as Space Lattice.

Crystal lattice :- 3-dimensional regular arrangement of atoms or molecules or ions in space is known as Crystal lattice.

→ Crystal lattice is also known as Space lattice.

Unit Cell :- Three-dimensional repeating group of lattice in space.

or: Unit cell is the smallest group of atoms possessing the symmetry of the crystal.

→ It is characterised by 6 parameters i.e. 3-edges ( $a, b, c$ ) and 3-angles ( $\alpha, \beta, \gamma$ ).

Crystal Structure :

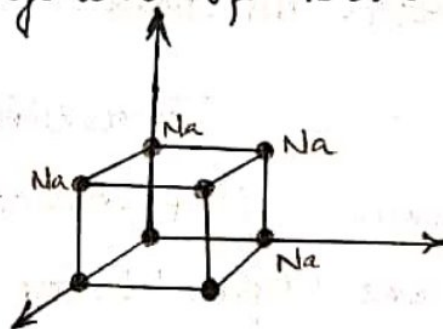
It is a solid in which (atoms, molecules, ions) are arranged in 3 dimensional patterns in space.

- Periodic arrangement of atoms over large atomic distance.
- Also crystal is defined as a lattice with basis added to each lattice site.

Crystal = Lattice + Basis

- Crystal is periodic arrangement of basis.

Ex: Na = BCC  
Al = FCC



BCC + Sphere  
(Lattice) (Basis)

- Usually basis consists of an atom, a group of atoms or molecules associated with each other

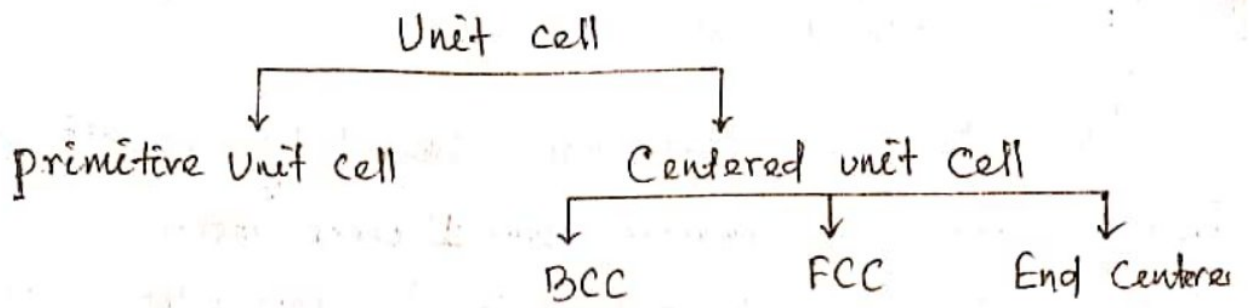
Types of Solids

↓  
Crystalline

If atoms are arranged in a regular fashion.

↓  
Amorphous

If the atoms are arranged in an irregular fashion.



End centered :

Unit particle is present at center of two opposite faces.



Primitive Unit Cell :

Primitive is a unit cell that contains exactly one lattice point per unit cell.

→ It is the smallest possible cell.

→ When particle (atom, molecules, ions) or a unit cell is so chosen that it contains lattice points only at its corner it is known as primitive unit cell.

→ Simple monoclinic, Triclinic, Simple cubic are known as primitive cells.

No. of atoms/unit cell :

An atom that is shared with "m" adjacent unit cell.

We only count a fraction of the atom " $\frac{1}{m}$ "

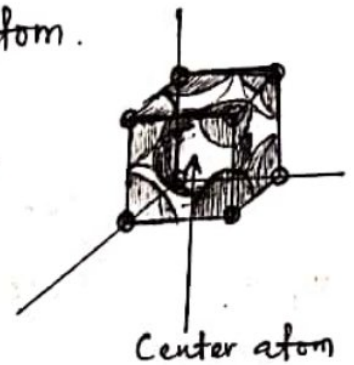
For BCC lattice number of atoms/unit cell :-

In BCC, 8 corner atom shared by = 8 unit cells  
i.e 8 unit cells shared with 1 corner atom  
1 unit cell shared with  $\frac{1}{8}$  corner atom.

$$\text{For 8 corner} = 8 \times \frac{1}{8} = 1 \text{ atom}$$

$$1 \text{ center atom} = 1 \text{ atom}$$

$$\text{Total} = \boxed{1 + 1 = 2}$$

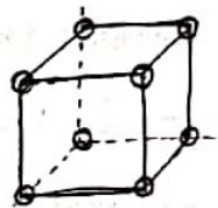


$\therefore$  The unit cell of BCC structure contains 2 atoms.

For Simple Cubic, number of atom/unit cell :-

There are 8 corners of the cube and

Each corner there is 1 atom.



Each corner is shared by 8 adjacent cubes.

$$\text{Therefore, the share of the cube} = \frac{1}{8} \times 8 = 1$$

$\therefore$  Total number of atoms in a simple cubic unit cell is 1

For FCC, number of atoms/unit cell :-

In FCC,

8 corners shared by 8 unit cells

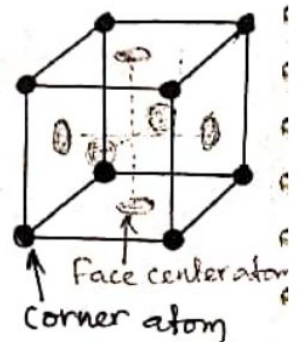
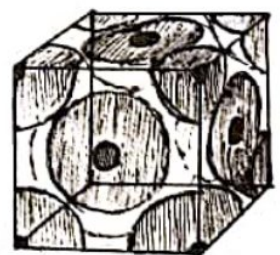
$$= 8 \times \frac{1}{8} = 1$$

2 adjacent unit cell shared by 1 face atom.

1 adjacent unit cell shared by  $\frac{1}{2}$  atom.

6 face atom shared by =  $6 \times \frac{1}{2} = 3$  atom.

$$\text{Total} = \boxed{3 + 1 = 4}$$



$\therefore$  The unit cell of FCC structure contains 4 atoms.

For HCP, number of atoms/unit cell :

In HCP,

$$12 \text{ corner (6 top + 6 bottom)} = 12 \times \frac{1}{6} = 2$$

$$2 \text{ atoms at face center} = 2 \times \frac{1}{2} = 1$$

$$3 \text{ atoms at interior} = 3$$

$$\therefore \text{Total} = \boxed{3 + 2 + 1 = 6}$$

$\therefore$  The unit cell of HCP structure contains 6 atoms.

Co-ordination Number :

It is defined as total no. of nearest neighbouring atoms.

— The coordination number of Simple cubic is 6.

— The co-ordination number of BCC is 8.

— The co-ordination number of FCC is 12.

— The co-ordination number of HCP is 12.

Difference between Isotropy and Anisotropy :

Isotropy

→ When properties of material is same in all crystallographic direction material is said to be isotropy.

→ It is independent of direction.

→ It exhibits consistent and uniform chemical bond.

Ex:- Glass, Metal

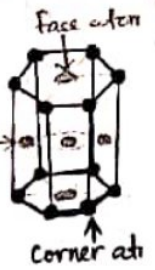
Anisotropy

→ If properties of different direction material is said an isotropic in nature.

→ It is dependent of direction.

→ No consistent and uniform chemical bond.

Ex:- Wood, Composite.



## Example of BCC :-

All Alkali earth Metal (IIA)

i.e. Na, Cr, Mo, V, W etc.

## Example of FCC :-

Cu, Au, Al, Ag, Pt, ceramics and inert gas etc.

## Example of HCP :-

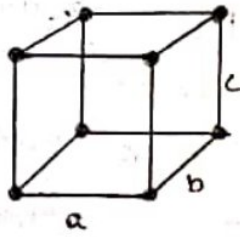
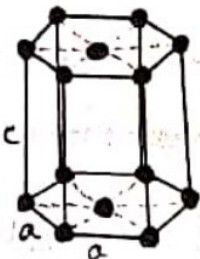
Zn, Ti, Zr, Mg, Cd, Be etc.

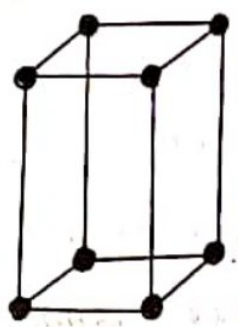
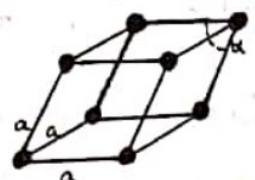
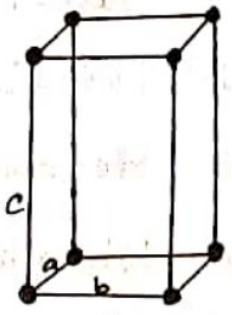
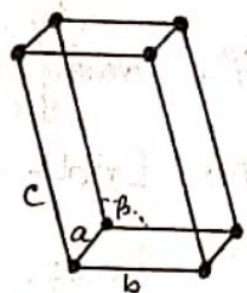
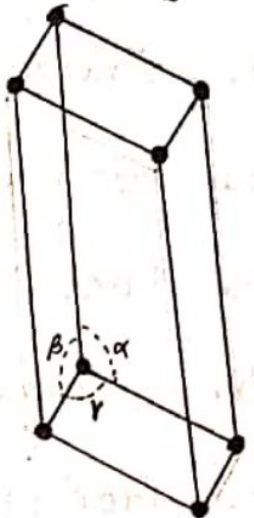
## Seven Crystal System :-

It is known as basic crystal system.

Bravais gave seven different kinds of lattice on the basis of point group symmetry i.e. 3-D periodic arrangement of points, about any of the point is identical with every respect (Dimension & Orientation) to that about any other point of arrangement.

The seven crystal systems are,

SI No.	<u>Crystal System</u>	<u>Axial Relationship</u>	<u>Interaxial Angles</u>	<u>Unit Cell Geometry</u>
1.	Cubic	$a=b=c$	$\alpha=\beta=\gamma=90^\circ$	
2.	Hexagonal	$a=b \neq c$	$\alpha=\beta=90^\circ, \gamma=120^\circ$	

<u>SI No.</u>	<u>Crystal System</u>	<u>Axial Relationship</u>	<u>Interaxial Angles</u>	<u>Unit Cell Geometry</u>
3.	Tetragonal	$a=b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
4.	Rhombohedral	$a=b=c$	$\alpha = \beta = \gamma \neq 90^\circ$	
5.	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
6.	Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$	
7.	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	

## Fourteen Bravais Lattices :-

Bravais lattices named after their originator Mr. Bravais, are the 14 distinguishable 3-dimensional Space lattices that can be generated by repeated translation of three non-coplanar vectors  $a, b$  &  $c$  of a unit cell in three dimensional Space.

The fourteen Bravais lattices are given below:

1. Simple monoclinic
2. End-centered monoclinic
3. Triclinic
4. Hexagonal
5. Rhombohedral
6. Simple orthorhombic
7. Body-centered orthorhombic
8. End-centered orthorhombic
9. Face-centered orthorhombic
10. Simple cubic
11. Body-centered cubic
12. Face-centered cubic
13. Simple tetragonal
14. Body-centered tetragonal



## Miller Indices

The layers of atoms or the planes along which atoms are arranged are known as atomic or crystallographic planes. Miller indices is a system of notation that denotes the orientation of the faces of a crystal and the planes are direction of atoms within the crystal.

→ It is denoted by  $\{ \}$ ,  $( )$ ,  $[ ]$ ,  $\langle \rangle$

→ (-)ve number is represented by a bar over the number

i.e.  $(\bar{1}, \bar{2})$

Miller indices of planes:

Algorithm:

→ 1st read intercept  $a, b, c$  or  $x, y, z$

→ 2nd, take reciprocal of them.

→ Convert to Smallest integral value.

→ Enclose in given notation  $( )$ ,  $\{ \}$ .

Example:

Draw planes of vertices  $(1,1,2)$ ,  $(0,0,1)$  and  $(1,0,1)$ .

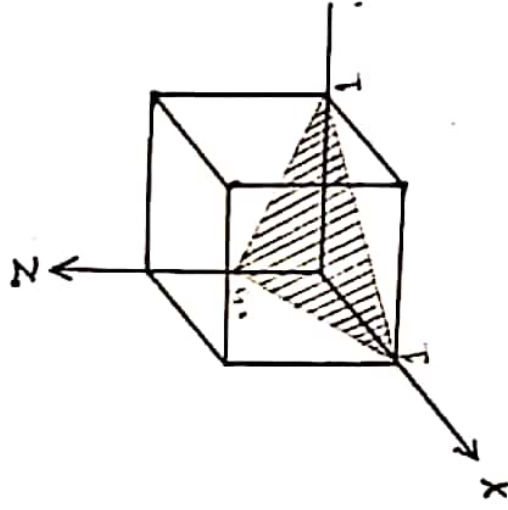
Ans:-  $(1,1,2)$  intercept =  $1, 1, 2$

Reciprocal =  $\frac{1}{1}, \frac{1}{1}, \frac{1}{2}$

=  $1, 1, 0.5$

Miller indices (MI) =  $(1, 1, 0.5)$

The shaded region is the required plane.



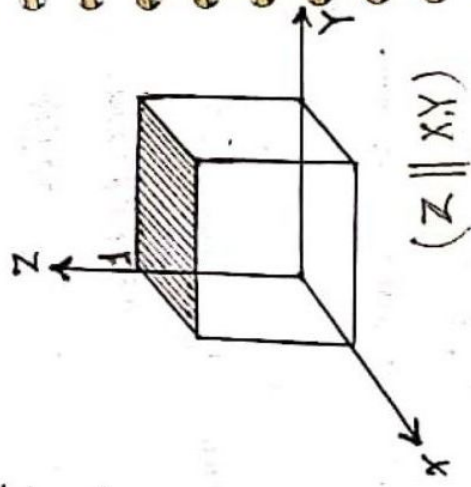
Similarly, for the 2nd point,

$$(001) \text{ intercept} = 0, 0, 1$$

$$\text{Reciprocal} = \frac{1}{0}, \frac{1}{0}, \frac{1}{1}$$

$$= \infty, \infty, 1$$

$$\therefore \text{MI} = (\infty, \infty, 1)$$



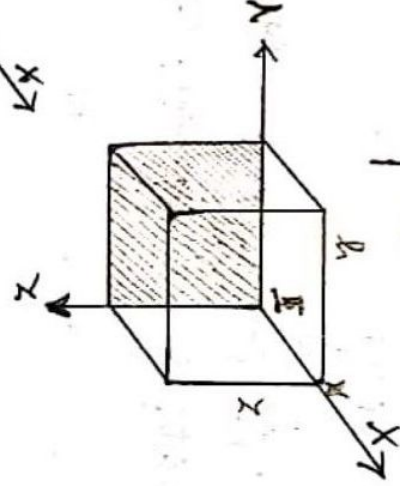
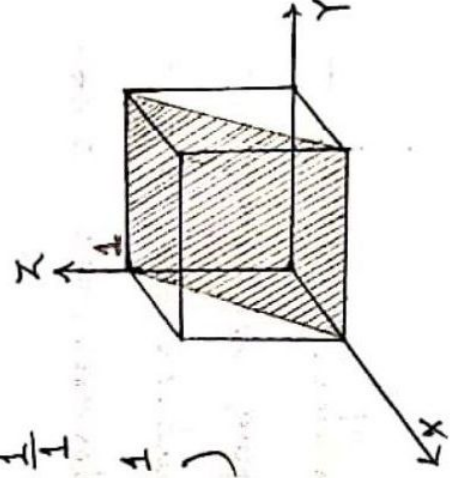
Similarly, for 3rd point,

$$(101) \text{ intercept} = 1, 0, 1$$

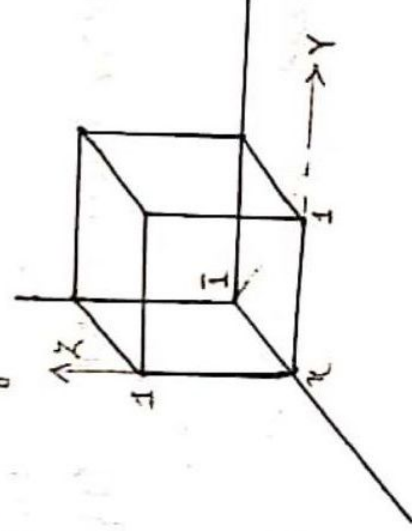
$$\text{Reciprocal} = \frac{1}{1}, \frac{1}{0}, \frac{1}{1}$$

$$= 1, \infty, 1$$

$$\text{MI} = (1, \infty, 1)$$



MI is  $(1, \infty, \infty)$



MI is  $(1, 1, 1)$

Example : 2

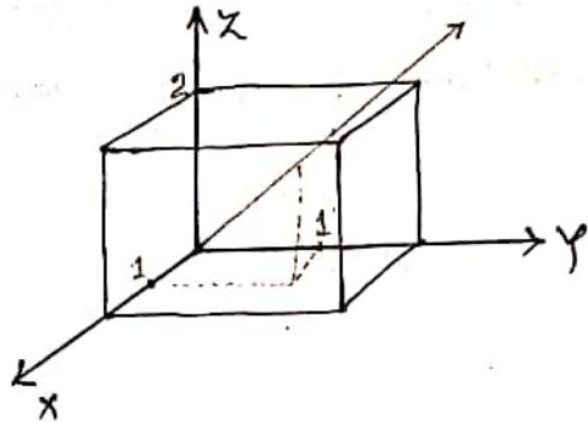
# Miller indices of Direction:

## Algorithm:

- 1st: Read intercept  $a, b, c$  or  $x, y, z$
- 2nd: Take reciprocal of these points.
- 3rd: Convert to smallest integral value.
- last: Enclose in given notation  $( )$ ,  $\{ \}$ .

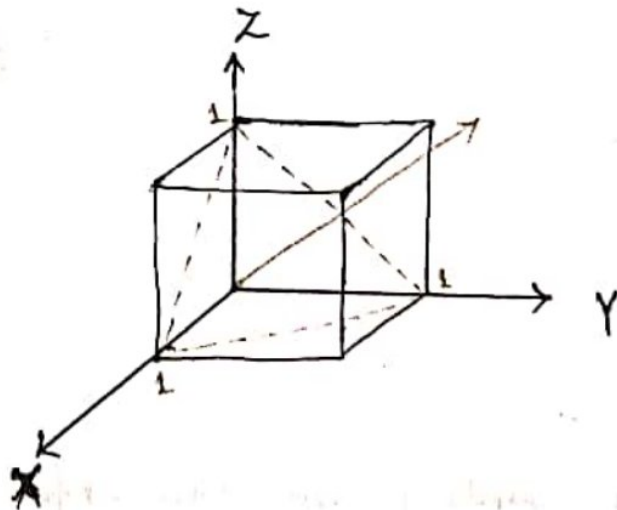
## Example:

MI is  $(112)$



## Example:

MI is  $(1,1,1)$

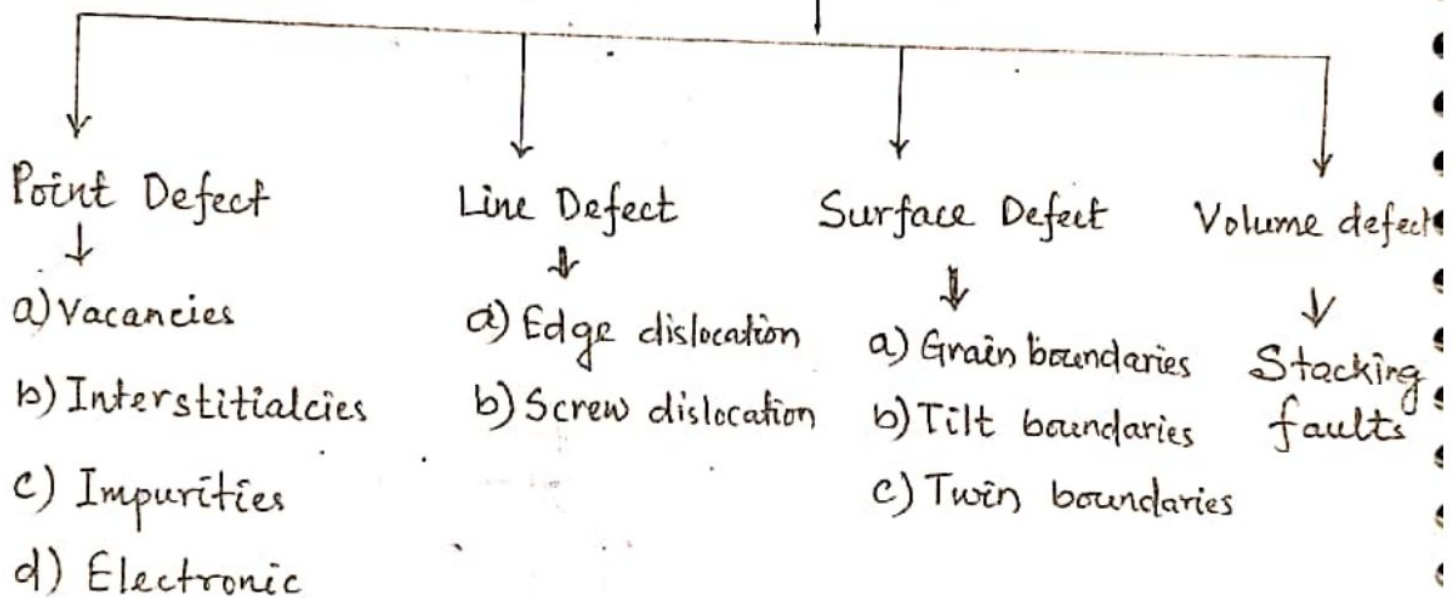


## Imperfection : / Defect

The perfectly regular crystal structures that have been considered upto now are called ideal crystals in which atoms are arranged in a regular way.

But, real crystals as in cast or welded objects are never perfect; lattice distortion and various imperfections irregularities or defects are general present in them.

### Crystal Imperfection



### Point defect :

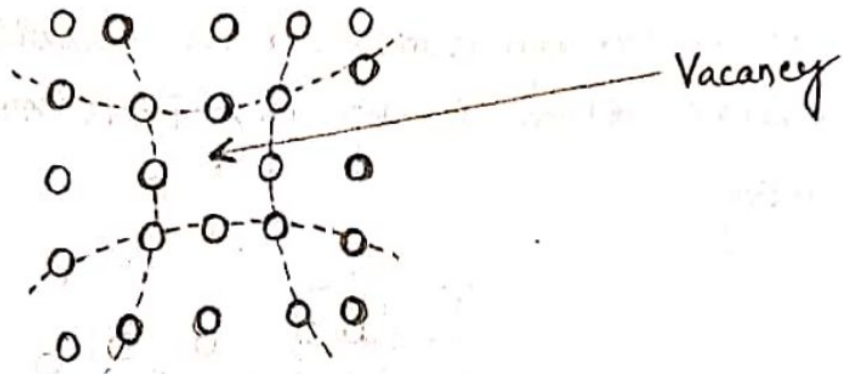
Point defects are imperfect point like regions in crystal.

- In a crystal lattice, point defect is one which is completely local in it's effect e.g. a vacant lattice site.
- The introduction of point defect into crystal increases it's internal energy as compared to that of the perfect crystal.

### a) Vacancies

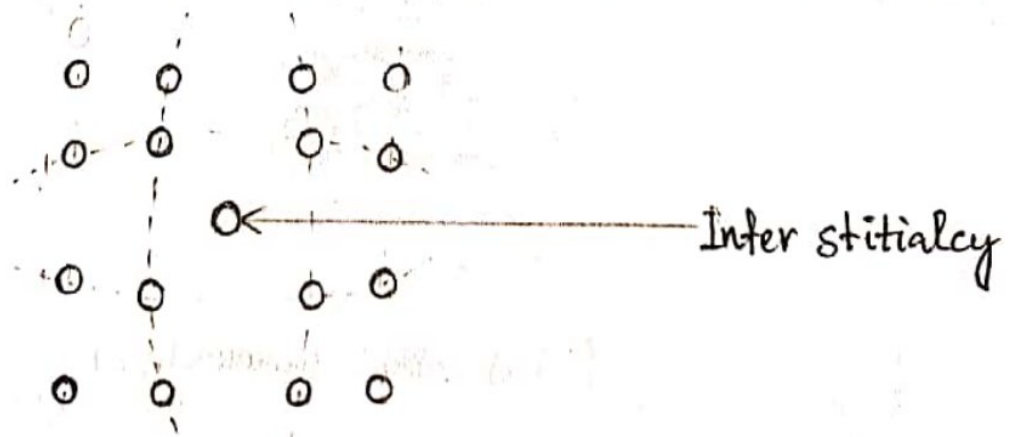
A vacancy is the simple point defect and involves a missing atom within a metal.

- = These defects may come up as a result of imperfect packing during the original crystallisation.
- They may also arise from thermal vibration of the atoms at high temperature.



### b) Interstitialcies

If a smaller atom occupies space between relatively larger atoms is known as interstitialcies impurity.



### c) Impurities :

Impurities may be small particles surrounded in the structure or foreign atoms in the lattice.

Foreign atoms generally have atomic radii and electronic structure differing from the main host atoms.

It is two types, i.e.

#### Substitutional impurity :

If a foreign atom occupies a lattice site from where a regular atom is missing, it is known as substitutional impurity.



( Substitutional impurity )

#### Interstitial impurity :

If a small atom occupies space between relatively larger atoms, it is known as interstitial impurity.



( Interstitial impurity )

## 1) Electronic defects :

Electronic defects are the result of errors in charge distribution in Solids.

- These defects are free to move in the crystal under the influence of an electrical field,

## 2) Line Defects :

The most important two-dimensional or line defect is

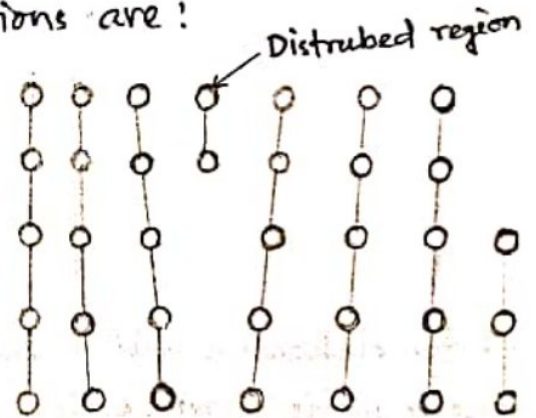
- the dislocation.

- A dislocation may be defined as a disturbed region between two substantially perfect parts of a crystal.

- The two basic types of dislocations are:

a. Edge dislocation

b. Screw dislocation



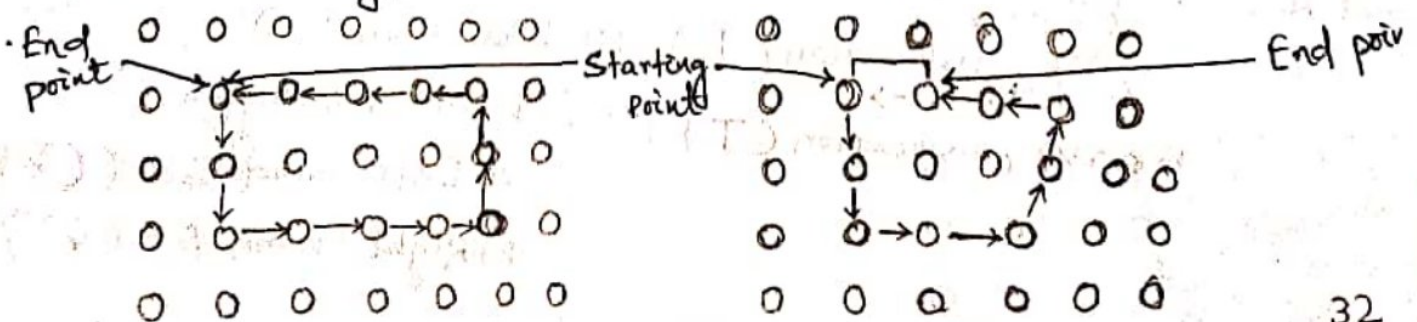
### a) Edge dislocation :

(Line defect)

An edge dislocation may be defined as an extra plane of atoms within a crystal structure.

- It is accompanied by zones of compression and of tension so that there is a net increase in energy along a dislocation.

- It is two types i.e. (+)ve dislocation (L) and (-)ve dislocation (T)



## b) Screw dislocation :

Screw dislocation may originate partial slipping of a section of crystal plane.

- In the screw dislocation, the distortion follows a helical or screw path & both right hand and left hand senses are possible.
- It is two types i.e. left hand screw dislocation and right hand S.D.

### Edge dislocation (E.D)

- Edge dislocation may be defined as the plastic movement of atoms in one plane, that can be seen on the edge of the crystal.

- E.D can be moved by climb.

- Speed of movement of E.D is more than S.D.

- E.D are two types

a) (+)ve dislocation (L)

b) (-)ve dislocation (T)

### Screw dislocation (S.D)

- Screw dislocation may be defined as the plastic movement of atoms among two separate planes that can be seen from the sides of the crystal.

- S.D can be moved by cross slip.

- Speed of movement of S.D is less than E.D.

- S.D are two types.

a) Left hand S.D ( $\curvearrowright$ )

b) Right hand S.D ( $\curvearrowleft$ )



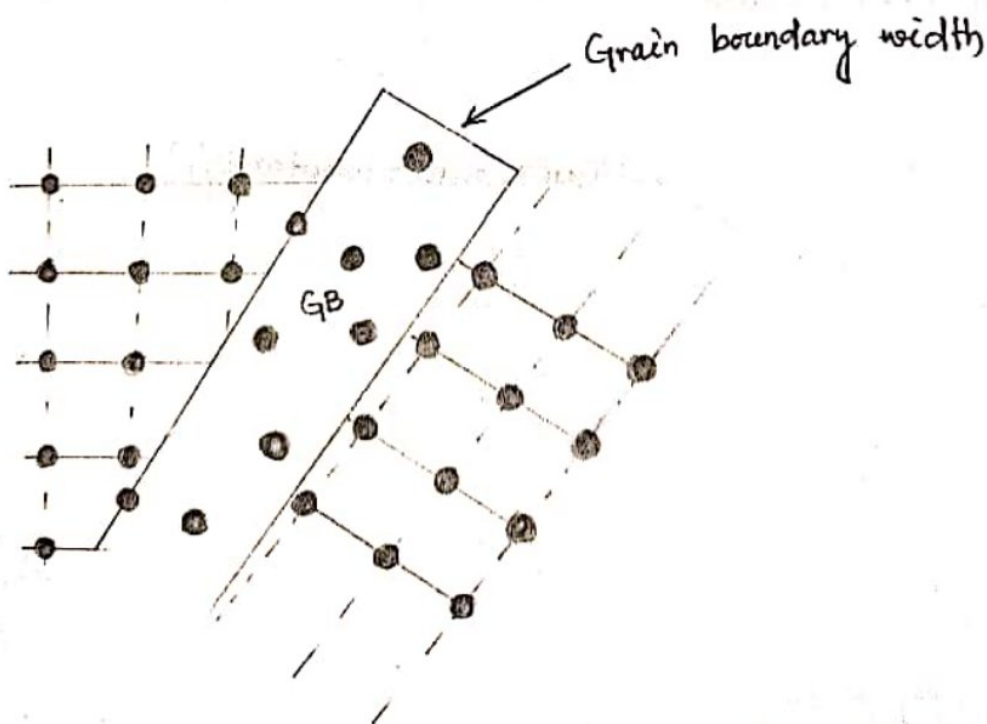
### 3. Surface Defects :

Surface defects are the two dimensional regions in a crystal. They arise from a change in the stacking of atomic planes on or across a boundary.

Surface defects are include grain boundaries, tilt boundaries and twin boundaries.

#### a) Grain boundary:

Grain boundaries are those imperfections which separate crystals or grains of different orientation, in polycrystalline aggregation during nucleation or crystallisation.



b) Tilt boundary :

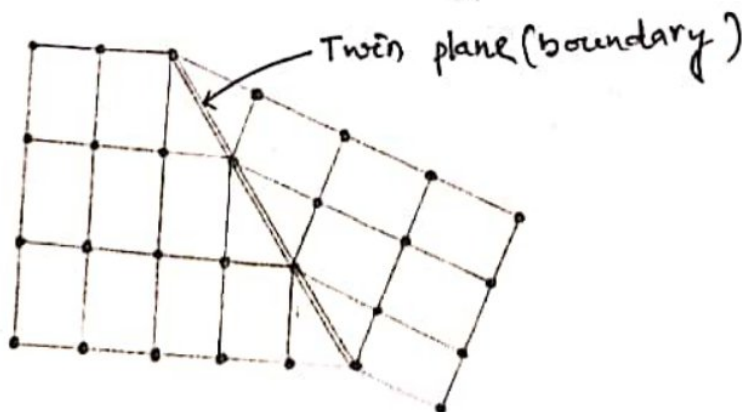
Tilt boundary is another surface imperfection and it may be regarded as any array of edge dislocation.

Tilt Boundary



c) Twin Boundary :

A twin boundary separates two parts of crystal having the same orientation and they look like mirror image of each other.



#### 4. Volume defects :

The important volume defect is stacking fault.

- It is found in HCP and FCC metals.
- Volume defects include pores, cracks, foreign inclusions and other phases.
- Volume defects are three-dimensional defects.