5.8.a) CRYSTAL IMPERFECTIONS

In ideal crystal (perfect crystal) the atomic arrangement is perfectly regular and continuous thought.

But in real crystal due to some reasons the regular orientation of atoms may be disturbed at a point, along a line or in a region.

Definition

The disturbance occurred in the regular orientation of atoms is called crystal defect of imperfections.

Some properties of crystal defects are structure sensitive i.e., properties such as mechanical strength, ductility,crystal growth,magnetic hysteresis, dielectric strength are greatly affected by relatively minor changes in crystal structure caused by imperfections.

Some other properties of crystals are structure–in sensitive i.e properties such as stiffness and density are not affected by the presence of imperfections.

Classification of crystal imperfections (or) Defects

Crystalline imperfections are classified on the basis of their geometry as follows.

1. **Point Defects**
   (a) Vacancies
   (b) Intersititials
   (c) Impurities
2. **Line Defects**
   (a) Edge dislocations
   (b) Screwdislocations
3. **Surface Defects**
   (a) Grain boundaries

(b) Tilt boundaries

(c) Twin boundaries

(d) Stackingfaults

4. **Volume Defects**

(a) Cracks

1. Point Defects

Point defects are crystalline irregularities of atomic dimensions.They are imperfect points like regions in crystal. One or two atomic diameter is the typical size of point imperfection.

Point defect takes place due to imperfect packing of atoms during crystallisation. They produced distortion in side the crystal structure.

Types of Point Defects

(a) Vacancies

(b) Intersititials

(c) Impurities

(a) Vacancy

In crystallography, a vacancy is simplest a type of point defect in a crystal. A defect in which an atom is missing from one of the lattice sites is known as a "vacancy" defect.

Whenever one or more atoms are missing from a normally occupied position as shown in figure,the defect caused is known as vacancy.

The atoms surrounding the vacancies are displaced inward thereby distorting the regularity of arrangement.There are different kinds of vacancies like Frenkel defect,Schottky defect,Colour centre,etc.

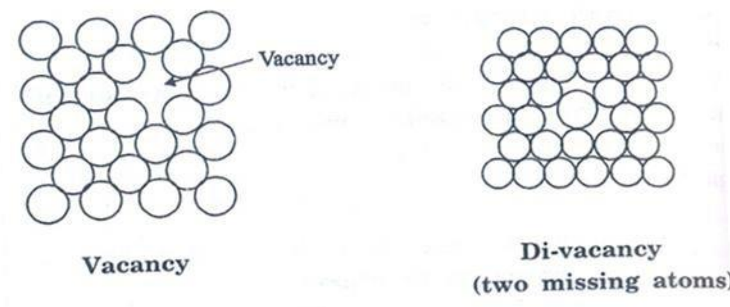

Fig:5.8.1 Vacancy

(i) Schottky Defect

It refers to the missing of pair of positive and negative ions in an ionic crystal.

A neutral defect that involves paired vacancies on the cation and anion sub lattices is called a **Schottky defect**.

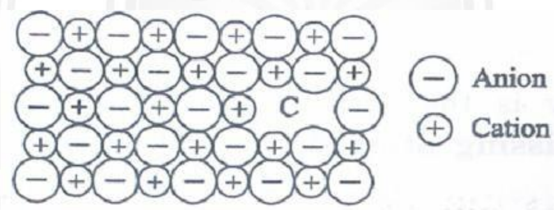

Fig 5.8.2 Schottky Defect

(ii) Frankel Defects

A vacancy associated with interstitial impurity is called Frenkel defect.

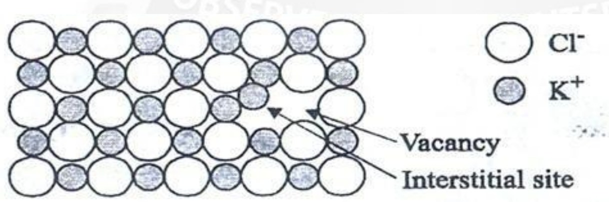

Fig 5.8.3 **Frankel Defects**

Here a missing atoms occupies interstitial position .This defect always occurs in ionic crystal, If a positive ion moves into an interstitial site in an ionic crystal, a cation vacancy is created in normal site, this ***vacancy- interstitial*** pair is known as ***Frenkel defect.***

(b) Interstitial Defect

When an extra atoms occupies interstitial space with in the crystal structure without removing parent atom,the defect is called interstitial defect.

Types of interstitial defect

(i) Self-interstitial

(ii) Foreign interstitial

(i) Self-interstitial

If an atom from same crystal occupies interstitial site,then it is called self-interstitial.

(ii) Foreign interstitial

If impurity atom(foreign atom) occupies the interstitial position without replacing the parent atom, it is called foreign interstitial.

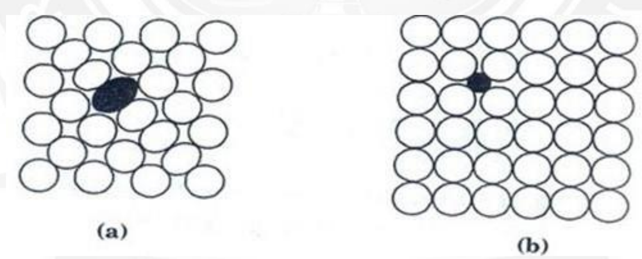

Fig 5.8.4 Foreign interstitial

- These can exist only ionic and covalent crystals.
- Here the impurity atom has very small size as that of the host atoms.

(c) Impurities

When the foreign atoms(impurities) are added to crystal lattices,they are known as impurities.The defect is called impurity defect.

The impurity atoms may fit in the structure in two ways giving rise to two kinds of impurities defects.They are

(i) Substitutional impurity defect

(ii) Interstitial impurity defect

(i) Substitutional Impurities

A substitutional impurity refers to a foreign atom that replaces a parent atom in the Lattice.

Substitutional impurities chances the electrical properties enormously.

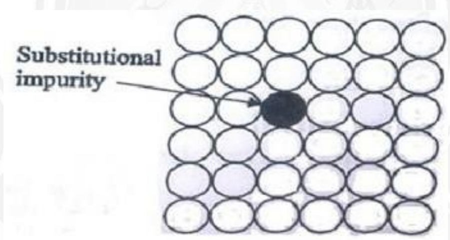

Fig 5.8.5- Substitutional impurities

Example

1. n-type and p-type semiconductor have substitutional impurities from Vth group and IIIrd group elements. This is used to producing many electronic devices like diode and transistors.
2. During the production of brass alloy, zinc atoms are doped in copper lattice. Here zinc atoms are called as substitutional impurities.

ii)Interstitial impurity defect

Fig 5.8.6**- Interstitial impurity defect**

An interstitial impurity is a small size atom occupying the empty space(interstitial) in the parent crystal,without dislodging any of the parent atoms from their sites.

An atom can enter into interstitial or empty space only when it is substantially smaller than parent atom.

Example

In FCC iron, the atomic radius of iron atom is 0.225nm. The carbon atoms with atomic radius 0.078nm can occupy empty space in FCC lattice as interstitial impurities.

5.1. Line defect or dislocation: (one dimensional Effect)

This defect due to dislocation or distortion of atoms along a line are known as line defects.

In line defect,a portion of line of atoms is missing or displaced from its regular site.

Types of line defects

There are two types of line defects

(a)Edge dislocation and

(b)Screw dislocations

(a) Edge Dislocation

An edge dislocation arises when one of the atomic planes forms only partially and does not extend through the entire crystal.

The atomic plane AB abruptly terminates at B.It is viewed as an extra plane inserted in between a set of parallel planes.

The edge of such a plane forms aline defect and it is called an edge dislocation.

The atomic row1 passing through paint B has one atom more than row 2 adjacent to it.

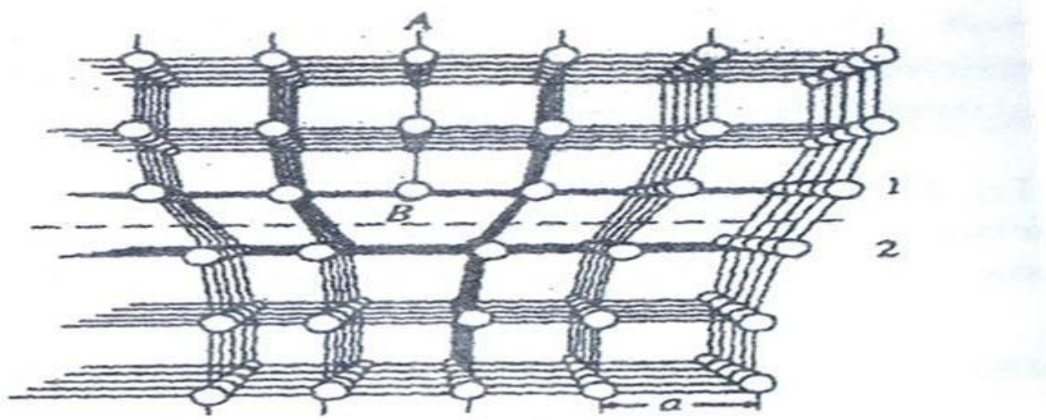

Fig 5.8.7- Edge Dislocation

Classification of edge dislocation

Edge dislocations are symbolically represented by or depending on whether the incomplete plane starts from top or bottom of the crystal.

There are two configurations are referred as

(i) Positive edge dislocation

(ii) Negative edge dislocations

(i) Positive edge dislocation

If the extra plane of atoms in above the slip plane of the crystal than the edge dislocation is called positive an shown in figure.It is denoted by the symbol $\perp$.

(ii) Negative edge dislocations

If the extra plane of atoms is below the slip plane than the edge dislocation is called negative.It is denoted by the symbol $\top$.

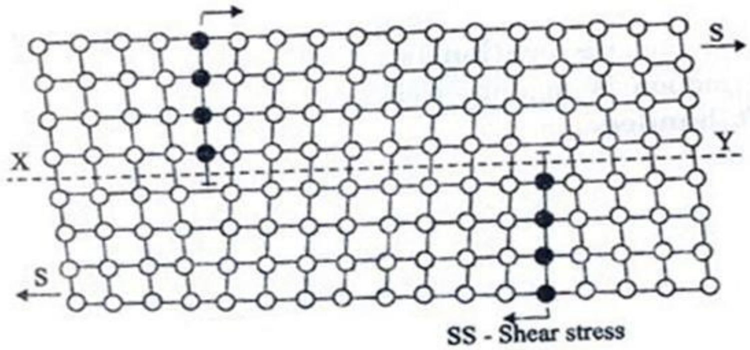

Fig 5.8.8- Negative edge dislocations

(iii)Screw dislocations

Screw dislocation is due to a displacement of atoms in one part of a crystal relative to rest of the crystal.

The displacement terminates with in crystal.This dislocation forms a spiral ramp around dis location line.

In screw dislocation,the reisaline of atoms about which crystal planes are warped to give an effect similar to threads of screw.

The row of atoms marking the termination of the displacement is the screw dislocation.EF indicates the dislocation line

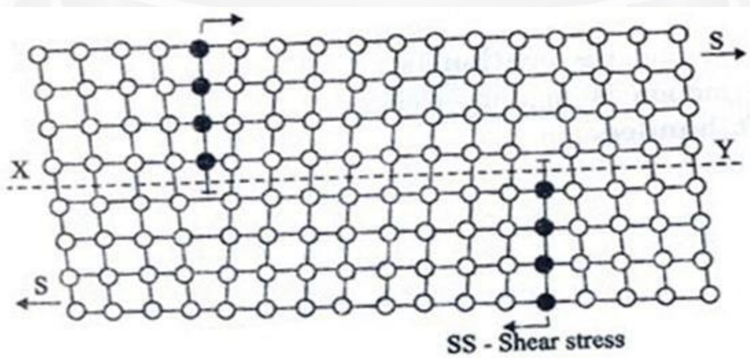

Fig 5.8.9- Screw dislocations

The term screw represents that one part of the crystal is moving in spiral manner about dislocation line.

BURGER'S VECTORS

The dislocation lines are expressed by a burger vector. It indicates the amount and direction of shift in lattice on slip plane. The figure shows a perfect crystal and crystal with a positive edge dislocation.

Consider a point starting from p in figure (b) which moves in particular direction as shown and it completes atomic distance in the form of a circuit called Burger circuit or burger loop.

If the same circuit is drawn starting from pin figure. Then the circuit would not complete, this is because of the presence of a dislocation.

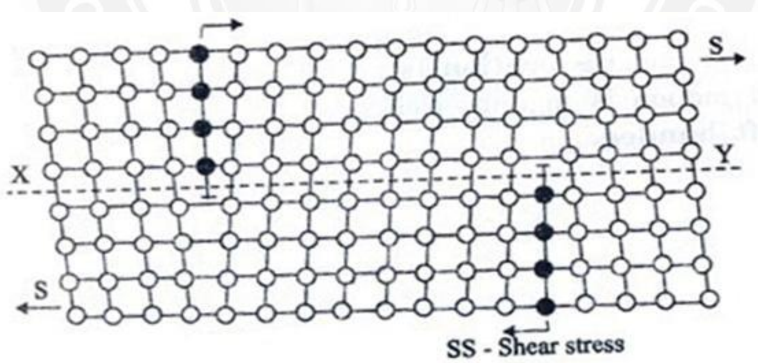

Fig 5.8.9- Burger'svectors

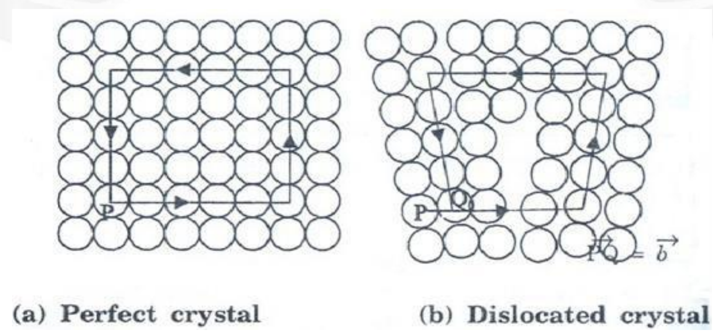

Fig 5.8.10 –a)Perfect Crystal and b)Dislocated Crystal

If we wish to arrive at starting point p from Q, then we must move an extra distance bas shown in figure The vector b+PQ connects end point with starting point. This is Burger'svector of the dislocation.

SURFACE DEFECTS(PLANEDEFECTS)

The defects on the surface of material are called as surface defector plane defects.

They are also known as two dimensional imperfections.

Surface defects are due to a change in the stacking of atomic planes on or across a boundary.Some important internal surface defects.

(i) Grain boundaries

(ii) Tilt and twist boundaries

(iii) Twin boundaries

(iv) Stacking fault

(v) Grain boundaries

(i) Grain boundaries

When ever the grains of different orientations separate the general pattern of atoms and exhibits a boundary the defect caused is called grain boundary.

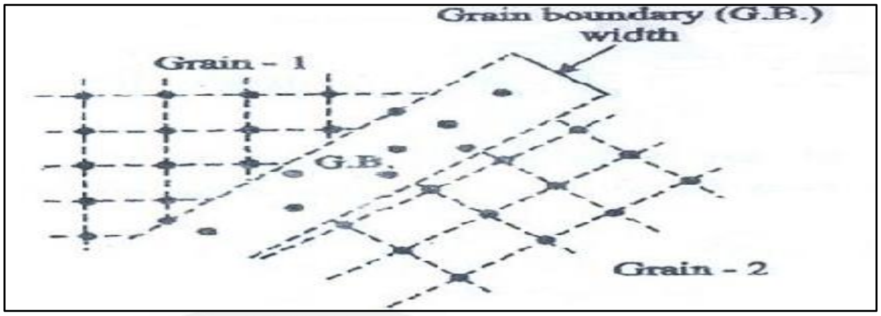

Fig 5.8.11- Grain boundaries

A grain boundary is formed when two growing grain surface meet.The shape of the grainis usually influenced by the presence of surrounding grains.

(i) Tilt and twist boundaries

Tilt boundary is another surface imperfection.It is an arry of parallel edge dislocations of same sign(i.e.either) arranged one above other in an array or series.

Tilt boundary is a type of low angle boundary(lessthan10)

By rotation of an axis in the boundary,it is possible to bring the axis of two bordering grains into coincidence,then

Angle of tilt, $\tan\theta = \frac{b}{D}$

D-dislocation spacing

b-length of Burger's vector

When angle very small,then $\tan\theta = \theta$,

$$\theta = \frac{b}{D}$$

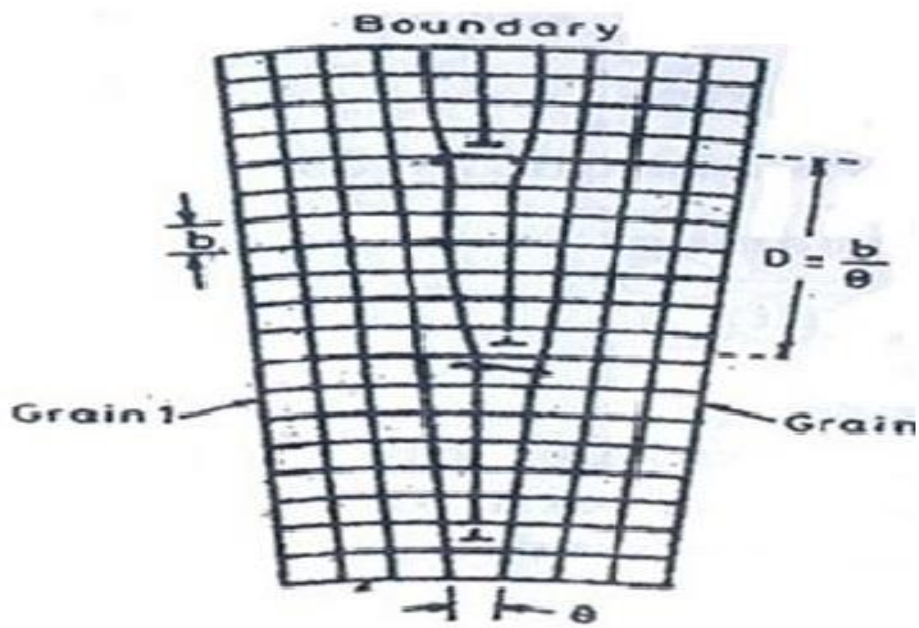

Fig 5.8.12- Tilt and twist boundaries

Twist boundaries

Twist boundaries are another type of low angle boundaries. It consists of at least two sets of parallel screw dislocations lying in the boundary. In two boundaries,the rotationis about an axis normal to boundary.

(ii)Twin boundaries

Twin boundaries are another surface imperfections

If the boundary in which the atomic arrangement on one side of the boundary is some what a mirror image of the arrangement of atoms of the other side. This defect caused is called twin boundary.

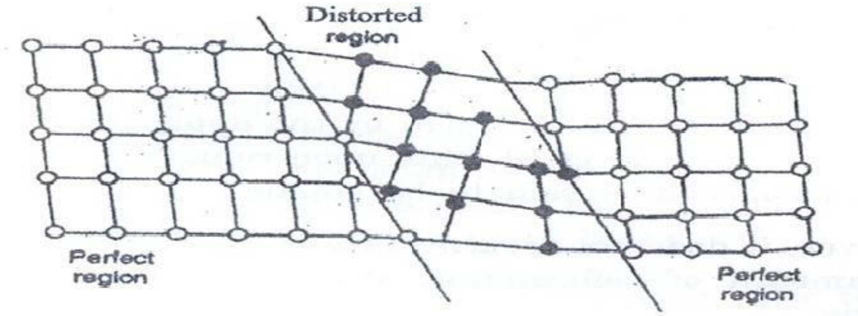

Fig 5.8.13- Twin boundaries

STACKING FAULTS

It is the kind of surface imperfection.Whenever the stacking of atoms is not in proper sequence thought the crystal,defect caused is called stacking effect.

Explanation

Figure shows that the proper sequences of atomic plans if we read from bottom to top A-B-C-A-B-C-A-B-C.

But figure(b)shows the sequence of atomic planes as A-B-C-A-B-A-B-A-B-C

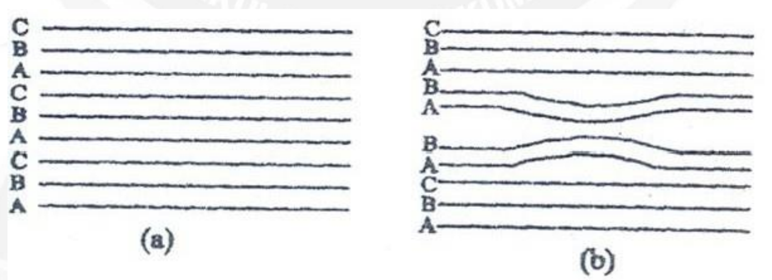

Fig:5.8.14 - stacking faults

The region in which the stacking fault occurs (A-B-A-B)forms a thin region of hexagonal close packing in FCC crystal.

5.8-b)ROLE OF IMPERFECTION IN PLASTIC DEFORMATION

Dislocation sand plastic deformation

Suppose a crystal is deformed by the application of stresses. Now it returns to its original state upon removal of the stresses, then the deformation is said to be elastic.

However, it does not return to its original state, i.e., retains a certain amount of deformation is said to be elastic.

It is generally believed that in most of the crystals the plastic deformation results from the slip of one part of the crystal relative to another.

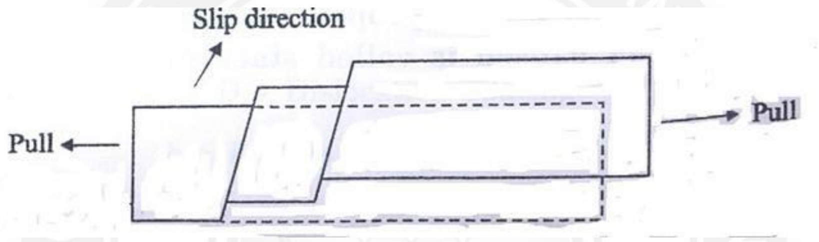

Fig:5.8.14 - Dislocation

If we confine ourselves with the plastic deformation which is composed of an increase in length only, then the figure is used to explain how such a process may lead to an increase in length of a crystal under the influence of tension.

Since slip is caused by the presence of dislocation, connections between plastic deformation and dislocations must obviously exist.