

CRYSTAL IMPERFECTIONS

WHY SHOULD WE STUDY CRYSTAL IMPERFECTIONS?

Technically important properties such as mechanical strength.

Ductility' Crystal growth, magnetic hysteresis, dielectric strength, conduction in Semiconductors are greatly affected by relatively minor changes in crystal Structure caused by DEFECTS/ IMPERFECTIONS.

Crystal Imperfections are the defects in the regular geometrical arrangement of the atoms in a Crystalline solid.

A Perfect Crystal is an idealization; there is no such thing in nature.

The defects may be the results of the crystal deformation or rapid cooling from high temperature or high energy radiation striking the solid.

The defects influence the mechanical, electrical, and optical behavior of the crystal.

The imperfections may be classified widely as:

- Point Defects
- Line Defects
- Surface Defects
- Volume Defects

1. POINT DEFECTS

These are the lattice errors at isolated points , takes place due to the imperfect packing of atoms during crystallization or due to the vibrations of atoms at high temperatures.

number of defects at equilibrium concentration , at a certain temperature is given by

$$n = N * \exp [-E_d/k_bT]$$

Where

n —number of imperfections

N—number of atomic sites per mole

E_d—free energy required to form defects

k_b—Boltzmann's constant (k_b= 8.62*10⁻⁵ eV/K)

T —Absolute temperature

(a)VACANCIES

A simplest point defects in a crystal.

Refers to missing atom or vacant atomic site.

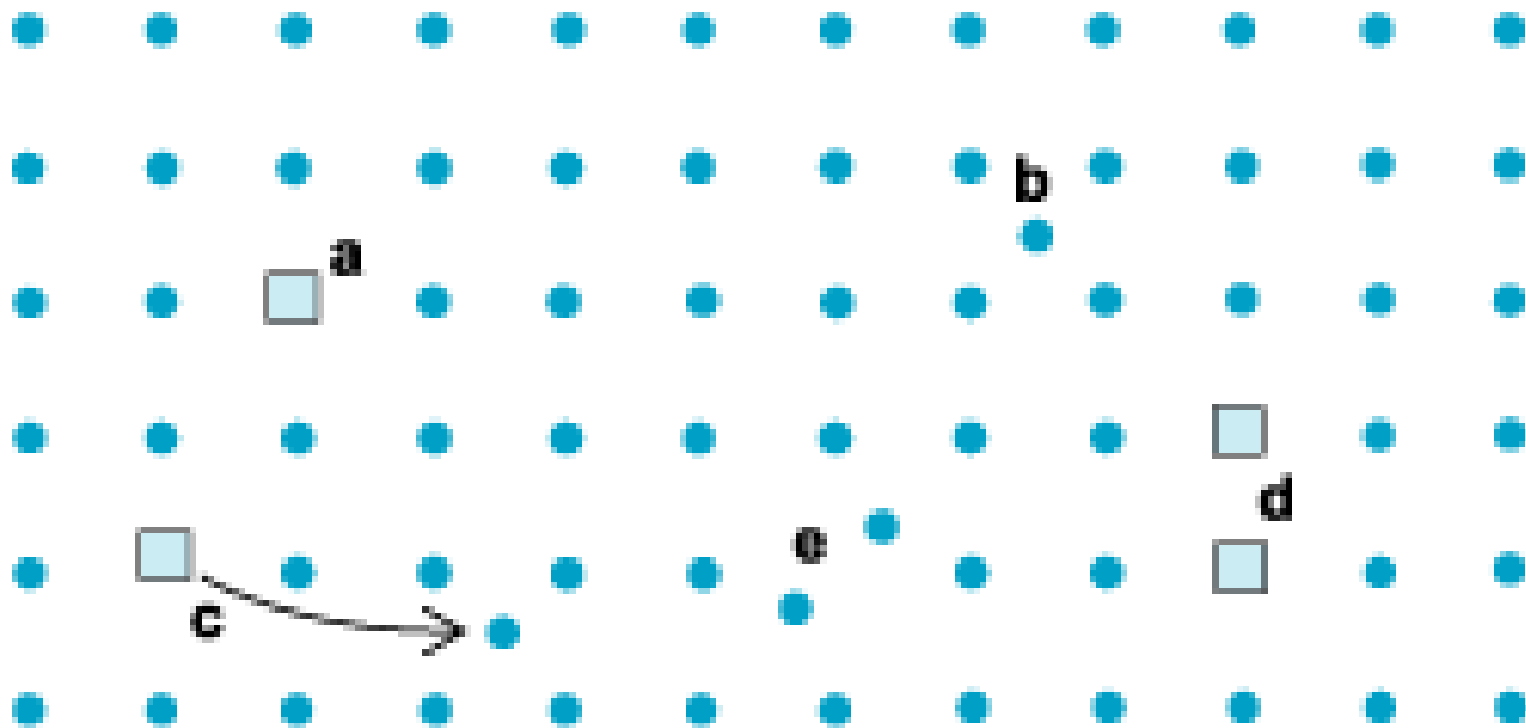
Arise either from imperfect packing during original crystallisation or from thermal vibrations at high temperatures.

(b)FRENKEL DEFECT

It is formed by a cat ion leaving its normal position and moving into an interstitial site.

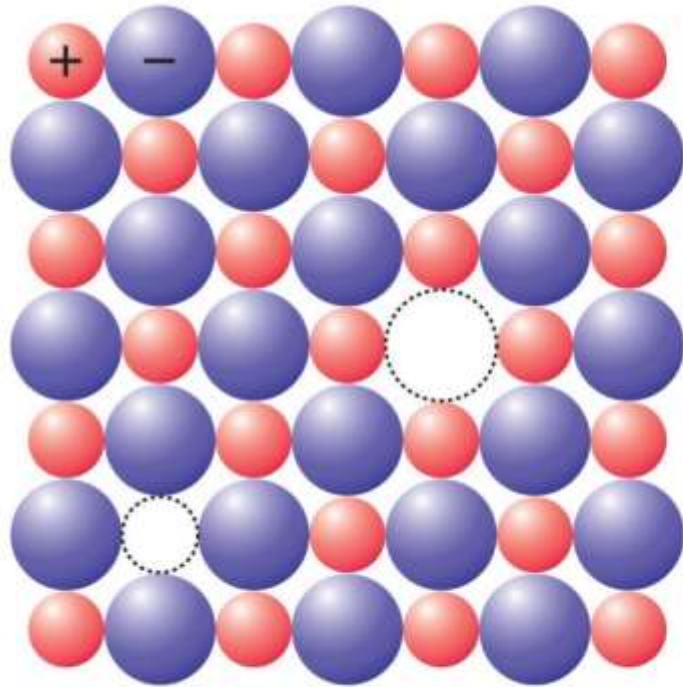
(c)SCHOTTKY DEFECT

It is formed by removing one cat ion and one anion from the interior of the crystal and then placing them both at an external surface.

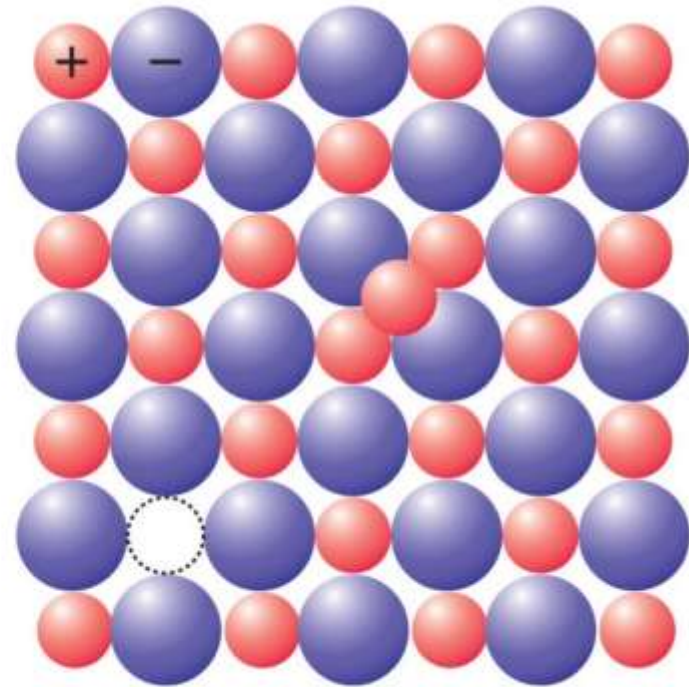


Key:

- a = vacancy (Schottky defect)**
- b = interstitial**
- c = vacancy-interstitial pair (Frenkel defect)**
- d = divacancy**
- e = split interstitial**
- = vacant site**



(a) Schottky defect



(b) Frenkel defect

(d) COMPOSITIONAL DEFECTS

- These arise from impurity atoms during crystallisation.
- They occur on lattice point as a **Substitutional** impurity or as an **interstitial** impurity.
- Substitutional impurity is created when a foreign atom substitutes for a parent atom in the crystal lattice.
- Interstitial impurity is a small sized foreign atom occupying an interstitial position between the regularly positioned atoms.

(e) ELECTRONIC DEFECTS

- These are the errors in charge distribution in solids.
- These are primarily necessary in electrical conductivity & related phenomenon
- Prominent example is pn junction formation and transistor junction formations.

2. LINE IMPERFECTIONS/ DISLOCATIONS

- 1-D defects around which some of the atoms are misaligned.
- These are responsible for the useful property of ductility in metals, ceramics and crystalline polymers.
- Types :- Edge Dislocations and Screw Dislocations.

(a)EDGE DISLOCATIONS

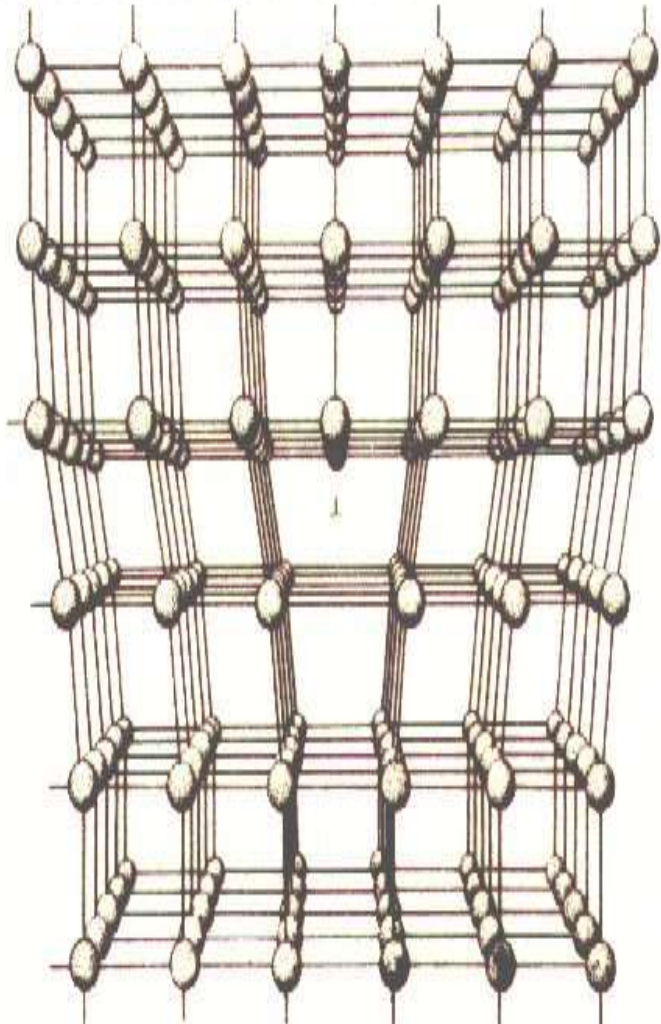
- The perfect crystal is considered to be made up of vertical planes parallel to one another and to the side faces. If one of these vertical planes doesn't extend from top to bottom of the crystal but ends partway within the crystal then there exists a Dislocation.
- The bond lengths above the slip plane are compressed to smaller than that of the equilibrium value. And below the slip plane bond lengths are found to be pulled apart and are in a state of tension.

(b) SCREW DISLOCATIONS

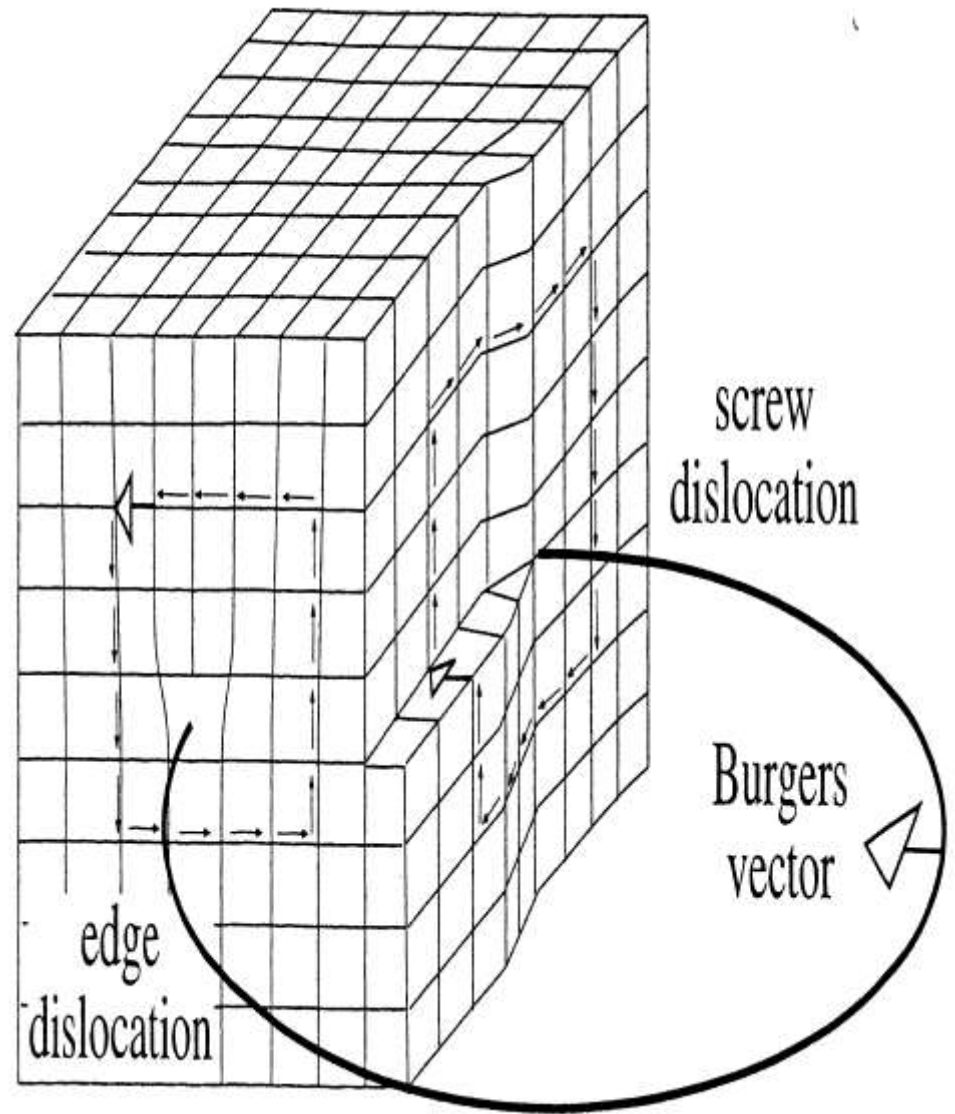
- It is formed by a shear stress that is applied to produce the distortion. The upper region of the crystal is shifted one atomic distance to the right relative to bottom portion.

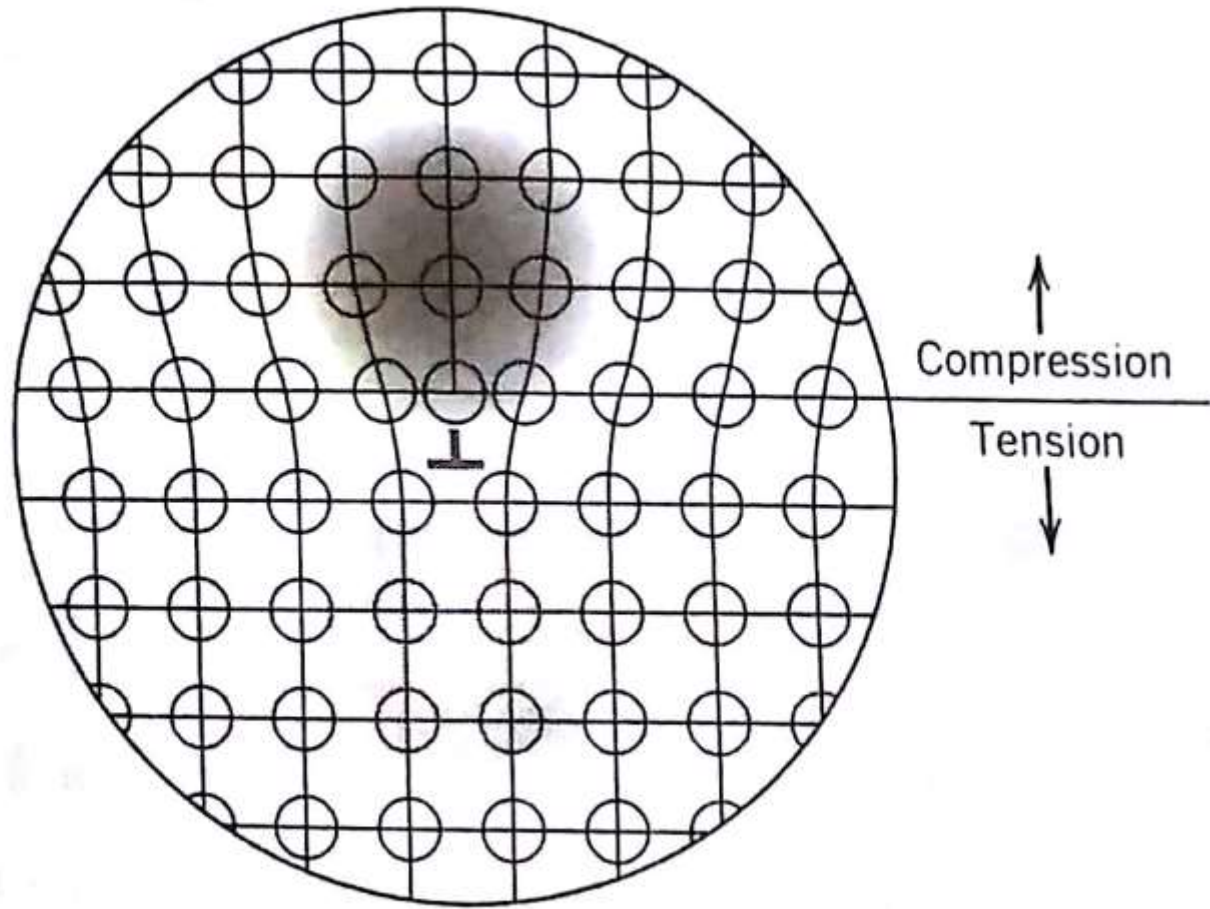
***BURGERS VECTOR.**

- The magnitude & direction of the lattice distortion associated with a dislocation is expressed in terms of a BURGERS VECTOR.
- If The BURGERS Vector and the orientation of the dislocation line are known , then the dislocation is completely described.
- This vector indicates how much and at what direction the lattice above the slip plane appears to have been shifted with respect to the lattice below the plane.
- The burgers vector is perpendicular to the dislocation line in Edge Dislocations and it is parallel to the dislocation line in Screw Dislocations.



Edge dislocation





Edge dislocation

3. SURFACE IMPERFECTIONS

- Two Dimensional defects.
- These arise from a change in the stacking of atomic planes on or across a boundary.

(a) External surface imperfections

- Imperfections represented by a boundary.
- The external surface of a material is an imperfection itself because the bonds do not extend beyond it since surface atoms are not entirely surrounded by other atoms on other side, they possess higher energy than that of internal atoms.

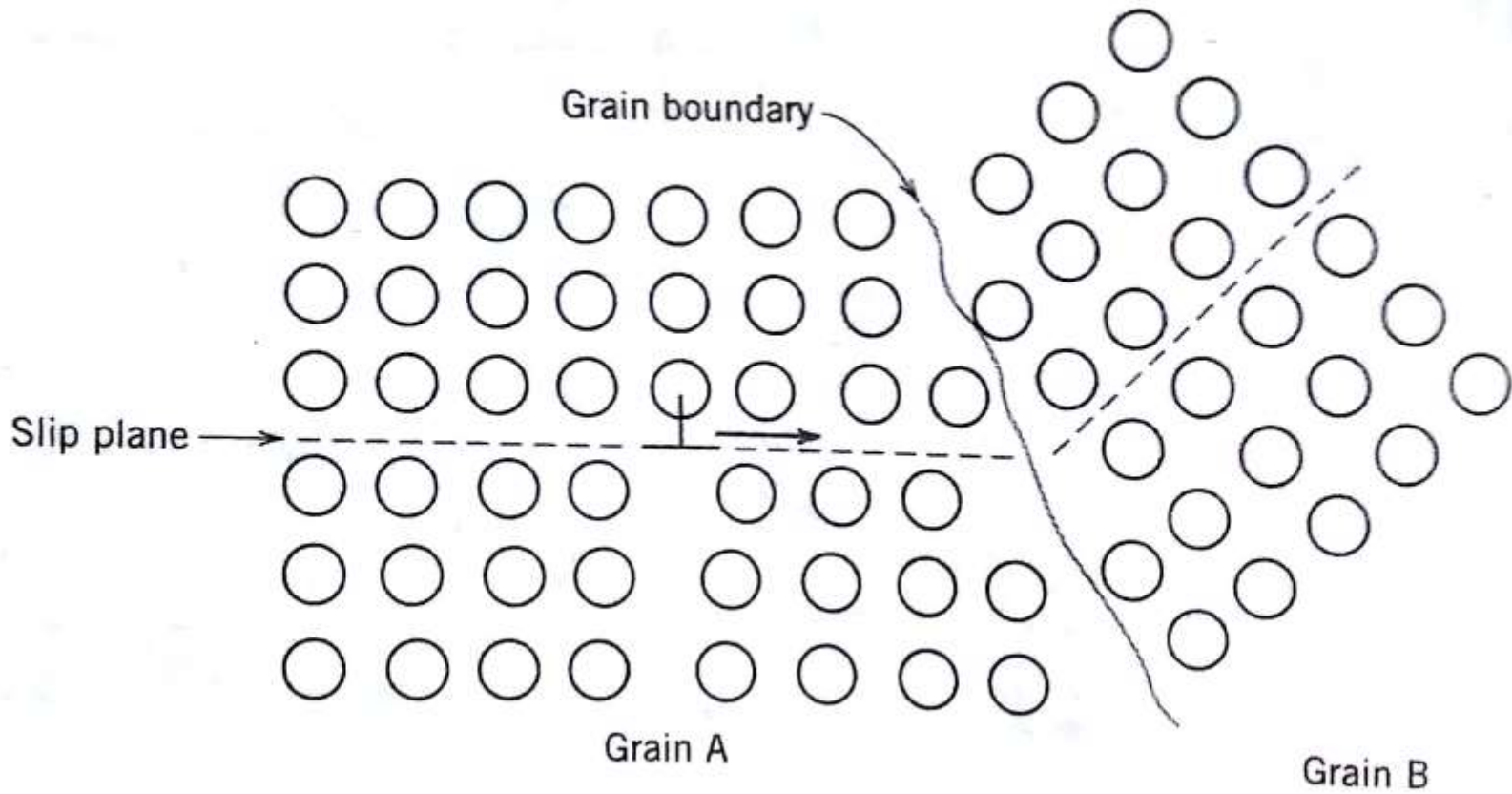
(b) Internal surface imperfections

These are manifested by such defects as Grain boundaries, Tilt boundaries, Twin boundaries, Stacking faults.

Grain boundaries: These separate crystals/ grains of different orientation in a polycrystalline material during crystallisation. The shape of a grain is usually influenced by the presence of surrounding grains. Hence a region of transition exists in which the atomic packing is Imperfect.

- In the boundary where the crystal or grains change abruptly, the orientation of difference between neighboring grains is more than 10° - 15° ,& the boundaries are known as high angle grain boundaries.
- The boundary between 2 crystals which have different crystalline arrangements or different compositions is called an interface.

Grain boundaries



Tilt Boundaries

- This is a low angle boundary as the orientation difference is between 2 neighboring crystals is less than 10°
- this is composed of edge dislocation lying one above the other.
- The tilt angle,
- Where, b —magnitude of Burgers vector,

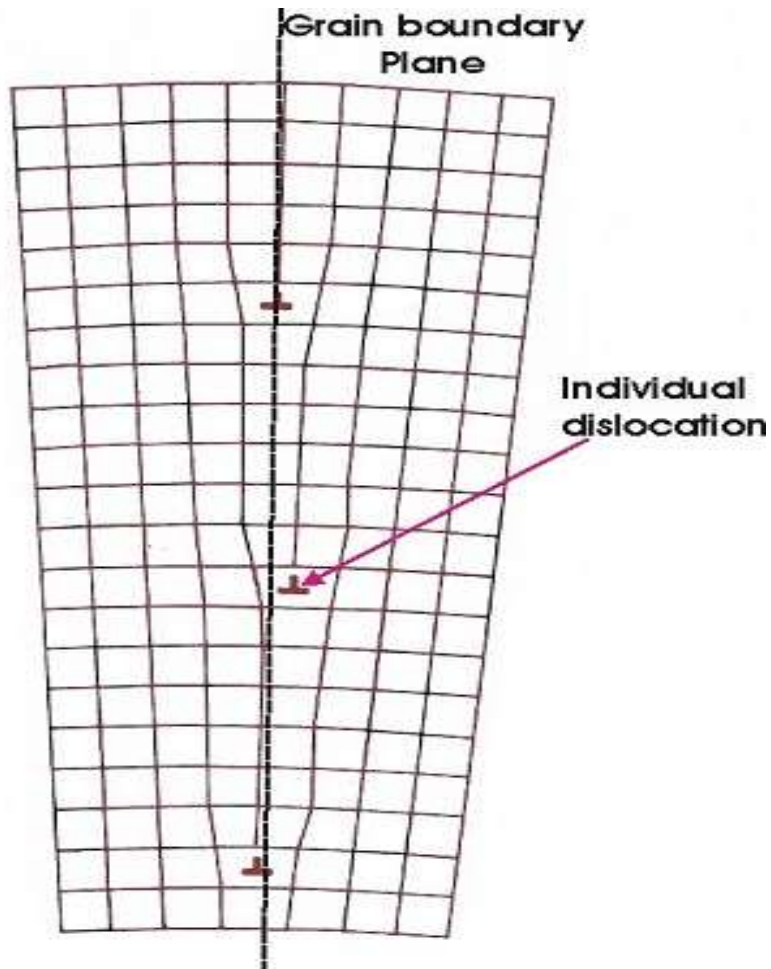
Twin Boundaries

- The atomic arrangement on one side of a twin boundary is a mirror reflection of arrangement on the other side.
- These occur always in pairs such that the orientation change introduced by one is restored by another.

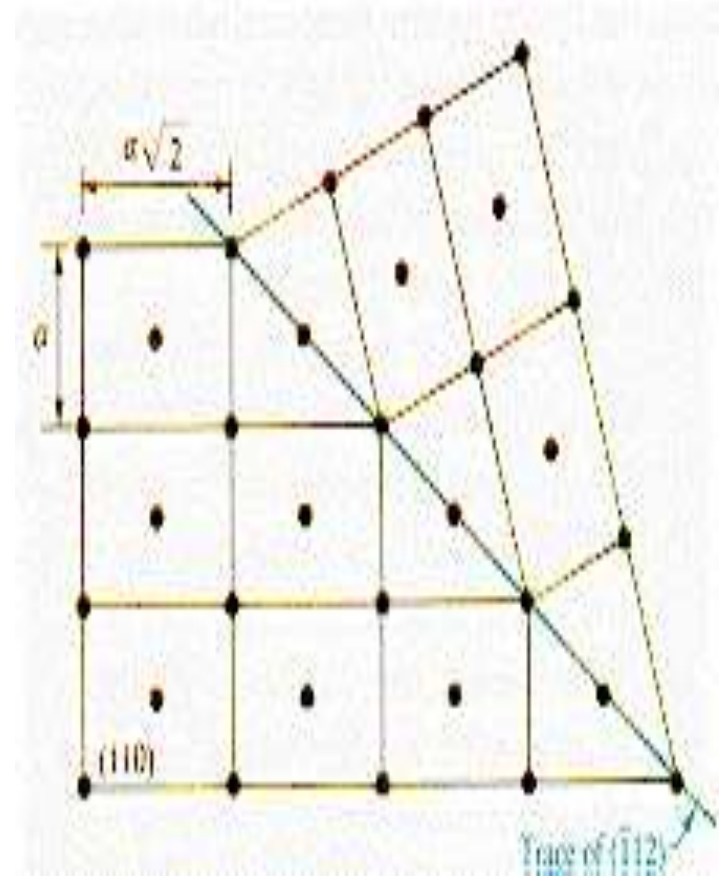
Stacking Defects

- This type of fault arises from the stacking of one atomic plane out of sequence on another while the lattice on either side of the fault is perfect.

Tilt boundaries



Twin boundaries



4. VOLUME IMPERFECTIONS

- 3 Dimensional Imperfections
- These may arise when there is only a small electrostatic dissimilarities b/w the stacking sequences of close packed planes in metals. For example cracks.
- When clusters of atoms are missing, a large vacancies or voids are created which are also the volume imperfections.

Reference

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- Callister's MATERIALS SCIENCE AND ENGINEERING Adopted by R Balasubramaniam