Crystal Imperfections

- A crystal is a solid composed of atoms, ions or molecules arranged in a pattern which is repetitive in three dimensions.
- In an ideal crystal, the atomic arrangement is perfectly regular and continuous throughout. An ideal crystal is perfect. But in real crystals as in cast or welded objects are never perfect.
- Lattice distortion and various imperfections, irregularities or defects are generally present in them.
- Because of these defects the physical and mechanical properties of engineering metals and alloys are profoundly affected by the imperfections in the crystals.

Classification of crystal imperfections

(1) Point defects

(2) Line defects

(3) Surface defects

(4)Volume defects.

Point defects

- Vacancies
- Interstitial impurities
- Substitutional impurities
- Electronic defects (errors in charge distribution in solids)

Line defects

- Edge dislocation
- Screw dislocation

Surface defects

- Grain boundries
- Tilt boundries
- Twin boundries
- Stacking faults

Volume defects

- **Cracks, blow holes, foreign inclusions.**

Point defects:

In a crystal lattice, point defects is one which is completely local in its defect. Example: a vacant lattice site.

Vacancies

Vacancies may occur as a result of imperfect packing during the original crystallisation or they may arise from thermal vibrations of atoms at elevated temperatures.

Because as thermal energy is increased there is a higher probability that individual atoms will jump out of their position of lowest energy.

The atoms surrounding a vacancy tend to be closer together, thereby distorting the lattice planes.

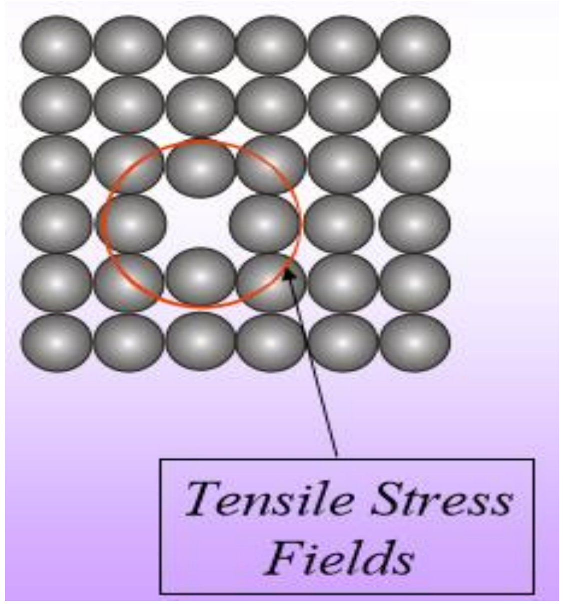
Vacancy – An atom missing from regular lattice position. Vacancies are present invariably in all materials.

Interstitialcy – An atom trapped in the interstitial point (a point intermediate between regular lattice points) is called an interstitialcy.

An impurity atom at the regular or interstitial position in the lattice is another type of point defect.

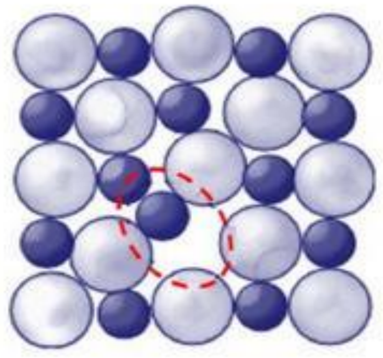
Vacancy

- Missing atom from an atomic site
- Atoms around the vacancy displaced
- Tensile stress field produced in the vicinity

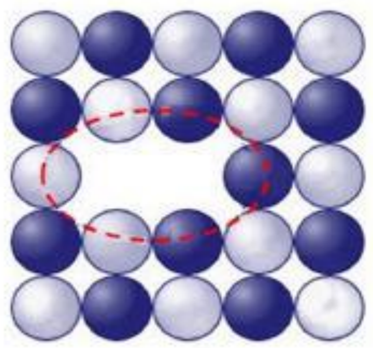


Schottky defect

- is closely related to vacancies and is formed when an atom or ion is removed from the normal lattice site and replaced in an average position on the surface of the crystal.
- In other words, when vacancies are created by movements of atoms from positions inside the crystal, a Schottky defect is said to have been formed.



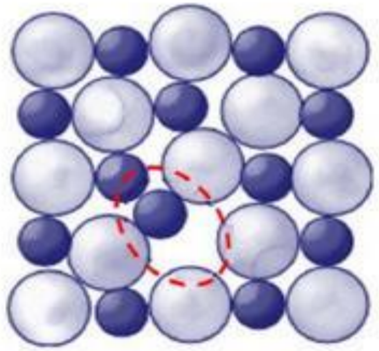
Frenkel defect



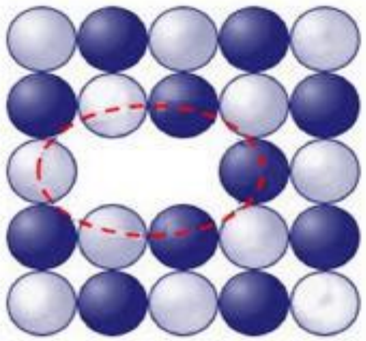
Schottky defect

Point defects

In ceramic materials point defects occur in pair to maintain the electro neutrality. A cation-vacancy and a cation-interstitial pair is known as **Frenkel** defect. A cation vacancy-anion vacancy pair is known as a **Schottky** defect.



Frenkel defect



Schottky defect

Interstitialcy

An interstitial defect arises when an atom occupies a definite position in the lattice that is not normally occupied in the perfect crystal.

In interstitialcies, atoms occupy positions between the atoms of the ideal crystal. This interstitial atom may be either a normal atom of the crystal or a foreign atom.

The interstitial atom may be lodged within a crystal structure, particularly if the atomic packing factor is low. (example: APF-SC=0.52 and BCC=0.68)

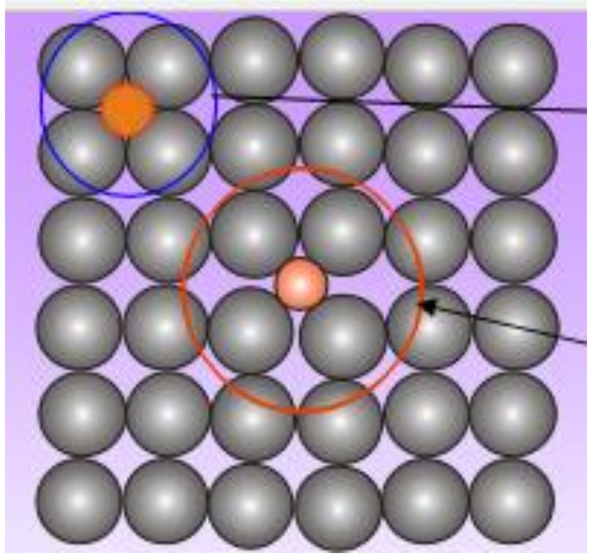
Interstitialcy produces atomic distortion because interstial atom tends to push the surrounding atoms farther apart, unless interstial atom is smaller than the rest of the atoms in the crystal.

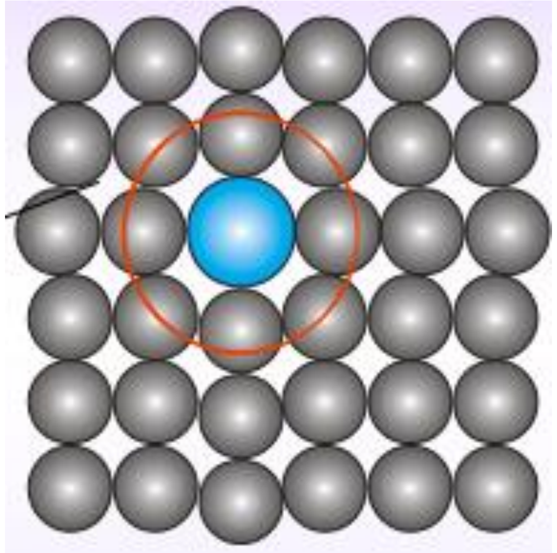
Impurities:

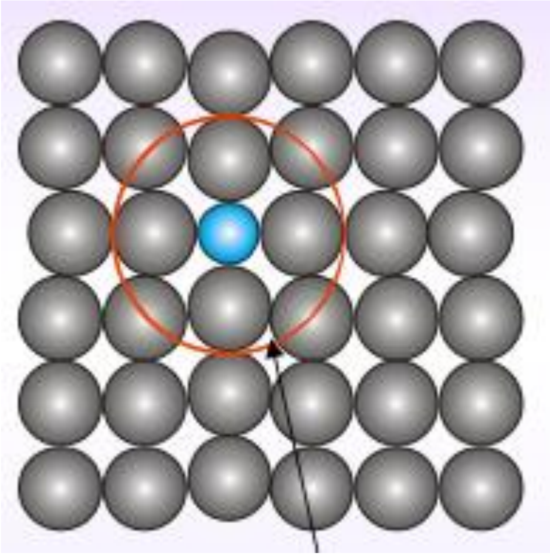
Impurities gives rise to compositional defects. Impurities may also be small particles (such as slag inclusions in metals) embedded in the structure, or foreign (metal) atoms in the lattice.

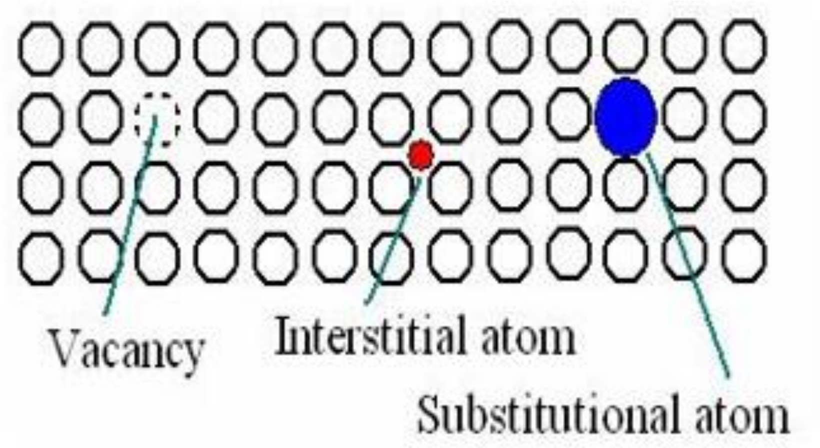
Impurity (foreign atoms) atoms are introduced into crystal structure as substitutional or interstitial atoms i.e., foreign atoms either occupy lattice sites from which the regular atoms of the ideal crystal.

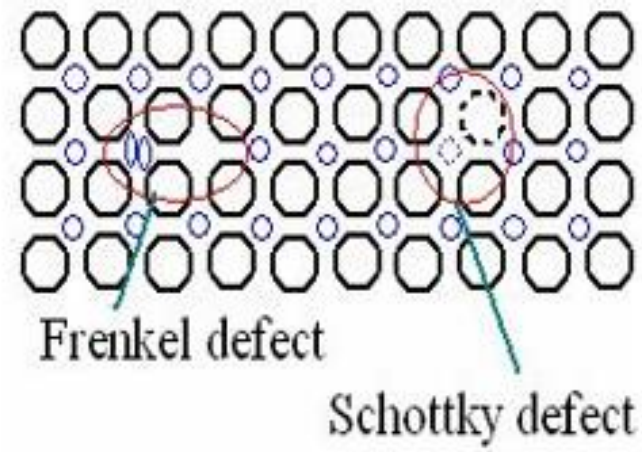
Impurities may considerably distort the lattice.








Vacancy
Interstitial atom
Substitutional atom


Frenkel defect
Schottky defect

Line defects

Line imperfections or dislocations, in crystalline solids are defects that cause lattice distortion centred around a line. dislocations are created during the solidification of crystalline solids.

They are also formed by permanent or plastic deformation of crystalline solids and by vacancy condensation and by atomic mismatch in solid solutions.

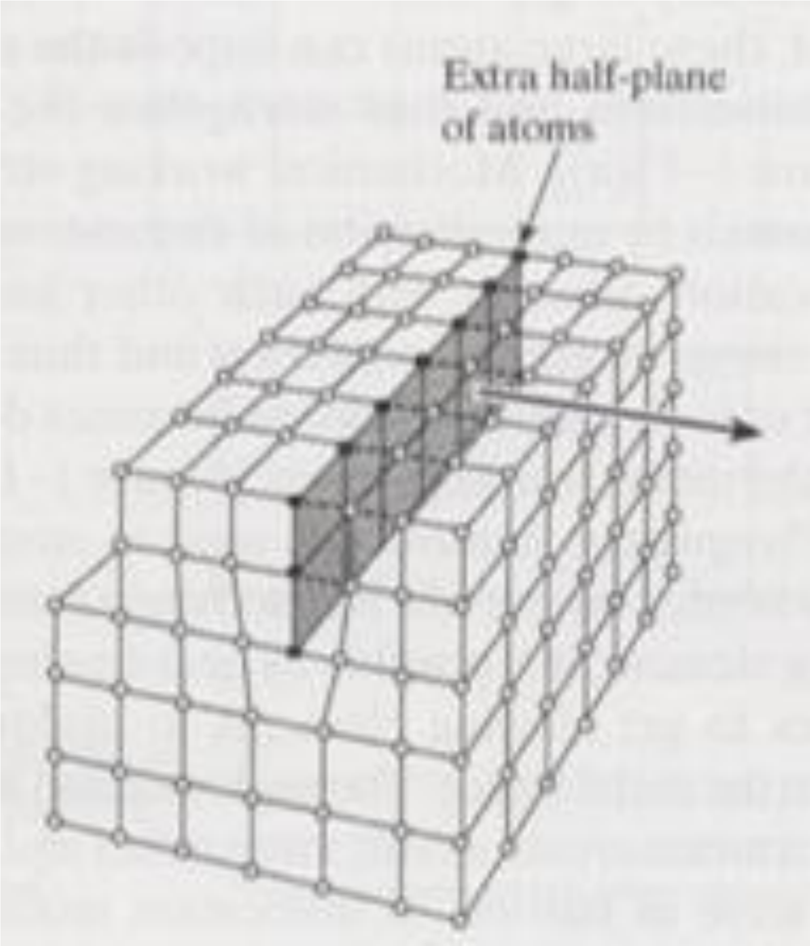
Two main types of dislocations are:

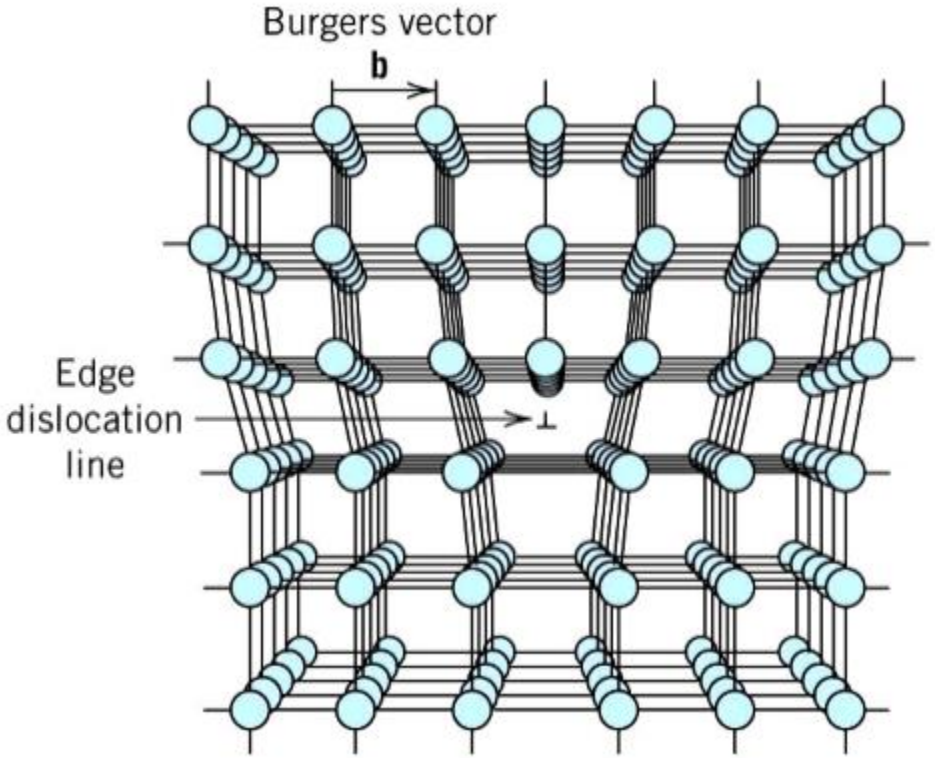
1. Edge dislocations

2. Screw dislocations

Edge dislocations

- An edge dislocation is created in a crystal by the insertion of an extra half plane of atoms **as shown.** The magnitude and direction of displacement of atoms in a dislocation is defined by a vector called burger’s vector.
- The displacement distance of the atoms around the dislocation is called the slip or burger's vector b and is perpendicular to the edge dislocation line. Dislocations are non-equillibrium defects and store energy in the distorted region of the crystal lattice around the dislocation.
- The edge dislocation has a region of compressive strain where the extra half plane is and a region of tensile strain below the extra half plane of atoms.


Extra half-plane
of atoms

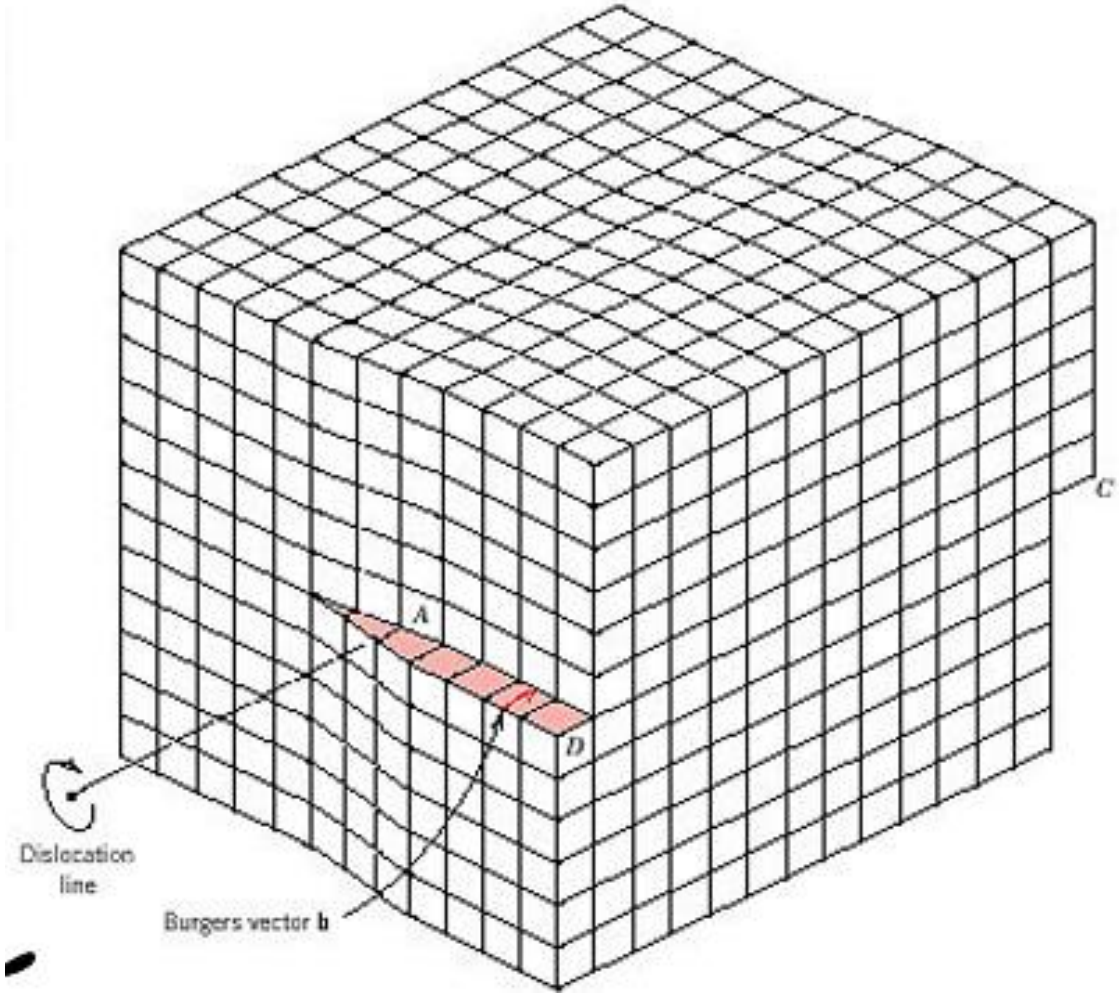

Burgers vector
b
Edge
dislocation
line

Screw dislocation

- The screw dislocation can be formed in a perfect crystal by applying upward and downward shear stresses to regions of a perfect crystal which have been separated by a cutting plane **as shown.**
- These shear stresses introduce a region of distorted crystal lattice in the form of a spiral ramp (slope joining two levels) of distorted atoms or screw dislocation **as shown.**
- A region of shear strain is created around the screw dislocation in which energy stored. The slip or burger’s vector of the screw dislocation is parallel to the dislocation line **as shown.**

- The name screw dislocation is given because it transforms successive atomic planes into the surface of helix around the dislocation line.
- The burger’s vector is parallel to the dislocation line. Such a dislocation has neither tensile nor compressive stresses but has shear stresses.
- In general, dislocations are more complicated, however, they can be resolved to obtain their edge and screw components. Dislocations come into the materials during the solidification or by mechanical processing of metals.

Screw dislocation



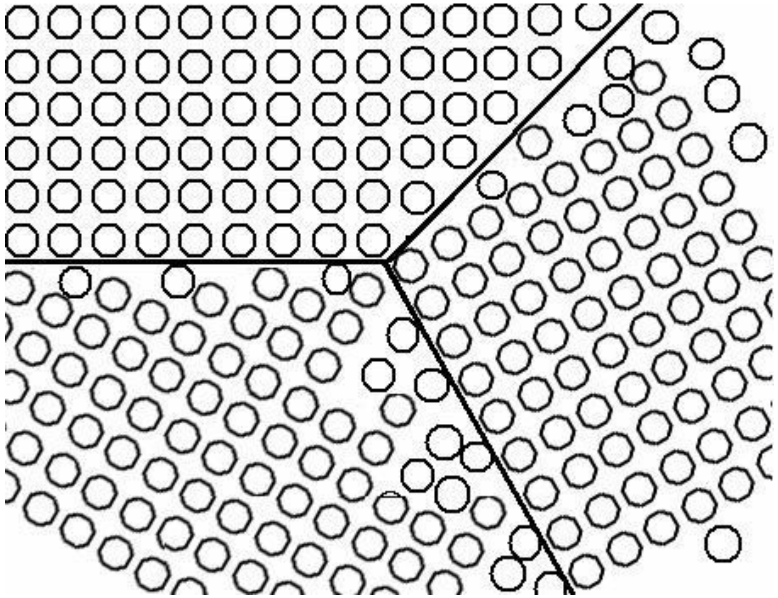
Surface defects

- Planar defects (surface imperfections) arise due to change in the stacking of atomic planes during solidification or mechanical and thermal treatments. The change may be of the orientation or of the stacking sequence of the planes.

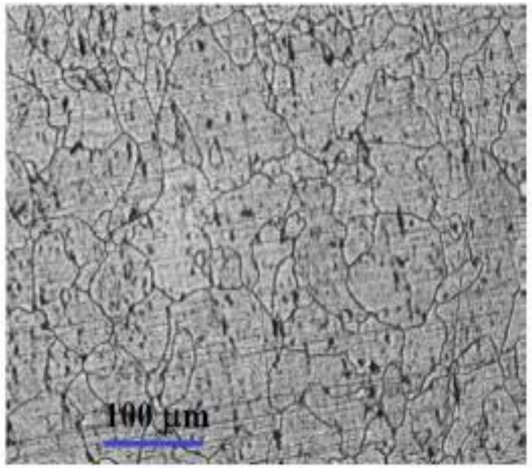
The various types of defects which belong to this type are

- Grain foundries
- Twin boundries
- Tilt boundries
- Stacking faults.

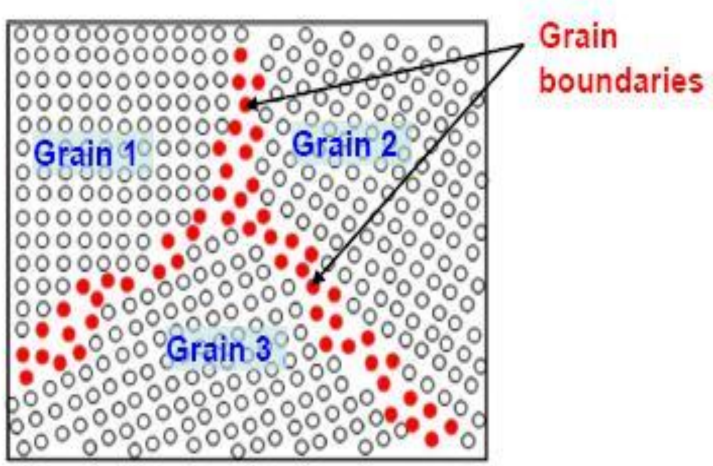
Grain boundaries: Crystalline solids are, usually, made of number of grains separated by grain boundaries. Grain boundaries are several atomic distances wide, and there is mismatch of orientation of grains on either side of the boundary as shown in *figure below.*



Schematic presentation of grain boundaries.



(a) Optical micrograph of a polycrystalline material



(b) Schematic of orientation change across the grain boundary

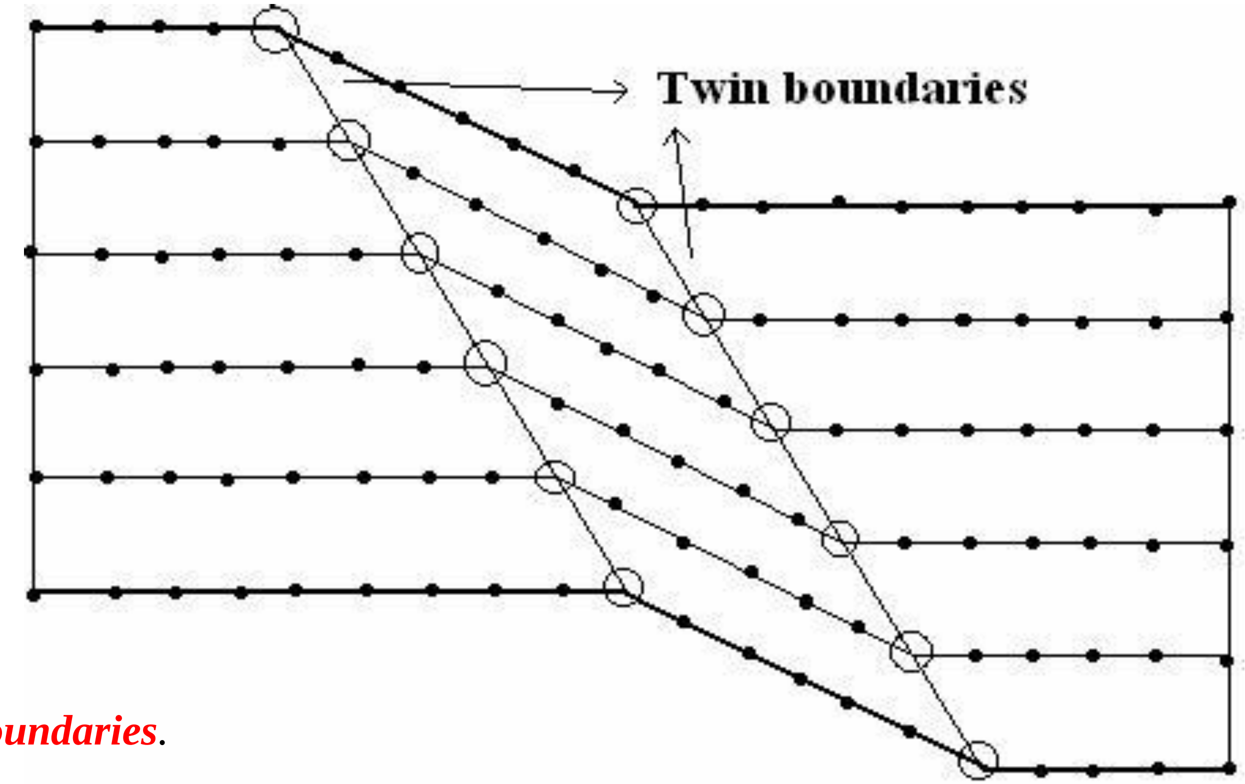
Twin boundries

- These are the boundries in the grains at which the atomic arrangement on one side of the boundry is the mirror image of the atoms on the other side.
- The volume of material which has an orientation similar to the mirror image of the matrix orientation is called a twin. The mirror is called the twinning plane or composition plane.
- Twins may form during solidification, deformation or during deformation and annealing of metals or mechanical working of metals.
- Twin boundries occur in pairs so that the change in orientation of two grains introduced by one boundry is restored by the other grain boundry **as shown.**

Twin boundaries

- It is a special type of grain boundary across which there is specific mirror lattice symmetry. Twin boundaries occur in pairs such that the orientation change introduced by one boundary is restored by the other as shown in figure.
- The region between the pair of boundaries is called the twinned region. Twins which forms during the process of recrystallization are called *annealing twins*, whereas *deformation twins* form during plastic deformation.
- Twinning occurs on a definite crystallographic plane and in a specific direction, both of which depend on the crystal structure.

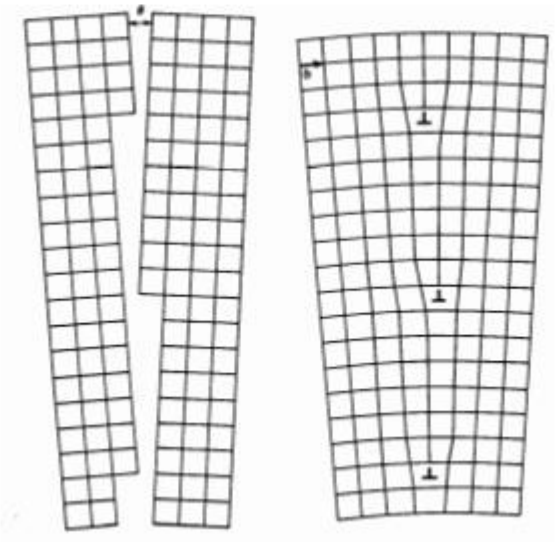
- Annealing twins are typically found in metals that have FCC crystal structure (and low stacking fault energy), while mechanical/deformation twins are observed in BCC and HCP metals.
- Annealing twins are usually broader and with straighter sides than mechanical twins. Twins do not extend beyond a grain boundary.

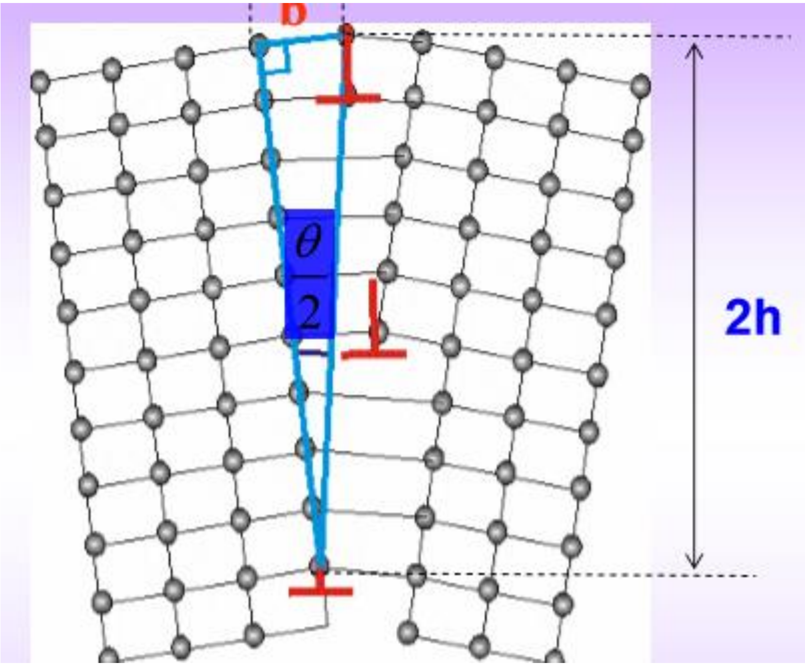


A pair of twin boundaries.

Tilt boundries

- It is also called low angle grain boundry where the orientation difference between two neighbouring crystals is less than 10º. The distorsion in the boundry is less and is limited to a few edge dislocations, located one below the other **as shown.**





***Stacking faults*:**

They are faults in stacking sequence of atom planes. Stacking sequence in an FCC crystal is ABC ABC ABC …, and the sequence for HCP crystals is AB AB AB…. When there is disturbance in the stacking sequence, formation of stacking faults takes place.

Volume imperfections

- Volume imperfections are those defects like blow holes, cracks, foreign inclusions etc. which are three dimensional and are much larger than other types of imperfections.
- They are normally introduced into solids during processing and fabrication (welding or casting) and have a considerable effect on the properties of materials. These defects are stress raisers and weaken the materials.

Thank You