5.15 CRYSTAL DEFECTS or (Crystal Imperfections)

Any deviation from a perfect periodic arrangement of atoms or molecule is called *imperfection* or *defect* in the crystal. In reality, defects are never perfect and contain various types of imperfections and defects which affect many of their physical and mechanical properties, which in turn affect many important engineering properties of materials such as the cold formability of alloys, the electronic conductivity of semiconductors, corrosion of metals, etc.

There are four types of defects. They are

i) Point defects (Zero dimension)

ii) Line defects (One dimension)

iii) Surface defects (Two dimension)

iv) Volume defects (Three dimension)

5.15.1 Point defect

In a crystal lattice, point defect is one which is completely local in its effect eg. a vacant site. The introduction of point defect into a crystal increases its internal energy as compared to that of a perfect crystal.

The point defects can be divided into four types, namely

a) Vacancies (Schottky defect)

b) Interstitial (Frenkel defect)

c) Impurities

d) Electronic defects

a) Vacancies

A vacancy refers to an atomic site from where the atom is missing as shown in Fig.(5.34).

Vacancies exist in a certain proportion in a crystal in thermal equilibrium, leading to an increase in the randomness of the structure.

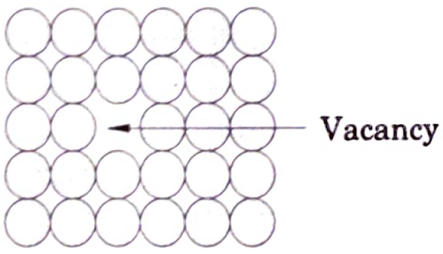


Fig. 5.34 Vacancy defect

Vacancies may occur as a result of imperfect packing during the original crystallization 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.

Vacancies may be single, or two or more of them may condense into a di-vacancy or tri-vacancy.

Schottky defect is closely related to vacancies and is formed when an atom or an ion is removed from a normal lattice site and replaced in an average position on the surface of the crystal (Fig.5.35).

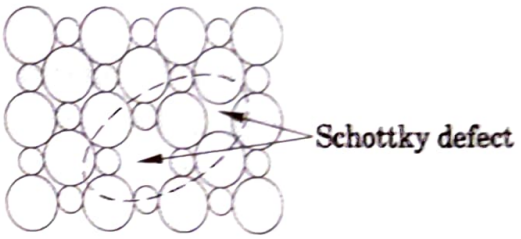


Fig. 5.35 Schottky defect

In other words, when vacancies are created by movement of atoms from positions inside the crystal to positions on the surface of the crystal, a Schottky defect is said to have been formed.

b) Interstitial

A small sized atom occupying the void space in the parent crystal without disturbing the parent atoms from their regular sites is an interstitial impurity. (Fig. 5.36)

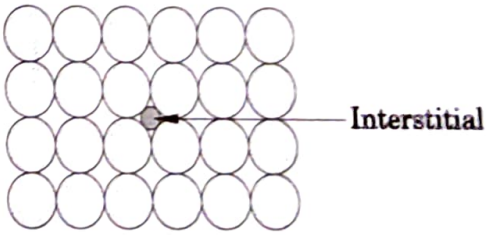


Fig. 5.36 Interstitial impurity

The interstitial atom may be either a normal atom of the crystal or a foreign atom. It may be dislodged within a crystal structure, particularly if the atomic factor is low.

Interstitial produces atomic distortion because interstitial atoms tend to push the surrounding atoms farther apart, unless the atom is smaller than the rest of the atoms in the crystal.

Frenkel defect is closely related to interstitialcies. An ion displaced from the lattice into an interstitial site is called a frenkel defect. (Fig.5.37)

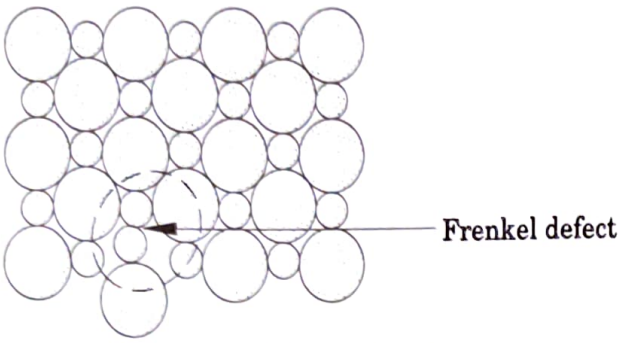
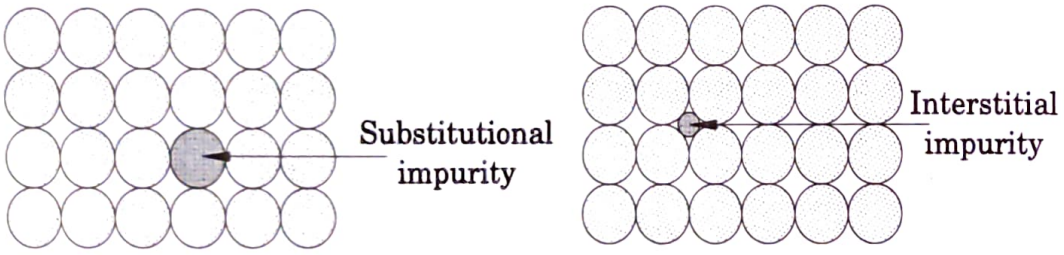


Fig. 5.37Frenkel defect

c) Impurities

Impurities may be small particles embedded in the structure, or foreign (metal) atoms in the lattice. Foreign atoms generally have atomic radii and electronic structures differing from those of the host atoms and therefore act as centres of distortion.

Impurity atoms are introduced into crystal structure as substitutional or interstitial atoms. i.e., foreign atoms either occupy lattice sites from which the regular atoms are missing or they occupy positions between the atoms of the ideal crystal. Impurities may considerably distort the lattice (Fig. 5.38(a) and 5.38(b).



(a) Substitutional impurity *(b) Interstitial impurity*

Fig. 5.38

Impurity defects occur in metallic, covalent and ionic solids and play a very important role in many solid state processes such as diffusion, phase transformation and electrical and thermal conductivity.

A controlled addition of impurity to a very pure crystal is the basis of producing many electronic devices.

d) Electronic defects

These 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, thereby

accounting for some electronic conductivity of certain solids and their increased reactivity.

A vacancy or an interstitial impurity may produce the excess or the deficit of positive or negative charges, by an excess of metal ions as in ZnO, where there is an excess of interstitial zinc ions.

The presence of a point imperfection introduces distortions in the crystal. If the imperfection is a vacancy, the bonds that the missing atom would have formed with its neighbours are absent which give rise to elastic strains.

In the case of impurity atom, because of its size difference, elastic strains are created in the regions surrounding the impurity atom. All these factors tend to increase the potential energy of the crystal called enthalpy. The work done for creation of such a point defect is called the enthalpy of formation of the point imperfection.

5.15.2 Line defects or Dislocation (One dimensional defect)

If a plane of atoms lies only partway through a crystal, the edge of such a plane is a defect in the form of a line, and is known as dislocation.

There are in general, two types of dislocation

a) Edge dislocation, and

b) Screw disloation.

Both these types are formed in the process of solidification or crystallisation of metals and mainly in the process of their deformation.

a) Edge dislocation

In the perfect crystal, the atoms are in equilibrium positions and all the bond lengths are of the equilibrium value. In the imperfect crystal on the right, just above the edge of the incomplete plane, the atoms are squeezed and are in a state of compression. The bond lengths have been compressed to smaller than the equilibrium value. Just below the edge, the atoms are pulled apart and are in a state of tension. The bond lengths have been stretched to above the normal values. The distorted configuration extends all along the edge into the crystal. Thus, as the region of maximum distortion is centered around the edge of the incomplete plane, this distortion represents a line imperfection and is called an edge dislocation.

It should be noted that the dislocation of figure represents a defect that rubs completely through the crystal front to back. This extra plane in Fig.(5.39) may be either above (PQ) or below (P'Q') the slip plane shown by the dashed line AC as shown in figure. In the former case, the dislocation(PQ) is said to be positive and is denoted by the symbol $\perp$, in the latter case it (P'Q') is said to be negative and is denoted by the symbol $\top$, where the horizontal line in the symbol represents the slip plane and the vertical line the incomplete plane. The magnitude and direction of the displacement are determined by a vector called the Burgers vector which is perpendicular to the dislocation line Fig.(5.39).

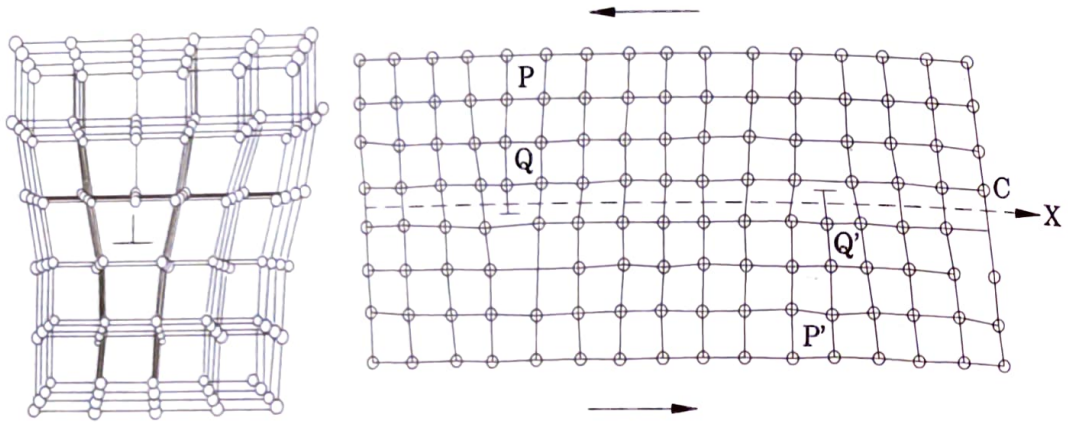


Fig 5.39 Positive and negative edge dislocation

b) Screw dislocation

The second basic type of dislocation is the screw or Burgers disloction. In this, the atoms are displaced in two separate planes perpendicular to each other.

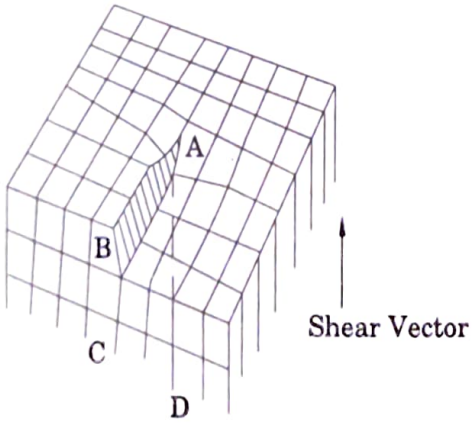


Fig. 5.40. Formation of screw dislocation

Fig.(5.40) is simple example of screw dislocation. The plane ABCD is the slipped area. The upper portion of the crystal has been sheared by an atomic distance

(as shown by the shaded area) to the right relative to the lower portion. No slip has taken place to the right of AD and AD is a dislocation line. Here, the dislocation is parallel to its Burgers vector of shear vector. The designation 'screw' for this lattice defects is derived from the fact that the lattice planes of the crystals spiral the dislocation line AD.

5.15.3 Surface defects (Two dimensional defect)

The defects in the materials arise from a change in the stacking of atomic planes on or across a boundary is known as surface defects.

There are dour different types of surface defects namely,

a) Grain boundary,
b) Tilt boundary,
c) Twin boundary, and
d) Stacking fault

a) Grain boundary

Whenever grains of different orientation separate the general pattern of atoms and exhibits a boundary, as shown in Fig.(5.41), the defect caused is known as grain boundary.

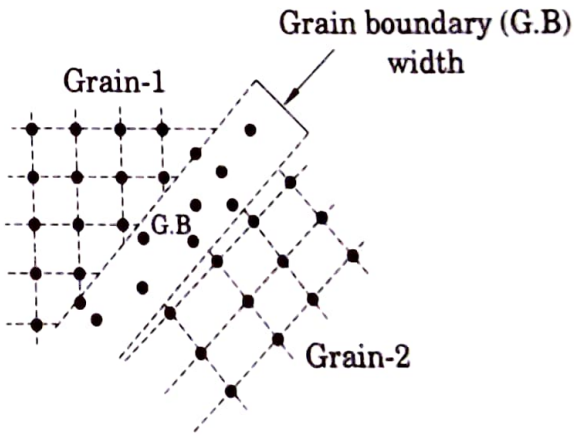


Fig. 5.41. Boundary between two grains

In simple terms, the boundary between the impinding crystal is called crystal or grain boundary. The shape of a grain is usually influenced by the presence of surrounding grains. This type of defect generally takes place during the solification of the liquid metal.

b) Tilt boundary

Tilt boundaries are low angle (i.e. less than 10°) grain boundaries and are considered as an array of parallel edge dislocations of dame sign (i.e. either T or) arranged one above the other in an array or series, as shown in Fig.(5.42)

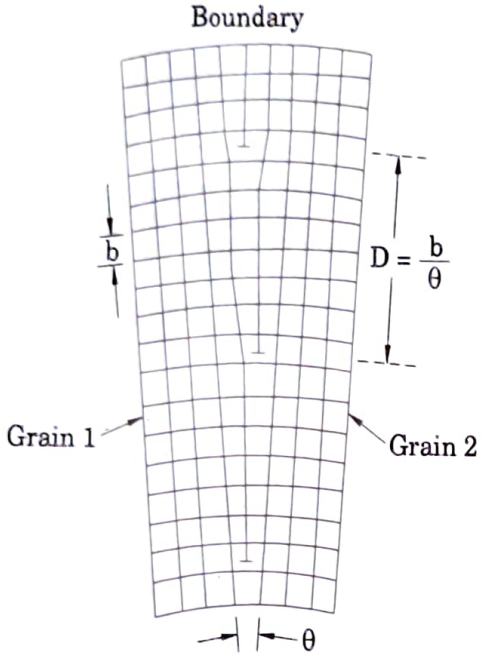


Fig. 5.42. Tilt boundary

The angle of tilt is given by, $\tan\theta = \frac{b}{D}$

when θ is very small, then $\tan\theta \approx \theta$

where, θ = Angle of tilt

D = Dislocation spacing, and

b = Length of Burger's vector

c) Twin boundary

Twist boundaries are also low angle grain boundaries. It consists of atleast two sets of parallel screw dislocations lying in the boundary.

When the boundaries 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, as shown in figure, the defect caused is known as twin boundary.

The region in which a twin boundary defect occurs is between the twinning planes as shown in Fig.(5.43).

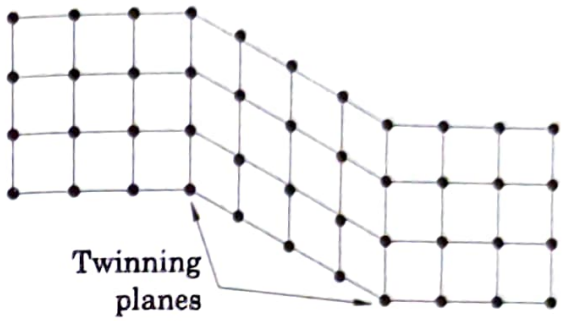


Fig. 5.43. Twin boundary

d) Stacking fault

Whenever the stacking of atoms is not in proper sequence throughout the crystal, the fault caused is known as stacking fault.

Description

Fig.(5.44 a) shows the proper sequency of atomic planes if we read from bottom to top as A-B-C-A-B-C-A-B-C. But Fig.(5.44 b) shows the sequence of atomic planes as A-B-C-A-B-A-B-A-B-C. The region in which the stacking fault occurs (A-B-A-B) forms a thin range of a hexagonal close packing in a FCC crystal.

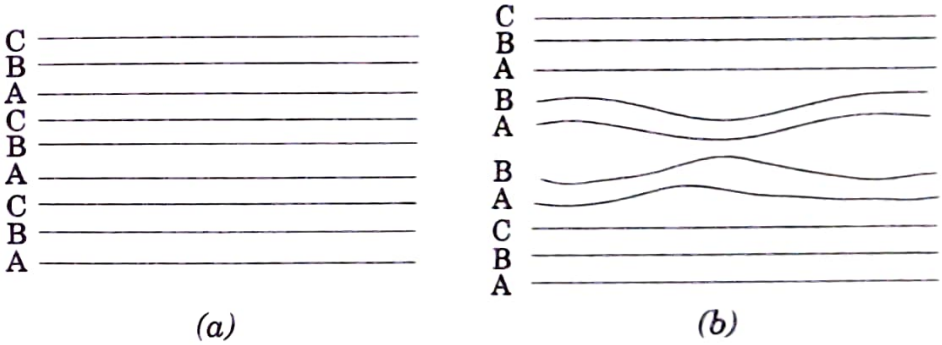


Fig. 5.44. Stacking fault

5.15.4 Volume defects

Volume defects such as cracks may arise in crystal either while being grown or while being used. While growing, any possible small electrostatic dissimilarity between the stacking layers may result in a crack. When the crystal is used for some device application, if it is subjected to sudden thermal waves, cracks generate.

Presence of a large vacancy or void such as clusters of atoms missing is also considered as a *volume imperfection*. While crystal is grown there is every possibility of inclusion of noncrystalline regions of atleast 10 to 30 AU. This is also called volume imperfection. Using optical microscopers, presence of volume defects can be detected. Interferometric techniques can also be applied to study such defeccts.

5.16 BURGER'S VECTOR

Definition

The vector which indicates the direction and magnitude of the shift of the lattice on the slip plane is called a Burger vector.

It is an important property of a dislocation because, if the Burgers vector and the orientation of the disclocation line are known, the dislocation is completely described. This indicates how much and in what direction the lattice above the slip plane appears to have been shifted with respect to the lattice below the slip plane.

i) Edge dislocation

Fig.(5.45) shows a method of determining the Burgers vector applied to an edge dislocation. It is first necessary to choose arbitrarily a positive direction for the dislocation and then to find out the vector which closes a circuit (line of arrows). In the present case a clock-wise of atom-to-atom steps is considered round a dislocation. It is seen that a fails to close the circuit when repeated in perfect lattice B unless completed by a closure vector equal to the Burgers vector b, which is found normal to the dislocation.

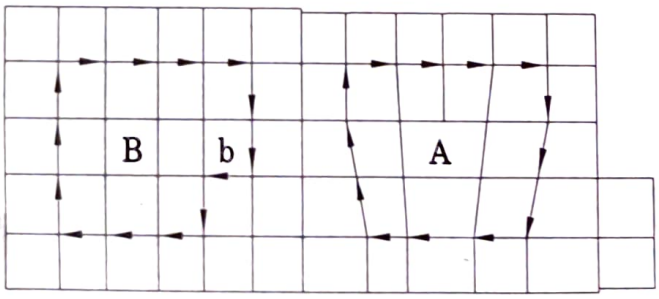


Fig 5.45 Burgers vector for edge dislocation

ii) Screw dislocation

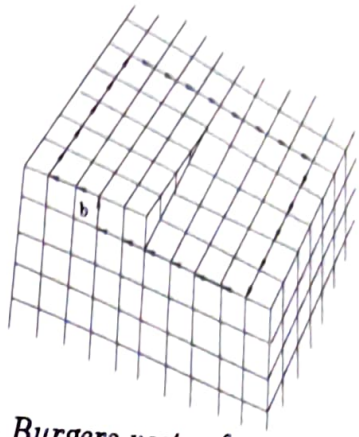


Fig. 5.46. Burgers vector for screw dislocation

In Fig.(5.46) for a screw dislocation, the Burgers circuit fails to close by the amount indicated by the Burgers vector b, which is parallel to the dislocation line.

SUMMARY

* *Crystals have directional properties and are anisotropic substances.*
* *The regular arrangement of the space positions of the atoms in a crystal is called space lattice.*
* *A crystal structure is developed by the combination of space lattice and its basis.*
* *An unit cell is defined as that volume of a solid from which the entire crystal can be constructed by translational repetition in three dimensions.*
* *The intercepts on the crystallographic axes a, b and c which define the dimensions of an unit cell and the interfacial angles α, β and γ are the basic lattice parameters.*
* *There are 7 crystal systems which can form in 14 Bravais lattices in three dimensions.*
* *Miller indices (hkl) are used to designate or name the crystal planes in a crystal lattice.*
* *FCC and HCP structures are close packed structures.*
* *The coordination number is the number of nearest neighbours at a distance '2r' from a corner atom.*
* *The packing factor* $= \frac{v}{V}$ *where v = total volume of atoms in the unit cell and V = volume of unit cell.*