



## **PH0101 UNIT 4 LECTURE-7**

- POINT IMPERFECTIONS
- LINE IMPERFECTIONS
- SURFACE IMPERFECTIONS
- VOLUME IMPERFECTIONS



## CRYSTAL DEFECTS AND IMPERFECTIONS

- An ideal crystal is a perfect crystal in which each atom has identical surroundings. Real crystals are not perfect.
- A real crystal always has a large number of imperfections in the lattice.
- Since real crystals are of finite size, they have a surface to their boundary.
- At the boundary, atomic bonds terminate and hence the surface itself is an imperfection.
- One can reduce crystal defects considerably, but can never eliminate them entirely.



## CRYSTAL DEFECTS AND IMPERFECTIONS

- The study of imperfections has a two fold purpose, namely,
- A better understanding of crystals and how they affect the properties of metals.
  - Exploration of possibilities of minimizing or eliminating these defects.

The term “*defect*” or “*imperfection*” is generally used to describe any deviation from the perfect periodic array of atoms in the crystal.



## CRYSTAL DEFECTS AND IMPERFECTIONS

Crystal imperfections can be classified on the basis of their geometry as,

- Point Imperfections,
- Line imperfections
- Surface (or) plane imperfections and
- Volume imperfections



## POINT IMPERFECTIONS

- They are imperfect point- like regions, one or two atomic diameters in size and hence referred to as ‘zero dimensional imperfections’.
- There are different kinds of point imperfections.  
**VACANCIES**
- If an atom is missing from its normal site in the matrix, the defect is called a *vacancy defect*.
- It may be a single vacancy, divacancy or a trivacancy.



## POINT DEFECT-VACANCY



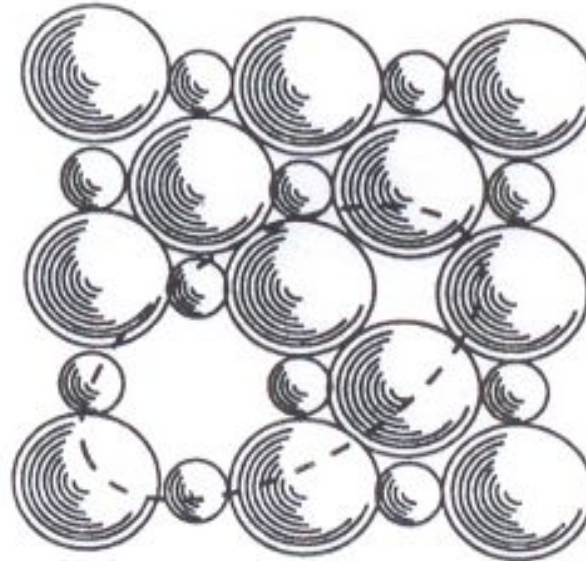


## POINT IMPERFECTIONS

- In metals vacancies are created by thermal excitation.
- When the temperature is sufficiently high, as the atoms vibrate around their regular positions, some acquire enough energy to leave the site completely.
- When the regular atom leaves, a vacancy is created.
- A pair of one cation and one anion can be missed from an ionic crystal. Such a pair of vacant ion sites is called *Schottky imperfection*.
- This type of defect is dominant in alkali halides.



## SCHOTTKY IMPERFECTIONS







## SUBSTITUTIONAL IMPURITY

- It refers to a foreign atom that substitutes for or replaces a parent atom in the crystal.
- Pentavalent or trivalent impurity atoms doped in Silicon or Germanium are also substitutional impurities in the crystal.



# SUBSTITUTIONAL IMPURITY





## INTERSTITIAL IMPURITY

- An interstitial defect arises when an atom occupies a definite position in the lattice that is not normally occupied in the perfect crystal.
- In crystals, packing density is always **less than 1**.
- If a small sized atom occupies the void space in the parent crystal without disturbing the parent atoms from their regular sites, then it is called as '***interstitial impurity***'.



## INTERSTITIAL IMPURITY



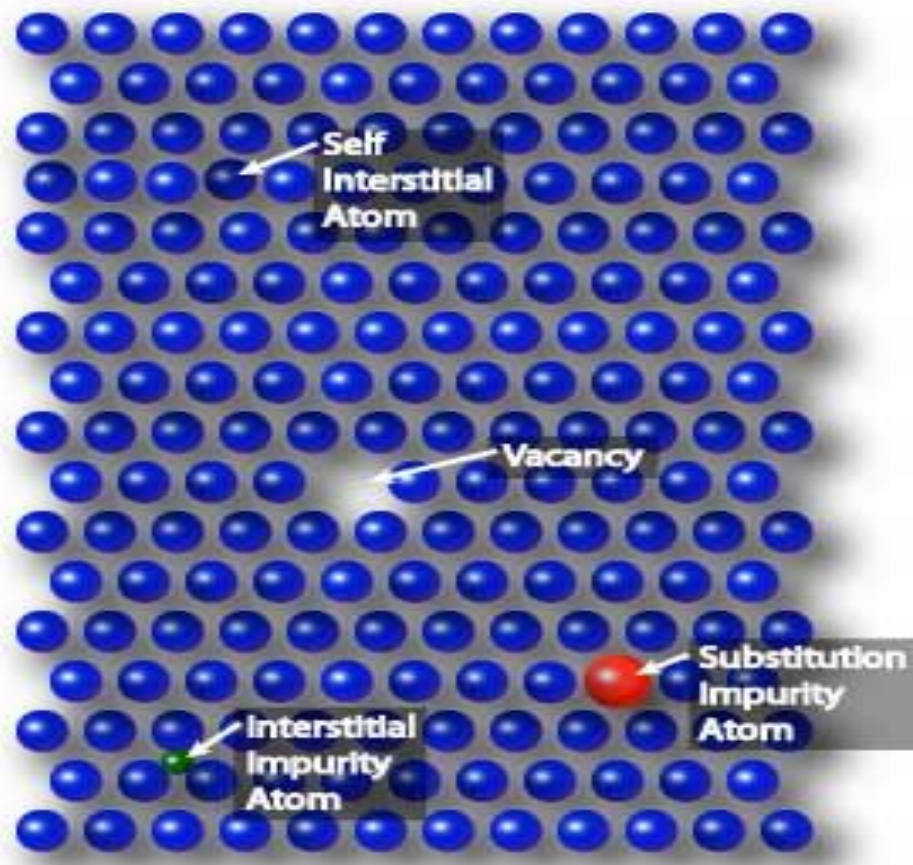


## INTERSTITIAL IMPURITY

- In ionic crystals, an ion displaced from a regular site to an interstitial site is called '*Frenkel imperfection*'.
- As cations are generally the smaller ones, it is possible for them to get displaced into the void space.
- Anions do not get displaced as the void space is too small compared to the size of the anions.
- A Frenkel imperfection does not change the overall electrical neutrality of the crystal. This type of defect occurs in silver halides and  $\text{CaF}_2$ .



# DIAGRAM SHOWING THE IMPERFECTIONS





## ELECTRONIC DEFECTS

- Errors in charge distribution in solids are called ‘*electronic defects*’.
- These defects are produced when the composition of an ionic crystal does not correspond to the exact stoichiometric formula.
- These defects are free to move in the crystal under the influence of an electric field.



## EFFECT OF POINT IMPERFECTIONS

- The presence of a point imperfection introduces distortions in the crystal.
- In the case of impurity atom, because of its difference in size, 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 the creation of such a point defect is called the '*enthalpy of formation*' of the point imperfection.





## LINE IMPERFECTIONS

- The defects, which take place due to dislocation or distortion of atoms along a line, in some direction are called as '*line defects*'.
- Line defects are also called dislocations. In the geometric sense, they may be called as 'one dimensional defects'.
- A dislocation may be defined as a disturbed region between two substantially perfect parts of a crystal.
- It is responsible for the phenomenon of slip by which most metals deform plastically.



## LINE IMPERFECTIONS

The two types of dislocations are,

- Edge dislocation
- Screw dislocation



## EDGE DISLOCATION

- In perfect crystal, atoms are arranged in both vertical and horizontal planes parallel to the side faces.
- If one of these vertical planes does not extend to the full length, but ends in between within the crystal it is called '*edge dislocation*'.
- In the perfect crystal, just above the edge of the incomplete plane the atoms are squeezed and are in a state of compression.
- Just below the edge of the incomplete plane, the atoms are pulled apart and are in a state of tension.

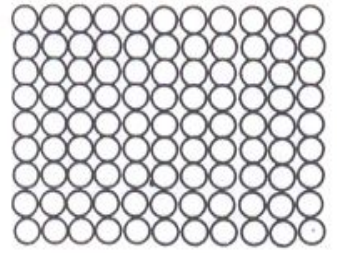
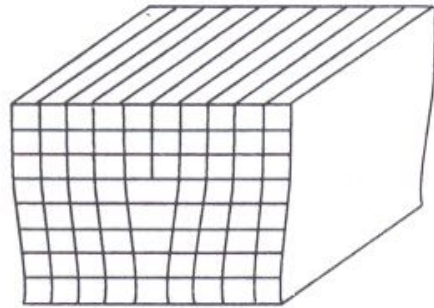
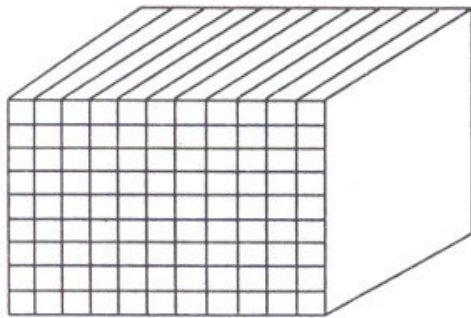


## EDGE DISLOCATION

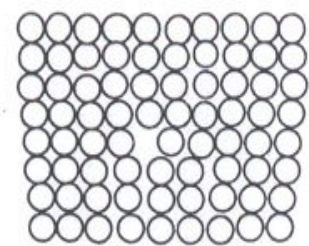
- The distorted configuration extends all along the edge into the crystal.
- Thus as the region of maximum distortion is centered around the edge of the incomplete plane, this distortion represents a line imperfection and is called an edge dislocation.
- Edge dislocations are represented by ‘ $\perp$ ’ or ‘T’ depending on whether the incomplete plane starts from the top or from the bottom of the crystal.
- These two configurations are referred to as positive and negative edge dislocations respectively.



# EDGE DISLOCATION



(a)



(b)



## BURGERS VECTOR

- The magnitude and the direction of the displacement are defined by a vector, called the *Burgers Vector*.
- In figure (a), starting from the point P, we go up by 6 steps, then move towards right by 5 steps, move down by 6 steps and finally move towards left by 5 steps to reach the starting point P. Now the Burgers circuit gets closed.
- When the same operation is performed on the defect crystal (figure (b)) we end up at Q instead of the starting point.

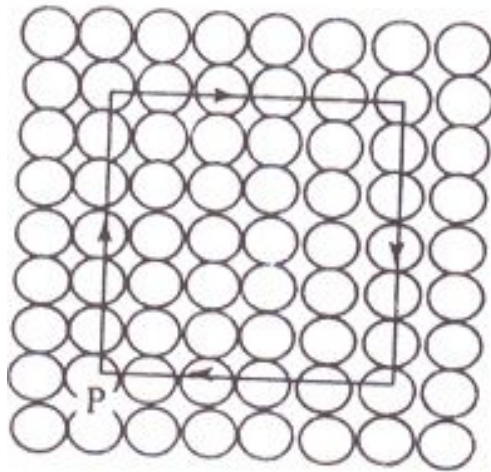


## BURGERS VECTOR

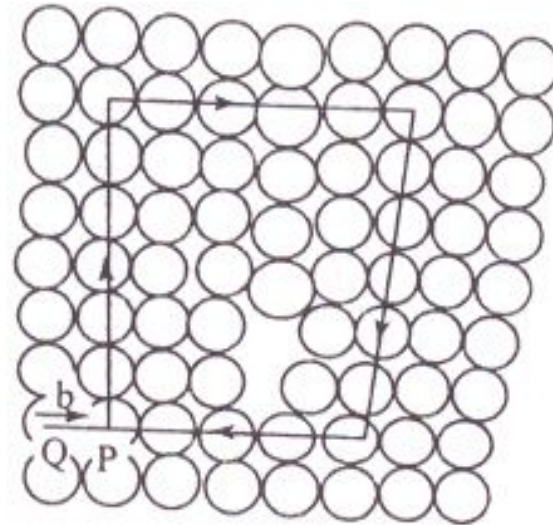
- So, we have to move an extra step to return to P, in order to close the Burgers circuit.
- The magnitude and the direction of the step defines the Burgers Vector (BV).
- $BV = \overline{QP} = b$
- The Burgers Vector is perpendicular to the edge dislocation line.



## BURGERS VECTOR



(a)



(b)



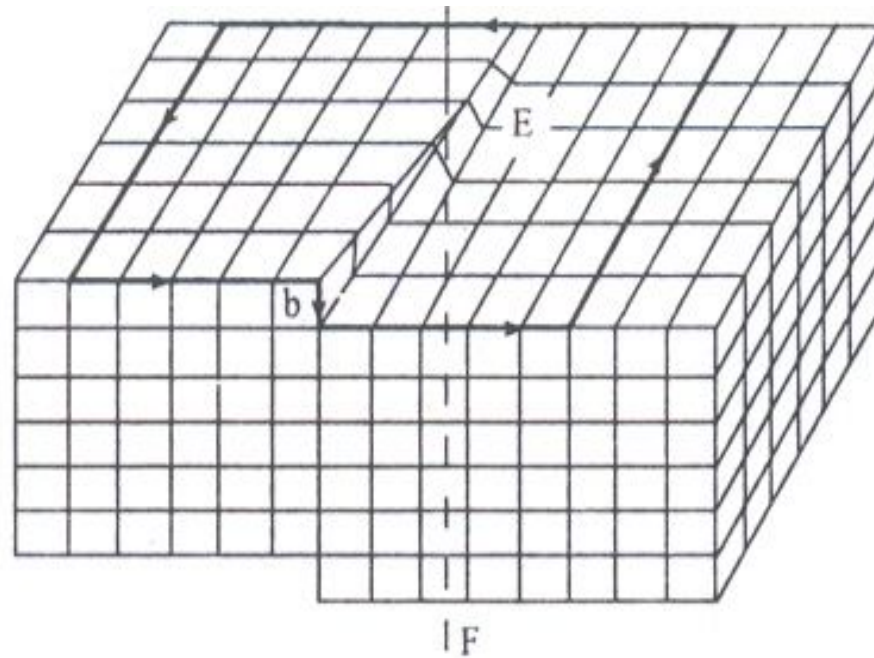


## SCREW DISLOCATION

- In this dislocation, the atoms are displaced in two separate planes perpendicular to each other.
- It forms a spiral ramp around the dislocation.
- The Burgers Vector is parallel to the screw dislocation line.
- Speed of movement of a screw dislocation is lesser compared to edge dislocation. Normally, the real dislocations in the crystals are the mixtures of edge and screw dislocation.



## SCREW DISLOCATION





## SURFACE IMPERFECTIONS

- Surface imperfections arise from a change in the stacking of atomic planes on or across a boundary.
- The change may be one of the orientations or of the stacking sequence of atomic planes.
- In geometric concept, surface imperfections are two-dimensional. They are of two types external and internal surface imperfections.

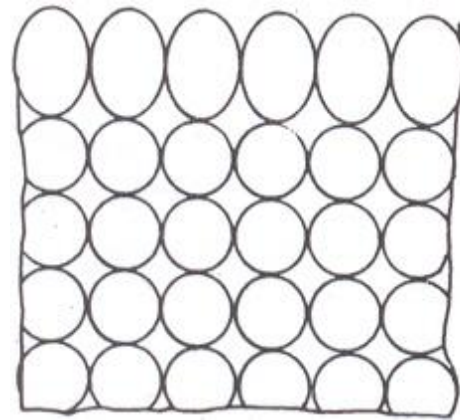


## EXTERNAL SURFACE IMPERFECTIONS

- They are the imperfections represented by a boundary. At the boundary the atomic bonds are terminated.
- The atoms on the surface cannot be compared with the atoms within the crystal. The reason is that the surface atoms have neighbours on one side only. Whereas the atoms inside the crystal have neighbours on either sides. This is shown in figure 4.38. Since these surface atoms are not surrounded by others, they possess higher energy than that of internal atoms.
- For most metals, the energy of the surface atoms is of the order of  $1\text{J/m}^2$ .



## EXTERNAL SURFACE IMPERFECTIONS





## INTERNAL SURFACE IMPERFECTIONS

- Internal surface imperfections are the imperfections which occurred inside a crystal.
- It is caused by the defects such as, grain boundaries, tilt boundaries, twin boundaries and stacking faults.



## GRAIN BOUNDARIES

- They are the imperfections which separate crystals or grains of different orientation in a poly crystalline solid during nucleation or crystallization.
- It is a two dimensional imperfection. During crystallization, new crystals form in different parts and they are randomly oriented with respect to one another.
- They grow and impinge on each other.
- The atoms held in between are attracted by crystals on either side and depending on the forces, the atoms occupy equilibrium positions.



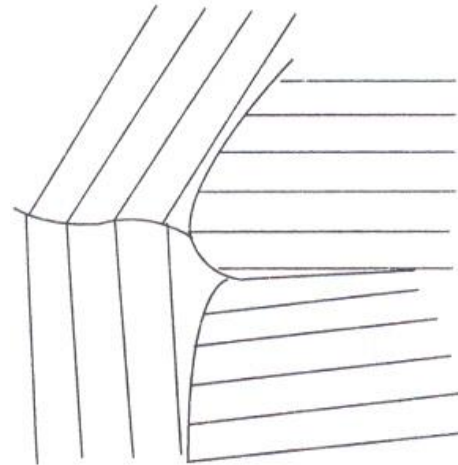
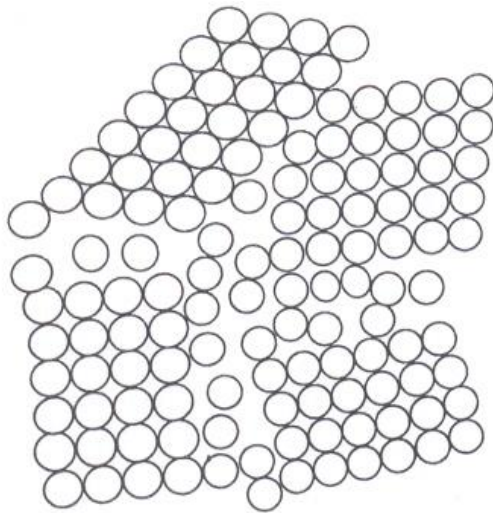
## GRAIN BOUNDARIES

- These positions at the boundary region between two crystals are distorted. As a result, a region of transition exists in which the atomic packing is imperfect.
- The thickness of this region is 2 to 10 or more atomic diameters.
- The boundary region is called a *crystal boundary* or a *grain boundary*.
- The boundary between two crystals which have different crystalline arrangements or different compositions, is called as interphase boundary or commonly an interface.





# GRAIN BOUNDARIES





## TILT BOUNDARIES

- This is called low-angle boundary as the orientation difference between two neighbouring crystals is less than  $10^\circ$ .
- The disruption in the boundary is not so severe as in the high-angle boundary. In general low-angle boundaries can be described by suitable arrays of dislocation.
- Actually a low-angle *tilt boundary* is composed of edge dislocation lying one above the other

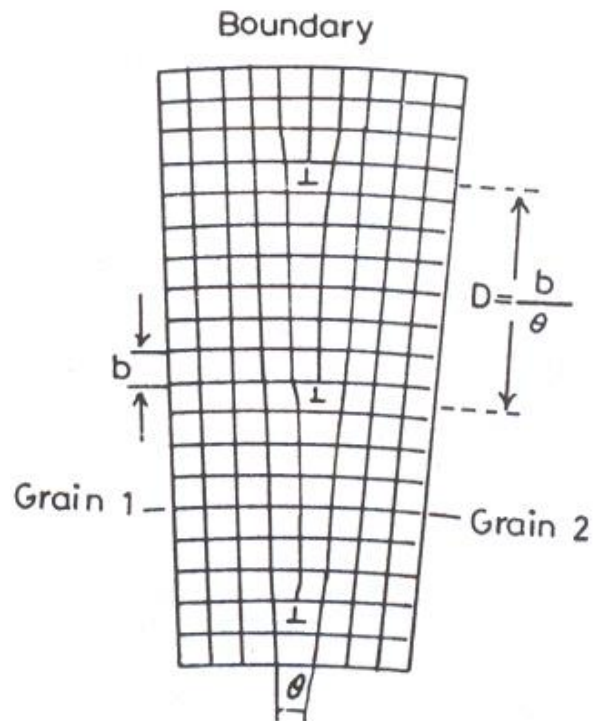
The angle or tilt will be 
$$\theta = \frac{b}{D}$$

where  $b$  = Burgers vector and

$D$  = the average vertical distance between dislocations.



# TILT BOUNDARIES



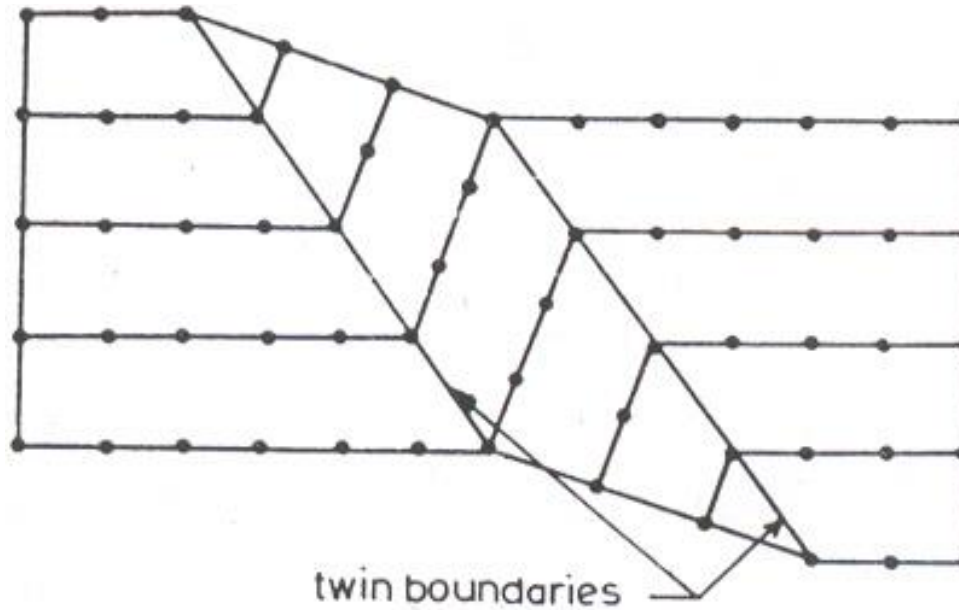


## TWIN BOUNDARIES

- If the atomic arrangement on one side of a boundary is a mirror reflection of the arrangement on the other side, then it is called as *twin boundary*.
- As they occur in pair, they are called twin boundaries. At one boundary, orientation of atomic arrangement changes.
- At another boundary, it is restored back. The region between the pair of boundaries is called the twinned region.
- These boundaries are easily identified under an optical microscope.



# TWIN BOUNDARIES



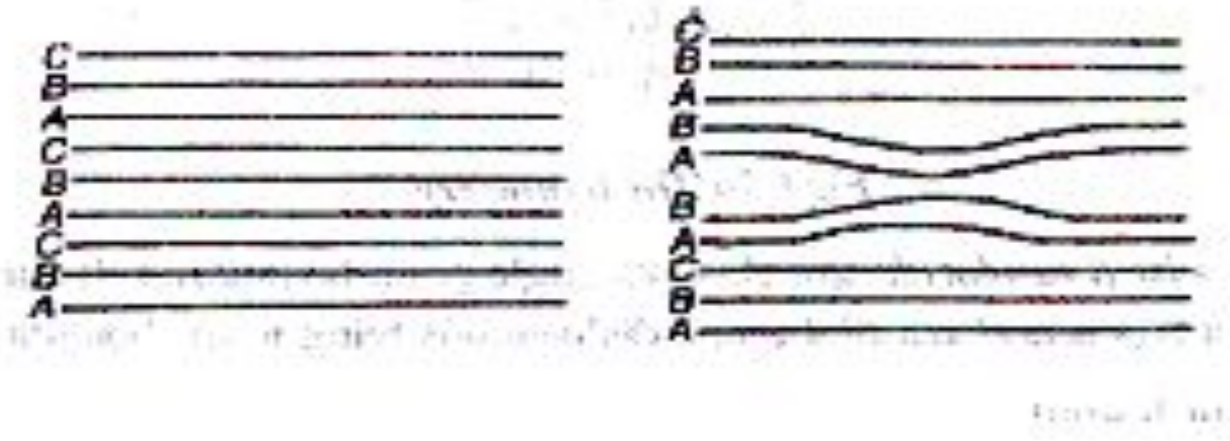


## STACKING FAULTS

- Whenever the stacking of atomic planes is not in a proper sequence throughout the crystal, the fault caused is known as *stacking fault*.
- For example, the stacking sequence in an ideal FCC crystal may be described as A-B-C-A-B-C- A-B-C-..... But the stacking fault may change the sequence to 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 region and it becomes HCP.
- This thin region is a surface imperfection and is called a stacking fault.



# STACKING FAULTS





## VOLUME IMPERFECTIONS

- Volume defects such as cracks may arise in crystals when there is only small electrostatic dissimilarity between the stacking sequences of close packed planes in metals. Presence of a large vacancy or void space, when cluster of atoms are missed is also considered as a volume imperfection.
- Foreign particle inclusions and non crystalline regions which have the dimensions of the order of 0.20 nm are also called as volume imperfections.





Physics is hopefully simple but Physicists are not