DEFECTS IN CRYSTALS

- **Introduction to Defects in Crystals:**
- An ideal crystal has a perfectly regular and continuous atomic arrangement.
- In a real crystal, this regular arrangement is disturbed at certain points, lines, or regions due to various reasons.
- **Definition:** A crystal defect is any deviation from the perfect, periodic arrangement of atoms in a crystal lattice. It is also known as imperfections.
- All crystals contain some form of defects; a perfectly flawless crystal does not exist.
- **Effects of Defects:**
- Defects significantly affect the properties of materials such as mechanical strength, ductility, crystal growth, magnetic hysteresis, and dielectric strength.
- Properties like stiffness and density are generally not affected by these defects.
- **Classification of Defects:**
- Crystal defects are categorized by their dimensions as

  1.Point defects (0-D)

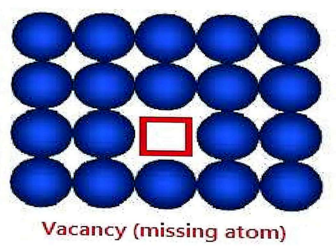
  2.Line defects (1-D)

  3.Surface defects (2-D)

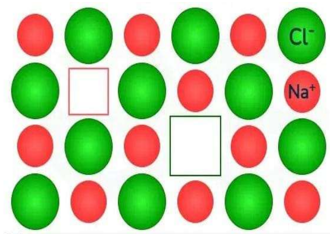
  4.Volume defects (3-D)

1.Point Defects

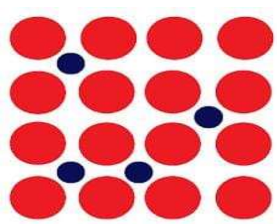
- **A point defect in a crystal occurs when an atom is missing or an impure atom or a matrix atom is in an irregular position within the lattice structure.**
- These are 0-D defects and are found in metallic and ionic crystals.
- They cause strain in a small volume of the crystal but don't affect distant parts of the crystal.
- **Types of Point Defects:**
- Point defects are categorized into 3 main types:
- **i.Vacancy Defect:**
- The simplest type of point defect where an atom is missing from a lattice site.
- This is often caused by imperfect packing during crystal formation or by thermal vibrations of atoms at high temperatures.



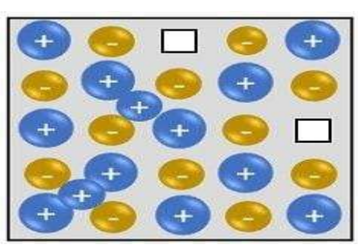
- **<u>A Schottky defect</u>** is a specific type of vacancy defect found in ionic crystals.
- It involves a **pair of vacancies one cation and one anion** to maintain charge neutrality.



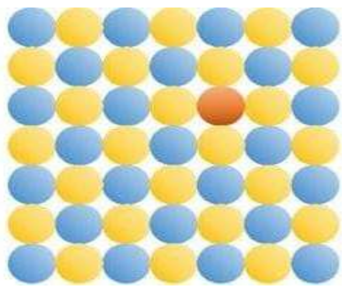
- **<u>Examples</u>** include **NaCl** and **CsCl**.
- **<u>ii.Interstitial Defect:</u>**
- An impurity atom occupies an interstitial space between the parent atoms without displacing them.
- The impurity atoms are typically much smaller than the host atoms.
- **An example** is carbon atoms in iron to make steel.
- It can be a self-interstitial (an atom from the same crystal) or a foreign interstitial (an impurity atom).



- **<u>A Frenkel defect</u>** is a special type of vacancy and interstitial defect in ionic crystals, where an ion moves from its regular lattice site to an interstitial site, leaving behind a vacancy.



- This defect maintains charge neutrality. **Examples** include AgBr and AgCl.
- **NOTE:** There are two types of point defects related to vacancies in ionic crystals: Schottky defect and Frenkel defect.
- **iii.Substitutional defect:**
- These defects arise when an impure(foreign) atom occupies the position of a parent(host) atom in its regular lattice site.
- The impurity atom is typically of a similar size to the parent atom and is common when the impurity atom is substantially smaller than the parent atoms.

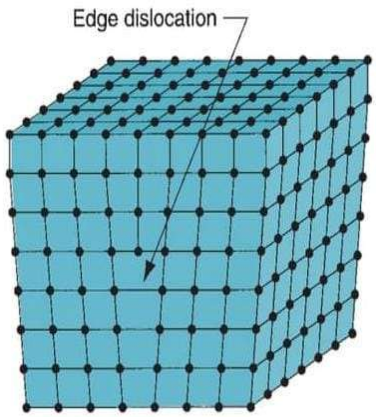


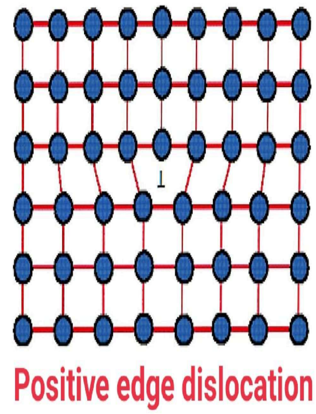
Examples: 1. zinc atoms in a copper crystal to form brass.

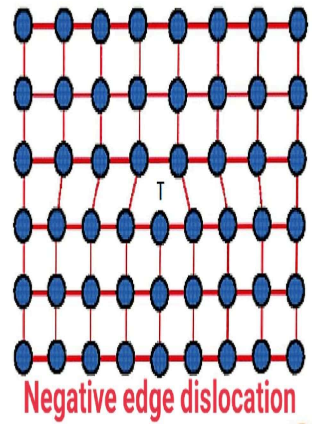
2.In FCC 0.225 nm of carbon atoms occupy a space in the 0.225 nm of iron.

2. Line Defects

- **A line defect in a crystal occurs when a portion of a line of atoms is missing or displaced from its regular site.**
- These are 1-D defects and also called linear defects or dislocations.
- They are generated in crystals due to Growth accidents,Thermal stresses, Phase transformations, etc.
- These defects are observed in crystalline materials using an electron microscope.
- **Types of Line Defects:**
- Line defects are categorized into 3 main types:
- **(i) Edge Dislocation:**
- Edge dislocation occurs when an extra atomic plane is inserted partially and does not extend through the crystal.
- The atoms above this incomplete plane are compressed, while those below are in a state of tension.
- **Types of edge dislocation**: Positive edge dislocation & Negative edge dislocation.



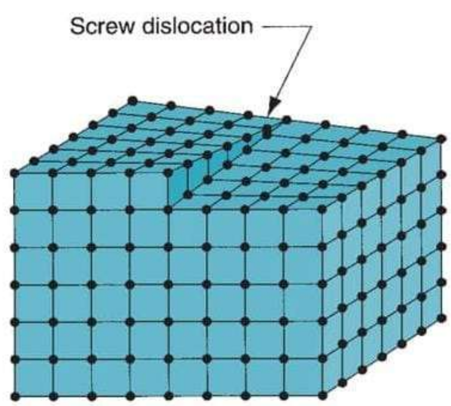




- ❖ Based on whether the incomplete plane starts from the top or bottom of the crystal.
- ❖ **Positive edge dislocation** is an incomplete plane that starts from the top of the crystal and represented by ⊥.
- ❖ **Negative edge dislocation** is an incomplete plane that starts from the bottom of the crystal and is represented by T.
- ❖ Edge dislocation lines are defined by a Burgers vector that is **perpendicular** to the dislocation line(axis).

❖ ii.Screw Dislocations:

- ❖ Screw dislocations arise due to the displacement of atoms in one part of a crystal relative to another, forming a spiral ramp around the dislocation line.
- ❖ Screw dislocations are also known as Burgers dislocations.

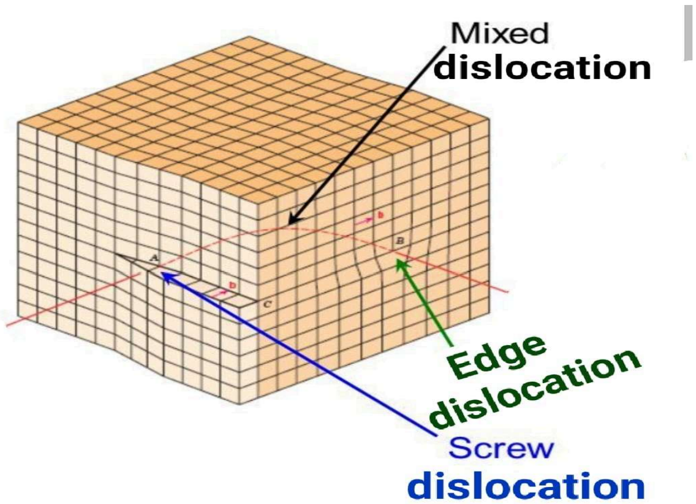


- ❖ Screw dislocation lines are defined by a Burgers vector that is **parallel** to the dislocation line(axis).

❖ iii.Mixed Dislocations:

- ❖ Most dislocations found in crystals are neither pure edge nor pure screw dislocations.

❖ Instead, they are mixed dislocations, which contain components of both edge and screw type dislocations.



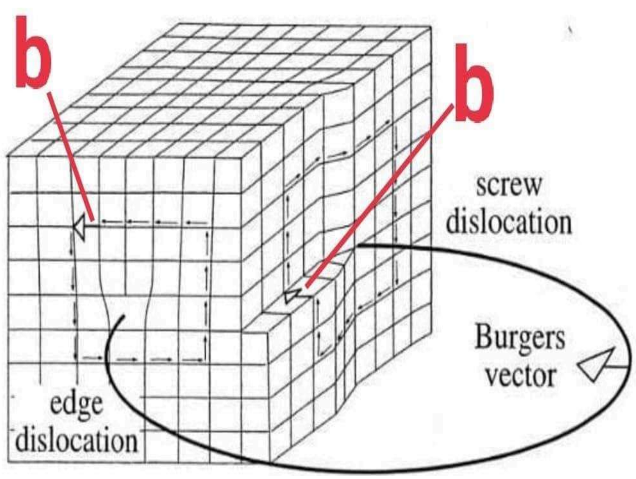
❖ Mixed dislocation lines are defined by a Burgers vector that has an arbitrary angle with a dislocation line(axis).

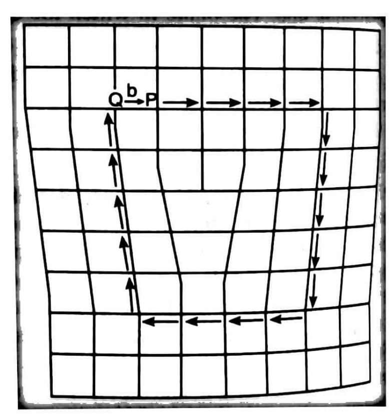
❖ **<u>Burgers Vector(b) :</u>**

❖ The Burgers vector is a vector that quantifies the magnitude and direction of the lattice distortion caused by a dislocation.

❖ The magnitude of the Burgers vector is found by drawing a closed circuit around the dislocation line, known as the **Burgers circuit.**

❖ When we draw a burger circuit around the dislocation, the circuit does not close and requires an extra step to return to the starting point. The vector of this extra step is the Burgers vector (which means, the vector that links the start and end points(P&Q) of the circuit in the perfect crystal is the Burgers vector) i.e., QP = b .





❖ For an **edge dislocation**, the Burgers vector is perpendicular to the dislocation line.
❖ For a **screw dislocation**, the Burgers vector is parallel to the dislocation line.
❖ For a **Mixed dislocation**, the Burgers vector has an arbitrary angle with a dislocation line.

3.Surface Defects

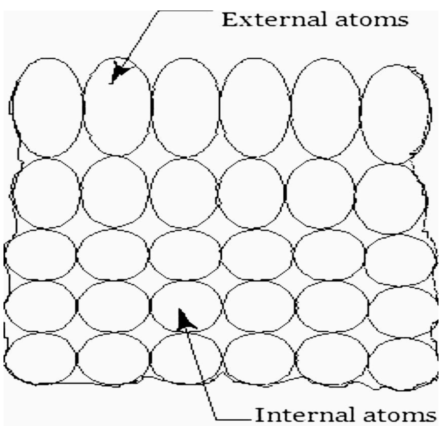
❖ **Surface defects in a crystal occur when regions of distortion lie on a surface with a thickness of a few atomic diameters.**
❖ These are 2-D and separate two regions of the crystal and are considered metastable.
❖ Many of these defects can disappear when the crystal is heated close to its melting point.

❖ Types of Surface Defects:

❖ Surface defects are categorized into 2 main types:

❖ i.External surface defects:

❖ Surface atoms are not fully surrounded and they possess higher energy than internal atoms.

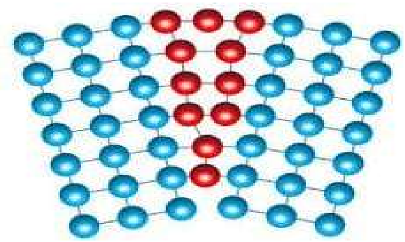


❖ This gives rise to surface energy ≈ 1.5 J/m² for most materials.

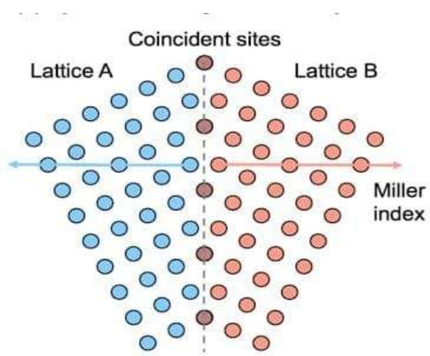
❖ ii.Internal surface defects:

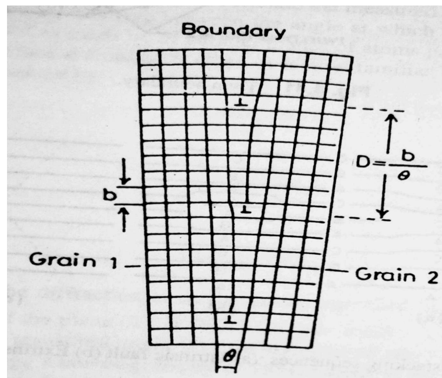
❖ An internal surface defect in a crystal occurs when the region within the bulk of a material where the regular lattice structure is disrupted.
❖ It is manifested as Grain boundaries , Tilt boundaries, Twist boundaries, Twin boundaries & Stacking faults.
❖ **The grain Boundaries** occur when grains of different orientations meet and separate the general pattern of atoms.

❖ The boundary formed during the growth of grains and influenced by surrounding grains.



❖ **The tilt Boundaries** by an array of parallel edge dislocations of the same sign, arranged in series.



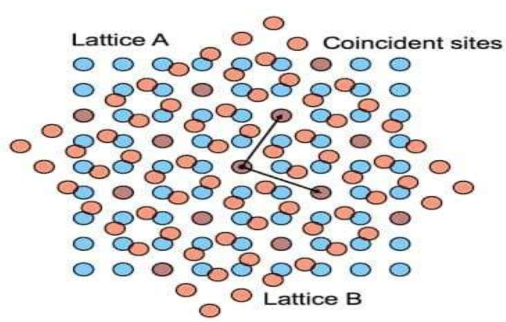


❖ Usually a low-angle boundary (<10°).

❖ **Angle of tilt: $\theta = b/D$** or **$D = b/\theta$**

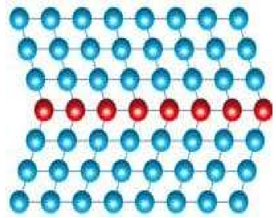
where b = Burgers vector length & D = dislocation spacing.

❖ **The twist boundary** consists of at least **two sets of parallel screw dislocations** lying in the boundary.

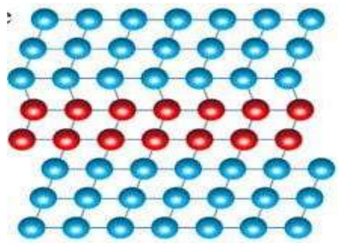


❖ Rotations occur about an axis normal to the boundary.

❖ **Twin boundaries are a boundary** where the crystal structure on one side is a mirror image of the structure on the other side.



❖ **Stacking defect** is caused by incorrect stacking sequence of atomic planes.

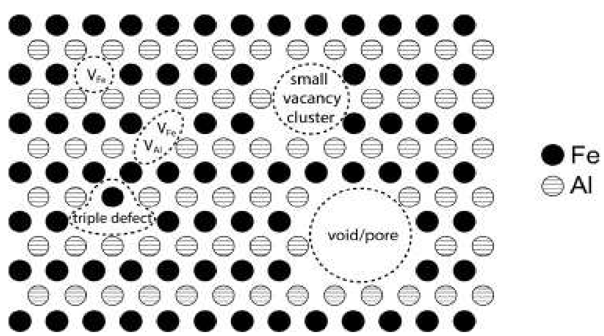


❖ **Example** in FCC crystal,Ideal sequence is ABC ABC ABC where as faulted sequence is ABC ABAB ABC

❖ The region with fault may form a thin hexagonal close-packed (HCP) region inside the FCC crystal.

4.Volume Defects

❖ **Volume defects in a crystal occurs due to irregularities within the crystal lattice, such as voids, cracks, inclusions of foreign particles, and precipitates of different phases**



❖ Volume defects also known as bulk defects, which occur within the crystal lattice in 3-D and have dimensions of the order of 0.20 nm.

❖ **Voids/Pores are** empty spaces or cavities within the crystal lattice where atoms should be.

❖ **Cracks** are fractures that extend through the crystal, forming a significant void.

❖ **Inclusions** are foreign atoms of a different substance embedded within the crystal.

❖ **Precipitates** are small particles of a different phase that form within the main crystal lattice.