Faculty of Engineering and Technology

University of Lucknow

Lecture Notes

Subject Code: EE–503

Electrical and Electronics Engineering Materials

Topic Name

(Crystal imperfection part 1)

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Crystal Defects

INTRODUCTION

- Crystals will have a regular periodic arrangement of atoms.
- Any deviation from this periodicity is known as defects or imperfections in crystals.
- ***Definition:*** ***The deviation from the perfect periodicity of atomic arrays in crystals is known as crystal defects.***

- The crystal defects affect their properties such as mechanical strength, ductility, crystal growth, dielectric strength, magnetic hysteresis, conductivity, etc.
- A perfect crystal, with every atom of the same type in correct position, does not exist.
- Thus, all crystals have some defects. The defects in crystals may be confined to a point, line, surface and volume.

The basic classes of crystal defects are:

1. **Point defects**
   (Zero-dimensional defects)

2. **Line defects**
   (One-dimensional defects)

3. **Surface defects**
   (Two-dimensional defects)

4. **Volume defects**
   (Three-dimensional defects)

1. Point Defects

- The point defects are zero-dimensional defects
- When an atom is missing or an atom is in an irregular place in the lattice structure, the corresponding defects are known as point defects.
- A point defect produces strain in a small volume of the crystal surrounding the crystal, but does not affect the perfections distant parts of the crystal.

- In general, point defects occur in metallic and ionic crystals.

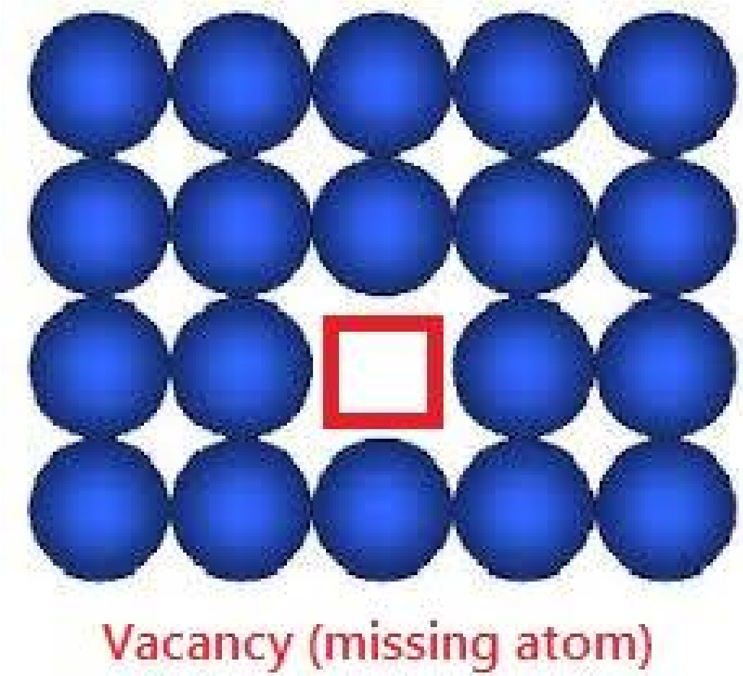
Point defects are of following types:

(1) Vacancies
(2) Interstitial defects
(3) Substitutional defects
(4) Frenkel's defect
(5) Schottky's defect

1.1. Vacancies

- Vacancies are simplest point defects in a crystal which refers to a missing atom at its site.
- **Definition:** *The defects due to the missing atoms at their lattice sites are called vacancies.*

A crystal lattice with vacancy defect is shown in figure.



- Vacancy defects are mainly due to the imperfect packing during the formation of crystal or due to thermal vibrations of atoms at high temperature.
- At high temperature atoms are frequently and regularly change their positions leaving empty lattice sites behind their positions.
- ***For most crystals, the thermal energy is of the order of 1 eV per vacancy.***

1.2. Interstitial defects

- **Definition:** ***When an impurity atom tries to settle in the interstitial space between the parent atoms of the crystal without displacing, then such a defect is known as interstitial defect.***
- Interstitial impurities are much smaller than the atoms in the bulk matrix.
- The formation of interstitial impurity defect is shown figure.

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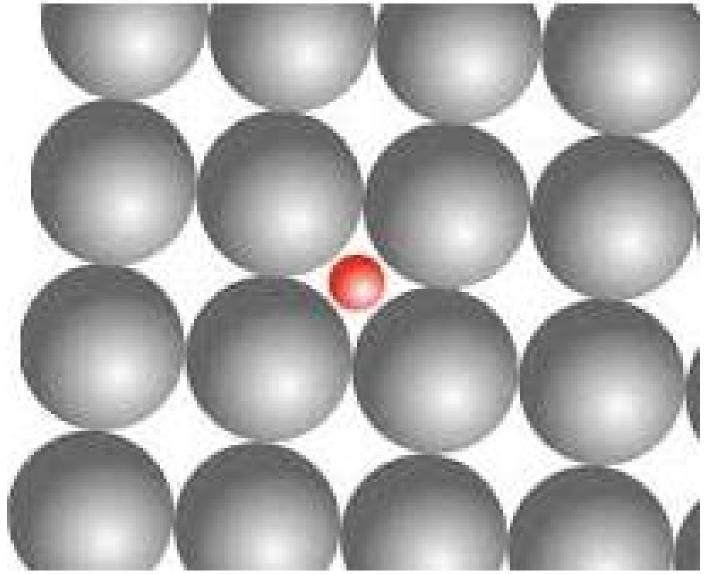


- **Example:**

Carbon atoms are interstitial impurity atoms that are added to Iron to make Steel. In steel, Carbon atoms with radius of 0.071 nm are well fitted in the interstitial spaces between the larger Iron atoms of radius 0.124 nm.

- The number of vacancies per unit volume of the crystal depends upon temperature.
- In most cases, diffusion (mass transport by atomic motion) can only occur because of vacancies.
- In case of ionic crystals, there are two types of point defects related to vacancies.
- **They are: (A) Schottky defects and**

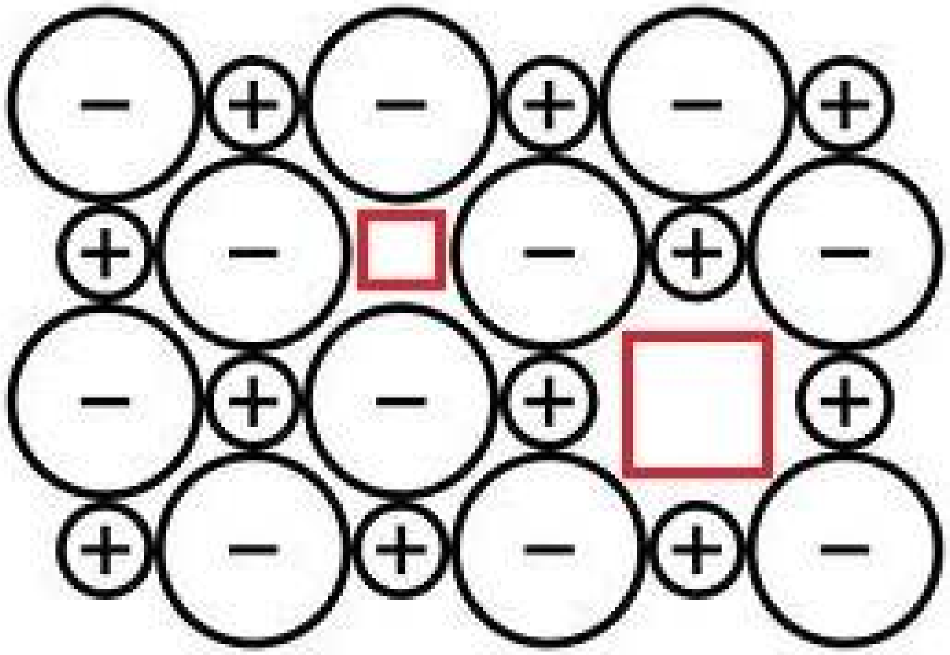
  (B) Frenkel defects

1.1.1. Schottky defects

- It is special case of vacancy defects in ionic crystals.
- **Definition:** *When a pair of vacancies is produced at one positive ion site and one negative ion site due to absence of positive and negative ions, then this type of defect is call the Schottky defect.*
- In ionic crystals, there are two types of possible vacancies, namely cation (+ve ion) vacancies and anion (–ve ion) vacancies.

- When a +ve ion from the interior of the lattice moves out of the crystal to its surface, then a +ve vacancy is formed at its site.
- The formation of +ve ion vacancy results in excess negative charge inside the crystal.
- To maintain charge neutrality, a –ve ion moves to the crystal surface creating a –ve ion vacancy at its site.

- NaCl, CsCl etc., exhibits Schottky defect
- The formation of vacancies is illustrated in the following figure.

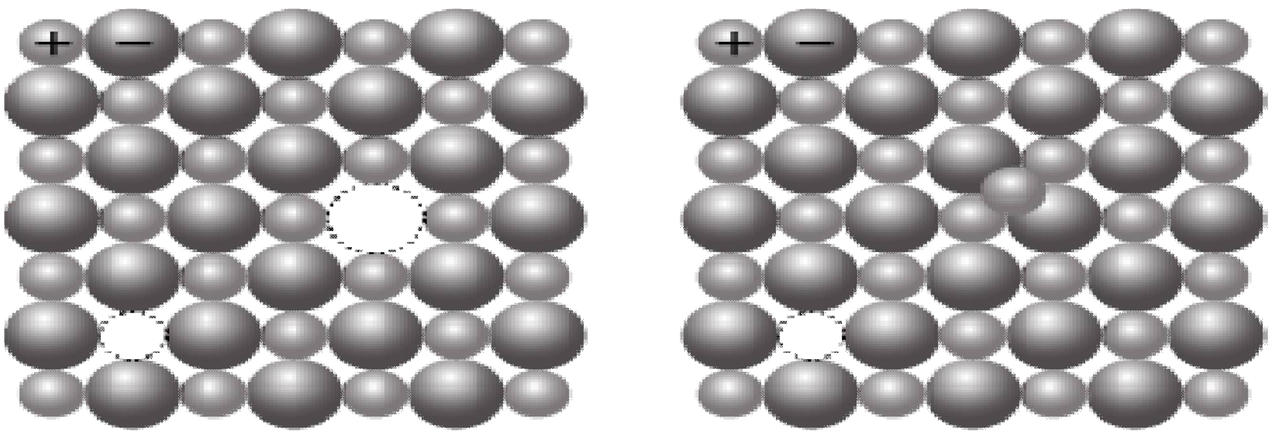


1.1.2. Frenkel defects

- It is special case of vacancy and interstitial defects in ionic crystals.
- **Definition:** *When an ion displaced from a regular location in the crystal lattice to an interstitial location in the crystal lattice , then this type of defect is called the Frenkel defect.*

- Consider the periodic distribution of +ve and –ve ions in an ionic crystal.
- When a +ve ion leave its site and settles in the interstitial position then it creates a vacancy in its position.
- Thus, a vacancy and interstitial defects are created. This pair of defects is known as Frankel defect.
- In case of Frankel defect also charge neutrality is maintained.

- AgBr, AgCl, ZnS etc., exhibits Frankel defects
- The formation of Frankel defects is described in the following figure.



(a) Schottky defect (b) Frenkel defect

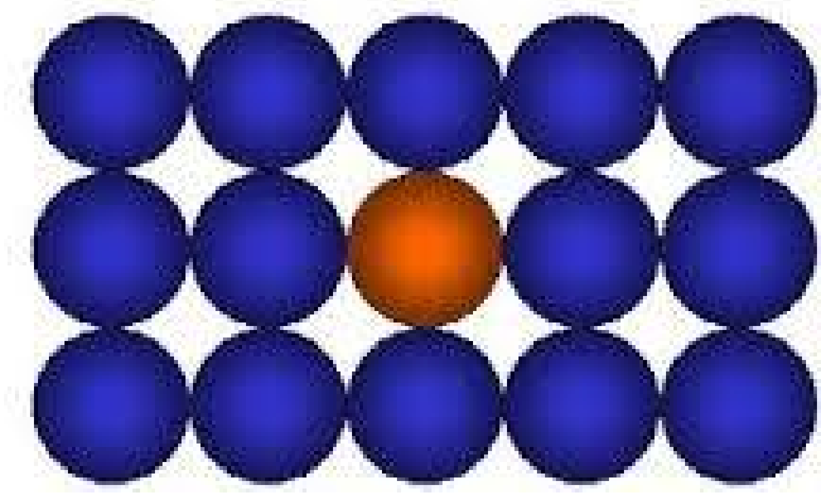
1.3. Substitutional defects

- **Definition:** *When an impurity atom occupies the one of the positions of the parent atoms of the crystal, then such a defect is known as substitutional defect.*

- A substitutional impurity atom is an atom of a different type than the bulk atoms.

- Usually, substitutional atoms are close in size (within approximately 15%) to the bulk atom.

- The formation of substitutional impurity defect is shown figure.



- **Example:** Zinc atoms are substitutional impurity atoms that are added to Copper to make Brass. In brass, Zinc atoms with radius of 0.133 nm have replaced some of the Copper sites of radius 0.128 nm.

2. Line Defects

- These are also called as linear defects or dislocations.
- These are one-dimensional defects
- **Definition**:

"Dislocations are areas where the atoms are out of position in the crystal structure"

(OR)

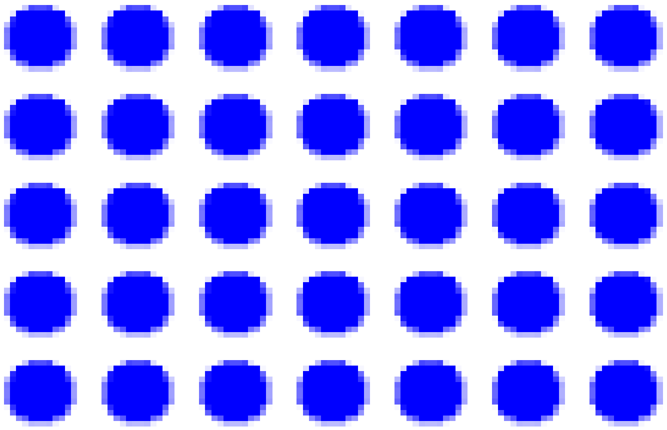
"A dislocation is a one-dimensional defect around which some of the atoms are misaligned".

- Thus, dislocations refer to a linear disturbance of the atomic arrangement in a crystal.
- Dislocations are generated in crystals due to growth accidents, thermal stress, phase transformation etc.
- They can be observed in crystalline materials with the help of electron microscope.

- They are two basic types of dislocations:
    - Edge dislocations and
    - Screw dislocations.
- **Most of the dislocations found in crystals are neither pure edge nor pure screw dislocations, but contain components of both these types. They are called mixed dislocations.**

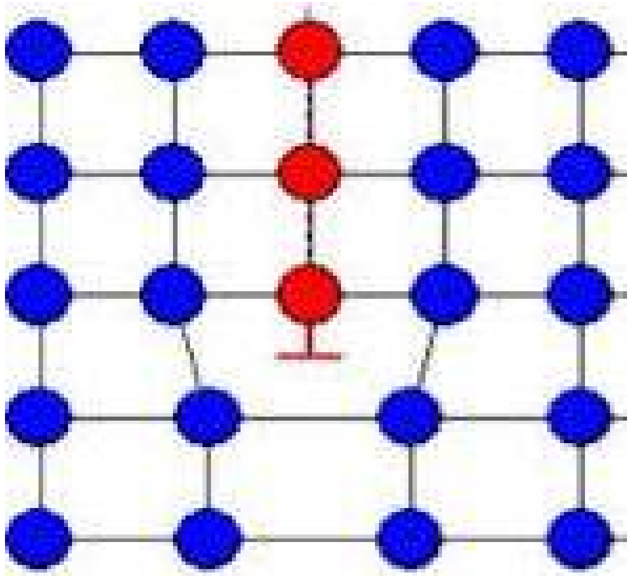
2.1. Edge dislocations

- If one of the vertical planes does not extended to the full length, but ends in between, within the crystal, then such a defect is known as edge dislocation.
- In perfect crystal, atoms are arranged in both vertical and horizontal planes as shown in Fig .



- From the figure it is clear that the atoms are in perfect equilibrium in their positions and all bond lengths are in equilibrium state.

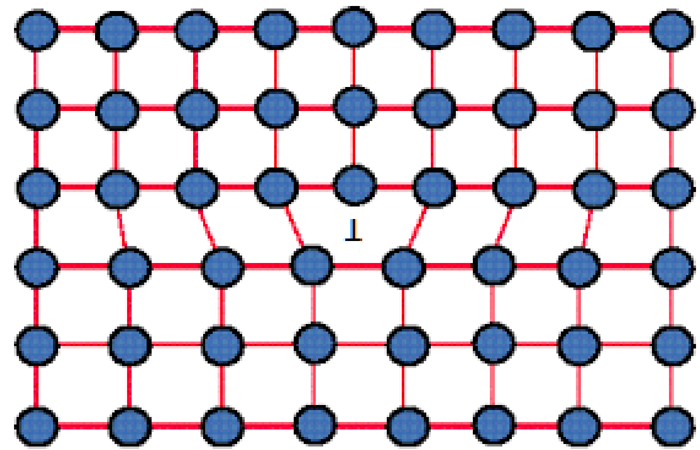
- If one of the vertical planes does not extend to the full length, but ends in between within the crystal as shown in Fig. it is called edge dislocation.



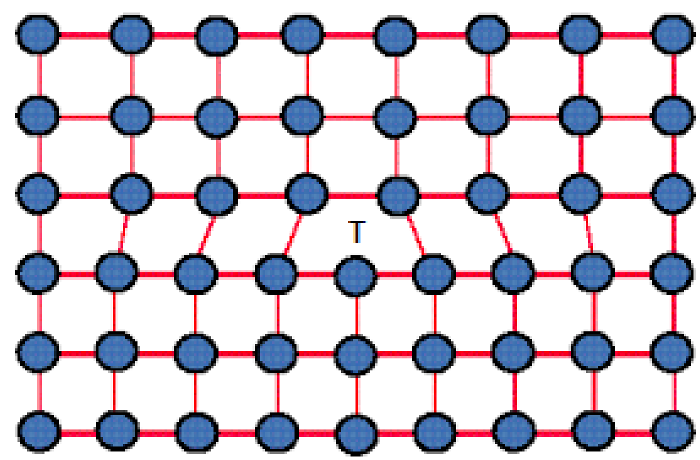
- Because of dislocation, (i) just above the discontinuity, the atoms are squeezed and are in state of compression and (ii) just below the discontinuity; the atoms are pulled apart and are in state of tension.

- The distorted configuration spreads all along the edge into the crystal.
- Thus, the 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 symbolically represented by $\perp$ or $\top$.

- When the incomplete plane starts from the top of the crystal, then it is called positive edge dislocation and is represented by "⊥" (see Fig. a)



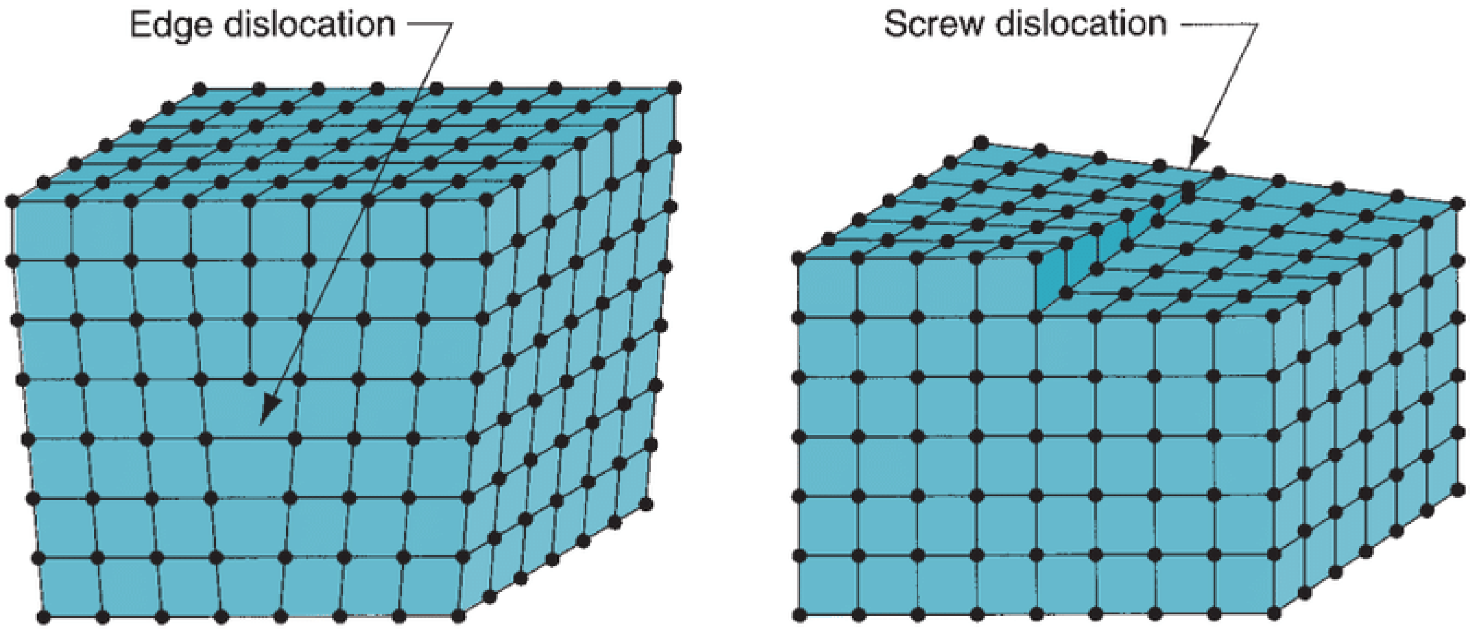
- When the incomplete plane starts from the bottom of the crystal, then it is called negative edge dislocation and is represented by "⊤" (see Fig. b).



2.2. Screw dislocations

- The screw dislocations are also known as Burger dislocations.
- These dislocations arise due to the displacement of atoms in one part of a crystal relative to the other part

  [forming a spiral ramp around the dislocation line].



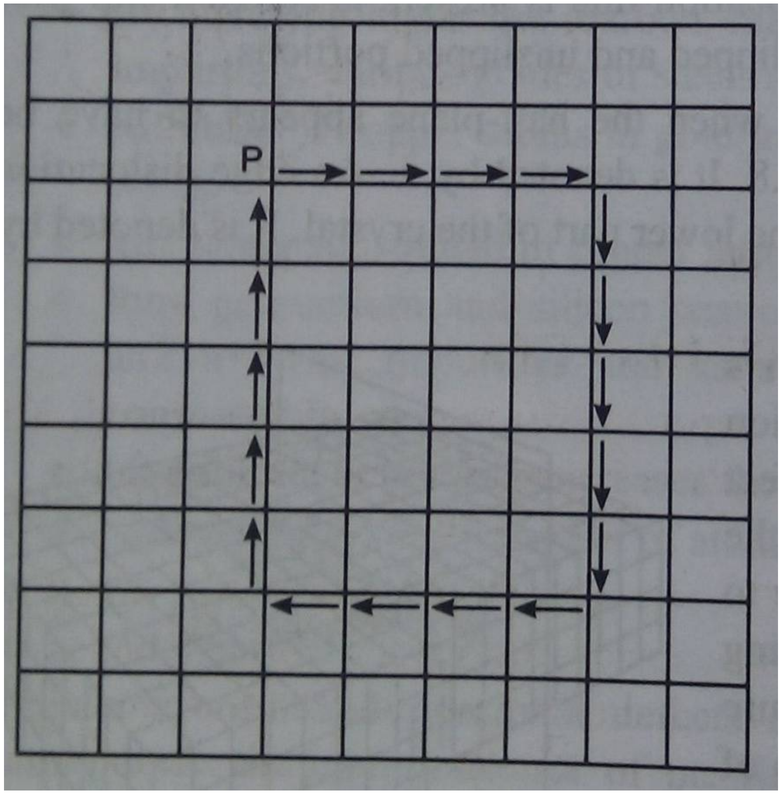
(a)

(b)

Burger Vector

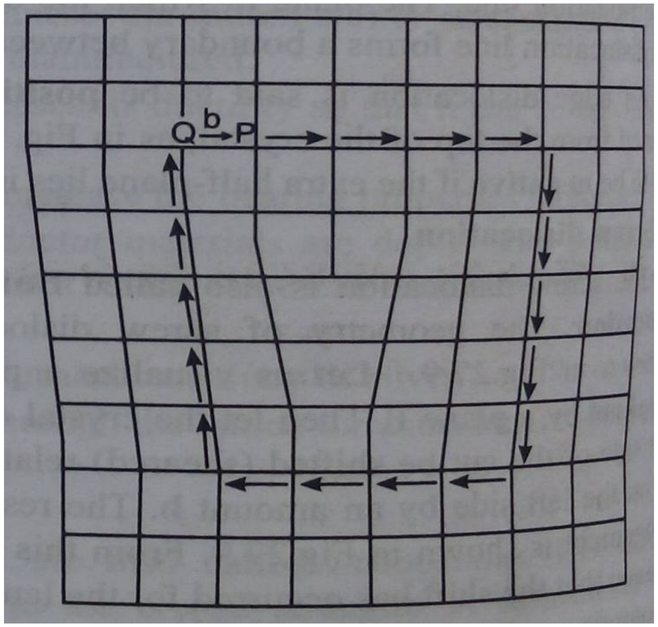
- The magnitude and direction of the lattice distortion associated with a dislocation is called **Burger vector**.
- Dislocations are quantitatively described by the Burger vector, and is donated by '**b**'
- **The magnitude of Burger vector is found by drawing a closed circuit around the dislocation line. This circuit is called Burger's circuit.**

- Consider a perfect crystal as shown in Fig.



- Consider the case of edge dislocated crystal shown in Fig.

- When the same operation is performed on the crystal, we end upto at point Q instead of the starting point P.



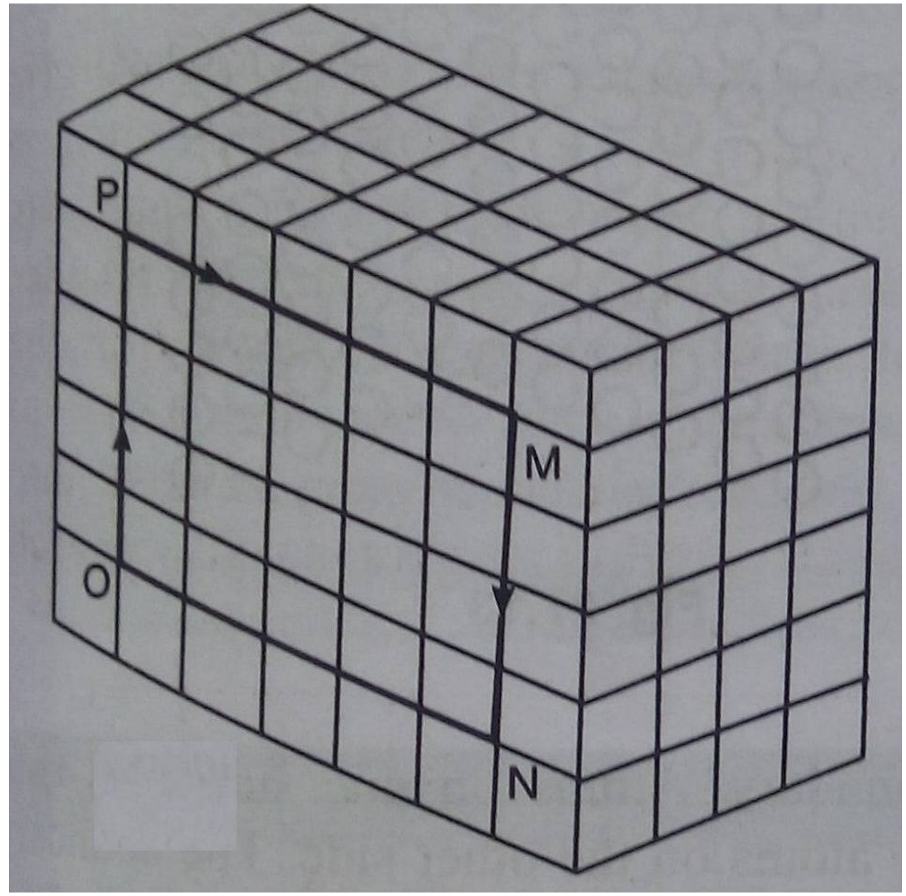
- Now, we have to move an extra step to return to point P in order to close the Burger circuit.

- The magnitude and direction of the step is called Burger Vector.

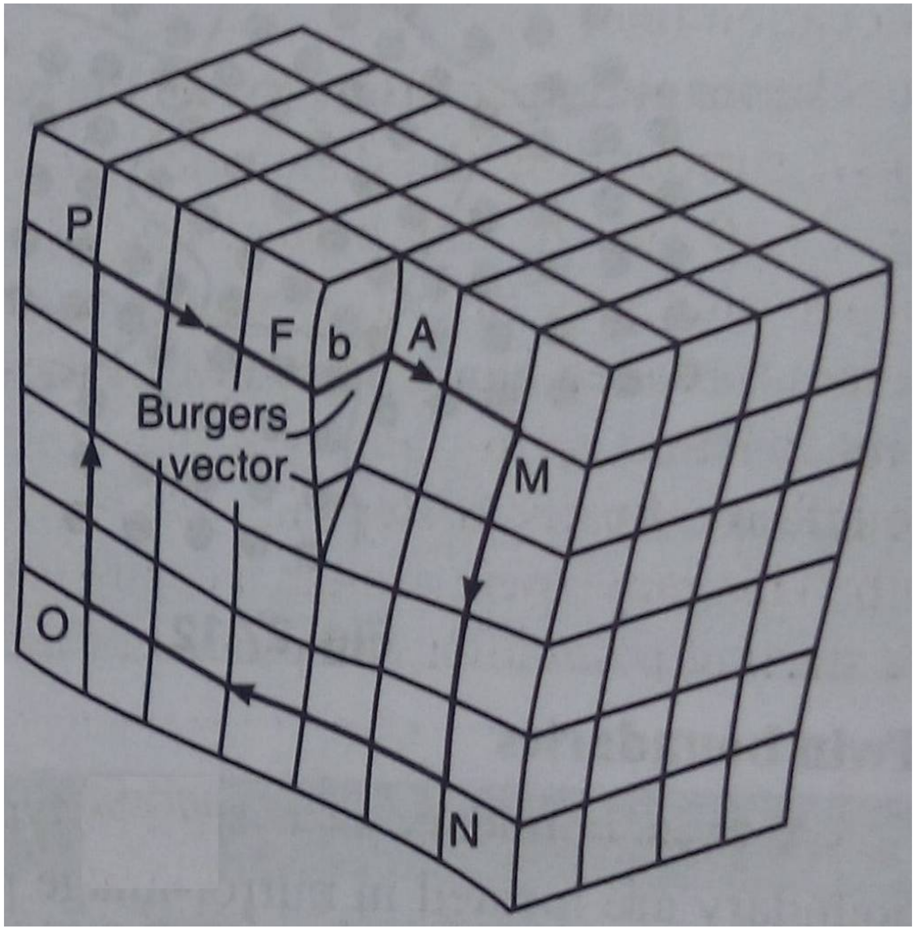
- Burger vector = $\vec{QP}$ = **b**

Note:
The Burger vector is perpendicular to the edge dislocation.

- Consider the Berger circuit in a crystal that contains screw dislocation.
- In the perfect crystal, starting from P, if we trace the Burger circuit, the circuit is closed path PMNOP as shown in Fig.



In case of a crystal with a screw dislocation shown in Fig. (b), the circuit would not be completed and requires an extra step **b = FA**, parallel to the dislocation axis to close the circuit. This additional vector **b** is called Burger vector.



Note:
The Burger vector is parallel to the screw dislocation.

3. Surface Defects

- These are two-dimensional defects
- The regions of distortions that lie about a surface having a thickness of few atomic diameters are known as surface defects.
- Surface defects are two-dimensional defects that separate two regions of the crystal.
- Surface imperfections are metastable imperfections.
- If the crystal is heated close to its melting point, many of the surface imperfections disappear.

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