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Imperfections in solids

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Abstract: solids have strong attraction forces hold their particles together in proper arrangement. Throughout solids microstructure, perfect arrangement of atoms does not exist. There are always imperfections which influence the material properties. Imperfections have different classifications according to geometry or dimensionality of the defect.

Keywords: imperfections, vacancy, dislocation, burgers vector.

Introduction:

Perfect solids do not exist; all solids contain large numbers of various defects or imperfections. This applies to both crystalline and amorphous solids.

Crystalline imperfections in solids**:**

Any deviation from the perfect order arrangement of atoms, ions or molecules in crystal is called crystalline imperfection or defect.

Crystalline defect is defined as a lattice irregularity having one or more of its dimensions on the order of an atomic diameter.[1]

Classification of crystalline imperfections: according to geometry or dimensionality of the defect.

- Point defect (0 dimensional)
- Linear defect (one-dimensional)
- Plane defect (two-dimensional)
- Volume defect (three-dimensional)[1]

Point defects: are the irregularities or deviations from ideal arrangement around a point or an atom in a crystal. Those are associated with one or two atomic positions. Point defects may be created or modified by external ionizing irradiation, either by photons or by high-energy particles.

Types of point defects:

1- **Vacancy**: which is the simplest form of the point defects; it is a vacant atomic site in the structure fig.1. In fact, it is not possible to create such a material that is free of these defects. It is possible to eliminate all point defects except vacancies, as they arise from thermodynamics (entropy).[1] As the temperature increases, the thermal vacancy concentration in pure metals dramatically increases, and makes an apparent contribution to different physical quantities of materials, such as heat capacity, melting point, diffusivity, thermal conductivity.[5]

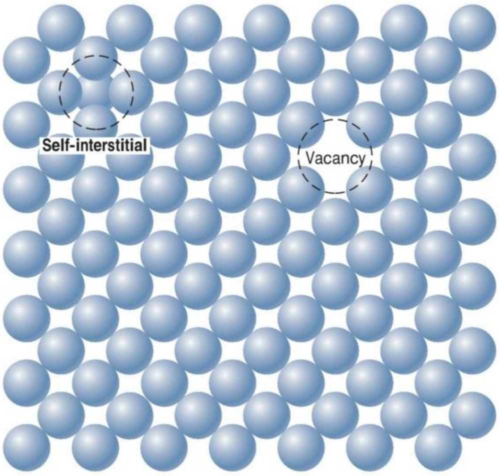

Fig.1 Two-dimensional representations of a vacancy and a self-interstitial.

The equilibrium number of vacancies (Nv) for a given quantity of material depends on the increase in temperature according to the following equation:

$$Nv= N \exp(- Qv/KT)$$

N is the total number of atomic sites, Qv is the energy required for the formation of a vacancy, T is the absolute temperature in kelvins, k is the gas or Boltzmann's constant=1.38 X 10^{-23} J/atom.

The number of vacancies is directly proportional to the temperature. For most metals, the fraction of vacancies Nv/N just below the melting temperature is 10^{-4}; that is, for each 10,000 atomic sites, there is only one site that is empty. [1]

2- **Self-interstitial:** is an extra atom from the crystal positioned between atomic sites (Fig.1). In metals, the atom is larger than the interstitial position in which it is situated, so there is a large distortion in the surrounding lattice. The equilibrium concentration of self-interstitials is very low compared to vacancies. [1]

3- **Impurities:** Metals cannot be obtained in a completely pure form; even with the most sophisticated manufacturing conditions, metals cannot be refined to purity greater than 99.9999%. Instead, they always contain small amount of impurities.[1]

There are two types of impurity point defects found in solid solutions: substitutional and interstitial.

a. Substitutional impurities: The impurity atoms replace the host or parent atoms (Fig.2). An example of a substitutional impurity is a copper atom preplacing or substituting a nickel atom from the nickel's lattice structure.
b. Interstitial impurities: Impurity atoms fill the voids or spaces between the host atoms (Fig.2). For metallic materials that have relatively high atomic packing factors, these interstitial positions are relatively small. In this case, the smaller atoms fit into interstitial spaces. Even very small impurity atoms

are larger than the interstitial sites, thus they introduce some lattice strains on the adjacent host atoms.

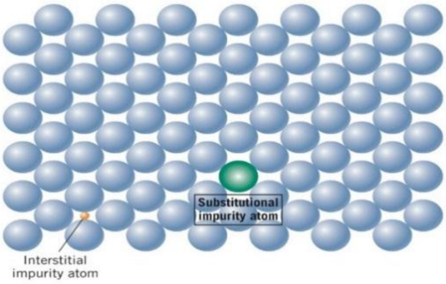

Fig.2 Two-dimensional schematic representations of substitutional and interstitial impurity atoms.

Point defects, whether interstitial atom, vacancy or impurity, cause space lattice distortion as shown in Fig. 3.

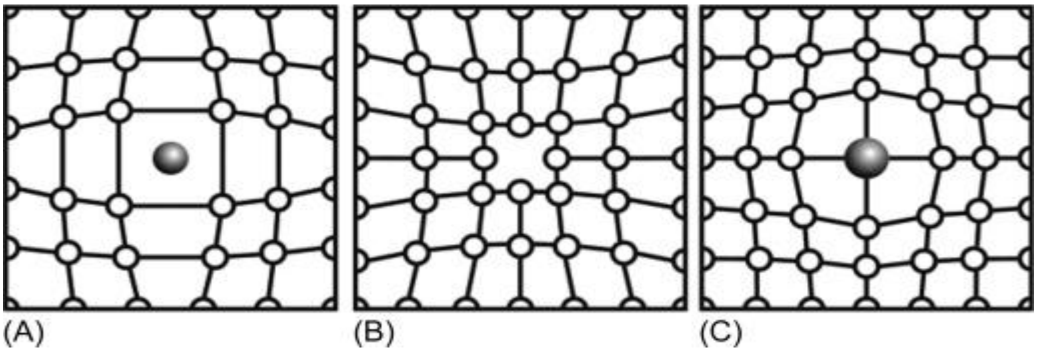

Fig.3. Schematic representation showing the space lattice distortion around interstitial atom (A), vacancy (B), and impurity atom (C)

Point defects in non-metallic crystals:

Point defects in non-metallic, particularly ionic, structures are associated with additional features (e.g. the requirement to maintain electrical neutrality and the possibility of both anion-defects and cation-defects existing).

- **Schottky defect:**

  It consists of a pair of an anion vacancy (an inion missing from the lattice site) and a cation vacancy (a cation missing from the lattice site). This maintains the charge neutrality (Fig.4.a)
- **Frenkel defect:**

  It consists of a pair of cations (positive ion) vacancy and a cation interstitial (Fig.4.b), or it may also be an anion (negative ion) vacancy and anion interstitial. However, anions are much larger than cations, so it is not easy for an anion interstitial to form.

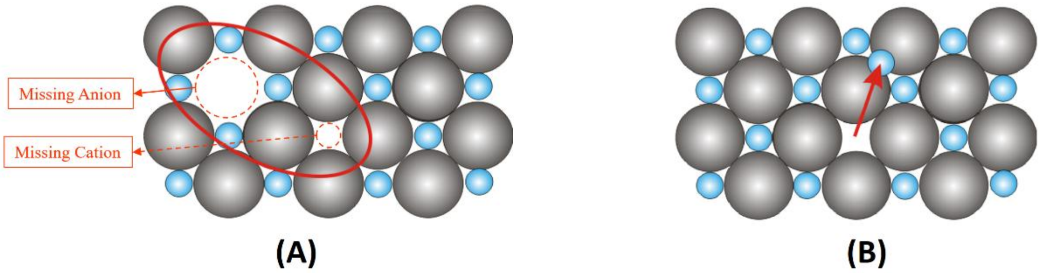

Fig.4. Schematic representation showing the Schottky defect (A) and Frenkel defect (B)

Linear defects / dislocations are defined as irregularities or deviations from ideal arrangement in entire row of lattice points, dislocation are a linear or one-dimensional defect around which some of the atoms are misaligned. [1]

There are three types of dislocations: edge dislocation, screw dislocation and mixed dislocation.

- **Edge dislocation/ dislocation line**: It is a linear defect that centers on the line that is defined along the end of the extra half-plane of atoms. At the region around the dislocation line, there is some localized lattice distortion which decreases as the distance from the dislocation line increases. Above the dislocation line in Fig.5 the atoms are squeezed together, and below the line, they are pulled apart; this results in a slight curvature in the vertical planes of atoms. [1]

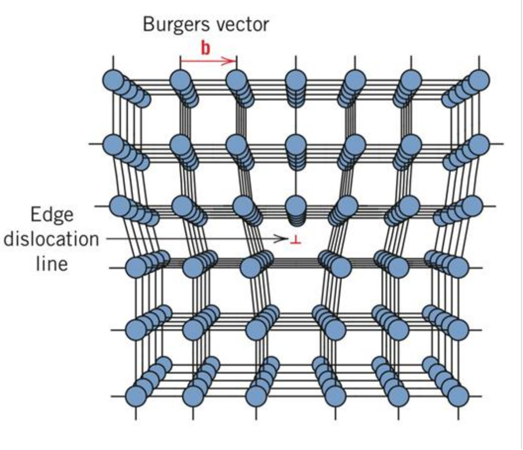

Fig.5. the atom positions around an edge dislocation; extra half-plane of atoms shown in perspective

Screw dislocation: Another type of dislocation may be thought of as being formed by a shear stress that is induced to produce the distortion shown in (Fig.6). The upper front region of the crystal is shifted one atomic distance to the right relative to the bottom portion. [1]

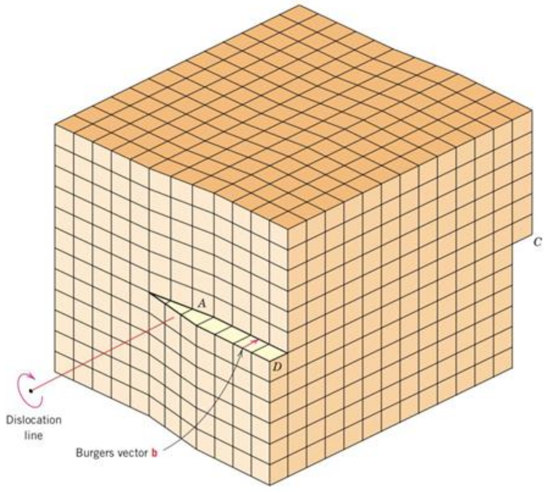

Fig.6 Screw dislocation within a crystal.

The atomic distortion associated with a screw dislocation is also linear and along a dislocation line. The screw dislocation derives its name from the spiral path that takes around the dislocation line. The motion of a screw dislocation that results from the induced shear stress is shown in (Fig.7). For a screw dislocation, lattice strains are pure shear only.[1]

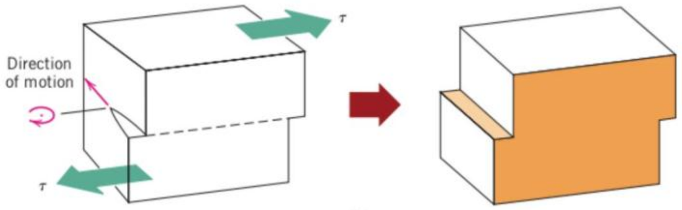

Fig.7. Formation of a step on the surface of a crystal by the motion of a screw dislocation

Comparison between edge dislocation and screw dislocation:[8]

Table.1. Comparison between edge dislocation and screw dislocation.

	Edge dislocation	Screw dislocation
Definition.	1-D line defect that is the edge of an extra half plane of atoms within the crystal lattice.	1-D line defect in which a path spirals around a dislocation line through individual parallel planes.
stresses	Tensile, compressive and shear stress fields my be present.	Only shear stress field exist.
Lattice disturbance	Region of lattice disturbance extends along an dislocation line.	Lattice disturbance extends in two separate planes at right angle to each others.
Burger's vector	Burger's vector is always **perpendicular** to the dislocation line.	Burger's vector is always **parallel** to the dislocation line.
Formation	Formed during formation and crystallization.	Formed during formation and crystallization.

Mixed dislocation: Most dislocations found in crystalline materials probably exhibit components of both edge and screw dislocation types; these known as mixed dislocations. All three dislocation types are represented schematically in (Fig.8); the lattice distortion that is produced away from the two faces is mixed, having varying degrees of screw and edge character.[1]

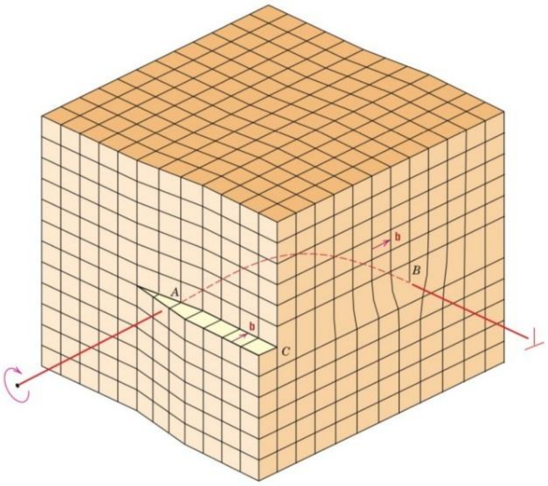

Fig.8. Schematic representation of a dislocation that has edge, screw, and mixed character.

Influence of point and plane defects on the material's properties and behavior:

1. Role of point defects in atomic diffusion
2. Effect of vacancies on thermal conductivity
3. Role of dislocations in plastic deformation of metals
4. Effect of dislocations and point defects on the electrical properties
5. Effect of dislocations and point defects on the optical properties

1. Role of point defects in atomic diffusion:

Point defects play an important role in atomic diffusion. Atomic diffusion can occur by two different mechanisms:

a) Vacancy Diffusion: It involves the interchange of an atom from a normal lattice position to an adjacent vacancy, as shown in (Fig.9). Of course, this process demands the presence of vacancies, and the extent to which vacancy diffusion can occur depends on the number of these defects are present.[1]

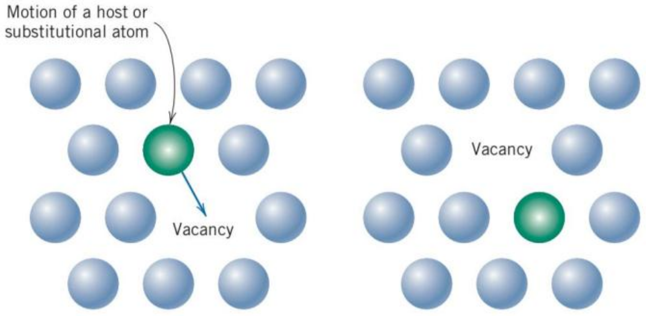

Fig.9. Schematic representation of vacancy diffusion

b) <u>Interstitial Diffusion:</u> The second type of diffusion involves atoms that migrate from an interstitial position to a neighboring one that is empty. This mechanism is found for inter-diffusion of impurities such as hydrogen, carbon, nitrogen, and oxygen, which have atoms that are small enough to fit into the interstitial positions (Fig.10). In most metal alloys, interstitial diffusion occurs much more rapidly than diffusion by the vacancy mode, because the interstitial atoms are smaller and thus more mobile. Furthermore, there are more empty interstitial positions than vacancies.[1]

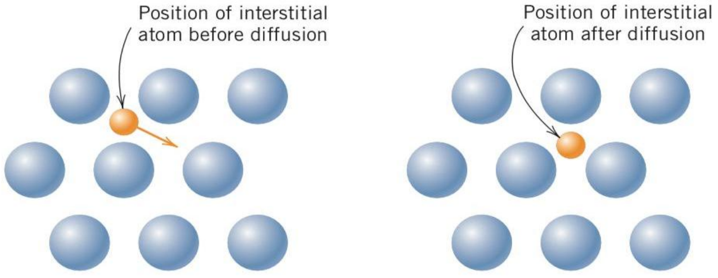

Fig.10. schematic representation of interstitial diffusion.

2. <u>Effect of vacancies on thermal conductivity:</u>

It was found that the thermal conductivity of the crystalline material decreases with the increase in the vacancy concentration. The presence of vacancies in the lattice structure elongates the "heat flux path" that the energy carriers follow during heat conduction.

3. <u>Role of dislocations in plastic deformation of metals:</u>

Dislocations are most significant in metals and alloys since they provide a mechanism for plastic deformation. Plastic deformation refers to irreversible change in shape that occurs when the force or stress that caused it is removed. In elastic deformation, the shape change is only a result of stretching of interatomic or interionic bonds, while in plastic deformation, the interatomic bonds are broken and new bonds are formed.[6]

A slip is the process by which plastic deformation is produced by dislocation motion. Slip between crystal planes result when dislocation moves, producing a permanent plastic deformation.

The vector representing the magnitude of the local slip, or more generally the difference in the amounts of local slip in neighboring regions, is known as the Burgers vector.[3]

An edge dislocation moves in response to a shear stress (Fig.11). Let the initial extra half-plane of atoms be plane A. When the shear stress is induced as shown in (Fig.11.a), plane A is pushed to the right; this in turn pushes the top halves of planes B, C, D, and so on, in the same direction (Fig.11.b). The extra half-plane, moves from left to right by successive and repeated breaking of bonds and shifting by interatomic distances of upper half-planes. Before and after the movement of a dislocation through some particular region of the crystal, the atomic arrangement is ordered and perfect; it is only during the passage of the extra half-plane that the lattice structure is disrupted. This extra half-plane may appear from the right surface of the crystal, forming an edge that is one atomic distance wide; this is shown in Fig. 11.c.[1].

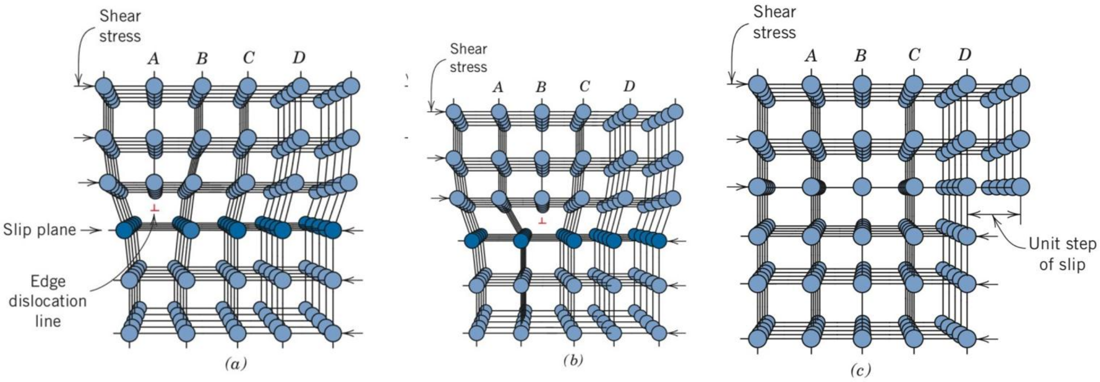

Fig.11. Atomic rearrangements that accompany the motion of an edge dislocation as it moves in response to an applied shear stress. (a) The extra half-plane of atoms is labeled A. (b) The dislocation moves one atomic distance to the right as A links up to the lower portion of plane B; in the process, the upper portion of B becomes the extra half-plane. (c)A step forms on the surface of the crystal as the extra half-plane exits.

It is noteworthy that in absence of dislocations (which is a hypothetical assumption), producing a permanent deformation in the metal would require breakage of bonds along an entire atomic plane. This would need an enormous amount of energy. On the other hand, in the presence of dislocations, the permanent deformation occurs by breakage of bonds along one row of atoms at a time, making the deformation much easier.

An often quoted analogy to show the effect of dislocations on facilitating slip movement is that of moving a carpet. Dragging the carpet across the floor is difficult because of the friction developed from the contact of the surface of the carpet with the floor. Imagine what would happen, however, if a wrinkle is put into the carpet, as shown in Fig.12. The carpet can now be moved by pushing the wrinkle across the floor, because only the friction between a small section of carpet and the floor has to be overcome. A similar phenomenon occurs when one plane of atoms moves past another by means of a dislocation defect. [6]

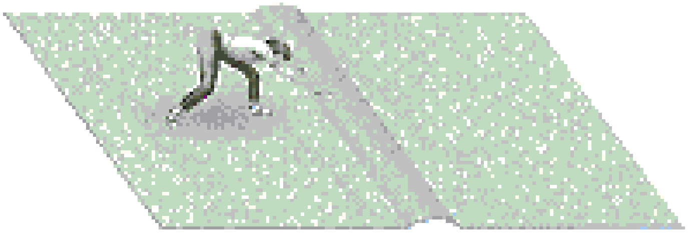

Fig.12. An analogy on how dislocation facilitates slip movement in metals

These dislocation-facilitated slip movements explain why the actual measured strength of metals is much lower than the predicted theoretical value calculated from the strength of the metallic bond (It was shown that the actual strength of metals is 10^3 to 10^4 times lower than their theoretical strength).[6]

Based on the previous discussion, it is clear that the slip provides ductility in metals. For example, if no dislocations were present, an iron bar would be brittle and could not be shaped by metal working processes. Material scientists actually make use of this fact when it comes to strengthening of metals. The mechanical properties of a metal or alloy can be increased by interfering with the movement of dislocations. An obstacle introduced into the crystal prevents a dislocation from slipping unless we apply higher forces. Thus, any mechanism that impedes dislocation motion makes a metal stronger.[6]

During the plastic deformation process, many dislocations move along the same slip plane until they encounter a barrier, such as a grain boundary, which prevents them from moving further. Thus, the dislocations pile up behind this barrier as shown in Fig.13. The interaction between these dislocations creates a back stress that makes it more difficult for further dislocation movements to occur. This explains the work hardening that metals experience during cold working.[7]

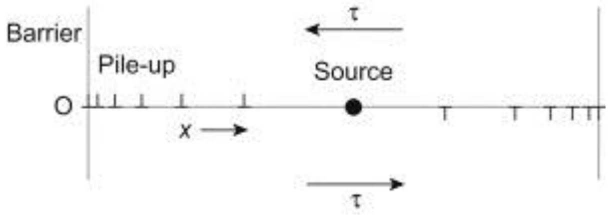

Fig.13 Linear arrays of edge dislocations piled-up against barriers under an induced shear stress τ

4. Effect of dislocations and point defects on the electrical properties:

Dislocations and other defects (including point defects) also influence the electrical properties of materials by interfering with the motion of charge carriers. This is why we make sure that the dislocation densities in single crystal silicon and other materials used in electrical applications are very small. Point defects also cause increased resistivity in metals.[6]

5. Effect of dislocations and point defects on the optical properties:

Both dislocations and some point defects act as light scattering centers within the material leading to an increase in its opacity. That is why the dislocation density affects the performance of photo detectors, light emitting diodes, lasers, and solar cells.

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