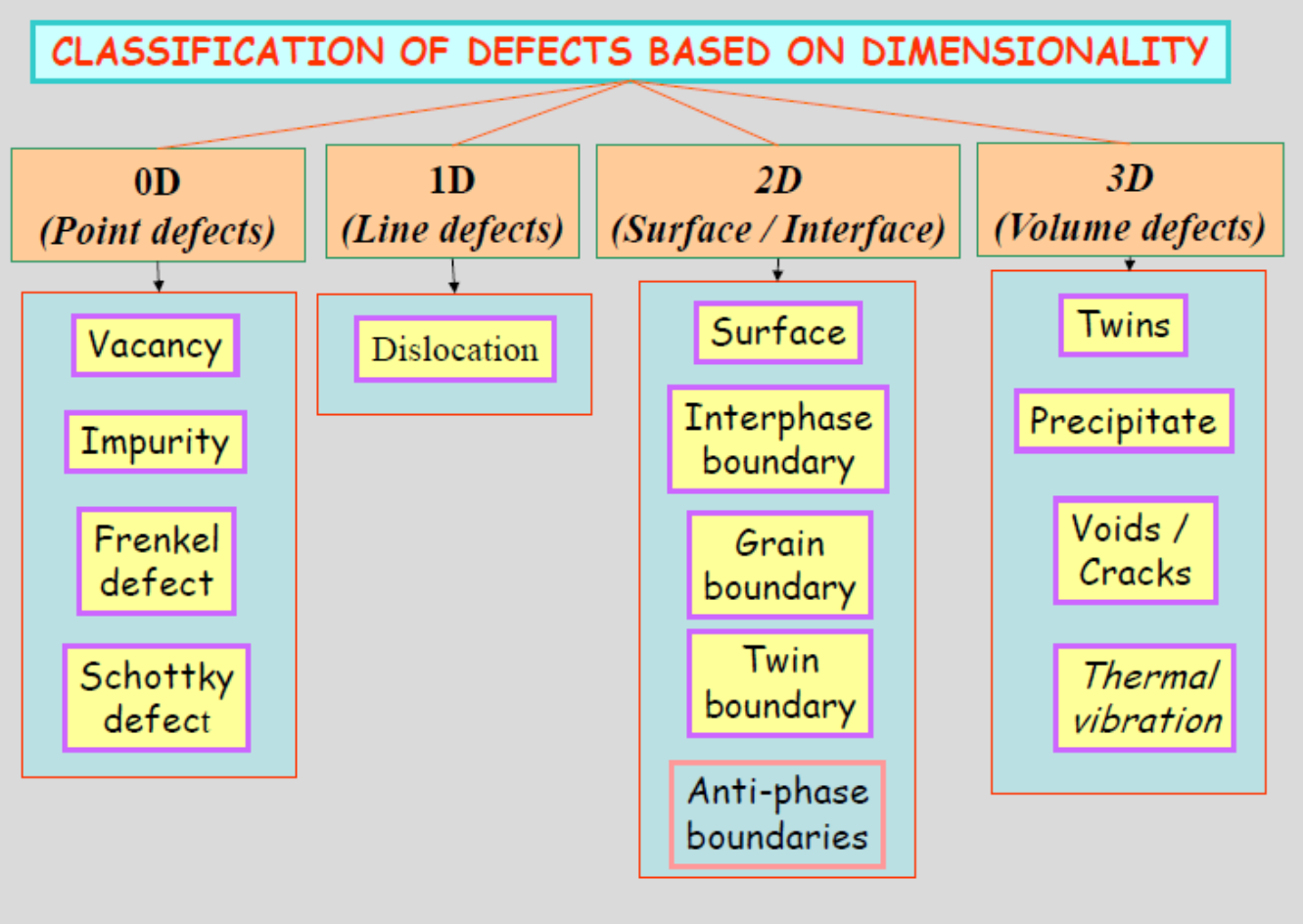
Atomic Defects in Metals

Crystalline structures in metals have many imperfections (defects). Atoms are not always where they should be if the crystal structure was adhered to. In reality there are often atoms missing, too many atoms, impure atoms, or distortions in the crystalline structure. These faults or defects are called crystal defects. **Defects** are imperfections which cause disruption in what otherwise would be a perfect lattice. Defects are classified based on their dimensionality into:

1. Point defects (**0-D**).
2. Line defects (**1-D**).
3. Surface defects (**2-D**).
4. Volume defects (**3-D**).



1. Point Defects (0-D)

An atom is missing or is in an irregular position in the lattice.

1.1 Vacancy Defect: As already mentioned, it is rare (uncommon) that an ideal crystalline structure exists in a metal. Sometimes an atom may be missing from a line or a row and the lattice is placed under strain. When this occurs, a vacancy exists.

The number of vacancies increases as the temperature goes up.

The number of vacancies:

$$N_v = N \exp\left(-Q_v / K.T\right)$$

N: Is the total number of sites in a crystal.
N_v: Is the number of vacancies.
Q_v: Is the activation energy for the formation of a vacancy, (1 eV/molecule = 96.49 kJ/mol).
K: Boltzmann's constant = (1.38×10^{-23} J/atom. K).
or = (8.62×10^{-5} eV/atom. K).
N_v: Goes up exponentially with temperature T.

1.2.1 Substitution Defect: When an atom from another element (which is not the same size as the other atoms) is present it also causes distortion in the lattice. This atom can be larger or smaller than the other atoms (i.e. one atom is replaced by as different type of atom).

1.2.2 Interstitial Defect: If an atom from an impurity finds its way into a space or interstice in the lattice the defect caused is called an Interstitial defect (i.e. extra atom is inserted (place in) into the lattice structure at a normally unoccupied position).

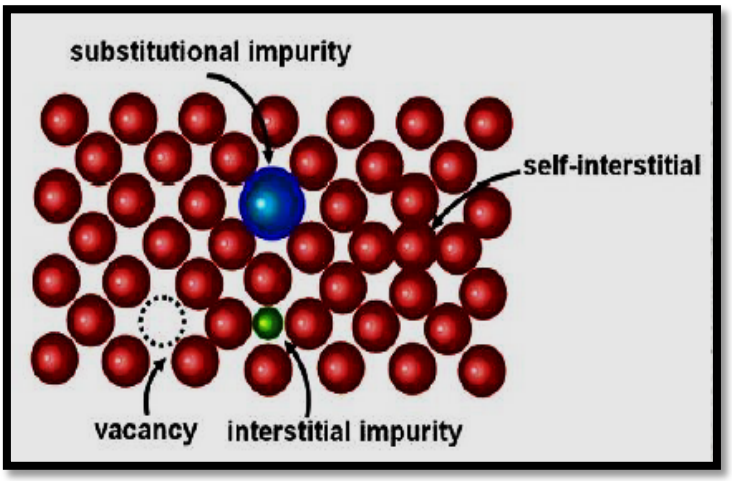


Figure 1. Points defects.

1.3 Frenkel defect: Anion jumps from a normal lattice point to an interstitial site, leaving behind a vacancy (vacancy-interstitial).

1.4 Schottky: Pair of vacancies in ionically bonded material. Both anion and cation must be missing from the lattice to maintain the crystal neutral.

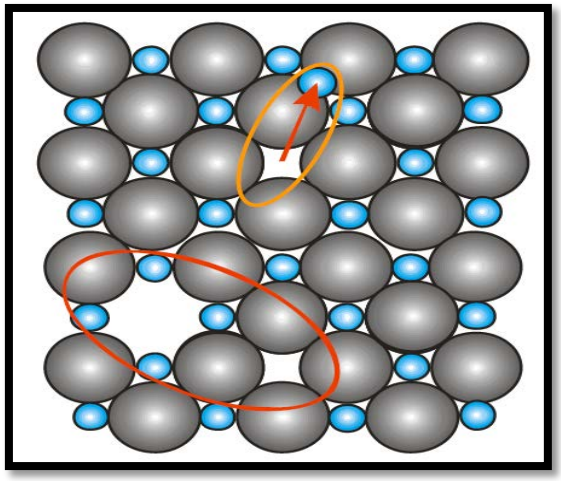


Figure 2. Frenkel defect (Cation vacancy + cation interstitial), Schottky defect (Cation vacancy + anion vacancy)

2. Line Defects in Crystals (1-D)

If atoms are out of line in the grain body, or lattice, this is known as a line imperfection, or line defect. Line defects are called dislocations. Dislocations allow the grains to distort or slip under shear stress. Slip in metals is largely due to the presence of dislocations. Ductility in metals is a result of the distortion allowed by slip in metals.

A method of restricting the movement of a dislocation is to alloy it with another element or to cold work the metal. Line imperfections (Dislocations) in a 2-D lattice:

1. Edge
2. Screw
3. Mixed

Dislocations: Boundary between two regions of a surface which are perfect themselves but are out of registry with each other. The resulting lattice distortion is centered along a line.

Burgers Vector, b: A vector by which the lattice on one side of an internal surface containing the dislocation line is displace (move) relative to the lattice on the other side.

There are two special cases of dislocations:

a. Edge Dislocation: b and normal vector along the dislocation line **L** are perpendicular.
b. Screw Dislocation: b and normal vector along the dislocation line **L** are parallel.

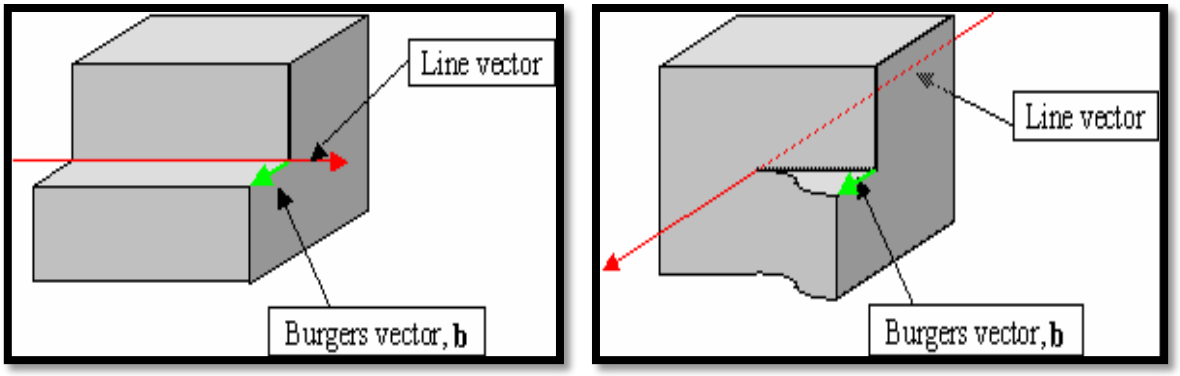


Figure 3. Burgers vectors in edge and screw dislocation.

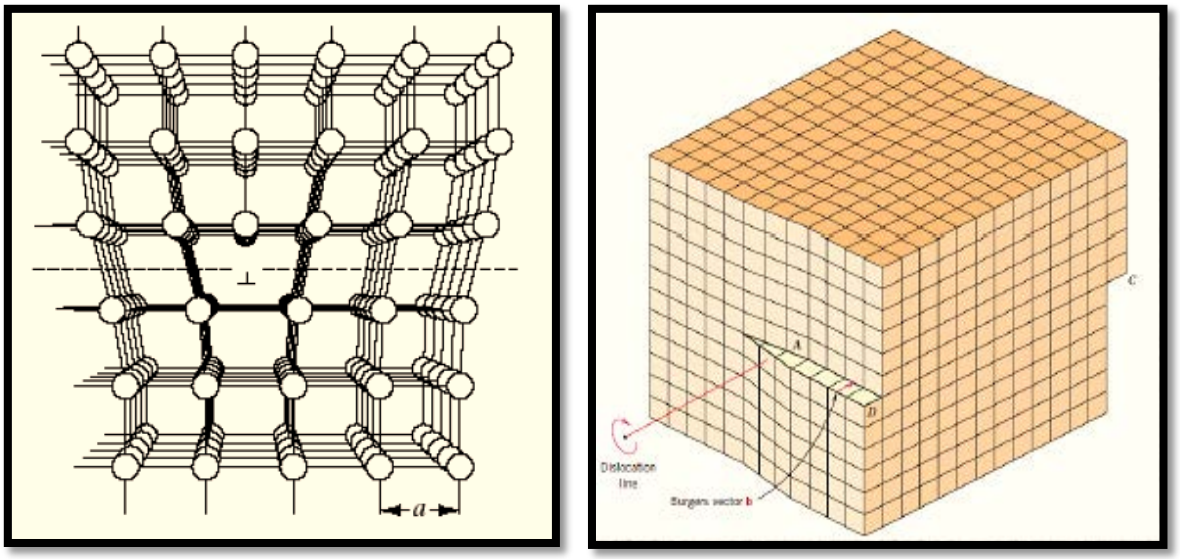


Figure 4. Line defect (edge and screw).

3. Planar (Surface) Defects (2-D): Interfaces between homogeneous regions of the material - grain boundaries, stacking faults, external surfaces.

4. Volume Defects (3-D): Other defects exist in all solid materials that are much larger than those heretofore discussed. These include pores, cracks, foreign inclusions, and other phases. They are normally introduced during processing and fabrication steps.

EXAMPLE

Calculate the equilibrium number of vacancies per cubic meter for copper at 1000°C. The energy for vacancy formation is 0.9 eV/atom; the atomic weight and density at (1000°C) for copper are 63.5 g/mol and 8.4 g/cm^3, respectively.

SOLUTION

$$N = \frac{N_A \rho}{A_{Cu}}$$

$$= \frac{(6.023 \times 10^{23}\ \text{atoms/mol})(8.4\ \text{g/cm}^3)(10^6\ \text{cm}^3/\text{m}^3)}{63.5\ \text{g/mol}}$$

$$= 8.0 \times 10^{28}\ \text{atoms/m}^3$$

Thus, the number of vacancies at 1000°C (1273 K) is equal to

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$

$$= (8.0 \times 10^{28}\ \text{atoms/m}^3) \exp\left[-\frac{(0.9\ \text{eV})}{(8.62 \times 10^{-5}\ \text{eV/K})(1273\ \text{K})}\right]$$

$$= 2.2 \times 10^{25}\ \text{vacancies/m}^3$$