Crystal defect (Imperfection)

Is imperfection in the regular geometrical arrangement of the atoms in a crystalline solid. These imperfections result from deformation of the solid by:

1-rapid cooling from high temperature

2- High-energy radiation (x-rays or neutrons) striking the solid

3- Foreign atoms

4- External stresses

5- Thermal effect.

These defects influence its mechanical, electrical, and optical behavior. Defects included:

1- Point defects
2- Linear defects
3- Surface defects

I- Point defects:

A point defect is a much localized disruption in the regularity of a lattice. It is a defect of dimensions just like a point (zero dimensions). The size of the defect could be one atom, or two atomic diameters. Point defects include: Vacancy types, impurity type Frenkel type, and the Schottky type.

1.1Vacancy:

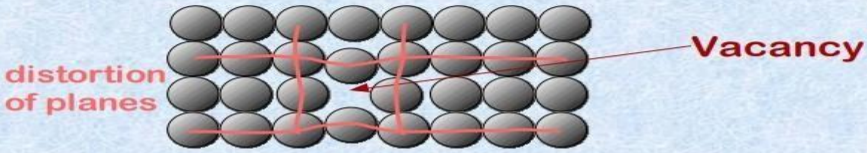
When an atom is missing from its lattice site in a crystal structure, it is called a vacancy The atoms surrounding a vacancy experience a **slight displacement** into the empty lattice site, and thus, a vacancy is a center of approximately spherical distortion in the lattice.

There could be di-vacancies (an association of two vacancies) or even tri-vacancies.

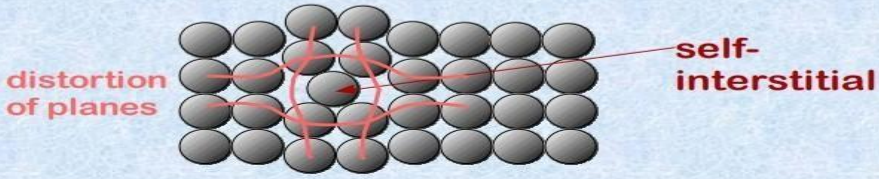
- The vacancies equilibrium concentration increases (**exponentially**) with the increase of temperature

Point Defects (I)

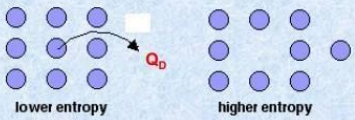
Vacancies: vacant atomic sites in a structure.



Self-Interstitials: "extra" atoms positioned between atomic sites



Equilibrium Concentration: Vacancies



Each lattice site is a potential vacancy site

$$N = \rho \times (N_A/A) \times V$$

where: ρ - density; A – atomic mass
V – volume and N_A – Avogadro number (6.02×10^{23} atom/mol)

$$\frac{N_D}{N} = \exp\left(\frac{-Q_D}{kT}\right)$$

where:
N - is number of sites
N_D - is number of defects
Q_D – is activation energy
T – is a temperature
k – Boltzmann's constant
1.38×10^{-23} J/atom K
8.62×10^{-5} eV/atom-K
1 eV =1.602 $\cdot 10^{-19}$ J

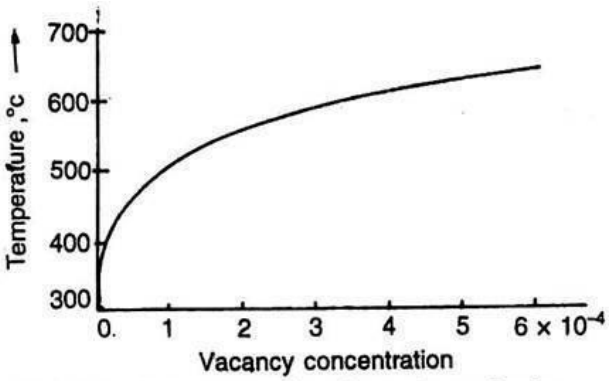


Fig. 4.8. Equilibrium concentration of vacancies as a function of temperature for aluminium.

Equilibrium Concentration of Vacancies

- **Find the equilibrium number of vacancies in 1m³ of Cu at 1000 °C.**

$\rho_{Cu} = 8.4$ g/cm^3 $\quad A_{Cu} = 63.5$g/mol

$Q_D = 0.9$eV/atom $\quad N_A = 6.02 \times 10^{23}$ atoms/mole

For 1 m^3, $\mathbf{N} = \rho \cdot N_A/A_{cu} \cdot 1\text{m}^3 = 8 \cdot 10^{28}$ sites

$$\frac{N_D}{N} = \exp\left(\frac{-Q_D}{kT}\right) = 2.7 \cdot 10^{-4}$$

Q_D: 0.9eV/atom; T: 1273K; k: 8.62×10^{-5} eV/atom-K

- **Answer:**

$N_D = 2.7 \cdot 10^{-4} \cdot 8.0 \times 10^{28}$ sites $= 2.2 \times 10^{25}$ vacancies

1.2 Impurity Atoms

a.Substitutional Type: an impurity (foreign) atom if present on the lattice by substituting the lattice site atom. Substitutional atoms may either be larger than the normal atom in the lattice (in which case, the surrounding atoms are compressed, or smaller (causing the surrounding atoms to be in tension). The number of defects is relatively independent of temperature.

b. Interstitially (self –Interstitial): an atom occupies an interstitial site (which is not its normal site), normally, it requires large energy to create an interstitially. The size of an interstitial site is very small, particularly in close- packed crystal structures are much more elastically strained (displaced) than around a vacancy. The small sized atoms present in the interstitial site. Therefore, the surrounding lattice is compressed and distorted.

- The number of interstitial atoms in the structure **remains constant**, even when the temperature is changed.
- Foreign atoms also play a role in changing the electrical conductivity of the semi-conductors.

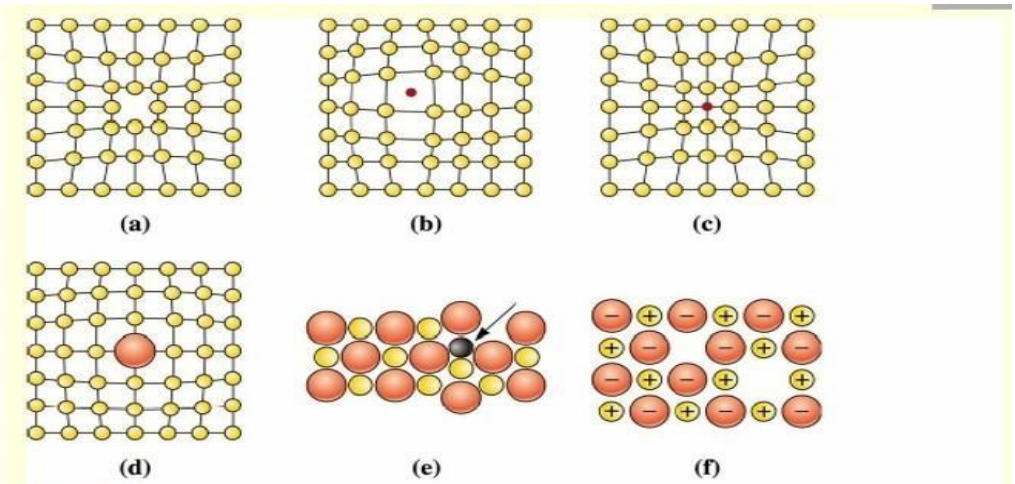


Figure 4-1 Point defects: (a) vacancy, (b) interstitial atom, (c) small substitutional atom, (d) large substitutional atom, (e) Frenkel defect, and (f) Schottky defect. All of these defects disrupt the perfect arrangement of the surrounding atoms.

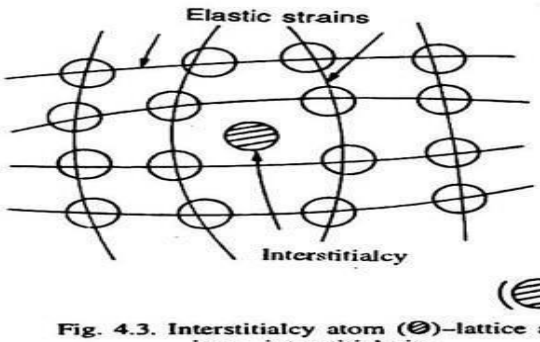


Fig. 4.3. Interstitialcy atom (⊘)–lattice atom in an interstitial site

1.3 Frenkel Defect: When an atom is shifted from a normal lattice site (thus creating vacancy) and is forced into interstitial position, the resulting pair of point defects (a vacancy as well as the interstitially) together is called a Frenkel defect.

1.4 Schottky defects: a missing of positive ion and negative ion from crystal.