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Lecture # 8

CHAPTER FOUR/IMPERFECTIONS IN SOLIDS

Introduction

The term ***defect***, or ***imperfection***, is generally used to describe any deviation from an orderly array of lattice points. When the deviation from the periodic arrangement of the lattice is localized to the vicinity of only a few atoms it is called a point defect, or point imperfection. However, if the defect extends through microscopic regions of the crystal, it is called a lattice imperfection.

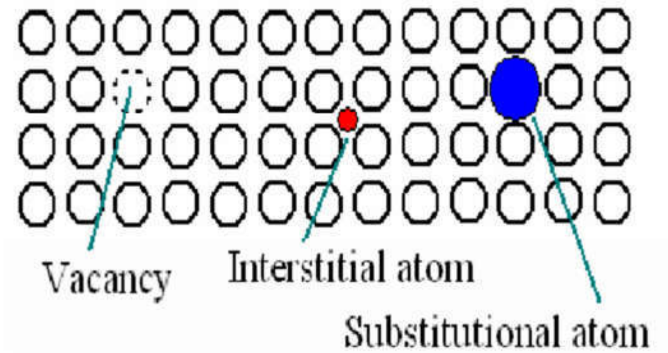
Imperfections in crystalline solids are normally classified according to their dimension as follows:

A. **Point defects** (zero-dimensional)
B. **Line defects** (single dimensional)
C. **Surface defects** (two dimensional)
D. **Volume defects** (three dimensional)

A. Point defects: lattice defects that involves a few atoms.

Point defects include: vacancies, interstitials or impurities. **Figure 1** illustrates three types of point defects.

- **Vacancy**: is a missing atom **or** is an irregular place in the lattice structure..
- **Interstitial**: atom at interstitial sites.
- **Substitutional impurity atom**: is a foreign atom occupying original lattice position by displacing the parent atom.



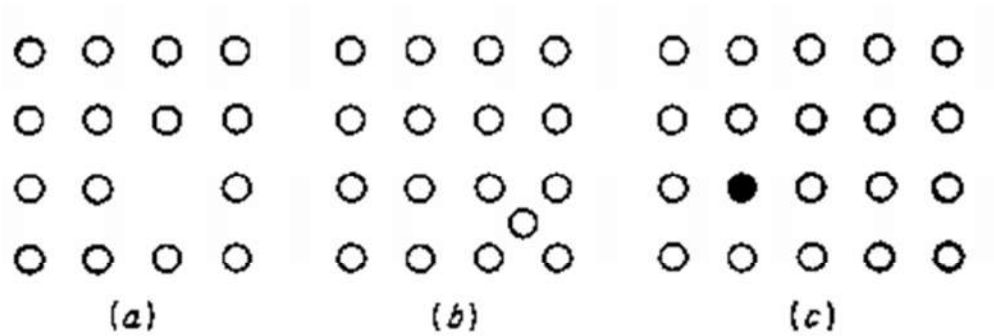


Figure 1 Types of point defects.
(a) Vacancy; (6) interstitial; (c) impurity atom.

In pure metals, small numbers of vacancies are created by thermal excitation, and these are thermodynamically stable at temperatures greater than absolute zero. At equilibrium, the fraction of lattices that are vacant at a given temperature is given approximately by the equation:

$$\frac{n_v}{N} = e^{\left(-\frac{Q}{RT}\right)} = e^{\left(-\frac{Q}{KT}\right)}$$

where;

n_v is the number of vacant sites
N total number of lattice sites

Q is the energy required to form vacancies (**J/mole**) or (**ev/atom).**
R Gas constant (**8.31 J/mol.K**).
K Boltzmann's constant **(1.38×10^{-23} J/mole.K)** or **(8.62×10^{-5} ev/atom.K).**
T is absolute temperature in kelvins.

- It is clear from the equation that there is an exponential increase in number of vacancies with temperature. When the density of vacancies becomes relatively large, there is a possibility for them to cluster together and form voids.
- We can use the same equation above to calculate the number of interstitial sites.

Point defects produced by:

1) Plastic deformation (cold work).
2) Rapid quenching from close of melting temperature.
3) Radiation of metal by high energy particles can produce high concentrations of point defects.

Number of Vacancies Computation at a Specified Temperature

EXAMPLE PROBLEM: 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: *Determine the value of N, the number of atomic sites per cubic meter for copper, from its atomic weight Mcu, its density , and Avogadro's number N_{av} , according to;*

ρ = 8.4 g/cm^3; **Atomic weight** = 63.5 g/mol, **N_{av}** is avogadro's number (6.022×10^{23} atoms/mol)

$$N = \frac{Nav \times \rho}{M} \qquad \textit{From Chapter } (2)$$

$$N = \frac{6.022 \times 10^{23} \text{ atoms/mol} \times 8.4 \text{ g/cm}^3}{63.5 \text{ g/mol}}$$

$$N = 8 \times 10^{22}\ \text{atoms/cm}^3\ ,\quad \mathbf{N = 8 \times 10^{28}\ atoms/m^3}$$

Determine the number of vacancies per cubic meter by eq.

$$\frac{n_v}{N} = e^{\left(-\frac{Q}{KT}\right)}$$

where;

Qv=0.9 eV/atom at 1000°C,

T= 1000+273=1273K

K= 8.62×10^{-5} ev/atom.K

$$n_v = 8 \times 10^{28}\ \text{atom/m}^3 \times exp\left(\frac{-0.9\ \text{eV/atom}}{8.62 \times 10^{-5}\ \text{ev/atom.K} \times 1273\text{K}}\right)$$

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

IMPURITIES IN SOLIDS

Alloy is a combination of two or more metals.

Solid solution: Homogenous crystalline phase that contains two or more chemical species. Either substitutional solid solution or interstitial solid solution.

Solute: One element or compound of a solution present in the minor concentration; It is dissolved in the solvent.

Solvent: One element or compound of a solution present in the greatest amount; solvent atoms are also called host atoms.

Substitutional solid solution: A solid solution where the solute or impurity atoms replace or substitute the host atoms. **An example**, zinc atoms in brass, make substitutional solid solution**.** a substitutional solid solution is also found for copper and nickel. <u>There are four conditions for substitutional solid solution</u>:

1) Atomic size factor; atomic radii difference about ± 15.
2) Same crystal structure.
3) Valences being equal..

4) Electronegativity; if one element is more electropositive and the other is more electronegative, they will form an intermetallic compound instead of a substitutional solid solution.

Interstitial solid solution: A solid solution where the small solute or impurity atoms fill the voids or spaces among the host atoms. **An example**, Carbon added in small amounts to iron to make steel which is stronger than pure iron. C is small interstitial atom in α-Iron make interstitial solid solution.

Solid Solution Strengthening: The introduction of solute atoms into solid solution in the solvent-atom lattice always produces an alloy which is stronger than the pure metal.

The factors playing an important role on strengthening effect:

1) Size of the solute
2) Concentration of solute
3) Elastic modulus of the solute (higher E → greater strengthening effect)
4) Nature of solute atoms (Interstitial or substitutional)

Computation of Composition

For an alloy that contains two hypothetical atoms denoted by 1 and 2, the concentration of 1 in **wt%**, $\mathbf{C_1}$, is defined as;

$$\mathbf{C_1} = \left[\frac{\mathbf{m_1}}{(\mathbf{m_1} + \mathbf{m_2})}\right] \times \mathbf{100}$$

The concentration of 2 in wt%, $\mathbf{C_2}$, is defined as;

$$\mathbf{C_2} = \left[\frac{\mathbf{m_2}}{(\mathbf{m_1} + m_2)}\right] \times \mathbf{100}$$

where $\mathbf{m_1}$ and $\mathbf{m_2}$ represent the weight (or mass) of elements 1 and 2, respectively.. The basis for **atom percent** (**at%**) calculations is the number of moles of an element in relation to the total moles of the elements in the alloy. The concentrations of elements 1 and 2 in atomic percentage (**at%**) are defined as;

$$\overline{C}_1 = \left[\frac{\mathbf{n_1}}{(\mathbf{n_1} + \mathbf{n_2})}\right] \times \mathbf{100}$$

$$\bar{C}_2 = \left[\frac{n_2}{(n_1 + n_2)}\right] \times 100$$

$\bar{C}_1$ = The concentration of element 1 in atomic percentage.

$\bar{C}_2$ = The concentration of element 2 in atomic percentage.

$$n_1 = \frac{m_1}{A_1} \quad , \quad n_2 = \frac{m_2}{A_2}$$

n_1 = The number of moles of an element **1**.

n_2 = The number of moles of an element **2**.

A_1 = The atomic weight of an element **1**.

A_2 = The atomic weight of an element **2**.

H.W (1) Find the relationship between atomic percent and weight percent?

$$\bar{C}_1 = \left[\frac{C_1 A_2}{(C_1 A_2 + C_2 A_1)}\right] \times 100$$

$$\bar{C}_2 = \left[\frac{C_2 A_1}{(C_1 A_2 + C_2 A_1)}\right] \times 100$$

H.W (2) Calculate the activation energy for vacancy formation in aluminum, given that the equilibrium number of vacancies at 500°C (773 K) is 7.57×10^{-23} m^{-3}.The atomic weight and density (at 500°C) for aluminum are 26.98 g/mol and 2.62 g/cm^3, respectively. [**$N = 5.85 \times 10^{28}$ atoms/m^3 , Q= 0.75 eV/atom**].

H.W (3) Calculate the fraction of atom sites that are vacant for lead at its melting temperature of 327°C (600 K). Assume an energy for vacancy formation of 0.55 eV/atom. [**$nv/N = 2.41 \times 10^{-5}$**]

H.W (4) What is the composition, in atom percent, of an alloy that consists of 30 wt% Zn and 70 wt% Cu?

EXAMPLE: Determine the composition, in atomic percent, of an alloy that consists of 97 wt% aluminum and 3 wt% copper.

Solution

If we denote the respective weight percent compositions as $C_{Al} = 97$ and $C_{Cu} = 3$, substitution into Equations 4.6a and 4.6b yields

$$C'_{Al} = \frac{C_{Al}A_{Cu}}{C_{Al}A_{Cu} + C_{Cu}A_{Al}} \times 100$$

$$= \frac{(97)(63.55 \text{ g/mol})}{(97)(63.55 \text{ g/mol}) + (3)(26.98 \text{ g/mol})} \times 100$$

$$= 98.7 \text{ at\%}$$

and

$$C'_{Cu} = \frac{C_{Cu}A_{Al}}{C_{Cu}A_{Al} + C_{Al}A_{Cu}} \times 100$$

$$= \frac{(3)(26.98 \text{ g/mol})}{(3)(26.98 \text{ g/mol}) + (97)(63.55 \text{ g/mol})} \times 100$$

$$= 1.30 \text{ at\%}$$