Lecture 11

6- Crystalline defects

No crystal is perfect !

The real crystal has a surface sets an upper limit on its perfection, and actually macroscopic samples of most solids include many crystallites, randomly oriented, with grain boundaries separating one crystal from the next.

explain why?

6.1 Point defects

Point defects are where an atom is missing. Point defects are defects that occur only at or around a single lattice point. They are not extended in space in any dimension. Point defects include **vacancies, self-interstitial atoms**, **interstitial impurity atoms**, and **substitutional atoms**.

1- Vacancy defect

A vacancy is produced when an atom is missing from a normal site see Fig.23. It is created when the solid is formed.

At R.T, very few vacancies are present, but this number increases exponentially as we increase the temperature (see Eq. 1).

2- Interstitial defect

An interstitial defect is formed when an extra atom is inserted into the lattice structure in a place between atoms

(see Fig.23). The number of this defects is independent of temperature

3- **Substitutional defect**

A substitutional defect is formed when an atom is replaced different type of atom. The substitutional atom remain at the original normal lattice point (see Fig.2). The number of this defects is independent of temperature.

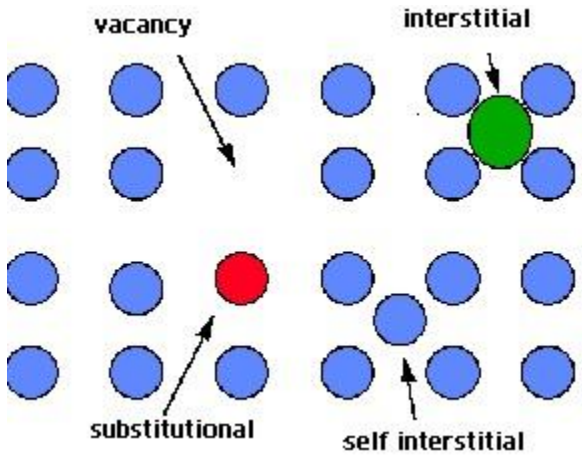

Fig.23.

4- Schottky defect

A vacancy can be formed by an atom migrating from a normal lattice site in the bulk to the surface of the crystal . This is known as a schottky defect (see Fig.24). Schottky defect occurs in ionic crystals such as NaCl.

Schottky got a mathematical relationship to calculate the concentration of the vacancies (n) in ionic crystals at different temperatures, so suppose that the real ionic crystals composed of equal numbers (N) of the positive and negative ions:

$$n = N\, e^{-E_p/2k_BT} \qquad (1)$$

Where n<<N

E_p represented energy required to form a pair of vacancies

∴ E = n E_p (E represented internal energy)

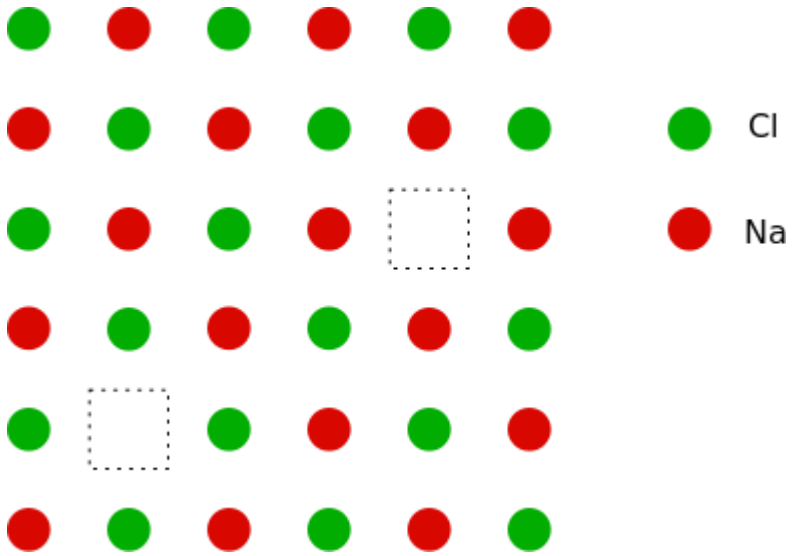

Fig.24 Schottky defect

5- Frenkel defect

A Frenkel defect is a vacancy-interstitial atom pair formed when an ion jumps from a normal lattice point to an interstitial site, leaving behind a vacancy see Fig.25. Frenkel defect occurs in metallic and semiconductor crystals.

Frenkel got a mathematical relationship to calculate the concentration of the number of pairs from the vacancy-interstitial at different temperatures:

$$n = \sqrt{NN_i}\, e^{-E_i/2k_BT} \qquad (2)$$

Where N_i is the number of intra-sites.

E_i represented energy required to form a pair of vacancy-interstitial atom.

∴ E = n E_i (E represented internal energy)

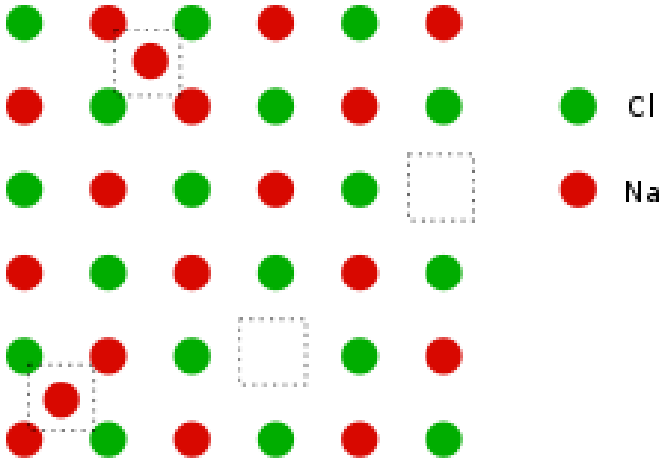

Fig.25 Frenkel defect

Figure -26- represents the crystalline defects group

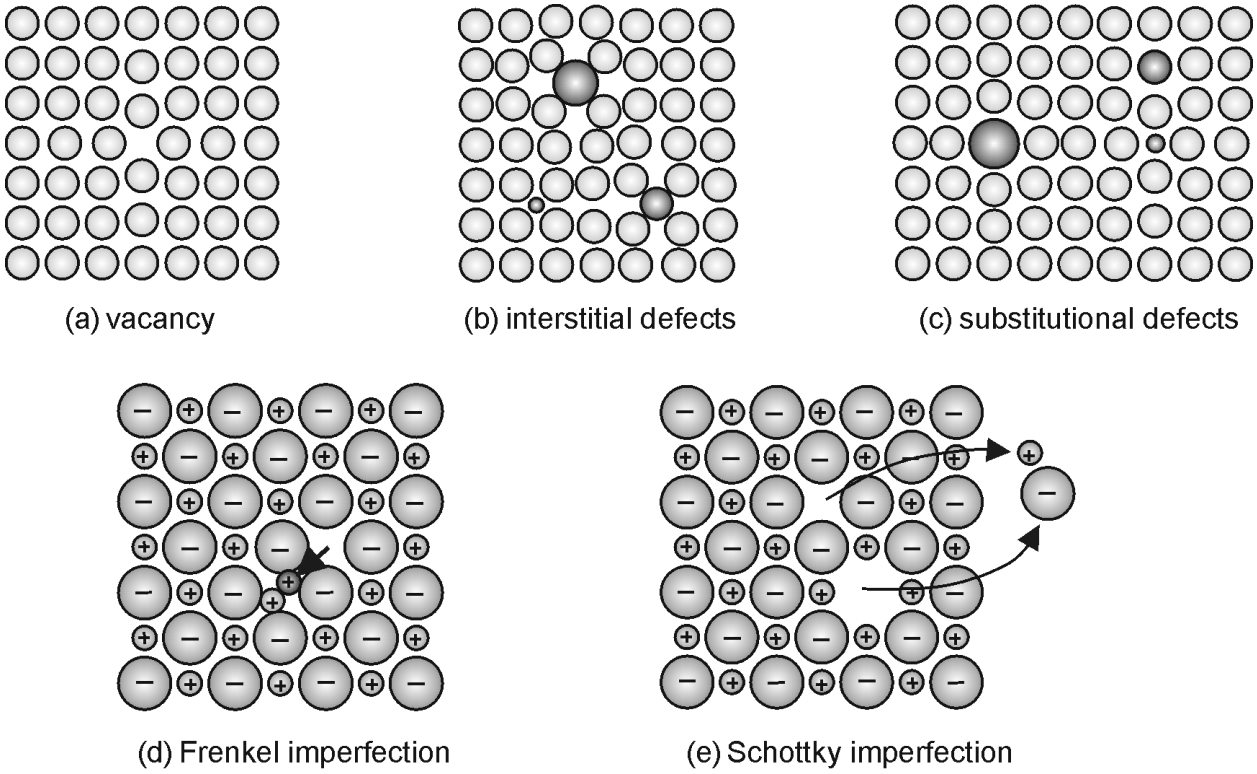

Fig.26

Exercise:

Why it was called point defects?

Solution:

Because the maximum dimension of a point defect in every direction is no more than a few atomic spacing's.

Exercise:

Calculate the number of vacancies per cubic centimeter and the number of vacancies per copper atom when copper is a (a) R.T and (b) 1084^0C.

About 20000 cal/mole required to produce a vacancy in copper.

Solution:

The lattice parameter of FCC coppert is $3.6151*10^{-8}$cm. The number of copper atoms or lattice points per cm^3 is:

N= $\frac{4}{(3.6151*10^{-8})^3}$ = $8.47*10^{22}$ copper atoms/cm^3

a) At room temperature, T=25+273=298K

$n = N\ e^{-E_p/2k_BT}$= $8.47*10^{22}$ exp $\frac{-20000}{(1.987)(298)}$

= $1.815\ 10^8$ vacancies/cm^3

$\frac{n}{N}$ = $\frac{1.815\ 10^8}{8.47*10^{22}}$ = $2.14\ 10^{-15}$

b) T=1084+273=1357K

$n = N\ e^{-E_p/2k_BT}$= $8.47*10^{22}$ exp $\frac{-20000}{(1.987)(1357)}$

= $5.09*\ 10^{19}$ vacancies/cm^3

$\frac{n}{N}$ = $\frac{5.09*10^{19}}{8.47*10^{22}}$ = $6\ *10^{-4}$