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Lecture for M. Sc. Physics IV Semester students

Paper-I: Condensed Matter Physics

Unit-2: Defects in Solid

Unit - 2

Defects or Imperfection in Solid :-

At absolute zero, crystal tends to have a perfectly ordered arrangement, this arrangement corresponds to state of lowest energy. As the temp. increase the crystal starts diverting from perfactly ordered arrangement. Any deviation from the perfectly ordered arrangment constitutes a defect or Imperfection.

There are imperfection from the perfect - periodic repeatition of atoms & this can be characterised geometrically according to weather the imperfection or a defect is at a point (zero dimension), along line (one-dim.), over a surface (two-dim.) & over a volume (3-dim). The study of these defects is useful in study of structure sensitive property like fracture strength, plasticity & thermal conductivity. In addition to this defects in the atomic arrangement of the crystal, It is also found that defect can occure on a subatomic scale in the electronic structure of the atom.

There are following types of defects :

1) Point defect
2) Line defect
3) Plane defect
4) volume defect

Point defect :-

A point defect is a very localised imperfection in the regularities of a lattice & it does not spread over more than one or more ~~than one~~ than two lattice spacing. The introduction of a point defect increases the internal energy of the

crystal as compared to perfect crystal. It is seen that the free energy of defected crystals may be decreases

The gibbs free energy is given as-

$$G = U + PV - TS \quad \text{——} (1)$$

Where, U stands for internal energy, P, V & T for pressure, volume & absolute temp. resp.

S - entropy of the system.

The term PV is negligible for solids under most of the circumstances.

$$G = U - TS \quad \text{——} (2)$$

At const. temp. the change in free energy, the addition of n_d vacancies to the lattice, is given by

$$dG = dU - T ds \quad \text{——} (3)$$

Let E_d be the formation energy of defect then $n_d . E_d$ is the increase in thermal energy i.e.,

$$dU = n_d E_d$$

as the no. of defects increases, the no. of possible arrangements increases, thereby increasing the entropy of the crystal. The entropy increases ds, when n_d vacancies formed, is given by

$$ds = k_B \log W \quad \text{——} (4)$$

Where W is the no. of distinct ways in which n_d distinguishable vacancies can be distributed along N total no. of atomic sides per mole this is given by

$$W = \frac{\lfloor N}{\lfloor n_d \lfloor (N - n_d)} \quad \text{——} (5)$$

∴ Although dU may increase, the effect of entropy increases ds. finally results in the decrease of dG. When the addition of more defects no longer lowers the value of G, The ~~equivalent~~ equilibrium state of minimum free energy has reach at this stage.

$$\frac{d(dG)}{dn_d} = 0$$

$$\frac{d(dU - Tds)}{d\,n_d} = 0$$

$$\frac{d}{dn_d}\left[n_d E_d - k_B T \log \frac{N!}{n_d!\,(N-n_d)!}\right] = 0 \quad \text{—⑥}$$

$$\log \lfloor x = x \log x - x \quad \text{—⑦}$$

Using Sterlings formula & differential eq. ⑥ we get,

$$E_d - k_B T \log \frac{N - n_d}{n_d} = 0 \quad \text{—⑧}$$

Since $n_d \ll N$

$N - n_d \approx N$

$$E_d - k_B T \log \frac{N}{n_d} = 0$$

$$\frac{E_d}{k_B T} = \log \frac{N}{n_d}$$

$$n_d = N e^{-E/k_B T} \quad \text{—⑨}$$

The structural pt. defect can be classified into three categories

(1) Interstitial (2) Vacancy (3) Impurity