Chapter One : Energy Bands in Solids

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1.1 Atomic Structure:

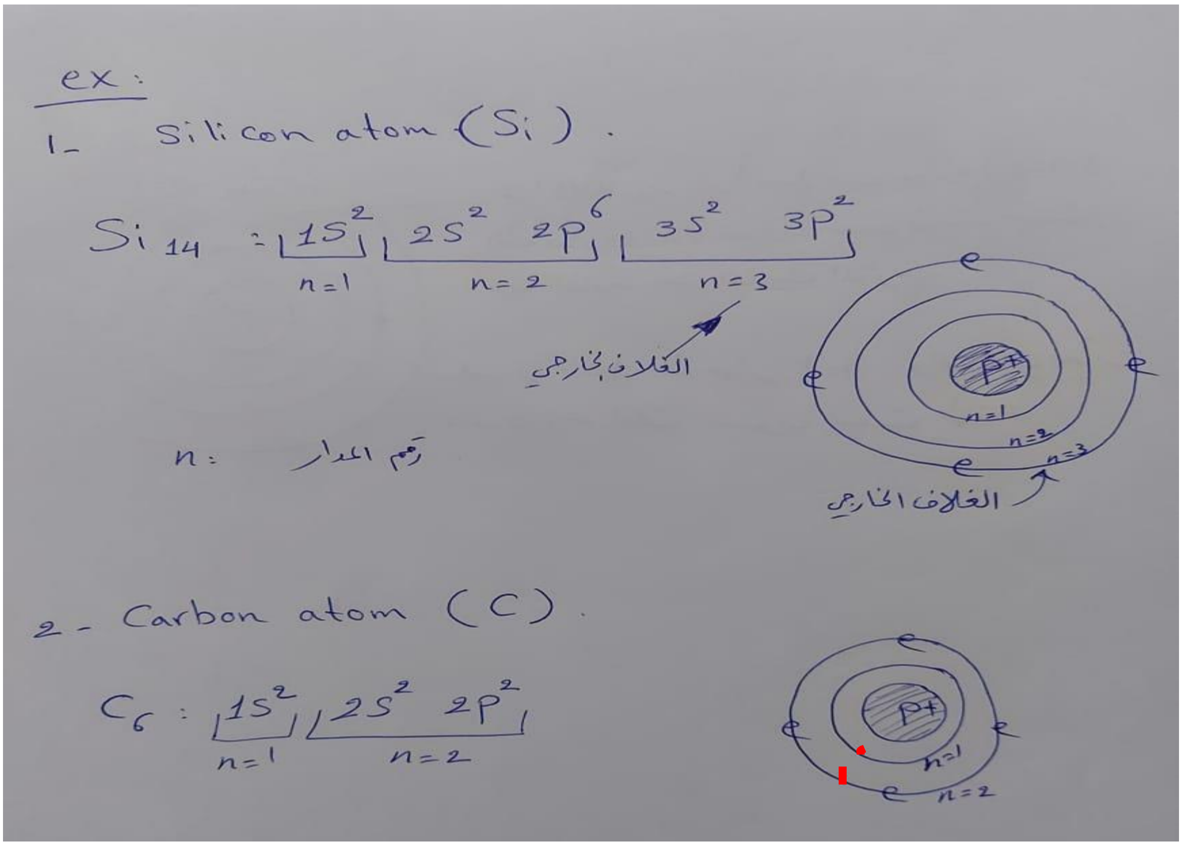
An atom is the smallest particle of an element that retains the characteristics of that element.

Atoms consist of three particles:

Protons, electrons and neutrons. The nucleus (center) of the atom contains the protons (positively charged) and the neutrons (no charge). The outermost regions of the atom are called electron shells and contain the electrons (negatively charged). Niels Bohr proposed an early model of the atom as a central nucleus containing protons and neutrons being orbited by electrons in shells.

- **Atomic Number and Mass Number**

The atomic number is the number of protons in an element, while the mass number is the number of protons plus the number of neutrons.



1.2 Energy Levels in Atom :

Energy levels (also called electron shells) are fixed distance from the nucleus of an atom where electrons may be found. Electrons move around positive nucleus at the center. They can occupy one energy level or another but not the space between energy levels.

The model in the Fig. 1.1 shows the first four energy levels of an atom. Electrons in energy level 1 (also called energy level K) have the least amount of energy. As you go farther from the nucleus, electrons at higher levels have more energy, and their energy increases by a fixed, discrete amount. Electrons can jump from a lower to the next higher energy level if they absorb this amount of energy. Conversely, if electrons jump from a higher to a lower energy level, they give off energy, often in the form of light.

For example: The energy of second state (level) is –3.4 ev and the energy of first state is -13.6ev. Then we required to 10.2 ev to raise the electron to second state as shown in Fig.1.1.

$$\triangle E = E_R \times \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \qquad \text{……..(1.1)}$$

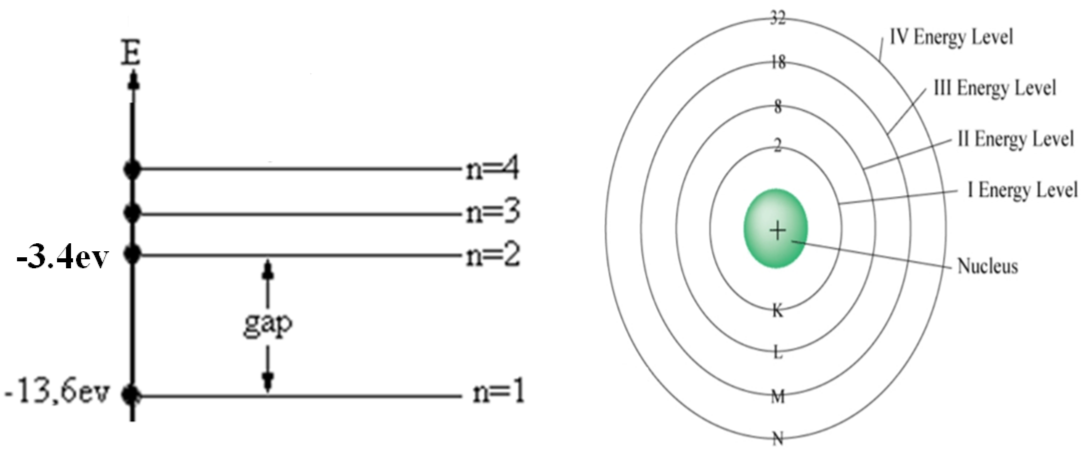


Fig. 1.1 Energy Levels in Atom.

example 1:

What is the energy which required moving an electron from the first orbit to the second orbit?

$$\Delta E = E_R \times \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) = \ 13.6 \times \left(\frac{1}{1^2} - \frac{1}{2^2} \right) = -10.2eV$$

➢ **Velocity of Electron**

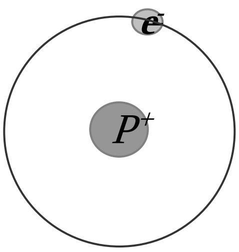
The electron velocity in orbit can be calculated by:

$$f_a \ = f_d$$

electro static

$$\frac{e^2}{4\pi\epsilon_o r^2} = \frac{m\,v^2}{r}$$

hydro static



$$v = \sqrt{\frac{e^2}{4\pi m\epsilon_o r}} \qquad \text{… …. (1.2)}$$

Where m: mass of electron, e: charge of electron, v: electron velocity.

r: a radius of orbit, ϵ_o: permittivity of space = 8.85*10^{-12} F/m.

The charge of electron (*e*) is : 1.6*10^{-19}C.

The mass of electron (*m*) is : 9.1*10^{-31}Kg.

According to eqn.(1.2) *__Bohr developed__* a model which contain three postulate :

1. The angular momentum ($m\ v\ r$) of the electron is quantized and should be an integer multiple by h/2π :

$$p = m\,v\,r = \ n\,\frac{h}{2\pi} \qquad \text{… … (1.3)}$$

h : is Plank's constant = 6.62 * 10^{-34} J.s.

2. Electromagnetic radiation is emitted if an electron initially moves from an orbit of total energy E_i to lower orbit of energy E_f. The frequency of the emitted radiation is equal to:

$$f = \frac{\Delta E}{h} = \frac{E_i - E_f}{h} \qquad \text{… … . (1.4)}$$

3. An atom has a finite state of energy. These states are separated and the electron in which state is stationary and non-radiating.

Hint:

If we want the radius of orbit (r) by the number of state (n) ,we can use:

From eqn.(1.2) and eqn.(1.3) we can write:

$$r_n = \frac{n^2\, h^2\, \epsilon_o}{\pi\, m\, e^2} \qquad \text{… … . . (1.5)}$$

From eqn. (1.5) When n =1

⇨ $r_1 = 5.29{*}10^{-11}$ m ➡ Bohr radius ≡ Hydrogen radius (a_o)

$$r_n = n^2 * a_o \qquad \text{……..(1.6)}$$

example 2:

What is the frequency of the electromagnetic wave which emitted from the electron transition from the third orbit to the second orbit?

$$\Delta E = E_R \times \left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right) = -13.6 \times \left(\frac{1}{3^2} - \frac{1}{2^2}\right) = 1.8eV$$

$$\Delta E = hf$$

$$f = \frac{\Delta E}{h} = \frac{1.8 \times 1.6 \times 10^{-19}}{6.62 \times 10^{-34}} = 4.5 \times 10^{14}\, Hz$$

example 3:

Calculate the radius of the orbit and the electron velocity in the second orbit of the boron atom?

$r_n = n^2 * a_o$

$r_2 = 2^2 * 5.29 * 10^{-11}$

$= 2.116 * 10^{-10}$ m

$$v = \sqrt{\frac{e^2}{4\pi m\varepsilon_o r}} = \sqrt{\frac{(1.6\times10^{-19})^2}{4\pi\times9.1\times10^{-31}\times8.85\times10^{-12}\times2.116\times10^{-10}}}(m/s)$$

example 4:

Find the orbital angular momentum of an electron in the second orbit?

$$P = mvr = n\frac{h}{2\pi} = 2\times1.05\times10^{-34} = 2.1\times10^{-34}\,J.s$$

1.3 Electron Energy in Orbit:

The total energy of electron in orbit around the nucleus is the sum of kinetic energy and electrostatic energy, that means:

E_{Total} = electrostatic (work) + kinetic energy

$$K.E. = \frac{1}{2}\,m\,v^2$$

Substituting about ***v*** from eqn.(1.2)

$$K.E. = \frac{e^2}{8\,\pi\,\epsilon_o r} \qquad \text{……. (1.7)}$$

The electrostatic energy represents the work, which required moving an electron from infinite to distance *r* from the positive nucleus. According to the laws of static electricity, the work is equal to:

$$W = \frac{-e^2}{4\pi\epsilon_o r} \qquad \ldots\ldots(1.8)$$

Then from eqn.(1.7) and eqn. (1.8) the total energy is:

$$E_{Total} = \frac{-e^2}{8\pi\epsilon_o r} \qquad \ldots\ldots(1.9)$$

Eqn. (1.9) shows that the electron energy is negative when it bounded to atom. If the total energy of electron is greater than zero, then the electron has enough energy to separate from atom.

Hint:

If we want total energy (E_{Total}) by number of state (n) :

By substituting about ***r*** from eqn.(1.5) we get:

1

$$E_{Total} = \frac{-me^4}{8h^2\epsilon_o^2} \times \frac{1}{n^2} \qquad \ldots\ldots(1.10)$$

The magnitude $\frac{-me^4}{8h^2\epsilon_o^2}$ is constant and equal to -13.6 eV which represents the energy of electron in ground state.

Then we can write eqn.(1.10) as:

2

$$E_{Total} = E_R \times \frac{1}{n^2} \qquad \ldots\ldots(1.11)$$

$\boldsymbol{E_R}$ **= -13.6 eV** .

Hint:

Electron Volt (*eV*) : Unit of Energy.

For energies involved in electron devices, '**joule**' is too large a unit. Such small energies are conveniently measured in **Electron Volt** (**eV**).

*The **electron volt** is the kinetic energy gained by an electron, initially at rest, in moving through a potential difference of 1 volt.* Since :

$e = 1.6 \times 10^{-19}$ Coulomb.

$1\ \text{eV} = 1.6 \times 10^{-19}\ \text{C} \times 1\ \text{V} = 1.6 \times 10^{-19}$ joule.

Electron Volt unit represent the energy of electron at potential equal 1 volt.

1.4 Potential Energy:

Potential energy is defined as the potential multiplied by charge:

$E = e * V.$

Where e : is the charge of electron and V : is the potential.

example 5:

An electron at rest is accelerated through a potential difference of 100 V. *Calculate its final kinetic energy in* J *and* eV. *What is the final velocity of the electron?*

Sol : The final kinetic energy of the electron is

$E_K = e \times 100 = 1.6 \times 10^{-19} \times 100 = 1.6 \times 10^{-17}\ \text{J} = 100\ \text{eV}.$

If v is the final velocity of the electron, we have

$$E_K = \frac{1}{2} m v^2$$

$$v = \sqrt{\frac{2E_K}{m}} = \sqrt{\frac{2 \times 1.6 \times 10^{-17}}{9.1 \times 10^{-31}}} == 5.92 \times 10^6 \, m/s$$

H.W:

An ion has a positive charge numerically equal to twice the electronic charge. The mass of the ion is 7360 *times that of an electron. The ion is initially stationary and accelerated through a potential difference of* 2 kV. *Calculate the velocity and the kinetic energy acquired by the ion.*

1.5 Energy Band Structure:

Due to intermixing of atoms in solids, instead of single energy levels, there will be bands of energy levels formed. These set of energy levels, which are closely packed are called "**Energy bands**".

Valence band (Ev): is the highest energy level filled by electrons at **0^{o}K temperature.**

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Conduction band (Ec): is the first unfilled band above the valence band as shown in Fig.1.2.

$$\mathbf{E_g = E_C - E_V}$$

E_g: energy gap.

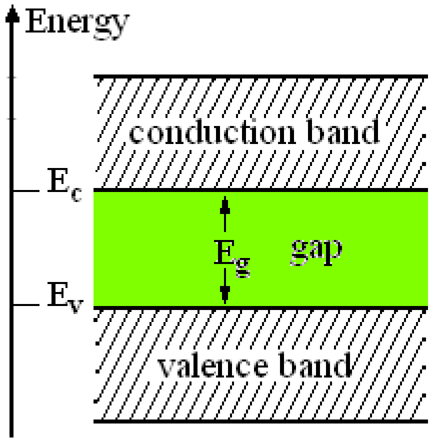

Fig.1.2 Energy Band Structure.

1.6 Insulator, Semiconductor and Conductor

On the basis of the band structure, crystals can be classified into insulators, semiconductors and conductors.

➢ **Insulator :**

Have a large forbidden gap $> 2ev$, separate the filled valence band from the vacant conduction band (Example: the forbidden gap for the carbon = 6ev).

The applied energy to an electron is too small to carry it from the filled band to the vacant band. So the conduction is impossible and the carbon is an ***Insulator***. The energy band structure of an insulator is shown in Fig. 1.3.

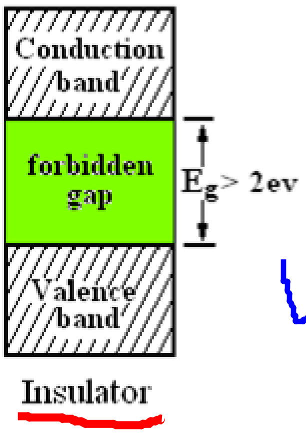

Fig. 1.3 Energy Band Structure in Insulator.

- **Semiconductor:**

The forbidden gap is small < **2ev** (Ge: germanium and Si: silicon) at 0^{o}K. Energy cannot be acquired from an applied field, so the valence band remains fill, and the conduction band empty, and it is ***insulator at low temperature***. At the temperature increase, some of these valence electrons obtain thermal energy greater than E_g , and the electrons move into conduction band. These are free electrons can move under the effect of a small applied field, and result a current. The Insulator has now become slightly conducting; it is a Semiconductor, which has a free electrons in a conduction band and a holes in a valence band. The band diagram of a semiconductor is given in Fig. 1.4.

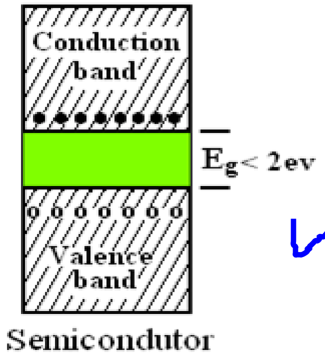

Fig. 1.4 Energy Band Structure in Semiconductor.

- **Conductor:**

Under the effect of an applied electric field, the electrons acquire additional energy and move into higher state. Since these mobile electrons result a current, this solid is ***a conductor***, and the filled region is the conduction band. Overlapping is happen between the valence and conduction bands. The band diagram of a conductor is given in Fig. 1.5.

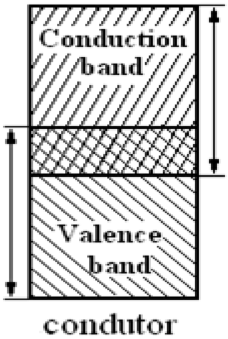

Fig. 1.5 Energy Band Structure in conductor.

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