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CHAPTER ONE (PHYSICS OF SEMICONDUCTORS)

In this chapter, the elementary theory and material properties of semiconductors will be studied as an introduction for Semiconductor Electronics.

Electron Configuration

Electrons are not placed at fixed positions in atoms, but we can predict approximate positions of them. **These positions are called energy levels or shells of atoms. The lowest energy level is 1 and it is denoted with integer $n = 1, 2, 3, 4, 5, 6, \dots$ or letters starting from K, L, M to Q. An atom can have a maximum of 7 energy levels and electrons can change their levels according to their energies.** Each energy level has a different number of electrons. For example, we find the number of electrons in an energy level with the following formula;

$$N_e = 2n^2 \quad \text{Eq.1.1}$$

Number of electrons in the 1st energy level (K) has; $N_{eK} = 2n^2 = 2 \times (1)^2 = 2$ electrons

Number of electrons in the 2nd energy level (L) has; $N_{eL} = 2n^2 = 2 \times (2)^2 = 8$ electrons

Number of electrons in the 3rd energy level (M) has; $N_{eM} = 2n^2 = 2 \times (3)^2 = 18$ electrons

Number of electrons in the 4th energy level (N) has; $N_{eN} = 2n^2 = 2 \times (4)^2 = 32$ electrons

Electrons are located energy levels starting from the first energy levels. If one of the energy level is full, then electrons placed following energy level.

1.1 ELECTRONS IN SILICON ATOM

Si contains 14 electrons distributed among 3 orbits K - L - M, the electrons within a given orbit occupy an electron energy shell, and each shell contains no more than a certain maximum number of electrons. The number of electrons in an orbit in silicon atom determined as:

$$N_K = 2 \times 1^2 = 2 \text{ electrons} \quad N_L = 2 \times 2^2 = 8 \text{ electrons} \quad N_M = 2 \times 3^2 = 18 \text{ electrons}$$



However, the third energy level for silicon not full, it has only four electrons. Each orbit subdivided to sub-shells as shown in figure (1- 2) ; the number of sub-shells in an orbit determined by its sequence in atom orbits. Each sub-shell has maximum number of electrons. In a defined material atom, the lowest energy state is the sub-shell (S) must be filled by its maximum electron capacity before beginning to fill the second lowest sub-shell and so on.

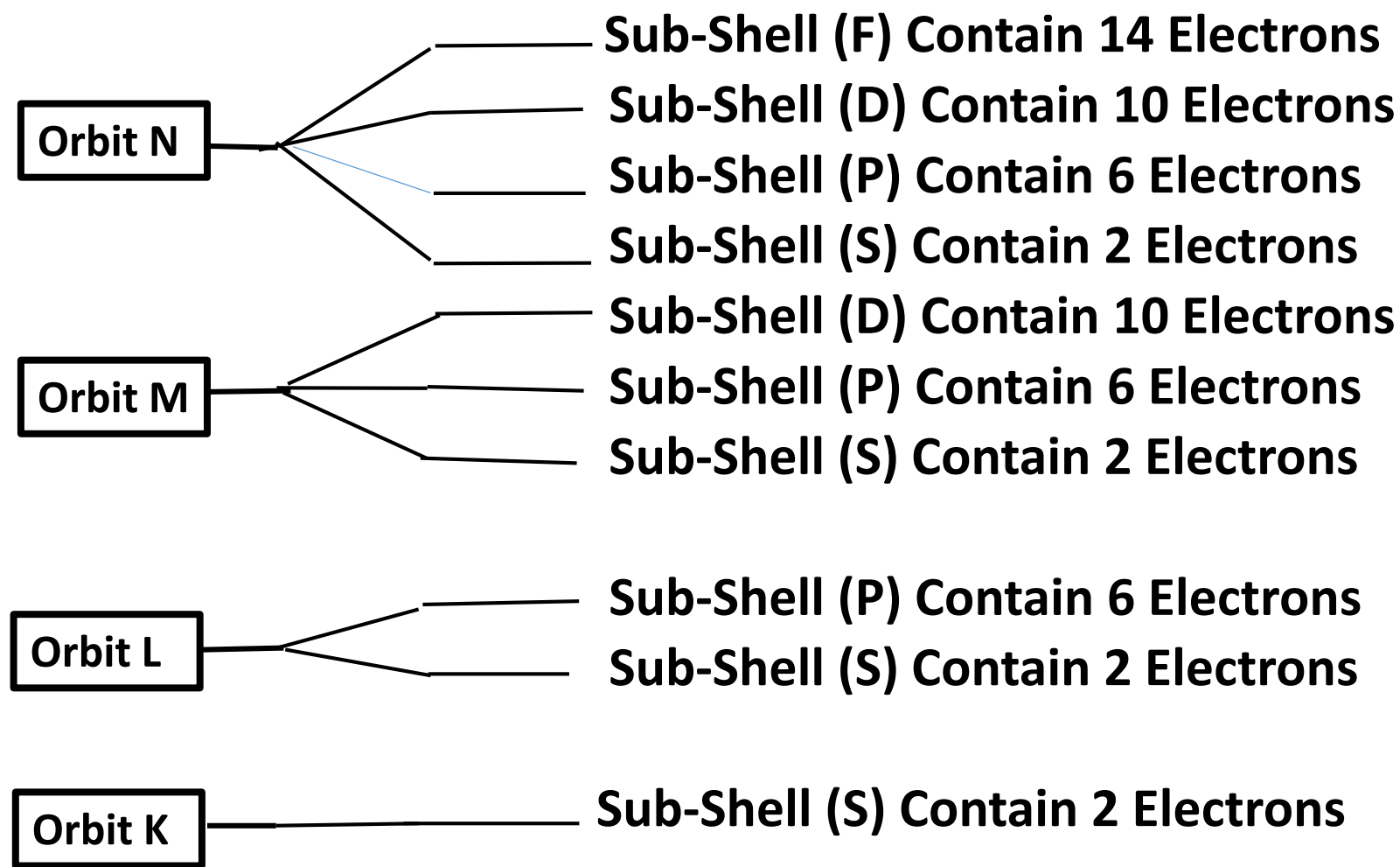


Figure 1-2 Orbits or Shells and Sub-Shells in Atom

The maximum electronic capacity for the sub-shells in atom is two electrons in sub-shell (S), six electrons in sub-shell (P), ten electrons in sub-shell (D), and fourteen electrons in subshell (F). The valance electrons in insulators are tightly bound to its nucleus, so that potential energy conserved in nucleus of insulators is more than that exists in nucleus of conductor atoms

WHY DO THE ELECTRON SHELLS BEGIN NAMED WITH K, L, M, N, O AND NOT WITH A, B, C?

The names of the electron shells come from Charles G. Barkla. He noticed that atoms appeared to emit two types of X-rays. The two types of X-rays differed in energy and Barkla originally called the higher energy X-ray type A and the lower energy X-ray type B. He later renamed these two types K and L since he realized that the highest energy X-rays produced in his experiments might not be the highest energy X-ray possible. He wanted to make certain that there was room to add more discoveries without ending up with an alphabetical list of X-rays whose energies mixed up. As it turns out, the K type X-ray is the highest energy X-ray an atom can emit. It produced when an electron in the innermost shell knocked free and then recaptured. This innermost shell now called the K-shell, after the label used for the X-ray.

Example (1):

Write the electronic configuration of silicon has 14 electrons in its atom, determine in which sub shell and in which orbit and how many electrons in the highest sub shell energy.

Solution:

The electronic configuration of silicon as follows,



The highest sub shell energy lies in (M) orbit, in the sub shell (p) which is not fully occupied, it has only 2 electrons

Example (2):

Write the electronic configuration of iodine (I) has 53 electrons in its atom, determine in which sub shell and in which orbit and how many electrons in the highest sub shell energy.

Solution:

The electronic configuration of iodine (I) as follows,



The highest sub shell energy lies in (N) orbit, in the sub shell (F) is not fully occupied, it has only seven electrons

If there is no way in the world to see an atom, then how do we know that the atom is made of protons, electrons, neutrons, the nucleus and the electron cloud?

There are three ways that, scientists proved these sub-atomic particles exist. They are direct observation, indirect observation or inferred presence and predictions from theory or conjecture.

The great Periodic Table of Elements by Mendeleev gave two very important things. The regularity of the table and the observed combinations of chemical compounds prompted to infer that atoms had regular repeating properties and may be had similar structures.

Theoretical predictions about what the nature of atomic structure really was. The weights of the elements to increase as the elements advanced through the periodic chart and there seemed to be a number, called the atomic number that explained the regular chemical properties. The other big thing is that, the chart predicts the elements that they had not found. The holes filled by inference, conjecture and discovery.

J.J. Thompson was the first to observe and understand the small particles called electrons. It quickly learned that electrons formed into beams and manipulated into images. The atomic number eventually identified as the charge of the nucleus or the number of electrons surrounding an atom, which usually found in a neutral, or balanced, state. The nucleus now better explained by using neutrons and protons to make up the atomic weight and atomic number. There were now electrons equal to the atomic number surrounding the nucleus made up of neutrons and protons; the amount of new science seems to be greater even as we probe to smaller dimensions. Current theories (if correct) imply that there is even more below the next horizon-awaiting discovery.

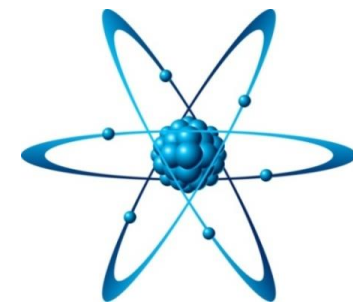
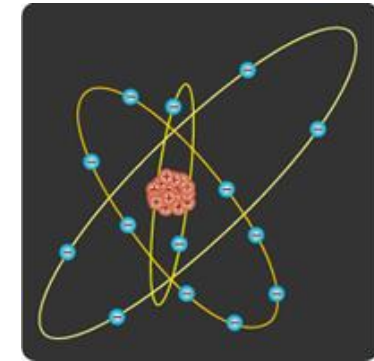
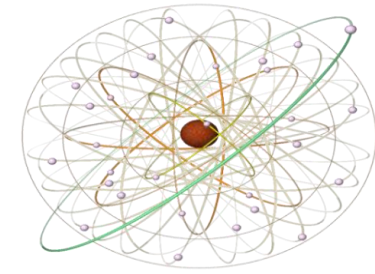
Figure 1-3a Conductor copper atom has 28 electrons in its 3 orbits and one valance electron in the fourth orbit

Figure 1-3b Semiconductor Germanium atom has 14 electrons in its two orbits and four valance electron in the third orbit

Figure 1-3c Insulator Sulfur atom has 16 electrons in its two inner orbits and six valance electron in the third orbit

1.2. SEMICONDUCTOR MATERIALS

Not all electronic devices constructed from semiconductor material. As the name implies, a semiconductor is neither an insulator like plastics nor a good conductor like copper. The mechanism by which charge flows through a semiconductor stems from the way its atoms interlock with each other to form the structure of the material. Recall that, conductors have nearly empty valance shells and tend to produce free electrons, while insulators tend to retain valance electron.



The valence shell in semiconductor atom is such that it can just fill an incomplete sub-shell, for example we find four valence electrons in the M orbit.

Semiconductor atom seeks state of stability and achieves it by sharing the valence electrons of four of its neighboring atoms, it in turn shares each of its own four electrons with its four neighbors and this contributes to the filling of their sub-shell. Every atom duplicates this process.

Therefore, every atom uses four of its own electrons, and one each of the four of its neighbors to fill its p sub-shell.

The result give stables tightly bond as crystals in lattice at regular interval because of their mutual forces. In fig.1.4, each pair of shared electron form

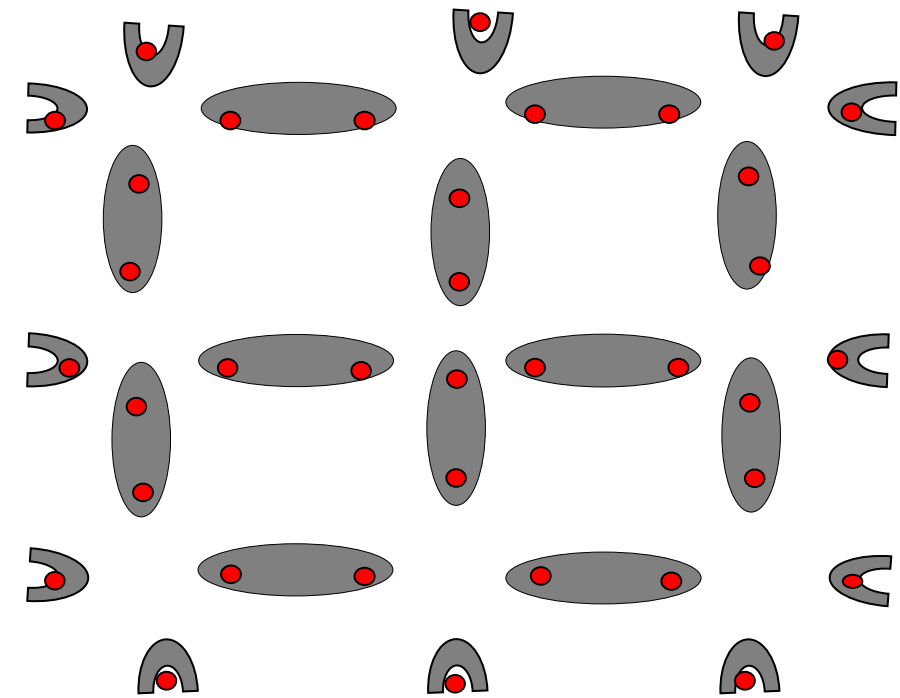


Figure 1-4 Covalent Bonding in a Semiconductor Crystal

Note only the center atom shown with a complete set of four covalent bonds, so the center atoms use its own four electrons and one from each of four neighbors. So it effectively has eight electrons in its M shell. The atoms of silicon, germanium, and carbon have the same covalent bonding, which is interlocking the atoms through electron sharing.

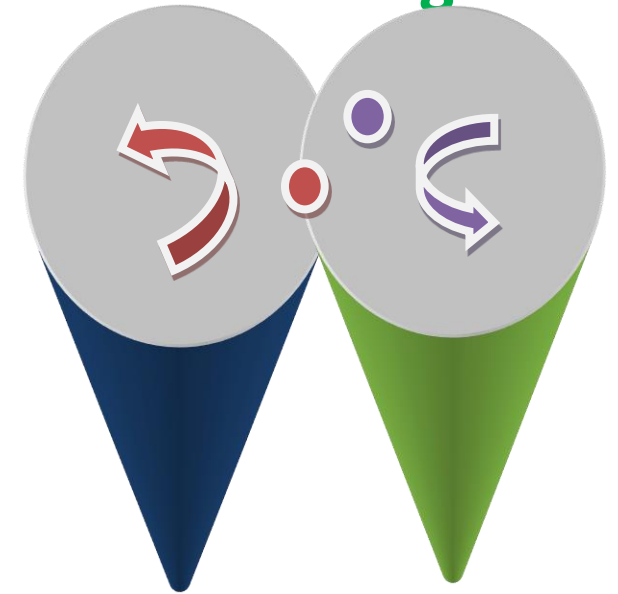
For electronic uses, **the most important property of semiconductor material is that its conductivity be modulate by external signals**, for example:

- 1-Conductivity (σ) directly proportional to the number of free charge carriers, negative electrons or positive holes, so σ regulates current in the device.
- 2- Concentration of electrons (n) or holes (p) is directly proportional to the electric field (ϵ) applied.
- 3- Light, heat, mechanical stress, magnetic fields, affect concentration of electrons (n) or holes (p).
- 4- Adding small quantities of dopants varies carrier concentration and the conductivity.

The motion of charge carriers is affected by crystal imperfections and by its presence nearby interfaces with metals, or insulator. The semiconductor to be discussed are solid mainly have single crystal structure. **Single crystal describes a solid with unusually high degree of perfection, and its atoms are located at coordinate system to form a pattern repeated itself through the solid.**

1.3. BAND THEORY OF SOLIDS

Atoms closed together. Metal atoms arranged at regular interval because of their mutual forces. **In the lattice, the atoms are so close to each other and its energy gap is very small mostly overlapped.** The electrons in the outer orbit overlap each other as in copper, figure (1.5).



Atom A Atom B
This Electron forget to which
atom it belongs

Figure 1- 5 Valance Electron in
Copper atom

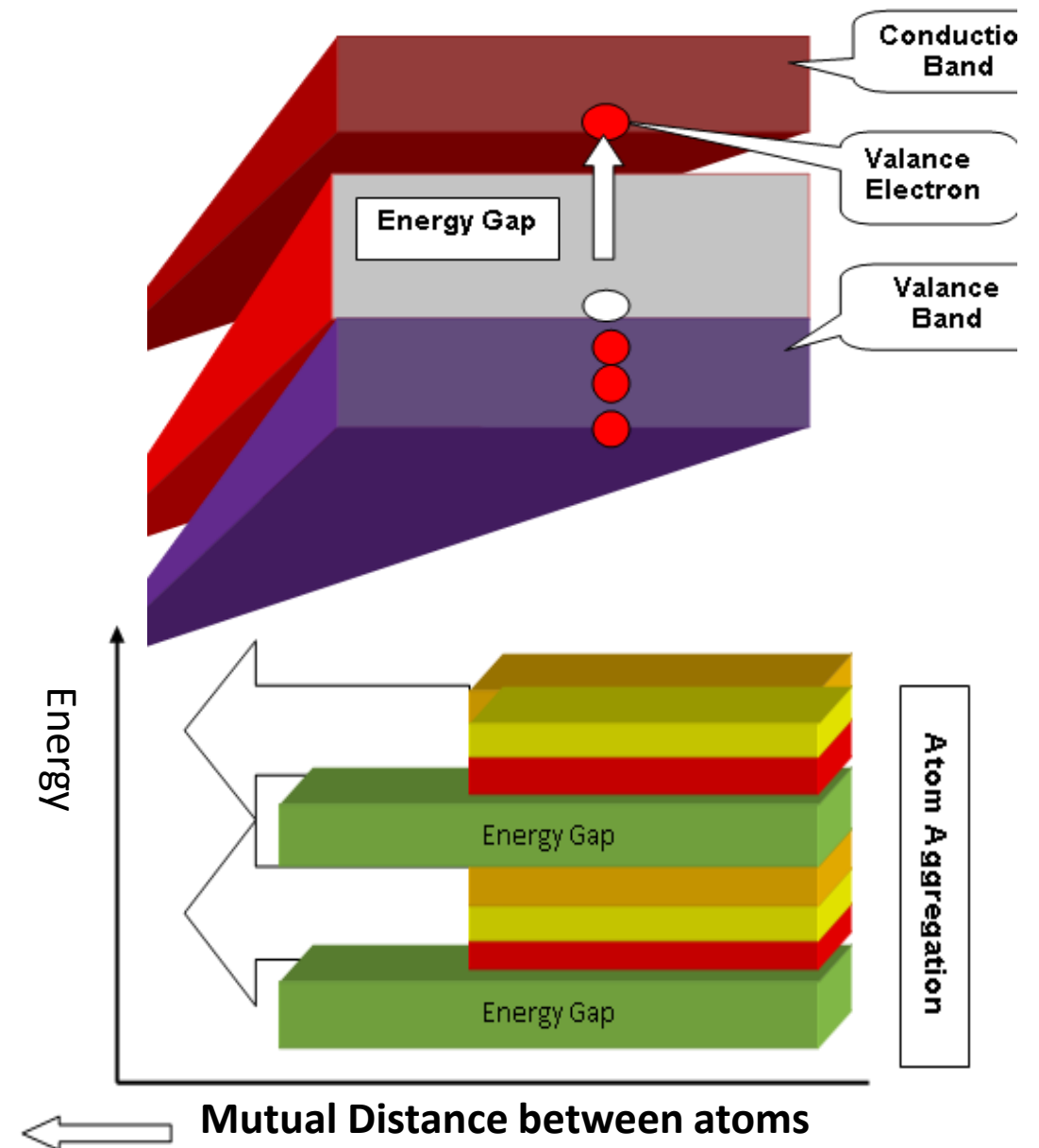
The electron in the outer orbit sometimes forgets to which atom it belongs, it can change its place with another electron from a neighboring atom. Consequently, valence electrons considered free to wander and cause conduction. In solids, the energy levels of electrons grouped into bands separated by forbidden gap as in figure (1 - 6). The lowest Energy State named valence band, and the highest one is the conduction band. In term of energy consideration this means that, conduction is possible only if we can impart kinetic energy to an electron or hole among the solid . If electric field ϵ applied, these electrons move toward the positive side, and electric current flow.

..

Figure 1.6 Energy band Diagram

Figure 1.7 Atom Structure in Solid State

In fig.1.7, the separate parallel lines correspond to energy levels of its shell and each electron has the equal probability to occupy any energy state, due to Pauli exclusion, where no two electrons have the same Energy State in the same atom in the same time. Metals are good conductors; mostly its outer orbit has only one electron. This quasi-free electron moves freely as described in figure (1- 5) before.



1.4. MATERIAL CLASSIFICATION

The material classified for three main types, **Conductors, Insulator, and Semiconductors**. The corresponding energy bands for these classifications are shown in figure (1-8) .

In Conductors, the valance electrons are free to move and constitute a sea of electrons, which are free to move upon the application of even small electric field.

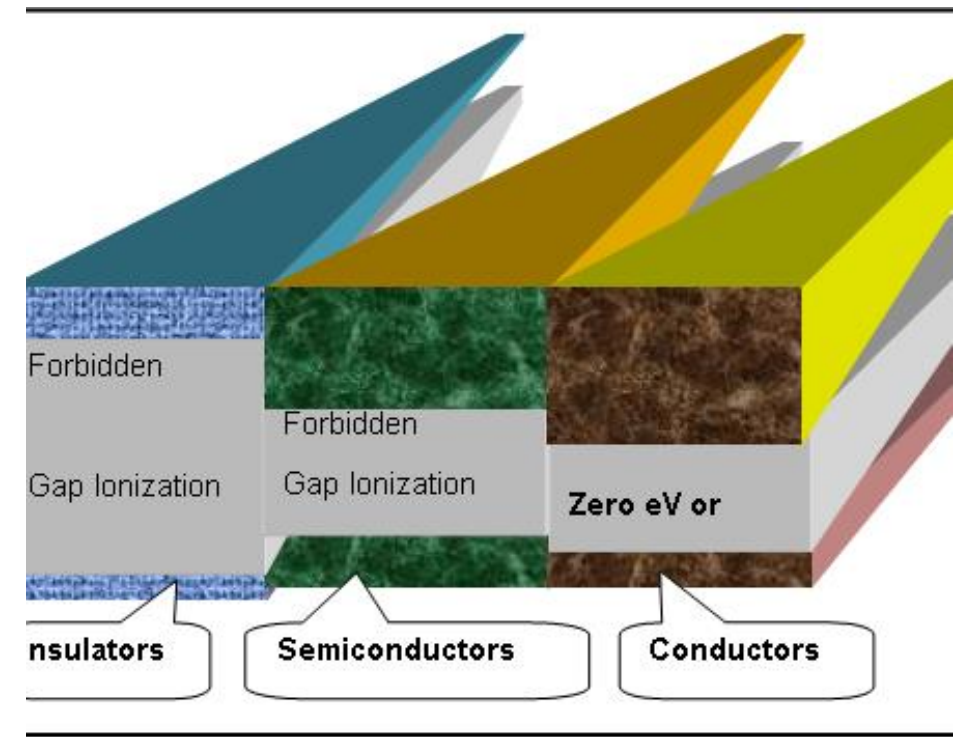
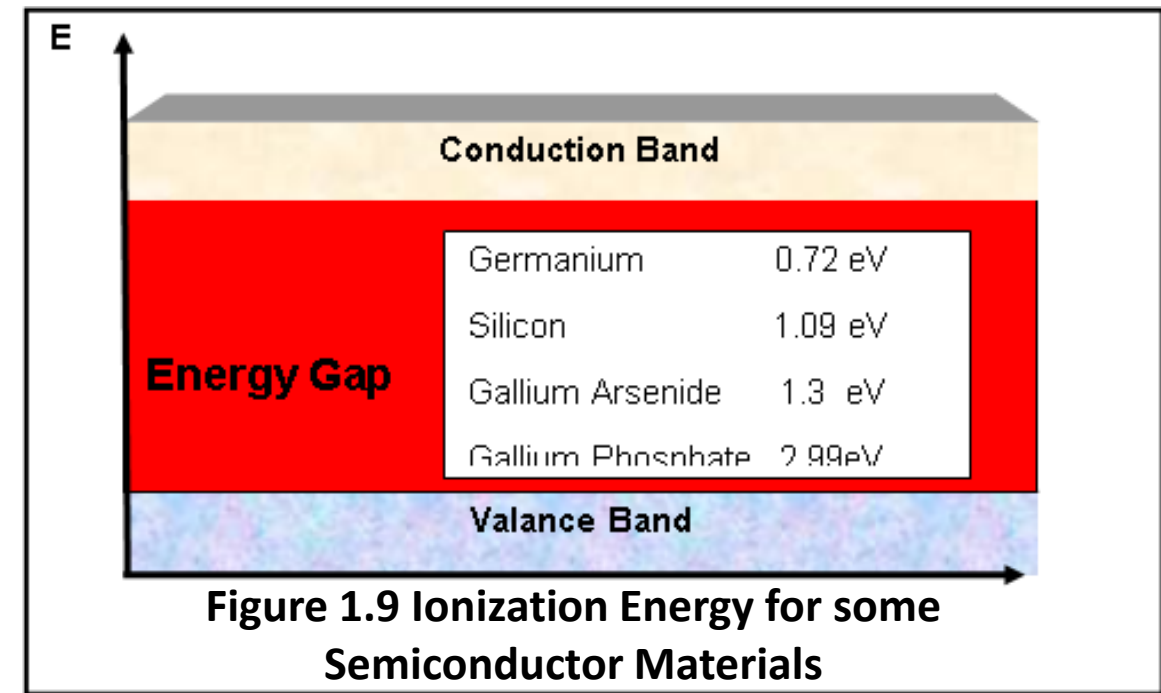


Figure 1.8 Energy Band Representations of Solids

The two bands for aluminum as an example for conductor are overlapped, thus there is no energy gap, so it is possible to move the topmost electron to the next levels, i.e., it is possible to impart a kinetic energy to the electron. Hence, conduction is possible. **In insulator such as a SiO_2 , the valance electron form strong bonds between neighboring atoms;**

these bonds are difficult to break and so, is no free electrons to participate conduction; and it has large energy band between the valance band and the conduction band. The ionization energy for some important materials to fabricate devices is showing in figure (1.9). For Si, the bonds between its atoms are moderately strong;



therefore, due to the thermal vibration some of their bonds will be broken at any temperature above absolute (-273°C); when a bond is broken, free electrons results and is able to conduction. The state where the electron had been before the bond is broken called hole. Valance electrons jump from neighboring bonds into the position of the hole and therefore additional conduction as the move of positively charged holes in the opposite direction.

gap of semiconductor is not as large as in insulators, so some of electrons will be able to jump to conduction band from valance band leaving behind holes in the valance band. Upon the application of electric field ϵ , electrons gain kinetic energy and conduct electricity..

Thus, when the energy of an electron increased, the electron will take a higher position in the direction of conduction band,

and when the energy of a hole increased, the hole will take a higher position in the direction of valance band. It is important to note that, the lowest level in conduction band designates the energy of a conduction electron at rest E_c and called the potential energy of the electron. It is important to note that, the lowest level in conduction band designates the energy of a conduction electron at rest E_c and called the potential energy of the electron.

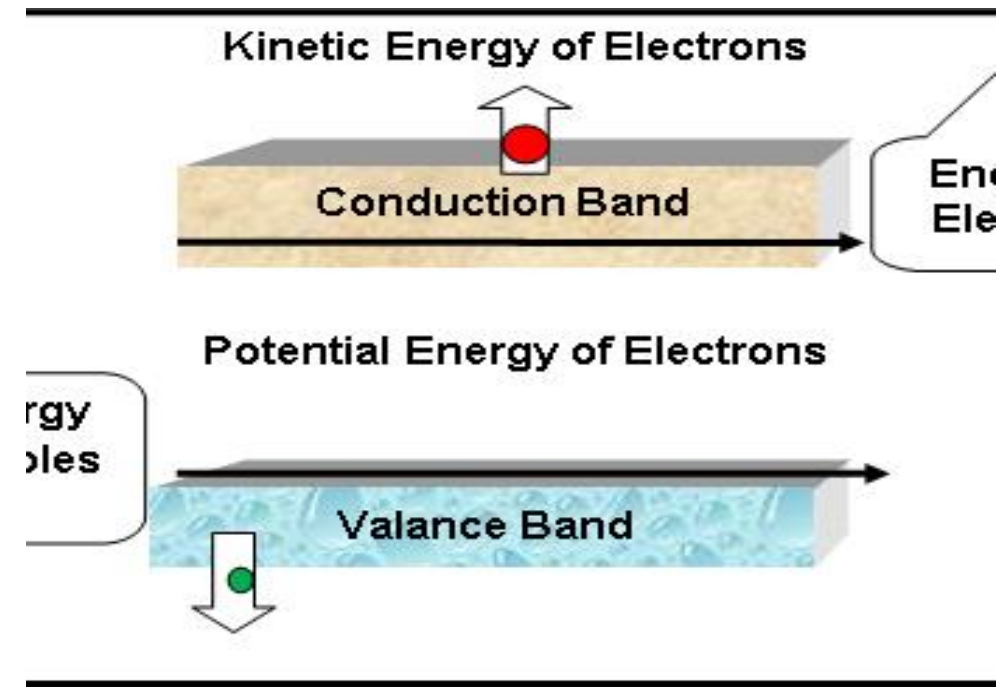


Figure 1.10 Potential and Kinetic Energies for Electrons and Holes in Energy Band Diagram

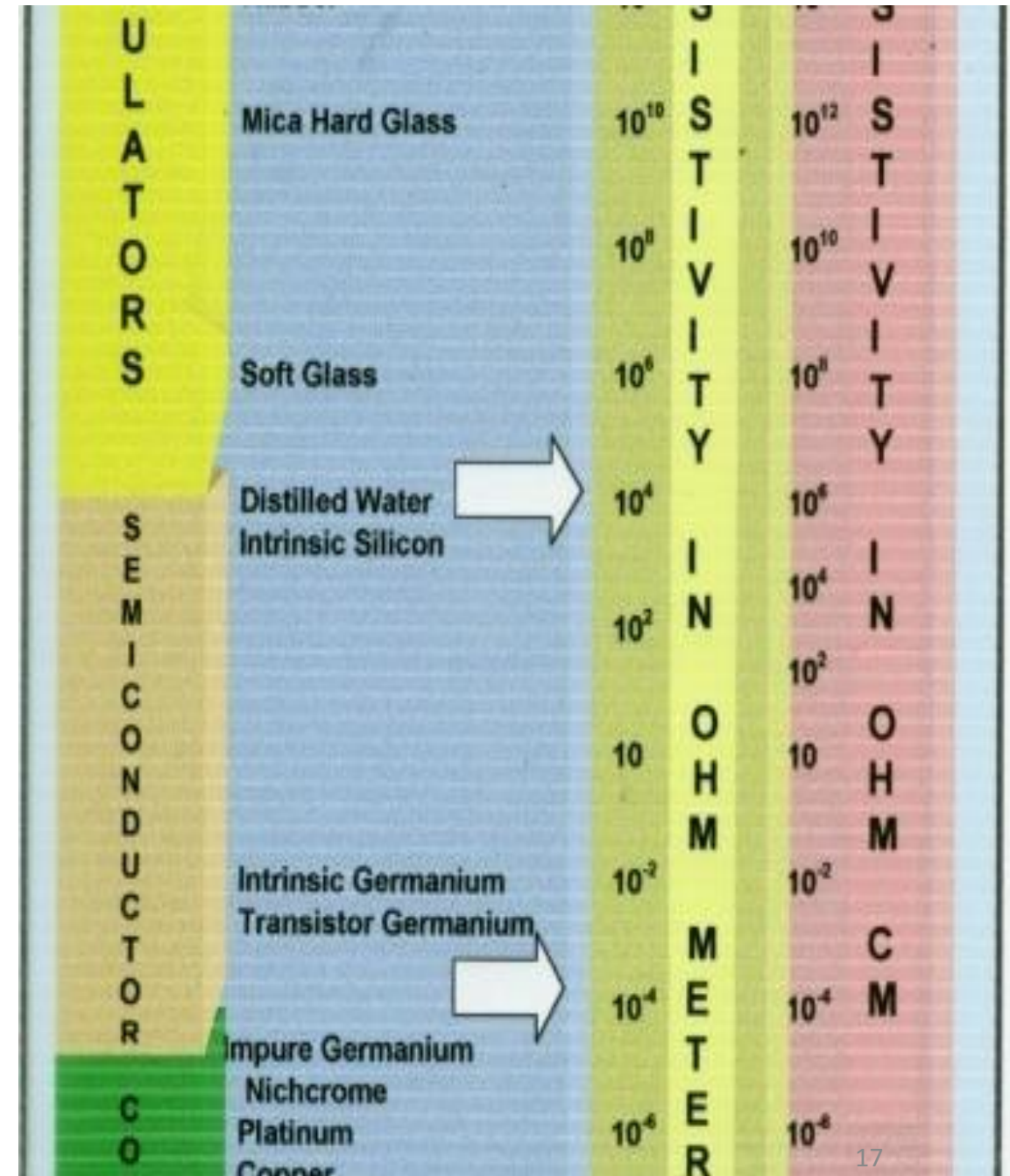
If the electron is at higher level than E_c or a hole at a lower energy than E_v , these electrons and holes have kinetic energy designates by the difference between their energies and the respective edge E_c for electrons and E_v for holes as shown in figure (1.10).

1.5. CONDUCTIVITY

Conductivity σ or resistivity ρ of a material investigated to control electric charges. The resistivity chart for common material is showing in figure (1-11). Insulators such plastics, glass, ceramic, diamond... have a very large resistivity in the order of $\Omega \cdot m$, or greater, and they have dielectric constants between One to ten. Amorphous material such as sulfur also is an insulator. Conductors have very low resistivity in the range of $10^{-8} \Omega \cdot m$ or less. Resistivity depends upon temperature. Semiconductors named because they fall between the insulator and conductors on the resistivity chart. There is no sharp dividing line; they have resistivity in the order of 10^{-4} to $10 \Omega \cdot m$ and dielectric constant in the range of 5 to 50. The electric properties of materials in third group are affecting by the purity.

Figure 1-11 Resistivity Chart for Common Materials

This is especially true for semiconductor group. Small amount of impurities is used to control the electrical properties of the material. The temperature coefficient of resistance of metals is positive at normal temperature; for semiconductors, it may be positive or negative and is nonlinear with temperature. The number of charge carriers in insulators is small but highly dependent on temperature, the number of charge carriers in semiconductors are small at low temperature but high at high temperature; in metals the number of charge carriers is always very large independent of temperature.



Example (6)

Calculate the conductivity and the resistivity of n-type silicon wafer, which contains 10^{16} electrons per cubic centimeter with an electron mobility of $1400 \text{ cm}^2/\text{Vs}$.

Solution:

The conductivity is obtained by adding the product of the electronic charge, q , the carrier mobility, and the density of carriers of each carrier type, or:

$$\sigma = q (n \mu_n + p \mu_p)$$

As n-type material contains almost no holes, the conductivity equals:

$$\sigma = q n \mu_n = 1.6 \times 10^{-19} \times 1400 \times 10^{16} = 2.24 \text{ } \Omega\text{cm}$$

The resistivity equals the inverse of the conductivity

$$\rho = \frac{1}{\sigma} = \frac{1}{q (n \mu_n + p \mu_p)}$$

In addition, equals $\rho = 1/\sigma = 1/2.24 = 0.446 \text{ } \Omega\text{cm}$

Example (7)

An n-type piece of silicon of length $L = 10$ micron has a cross sectional area $A = 0.001 \text{ cm}^2$. A voltage $V = 10$ Volts applied across the sample yielding a current $I = 100 \text{ mA}$. What is the resistance, R of the silicon sample, its conductivity, σ , and electron density, n ? If $\mu_n = 1400 \text{ cm}^2/\text{Vs}$

Solution

The resistance of the sample equals

$$R = V/I = 10/0.1 = 100 \text{ } \Omega.$$

Since , $R = L / (\sigma A)$

The conductivity obtained from:

$$\sigma = L/(R A) = 0.001/(100 \times 0.001) = 0.01 \text{ } 1/\Omega\text{ cm}.$$

The required electron density is related to the conductivity by: $\sigma = q n \mu_n$

so that the density equals:

$$n = \sigma / (q \mu_n) = 0.01 / (1.6 \times 10^{-19} \times 1400) = 4.46 \times 10^{13} \text{ cm}^{-3}.$$

1.6. ELECTRONS AND HOLES IN SEMICONDUCTORS

In pure semiconductor, conduction electrons and holes result through the breakage of bonds. Results equal concentration of electrons and holes $n = p$, these are named intrinsic electrons concentration or intrinsic holes' concentration and it is designated as n_i . This intrinsic concentration is in function of vibrations energy and material itself. Figure (1.12), shows intrinsic concentration density N_i as a function of temperature for three different semiconductor materials, Ge- Si- and Ga As, from the figure,

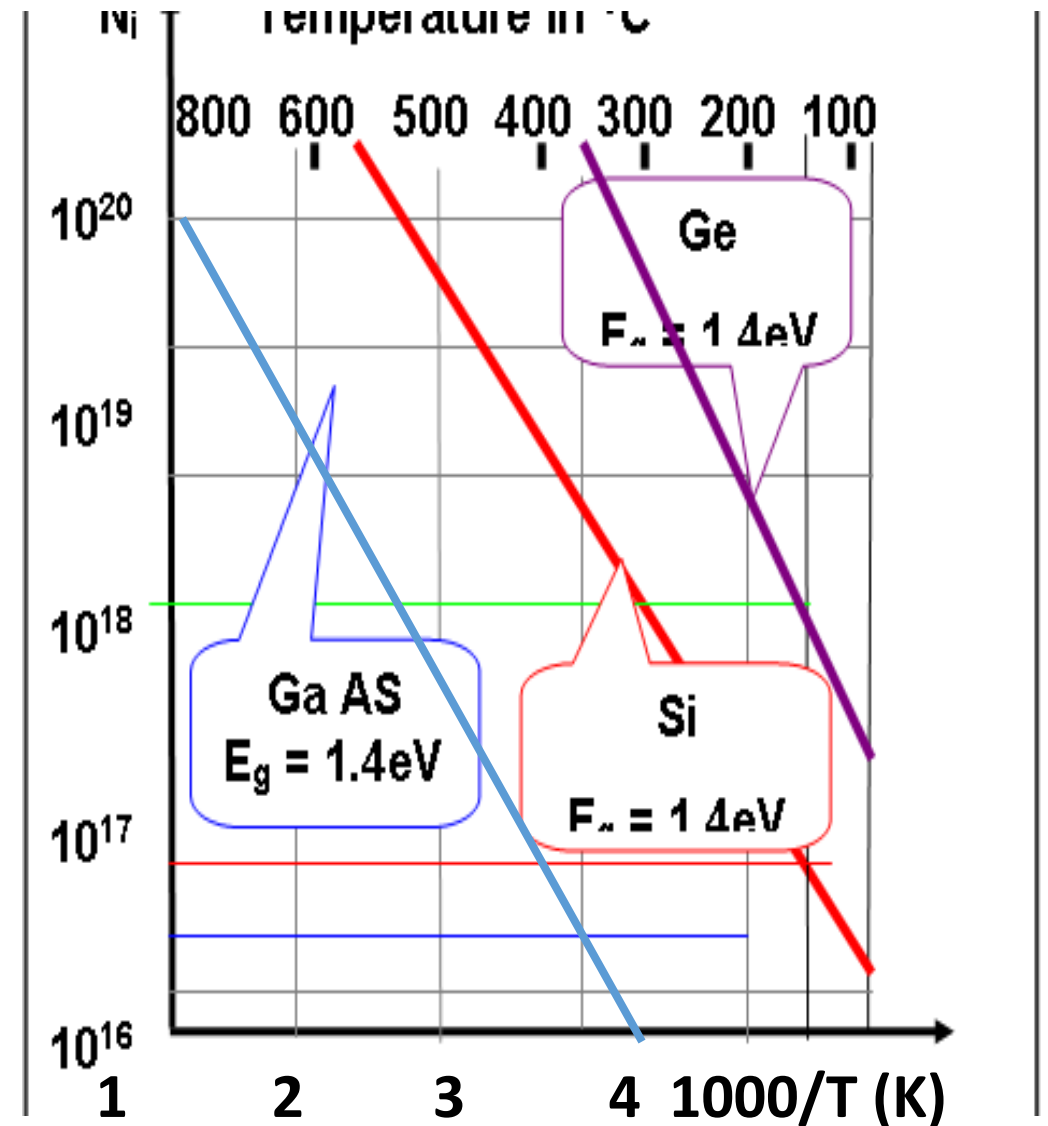


Figure 1.12 Carriers Densities as a Function to Energy Gap and Temperature)

we can indicate:

1- Intrinsic concentration densities increase very sharply with temperature.

2- Intrinsic concentration density decreases very sharply with energy gap.

$$E_a = \frac{1}{2} E_g \quad \text{Eq. 1.3}$$

This summarized by the exponential temperature dependence

$$n_i \propto e^{\left(- \frac{E_a}{KT} \right)} \quad \text{Eq. 1.2}$$

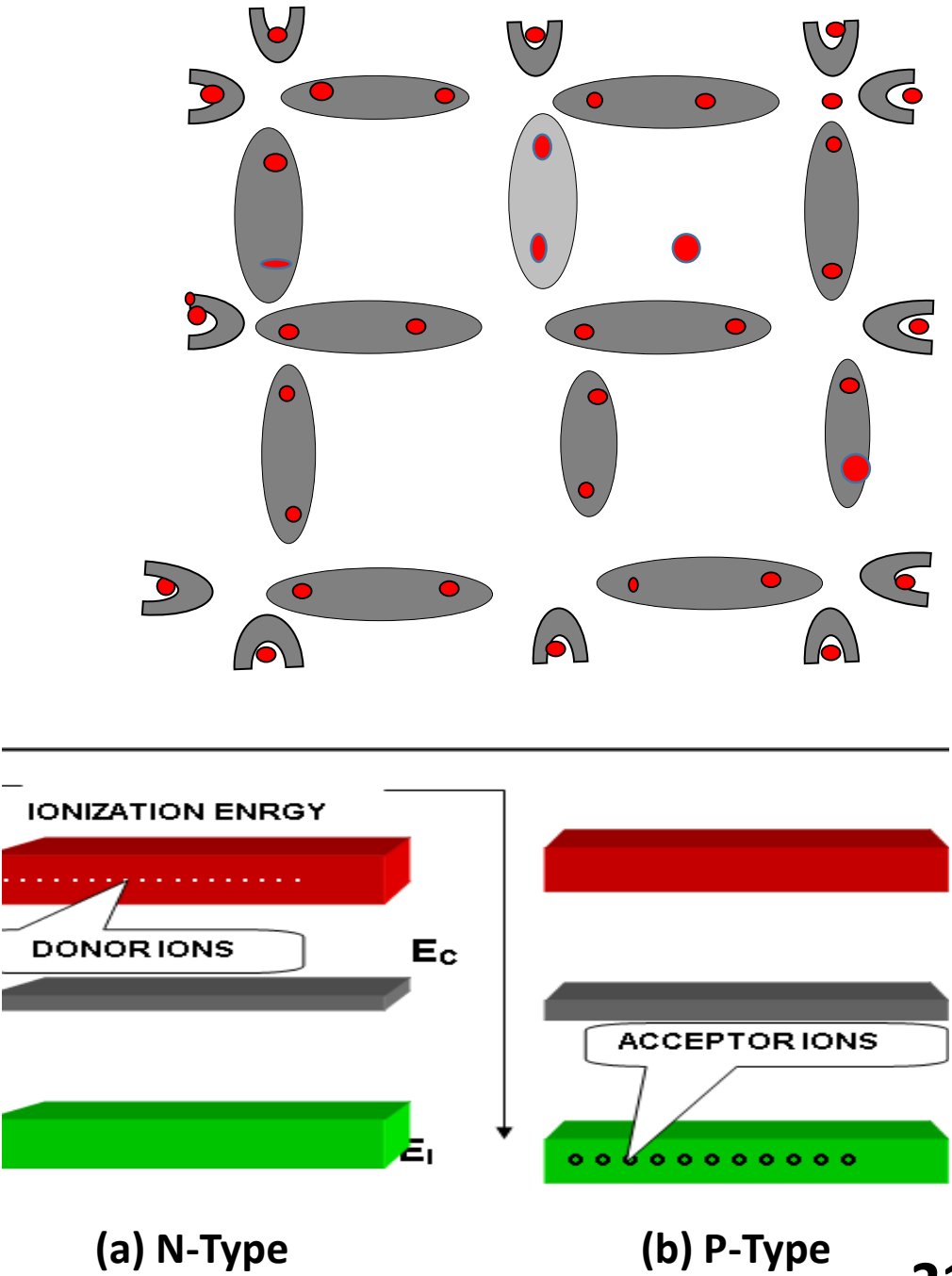
Where :

Let us now consider the case where a dopant is added to a semiconductor material, Si or Ge, which occupy a place in fourth column of the periodic table, in sense firstly the do pant will be from the fifth or the third column.

Figure 1.13 Structure Model for N - Type Material
 Fig.1.14 Energy Band Representation of Extrinsic Semiconductors

1.6.1. N-TYPE MATERIAL

If we add, a dopant has five valance electrons to which has four, figure (1.13), like Phosphorus, Antimony, Arsenic, the extra electron of the dopant cannot fit in the regular bond arrangement of the Ge or Si lattice. The ionization energy of such dopant is about 0.05 eV. At room temperature, there is enough energy to supply this amount. Column V materials in Ge or Si will be ionized at room temperature.



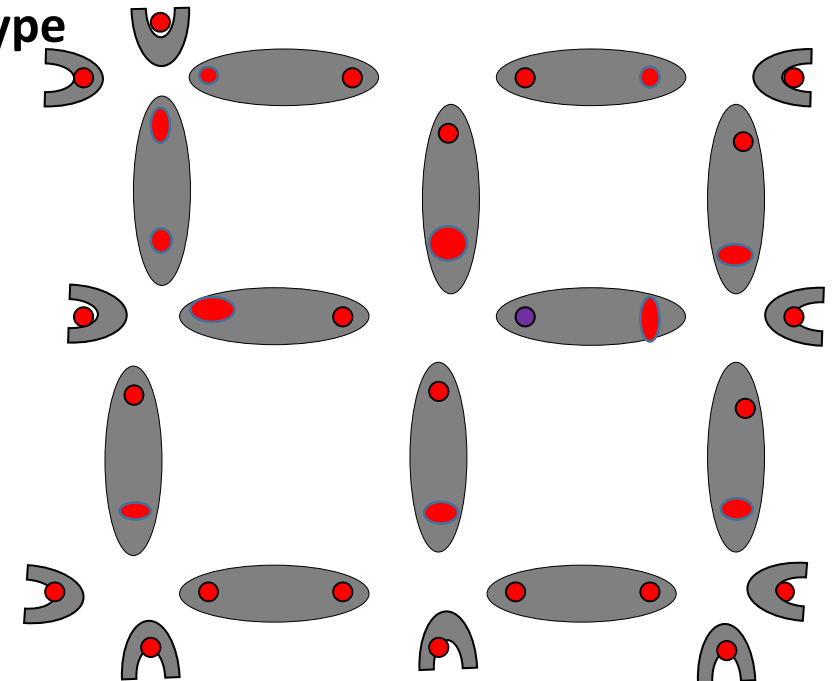
Providing equal number of conduction electrons. Such condition called complete ionization. Thus, under this condition, the density of electrons $n = N_D$ where N_D is the density of dopants from column V, and it called **DONORS** because they donate electrons to the conduction band of Ge or Si crystal. In the form of energy band representation, figure (1.14a), where conduction of electron and donor ions are equal as indicated. The donor ions denoted by positive charge slightly below the conduction band.

1.6.2. P-TYPE MATERIALS

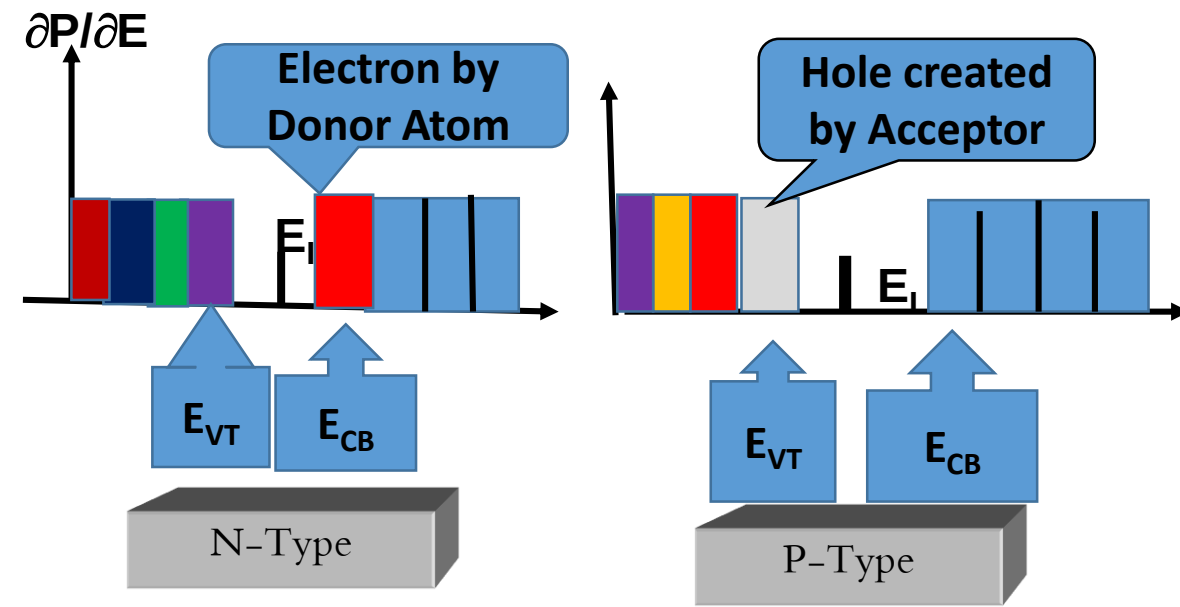
Semiconductor materials such Ge or Si doped with three valance electron materials, column III such as Boron, Aluminum, Gallium, Indium, figure (1.15). Since column III materials has one less electron than Ge or Si, we can consider it to carry a hole.

This hole removed easily with ionization energy of 0.05 eV.

Figure 1 - 15. Structure Model for P - Type



If the ionization is complete, the density of holes $p=N_A$ where N_A is the density of acceptor dopants, and it is called **ACCEPTOR** because they accept an electron from the valance band of Ge or Si crystal. As shown in figure.1.14 (b),



in case of complete ionization, the density of holes equals to density of the acceptor ions denoted by negative charge slightly above the acceptor , band energy level. In the n-type material, the concentration of electrons is much larger than of holes ($n>p$), and the current is due to electrons and the conduction is occurred in the conduction band. In the p-type material, the concentration of holes is much larger than of electrons ($p>n$), and the current is due to holes,

and the conduction is occurred in the valance band.

In general, the conduction type of the material determined by the dopant, which is present.

Concentration of majority carriers will be given by:

$$n = N_D - N_A \quad (\text{If } N_D > N_A) \quad \text{Eq. 1.4}$$

$$p = N_A - N_D \quad (\text{If } N_A > N_D) \quad \text{Eq. 1.5}$$

For N-Type, the free excess electron from the donor atom had energy sufficiently to place them in the bottom level of conduction band (E_{CB}), and the conduction occurs due to electrons in the conduction band. This means that in p-type material the conduction occurred due to holes in the valance band. If equal number of donor and acceptor atoms are added to a crystal of pure Si or Ge.

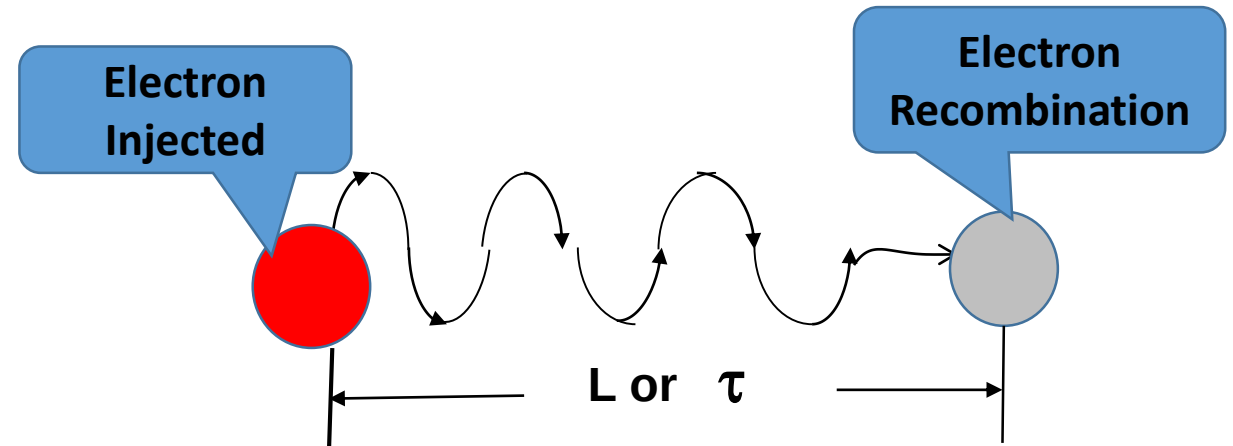


Figure 1.17. Electron Diffuses Then Recombine

Electrons from the donor atoms tend to fill the holes contributed by the acceptor atoms.

The electrical conduction approaches that of pure Si or Ge, the material then compensated. **The compensated material is an extrinsic material has the same property of intrinsic.** If an electron or hole injected to a semiconductor sample, it diffuses away from where it injected and then recombines after diffusion length L or lifetime τ as shown in figure (1.17). It observed that the injected carrier concentration decreases with time. It is diffusing in exponential function $e^{t/\tau}$ or $e^{-x/L}$. Eq.1.6, Eq.1.7, gives the average distance that the electrons or holes will diffuse before recombination.

For P-Type, the absence of one-electron leaves the valance band unfilled, so it allows transfer of electron from hole to hole, allowing the hole to change location.

• Example (11)

A germanium wafer is doped with a shallow donor density of $3n_i/2$. Calculate the electron and hole density.

Solution:

- The electron density obtained from equation

$$n_o = \frac{N_D^+ - N_A^-}{2} + \sqrt{\left(\frac{N_D^+ - N_A^-}{2}\right)^2 + n_i^2}$$

$$= n_i \left(\frac{3}{4} + \sqrt{\frac{9}{16} + 1} \right) = 2 n_i$$

And the hole density is obtained using the mass action law:

$$p_o = \frac{n_i^2}{n_o} = \frac{n_i}{2}$$

Problem (13)

Calculate the effective density of states for electrons and holes in germanium, silicon and gallium arsenide at room temperature and at 100 °C. Use the effective masses for density of states calculations.

Solution:

The effective density of states in the conduction band for germanium equals:

$$N_c = 2 \left(\frac{2 p m_e^* K T}{h^2} \right)^{3/2} =$$

$$2 \left(\frac{2 \times 0.55 \times 9.11 \times 10^{-31} \times 1.38 \times 10^{-22} \times 300}{(6.626 \times 10^{-34})^2} \right)^{3/2} = 1.02 \times 10^{19} \text{ cm}^{-3}$$

Where, the effective mass for density of states is used. Similarly, one finds the effective densities for silicon and gallium arsenide and those of the valence band, using the effective masses listed below:

The effective density of states at 100 °C (372.15 K) are obtain from:

$$N_c(T) = N_c(300k) \left(\frac{T}{300} \right)^{3/2}$$

	Germanium	Silicon	Gallium Arsenide
m_e/m_0	0.55	1.08	0.067
$N_c \text{ (cm}^{-3}\text{)}$	1.02×10^{19}	2.81×10^{19}	4.35×10^{17}
$N_v \text{ (cm}^{-3}\text{)}$	5.64×10^{18}	1.83×10^{19}	7.57×10^{18}

yielding

T = 100°C	Germanium	Silicon	Gallium Arsenide
$N_c \text{ (cm}^{-3}\text{)}$	1.42×10^{19}	3.91×10^{19}	6.04×10^{17}
$N_v \text{ (cm}^{-3}\text{)}$	7.83×10^{18}	2.54×10^{19}	1.05×10^{18}