Energy Bands in Solids

Objectives

After going through this module, the learners will be able to:

- Understand the formation of energy bands in solids
- Define forbidden gap, fermi level
- Distinguish between energy bands in conductors, semiconductors and insulators

Content Outline

- Unit syllabus
- Module Wise Distribution of Unit Syllabus
- Words You Must Know
- Introduction
- Energy Band Description of Solids
- Band in Silicon and Germanium
- Classification of Solids as Metals, Insulators and Semiconductors on The Basis of Energy Band Structure.
- Summary

Unit Syllabus

Unit 9: Electronic Devices

Chapter 14: Semiconductor electronic material, devices and simple circuits

- Energy bands in conductors, semiconductors and insulators (qualitative only)
- Semiconductors: intrinsic and extrinsic
- Semiconductor diode- I-V characteristics in forward and reverse bias, application of diode as a rectifier.
- Special purpose p-n junction diodes- LED, photodiode, solar cell, Zener diode and their characteristics, Zener diode as a voltage regulator
- Junction transistor, transistor action, characteristics of a transistor and transistor as an amplifier, common emitter configuration
- Basic idea of analog and digital signal, logic gates OR, AND, NOR, NOT, NAND

Keeping the needs of state boards in mind we have not changed the content

Module Wise Distribution Of Unit Syllabus - 10 Modules

Module 1	• Energy bands in solids • Forbidden gap • Fermi level • Energy bands in conductors, semiconductors and insulators
Module 2	• Uniqueness of semiconductors • Charge carriers in semiconductors electrons and holes • Intrinsic semiconductors • Extrinsic semiconductors p and n type • Why are p and n type semiconductors neutral?
Module 3	• p-n junction diode • Potential barrier • Depletion layer • Characteristics of p-n junction diode • forward and reverse bias, knee voltage, magnitude of bias voltages • To draw the I-V characteristics curve for a p-n junction in forward bias and reverse bias

Module 4	• Application of diode
	• Rectifier meaning and need of such device
	• half wave and full wave rectifier
	• Rectifier in our homes
	• Special purpose diode
	    ○ LED
	    ○ Photodiode
	    ○ Solar cells
	• Solar panels and future of solar energy

Module 5	• To identify a diode, a LED, a resistor and a capacitor • Use a multimeter to ○ See the unidirectional flow of current in case of a diode and a LED

	○ Check whether a given diode is in working order
Module 6	● Zener diode ● Characteristics of Zener diode ● To draw the characteristic curve of a Zener diode and to determine its reverse breakdown voltage ● How is a Zener diode different from other diodes? ● Zener diode as a voltage regulator ● Working of a Zener diode ● Zener diodes in our homes
Module 7	● Junction transistor ● Design of the transistor ● n-p-n and p-n-p ● Use a multimeter to ○ identify base of transistor ○ distinguish between n-p-n and p-n-p type transistor ○ check whether a given electronic component (e.g. diode, transistor or IC) is in working order ● Transistor action ● Characteristics of a transistor, n-p-n -common emitter
Module 8	● Understanding transistor characteristics and its applications ● To study the characteristic of a common emitter n-p-n and p-n-p transistor and to find the values of current and voltage gains ● Transistor as a switch ● Transistor as an amplifier
Module 9	● Transistor as an amplifier ● circuit diagram and understanding bias ● input and output waveforms ● Phase change

Module 10	● Analog signals ● logic gates ● truth tables ○ OR gate ○ AND gate ○ NOT gate ○ NAND gate ○ NOR gate

Module 1

Words You Must Know

- **Atom:** An atom is the smallest constituent unit of ordinary matter that has the properties of a chemical element. Every solid, liquid, gas, and plasma is composed of neutral or ionized atoms
- **Atomic Structure:** All substances are made from atoms. Each atom is made of a nucleus - containing protons and neutrons - surrounded by electrons.
- **Atomic Number:** Atomic number is the number of protons in an atom. The elements are arranged in the periodic table in ascending order of atomic number.
- **Mass Number:** The mass number of an atom is the total of protons plus neutrons.
- **Electron Orbits:** Electrons revolve around the nucleus in allowed energy states called orbits. The distribution of electrons in orbits is governed by quantum numbers.
- **Nucleus:** The **atomic nucleus** is the small, dense region consisting of protons and neutrons at the centre of an **atom**, discovered in 1911 by Ernest Rutherford based on the 1909 Geiger–Marsden gold foil experiment. ... Almost all of the mass of an **atom** is located in the **nucleus**, with a very small contribution from the electron cloud.
- **Energy Level: Energy levels** inside an atom are the specific energies that electrons can have when occupying specific orbitals. A quantum mechanical system or particle that is bound i.e., confined spatially—can only take on certain discrete values of energy. This contrasts with classical particles, which can have any energy. These discrete values are called energy levels
- **Bond Energy** is the measure of **bond** strength in a chemical **bond**.
- **Valency:** The valence or **valency** of an element is a measure of its combining power with other atoms when it forms chemical compounds or molecules. The concept of

valency developed in the second half of the 19th century and helped successfully explain the molecular structure of inorganic and organic compounds.

- **Heisenberg Uncertainty Principle: It is an** indeterminacy **principle**, stated and articulated (1927) by the German physicist Werner **Heisenberg**, that the position and the velocity of an object cannot both be measured exactly, at the same time, even in theory.
- **Pauli's Exclusion Principle:** The principle states that No two electrons in an atom can have the same set of four quantum numbers.
- **Kelvin:** Absolute scale of temperature
- **eV is a unit of energy equal to (approximately) 1.6×10^{-19} joules (symbol J). By definition, it is the amount of energy gained (or lost) by the charge of a single electron moving across an electric potential difference of one volt.**
- **0K** is lowest temperature, equivalent to -273 ^{0}C

Introduction

One of the main functions of **electronic and electrical circuits is to control the current** according to the application of the device. Circuits using current have devices in which a controlled flow of electrons can be obtained. These devices are the basic **building blocks** of all the electronic circuits.

Historically, before the discovery of transistors in 1948, such devices were mostly vacuum tubes (also called valves). Like the vacuum diode had two electrodes, viz., anode (often called plate) and cathode. Triode has three electrodes – cathode, plate and grid; tetrode and pentode have 4 and 5 electrodes respectively. In a vacuum tube, the electrons can be supplied by a heated cathode and the controlled flow of these electrons in vacuum is obtained by varying the voltage between its different electrodes. Vacuum is required in the inter-electrode space; otherwise the moving electrons may lose their energy on collision with the air molecules in their path. In these devices the electrons can flow only from the cathode to the anode (i.e., only in one direction). Therefore, such devices are generally referred to as valves. These vacuum tube devices are bulky, consume high power, operate generally at high voltages (~100 V) and have limited life and low reliability.

The seed of the development of modern solid-state semiconductor electronics goes back to the 1930's when it was realised that some solid state semiconductors and their junctions offer the possibility of controlling the number and the direction of flow of charge carriers through them.

Simple excitations by light, heat or small applied voltage can change the number of mobile charges in a semiconductor.

Note That

- The supply and flow of charge carriers in the semiconductor devices are **within the solid itself,** while in the earlier vacuum tubes/valves, **the mobile electrons were obtained from a heated cathode and they were made to flow in an evacuated space or vacuum.**
- No external heating or large evacuated space is required by the semiconductor devices.
- **Semiconductor devices are small in size, consume low power, operate at low voltages**
- **Semiconductor devices have long life and high reliability.**

Now even the Cathode Ray Tubes (CRT) used in television and computer monitors which work on the principle of vacuum tubes have been replaced by Liquid Crystal Display (LCD) monitors supporting solid state electronics. Much before the full implications of the semiconductor devices was formally understood, a naturally occurring crystal of ***galena*** **(Lead sulphide, PbS)** with a metal point contact attached to it was used as a detector of radio waves.

In this module we will introduce the basic concepts of semiconductor physics.

In subsequent modules of the unit we would discuss some semiconductor devices like junction diodes (a 2-electrode device) and bipolar junction transistor (a 3-electrode device). We will also consider few circuits illustrating their applications

Energy Band Formation in Solid

According to the Bohr atomic model, in an **isolated atom** the energy of any of its electrons is decided by the orbit in which it revolves. However, when the atoms come together to form a solid they are close to each other. So,The outer orbits of electrons from neighbouring atoms would come very close or could even overlap. **This would make the nature of electron motion in a solid very different from that in an isolated atom.**

Inside the crystal each electron has a unique position and no two electrons see exactly the same pattern of surrounding charges. Because of this**, each electron will have a different energy level.**

Band theory is based on quantum mechanics and comes from the theory of orbitals. If multiple atoms are brought together their atomic orbitals will combine to form a layer of orbitals each with a different energy. For a solid the energy levels are so close that they can be considered to form a continuum.

These different energy levels with almost continuous energy variation are called energy bands.

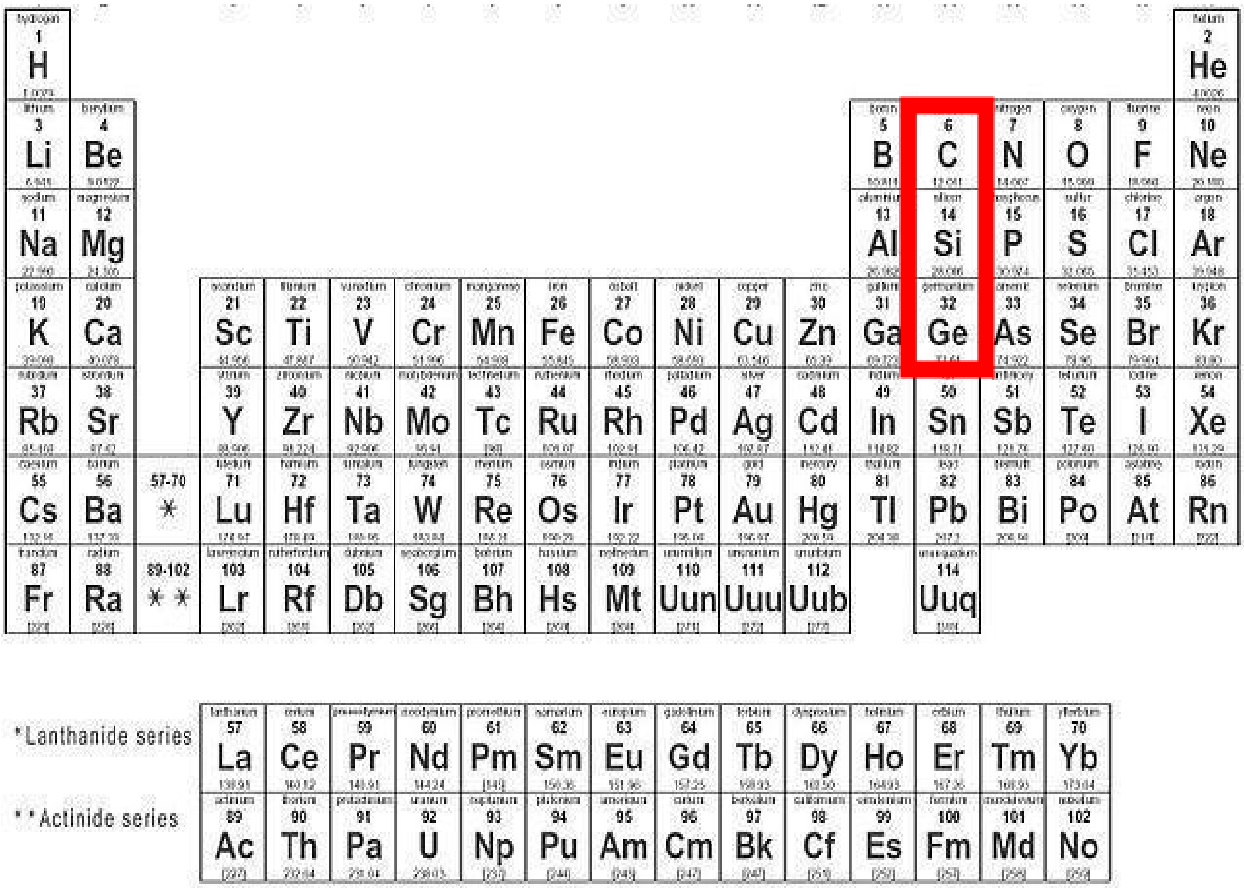
What is Means By Energy Bands

For an isolated atom, the field in which the electrons move is that due to the nucleus of the atom only. The discrete energy values of the electron therefore have sharp values which according to Bohr are called energy levels. In a solid, because of the closeness of different atoms, the outer (valence) electrons in a particular atom are under the influence of the nuclear fields of a large number of neighbouring atoms. The effective field value thus has a spread (range of close values) this causes the valence electron energy values to also have a spread. Because of the spread, and Pauli's exclusion principle and Heisenberg's uncertainty, there is a range of energy values that the collection of valence electrons may have. We therefore have energy bands, rather than sharp energy states for the outermost electrons in the solid.

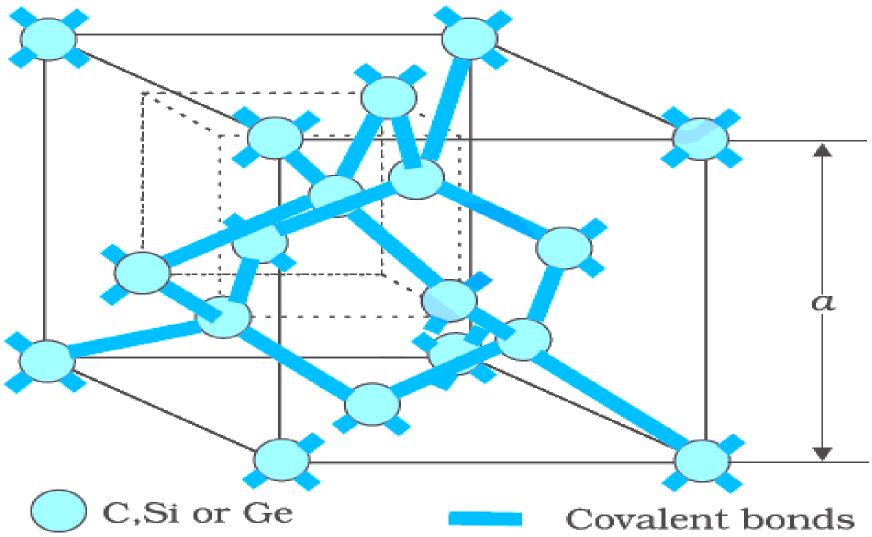
The inner electrons of one atom are not influenced by the neighbouring electrons of other atoms.

Band in Silicon and Germanium

The bonding in carbon, Si and Ge will be the same as the number of electrons in their outermost orbits are the same (four each). They form the stable inert gas configuration through covalent bonding



Si and Ge are the two semiconductors widely used for designing electronic devices



Three-dimensional diamond-like crystal structure for Carbon, Silicon or Germanium with respective lattice spacing equal to 3.56, 5.43 and 5.66 Å.

Think About This

- Why should Carbon, Silicon or Germanium have the same structure?
- In covalent bonding would you have a valence band, conduction band?
- It is possible that some of the electrons from the valence band may gain external energy to cross the gap between the conduction band and the valence band.

Then these electrons will move into the conduction band.At the same time, they will create vacant energy levels in the valence band where other valence electrons can move.

Thus **the process creates the possibility of conduction due to electrons in the conduction band as well as due to vacancies –these are called holes-so holes in the valence band.**

In the bond description of solids, the bonding **electrons and holes** have been considered as highly localized.

Considering the **Si or Ge crystal, say it contains N atoms**.

Electrons of each atom will have discrete energies in different orbits.

The electron energy will be same if all the atoms are isolated, i.e., separated from each

other by a large distance. However, in a crystal, the atoms are close to each other (at a separation of 2 to 3 angstrom) and therefore the electrons interact with each other and also with the neighboring atomic nucleus.

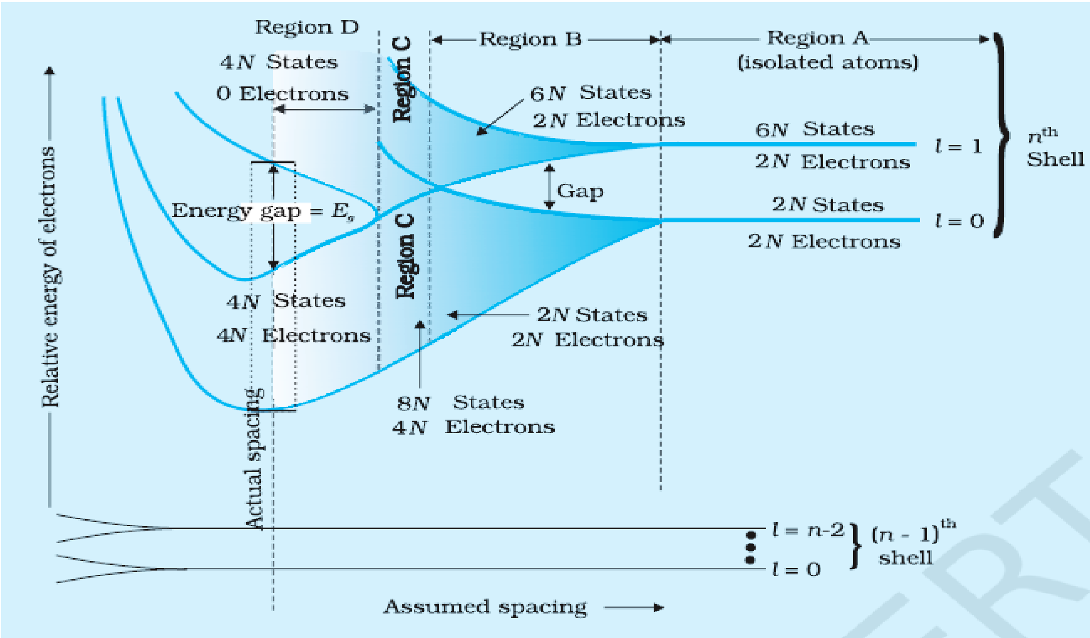
The overlap (or interaction) will be more felt by the electrons in the outermost orbit while the inner orbit (or core) electron energies may remain unaffected.

Therefore, for understanding electron energies in Si or Ge crystal, we need to consider the changes in the energies of the electrons in the outermost orbit only.

For Si, the outermost orbit is the third orbit (n = 3), while for Ge it is the fourth orbit (n = 4).

The number of electrons in the outermost orbit is 4 (2s and 2p electrons).Hence, the total number of outer electrons in the crystal is 4 N. The maximum possible number of outer electrons in the orbit is 8 (2s + 6p electrons).

So out of the 4N electrons, 2N electrons are in the 2N s-states (orbital quantum number $l = 0$) and 2N electrons are in the available 6N p-states.



Obviously, some p-electron states are empty as shown in the extreme right of the graphs. This is the case of well separated or isolated atoms (region A of figure)

Suppose these atoms start coming closer to each other to form a solid.

The energies of these electrons in the outermost orbit may change (both increase and decrease) due to the interaction between the electrons of different atoms, and the requirement of each electron to possess a unique and exclusive energy value.

The 6N states for l - 1, which originally had identical energies in the isolated atoms, split into a second band (carefully see the region B of figure) separated from the first one by an energy gap.

At still smaller spacing, however, there comes a region in which the bands merge with each other. The lowest energy state that is a split from the upper atomic level appears to drop below the upper atomic level that has come from the lower atomic level. **In this region (region C in figure), no energy gap exists and the upper and lower energy states get mixed.**

Finally, if the distance between the atoms further decreases, the energy bands again split apart and are separated by an energy gap E_g (**region D in figure**. The total number of available energy states (8N) has been **re-apportioned** between the two bands (4N bands).

Here the significant point is that there are exactly as many states in the lower band (4N) as there are available valence electrons from the atoms (4N).

Therefore, the **lower band** (called the **valence band**) is **completely filled** while the **upper band** is **completely empty**. The upper band is called the **conduction band.**

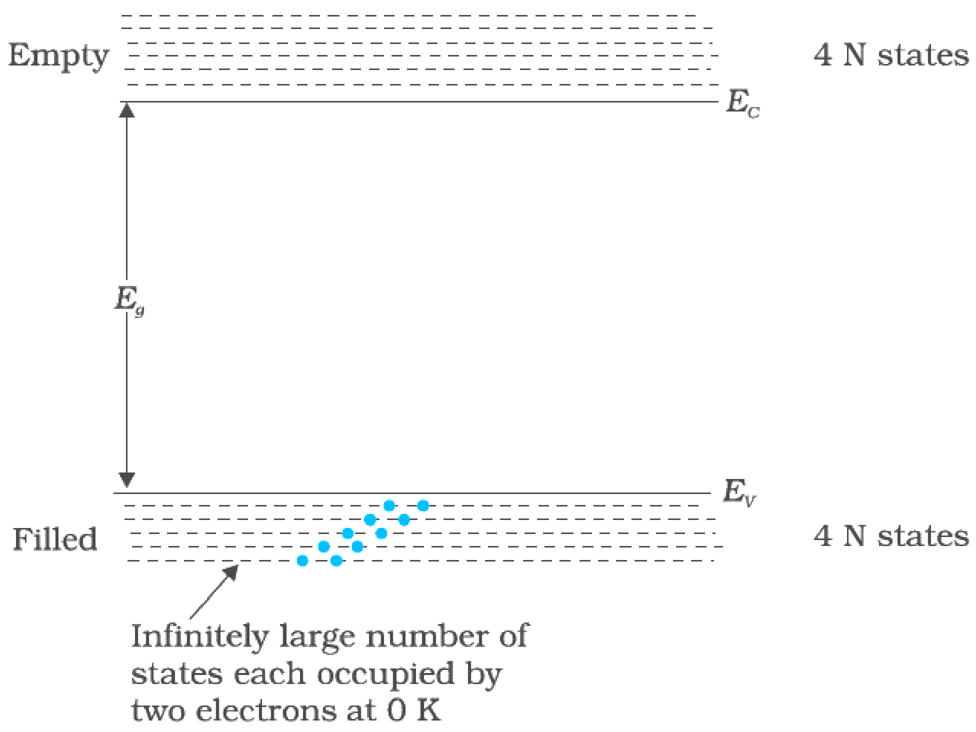
Note

The action of the electrons filling up the valence band corresponds to their forming all the bonds.

However, it is not correct to use the bond description to state that the electrons in the valence band would not move under the action of applied voltage or field. On the basis of quantum mechanics, we know that it is not possible to impart any net momentum to a completely filled band however for the motion of electrons under an electric field in solids (i.e. for an electric current) we need momentum to be given to the electrons in the direction of the field.

Therefore, the valence electrons do not conduct. The electrons in the upper band (or conduction band) can, however, gain momentum and move since there are closely spaced empty available states in the band.

It is important to realize that at equilibrium spacing, the lowest conduction band energy is Ec and highest valence band energy is E_v, Above E_c, or below E_v, there are a large number of closely spaced energy levels.



The energy band positions in a semiconductor at 0 K. The upper band, called the conduction band, consists of an infinitely large number of closely spaced energy states. The lower band, called the valence band, consists of closely spaced completely filled energy states.

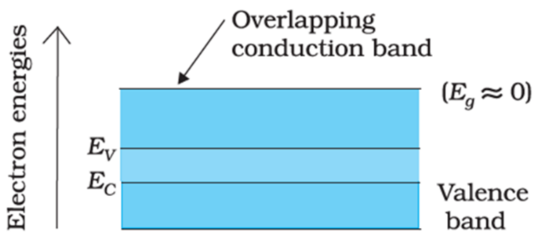
Maximum number of electrons in each energy level can be only two, according to Pauli's exclusion principle.

Classification of Solid as Metals, Insulators and Semiconductor on the Basic of Energy Band Structure

- The gap between the top of the valence band and bottom of the conduction band is called the **energy band gap (Energy gap)**.
- It may be large, small, or zero, depending upon the material. These different situations are depicted in Figure and discussed below:

Case (I): This refers to a situation, as shown in Fig. (i) and Fig (ii).

(i)



(ii)

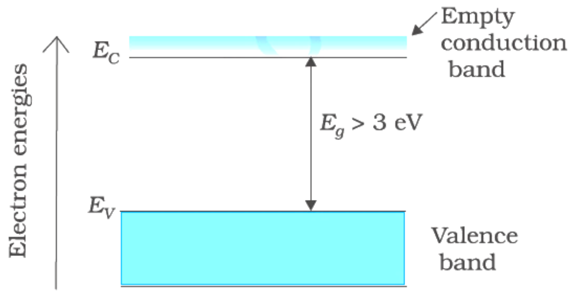
A material will be a metal

- **Either when the conduction band is partially filled and the valence band is partially empty or**
- **When the conduction and valence bands overlap.**
- **When there is an overlap, electrons from the valence band can easily move into the conduction band.**

This situation makes a large number of electrons available for electrical conduction. When the valence band is partially empty, electrons from its lower level can move to higher level making conduction possible.

Therefore, such materials are conductors the resistance of such materials is low, or the conductivity is high.

Case (II):



(b)

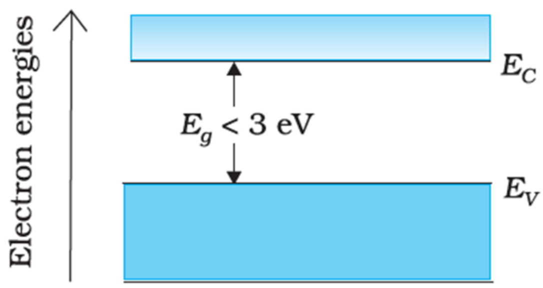
In this case, as shown in Fig (b),

- **A large band gap (Eg.) exists (Eg. > 3 eV)**

  There are no electrons in the conduction band, and therefore
- **No electrical conduction is possible.**
- **The energy gapEg is so large that electrons cannot be excited from the valence band to the conduction band by thermal excitation.**

  This is the case of insulators.

Case (III): This situation is shown in Fig. (c).



(c)

Here

- **A finite but small energy band gap($E_{.g.} < 3$ eV) exists.**
- **Because of the small band gap, some electrons can be thermally excited to the conduction band (according to Boltzmann law $n \propto \exp\{-E_g/2kT)$.**

- **These thermally excited electrons (though small in number) can move in the conduction band. Hence,**
- **The resistance would not be as high as that of the insulators.**
  This is the case of semiconductors.

We have implicitly said above, while describing the semiconductor in terms **of band gap**, that the conduction band is completely empty, in the absence of thermal energy at 0 K
Hence, we describe an **intrinsic semiconductor as one which will behave like an insulator at T = 0 K.**
It is the thermal energy at high temperatures (T >> 0 K), say close to room temperature, which excites some electrons from the valence band (thus creating an equal number of holes in the valence band) to the conduction band.
Example of Semiconductors

- **Elemental semiconductors: Si and Ge**
- **Compound semiconductors:**
- **Inorganic**: CdS, GaAs, CdSe, InP, etc.
- **Organic:** anthracene, doped phthalocyanines, etc.
- **Organic polymers**: polypyrene, polyaniline, polythiophene, etc.

Most of the currently available semiconductor devices are based on elemental semiconductors, Si or Ge and compound inorganic semiconductors.

  - However, after 1990, a few semiconductor devices using organic semiconductors and semiconducting polymers have been developed signalling the birth of a futuristic technology of polymer electronics and molecular-electronics.
  - In this unit, we will restrict ourselves to the study of inorganic semiconductors, in particular elemental semiconductors Si and Ge.
  - The general concepts introduced here for discussing the elemental semiconductors, by-and-large, apply to most of the compound semiconductors as well.

Fermi Level

Fermi level is the term used to describe the top of the collection of electron energy levels at absolute zero temperature. This concept comes from Fermi-Dirac statistics. Electrons are fermions and by the Pauli Exclusion Principle any two electrons cannot exist in identical energy states.

Fermi energy is often defined as **the highest occupied energy level of a material at absolute zero temperature**. In other words, **all electrons in a body occupy energy states at or below that body's Fermi energy at 0K.**The fermi energy is the difference in energy, mostly kinetic.

In metals this means that it gives us the velocity of the electrons during conduction. So during the conduction process, only electrons that have an energy that is close to the value of the fermi energy can be involved in the process.

This concept of Fermi energy is useful for describing and comparing the behaviour of different solids as classified above on the basis of band theory namely conductor, semiconductors and insulators. For example: a conductor will have a Fermi energy close to the conduction band, whereas a semiconductor will have a Fermi energy close to the valence band.

As the temperature of material rises above absolute zero, the probability of electrons existing in an energy state greater than the Fermi energy increases, and there is no longer any constant highest occupied level. So, it is clear, therefore, that even though the material's Fermi energy may be useful as a reference, it is not very useful at real temperatures.

Example

For a single atom the electrons move in distinct energy states. If a solid piece has N atoms,why do we say the distinct energy levels become an energy band and hold a collection of allowed energy states?

Answer

All atoms of the solid must have the same energy states, forming a shell in 3 D space.

However, the individual electrons in the outer orbits modify their energies slightly to remain in a collection of allowed energy states. Each follows the exclusion principle.

Hence a band is actually a collection of a large number of energy states.

Consider These

- **What occupies the region between the energy bands?**

  Ans: Vacuum

- **What the different ways to classify solids as metals and insulatorsn the basis of electrical conductivity**

  Ans: Metals: They possess very low resistivity (or high conductivity).

  $\rho \sim 10^{-2} – 10^{-8}$ W m

$\sigma \sim 10^{2} - 10^{8}$ S m^{-1}

Insulators: They have high resistivity (or low conductivity).

$\rho \sim 10^{11} - 10^{19}$ W m

$\sigma \sim 10^{-11} - 10^{-19}$ S m^{-1}

The values of ρ and σ given above are indicative of magnitude and could well go outside the ranges as well.It could be on the basis of heat conductivity

- **If the valency of sodium is 1, how many electrons occupy the valence band? The conduction bands per atom?**

  Ans: One

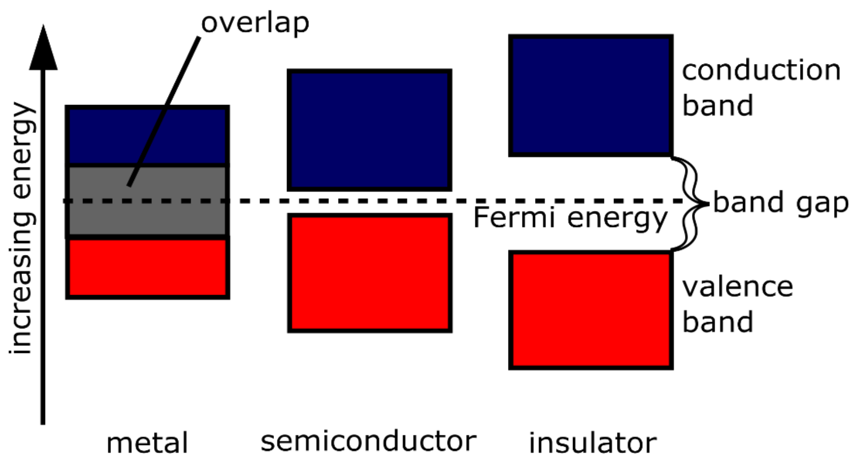
- **Why is study of semiconductors important for their electrical properties?**

  Ans: The supply and flow of charge carriers in the semiconductor devices are *within the solid itself*, while in the earlier vacuum tubes/valves, the mobile electrons were obtained from a heated cathode and they were made to flow in an *evacuated* space or vacuum.

- No external heating, or large evacuated space is required by the semiconductor devices.
- They are small in size, consume low power, operate at low voltages and
- They have long life and high reliability
- **What is the difference between conduction and valence band?**

  Ans: The outermost electrons of atoms making up a solid occupy the valence band. The conduction band is the band of higher values of allowed energies. This means that if the electron in the valence band acquires enough energy they can reach the set of energy states in the conduction band.

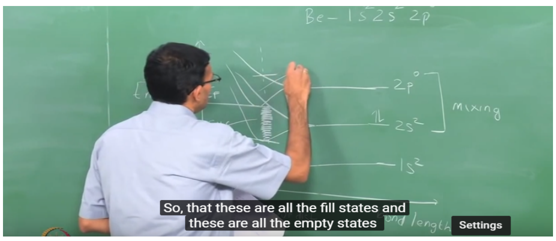
- **Study the comparative energy band diagram for metals, semiconductors and insulators.**
  a) **In which band electrons will have more energy?**
  b) **Is it necessary that the width of conduction and valence band be equal to each other?**



a) **In the conduction band**
b) **No they can have different widths**

- **Where does the Fermi level lie in a conductor, insulator and semiconductor?**
  Ans : The Fermi level in conductors lies in the conduction band, in insulators it lies in the valence band and in semiconductors, it lies in the gap between the conduction, and valence band.
- **Why does diamond behave like an insulator?**
  Ans: There is a large forbidden band of 6 eV in diamond. It is difficult to excite the electrons from valence band to conduction band. Due to the absence of free charge carriers, diamond behaves as an insulator.
- **Why does the conductivity of a semiconductor increase with rise of temperature?**
  Ans: When a semiconductor is heated, more and more electrons jump across the forbidden gap from the valence band where these are free to conduct electricity. Hence the conductivity increases with the increase in temperature.
- **The forbidden energy band of silicon is 1.1 eV. What does it mean?**

Ans: This means that if energy of 1.1 eV is given to an electron in the valence band, it will jump to the conduction band



https://www.youtube.com/watch?v=G41t_0CqPzY

and

https://www.youtube.com/watch?v=OsBoAVZUirg

Try and Answer These

a) What is ‘controlled flow of electrons’?

b) What is the difference between electronic and electric circuits?

c) Why are semiconductors specifically called solid state devices?

d) What are those general properties following which even inorganic compounds (CdS, GaAs, CdSe, InP), organic compounds and organic polymers work as a semiconductor?

e) How can overlapping of orbits from neighboring atoms affect the motion of electrons?

f) What is the reason for the formation of the balance band and conduction band?

g) What is meant by ‘splitting of energy levels’?

h) What is the reason for widening of energy levels when atoms come closer to each-other?

i) Are the numbers of energy states in Valence and conduction bands equal or not?

j) Is there any possibility of an electron being in conduction band while the atom is in ground state?

k) While the energy states of electrons from different atoms are overlapping each-other, how can there be any energy gap?

l) Between Ge and Si, which is the better conductor of electricity?

m) Can an electron from a neighboring atom fall in the vacancy of other atom creating a hole in its own site?

n) Where are free electrons found in a metal?

Summary

In this module we have considered

- In a bulk solid, instead of having discrete energies as in the case of free atoms, the available energy states form bands.
- The inner electrons of an atom are hardly influenced by the electrons of neighbouring atoms.
- The outer electrons form valence band and the next higher allowed energy states form the conduction band.
- Crucial to the conduction process is whether or not there are electrons in the conduction band where the electrons may be free to move.

- In insulators the electrons in the valence band are separated by a large gap from the conduction band. This gap is called a forbidden gap and its value is different for different materials.
- In conductors like metals the valence band overlaps the conduction band, and
- In semiconductors there is a small enough gap between the valence and conduction bands, thermal or other excitations can bridge the gap.
- An important parameter in the band theory is the Fermi level, the top of the available electron energy levels at low temperatures. The position of the Fermi level with the relation to the conduction band is a crucial factor in determining electrical properties.