UNIT 4

Solid State Physics

4.1 THE BAND THEORY OF SOLIDS

4.1.1 Formation of Energy Bands in Solids

In the case of a single isolated atom, the electron in any orbit, as shown in Figure 4.1, has a definite energy. As a result, they occupy discrete energy levels, as shown in Figure 4.2(a).

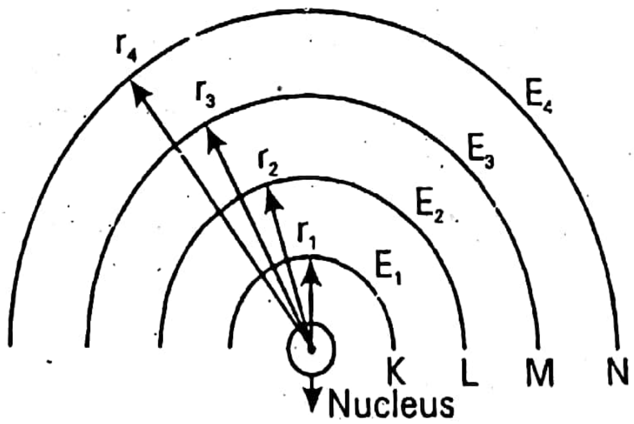

Figure 4.1: The energy levels of a single isolated atom

The Pauli exclusion principle allows each energy level to contain only two electrons. For example, the 2s level of a single atom contains one energy level with two electrons and 2p level contains three energy levels with two electrons in each level thus, with a total of six electrons, as shown in Figure 4.2(a).

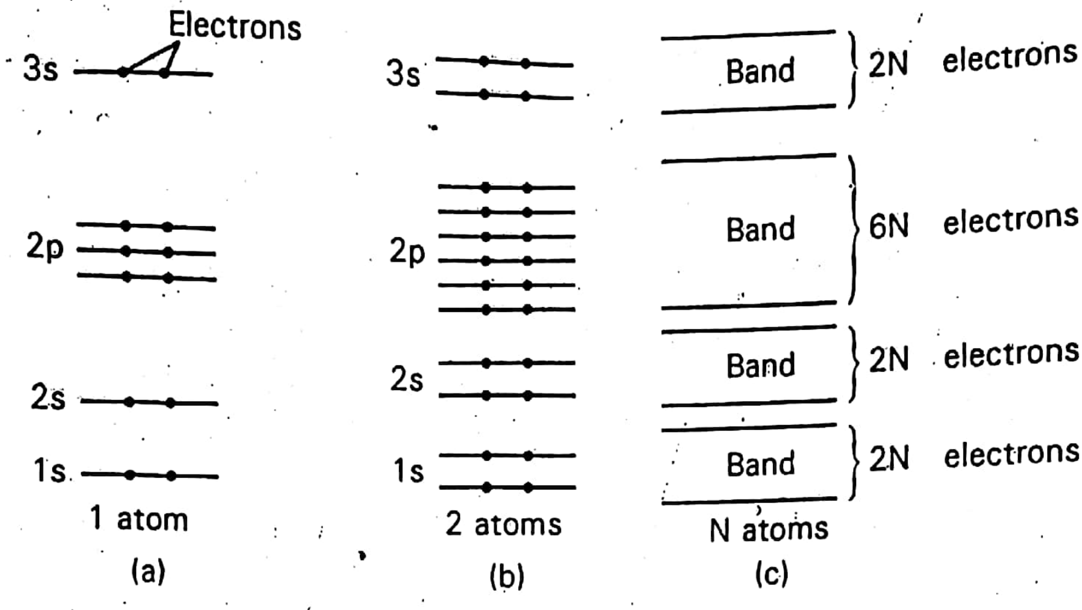

Figure 4.2: The energy levels broaden into energy bands

4.1.2 Band Structure in Solid

Let us consider the formation of bands in a solid sodium.

The single energy level of an isolated sodium (Z = 11) based on the electron configuration $1s^2\ 2s^2\ 2p^6\ 3s^1$ is shown in Figure 4.2(a).

When another sodium is brought close to it, the electrons will be subjected to the effect of an additional field. As a result, each energy level is split into two, as shown in Figure 4.2(b). Similarly, when three atoms come close together, the original level splits into three levels and so on.

More generally, when a solid is formed by bringing N atoms together, the Pauli exclusion principle still demands that only two electrons in the entire solid should have the same energy. Hence, in a solid the different split energy levels of electrons come together to form continuous bands of energies, as shown in Figure 4.2(c).

Consequently, the 2s band in a solid sodium contains N discrete energy levels and 2N electrons, two in each energy level. Similarly, each of the 2p level contains N energy levels and 2N electrons. Hence, a broad 2p band will contain 3N energy levels and 6N electrons since the three 2p bands overlap.

Hence in general, each energy band has a total of N individual levels and can hold a maximum of $2(2l + 1)$ N electrons.

[Each energy level can hold $2\ (2l + 1)$ electrons. The number 2 corresponds to the electrospin and $(2l + 1)$ corresponds to the orientation of the electron orbital angular momentum].

The result is that electrons in any orbit of atom within a solid can have a range of energies rather than a single value. *Thus, the range of energies possessed by an electron* *in a solid is known as energy band,* i.e., Each energy level of an isolated atom becomes a band in a solid, as shown in Figure 4.2(c).

Note:

- In general, it is the outermost energy levels that are mostly affected, whereas the innermost levels barely suffer any splitting during the formation of a band. In the case of sodium it is the outermost energy levels, i.e., 3s and 3p energy levels that are mostly affected, whereas the 1s, 2s and 2p levels barely suffer any splitting during the formation of a band.

4.2 ENERGY BANDS IN SOLIDS

As explained in the case of solid sodium, the discrete energy levels of an atom becomes bands during the formation of solid due to the influence of the constituent atoms. Each band consists of a large number of energy levels which correspond to a range of energy values. The energies within the bands depend on the spacing between the atoms.

The highest occupied band is called the valence band below which all the lower bands are occupied fully. The valence band may even be partially filled. In the case of sodium, the 3s energy levels are the valence band which is partially filled.

The empty band which is immediately above the valence band is called the conduction band. In the case of sodium atom the empty 3p energy levels which are separated from the 3s band by an energy gap is the conduction band.

The gap between the valence band and conduction band is called the forbidden band or the energy gap.

The following are the important energy bands in the solids:

1. Valence band
2. Forbidden band or Energy gap
3. Conduction band

4.2.1 Valence Band

The band of energies occupied by the valence electrons is called as valence band.

The electrons in the outermost orbit of an atom are known as valence electron. In a normal atom valence band posseses electrons of higher energy. This band may be completely or partially filled. Electrons can be moved from the valence band to the conduction band by the application of external energy.

4.2.2 Forbidden Energy Gap

The gap between the valence band and the conduction band on the energy-level diagram is known as forbidden band or energy gap. Electrons are never found in this gap. Electrons may jump back and forth from the bottom valence band to the top conduction band. But they never come to rest in the forbidden band.

4.2.3 Conduction Band

The band of energies occupied by conduction electrons is known as conduction band. This is the uppermost band, and all electrons in the conduction band are free electrons. The conduction band is empty for insulators and partially filled for conductors.

4.3 CLASSIFICATION OF SOLIDS INTO METALS SEMICONDUCTORS AND INSULATORS ON THE BASIS OF BAND THEORY

Depending upon the ability to conduct electricity, materials are classified into three types. They are conductors, semiconductors and insulators. The extent of forbidden gap determines whether the substance is conductor, semiconductor or insulator.

The distinction between them on the basis of the forbidden band or energy gap is discussed in the following section.

4.3.1 Conductors

Conductors are characterised by high electrical conductivity. These are the solids in which plenty of free electrons are available for electrical conduction. **Example:** silver, copper, iron, aluminium, etc. In general, the resistivity of conductors lies in the range of 10^{-9} Ωm at room temperature.

In a conductor the conduction band and the valence band overlap each other, as shown in Figure 4.3(a), so that the electrons can readily pass into the conduction band, i.e., the electrons can readily move under the influence of applied field. ***For conductors the energy gap is of the order of 0.01 eV.***

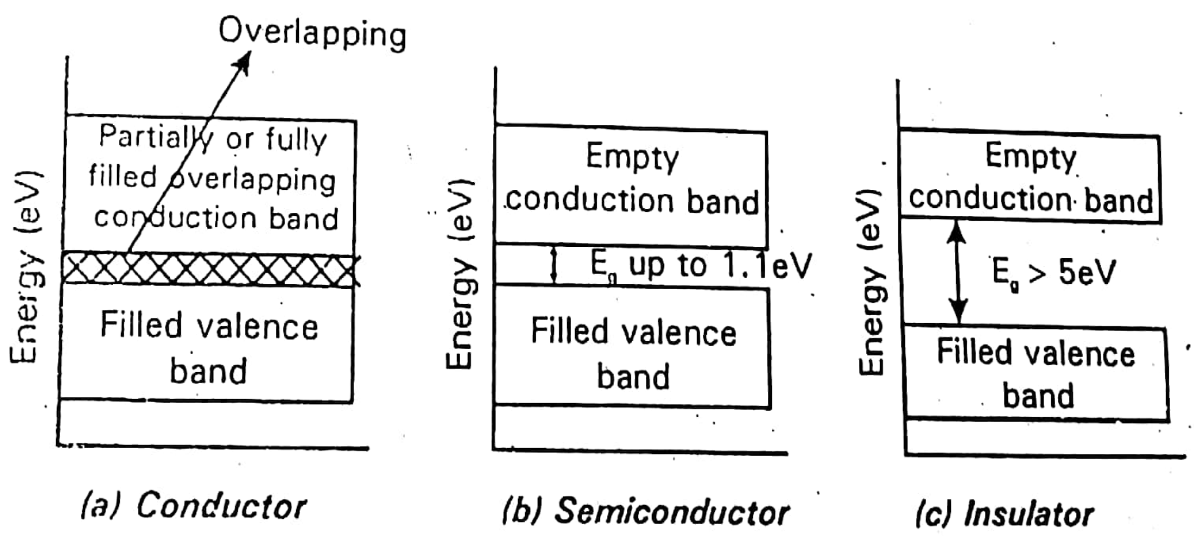

Figure 4.3: Schematic representation of band structure of solids

4.3.2 Semiconductors

These are the solids whose electrical properties lie in between those of conductors and insulators. Example of semiconductors are germanium and silicon.

The resistivity of semiconductors lies between $10^{-4}\ \Omega$ m to $10^{3}\ \Omega$ m at room temperature.

In terms of energy bands semiconductors can be defined as those materials which have almost an empty conduction band and an almost filled valence band, with a very narrow energy gap separating the two bands ≈ 1 eV.

At low temperatures, the valence band of a semiconductor is completely filled and the conduction band is completely empty, as shown in Figure 4.3(b). Therefore a semiconductor virtually behaves like an insulator at low temperatures. However, at room temperature some electrons cross over to the conduction band, giving a little conductivity to the semiconductor.

As temperature is increased more valence electrons cross over to the conduction band and conductivity increases. This shows that electrical conductivity of a semiconductor increases with the increase of temperature, i.e., a semiconductor has negative temperature coefficient of resistance.

The forbidden energy gap for germanium is 0.7 eV and for silicon it is 1.1 eV.

4.3.3 Insulators

In an insulator the energy gap between valence band and conduction band is very large and approximately equal to 5 eV or more, as shown in the Figure 4.3(c). Therefore, a very high energy is required to push the electrons to the conduction band. For these reasons the electrical conductivity of the insulator is extremely small and may be regarded as nil under ordinary conditions (room temperature).

The resitivity of insulators lies between 10^{3} to $10^{17}\ \Omega$ m at room temperature.

At room temperature, the valence electrons of the insulators do not have enough energy to cross over to the conduction band. However when the temperature is raised, some of the valence electrons gain enough energy to cross to the conduction band. Hence, the resistance of the insulator decreases with increase of temperature, i.e., an insulator has negative temperature coefficient of resistance.

For an insulator, such as diamond, the forbidden gap is ≈ 6 eV and for glass it is ≈ 10eV.