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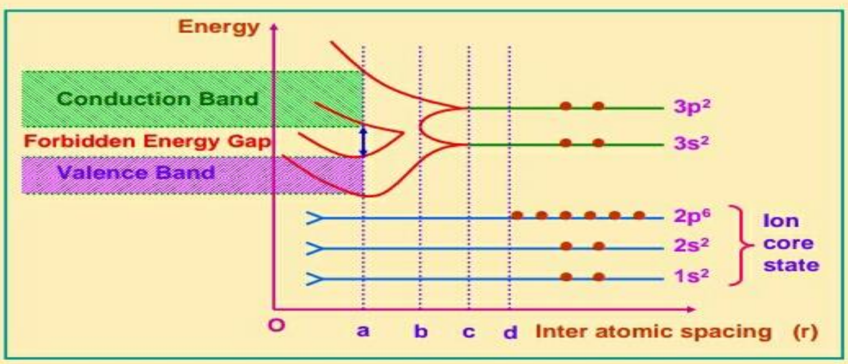
Energy Bands in Solids:

- According to Quantum Mechanical Laws, the energies of electrons in a free atom can not have arbitrary values but only some definite (quantized) values.
- However, if an atom belongs to a crystal, then the energy levels are modified.
- This modification is not appreciable in the case of energy levels of electrons in the inner shells (completely filled).
- But in the outermost shells, modification is appreciable because the electrons are shared by many neighbouring atoms.
- Due to influence of high electric field between the core of the atoms and the shared electrons, energy levels are split-up or spread out forming energy bands.

Consider a single crystal of silicon having N atoms. Each atom can be associated with a lattice site.

Electronic configuration of Si is $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^2$. (Atomic No. is 14)

Formation of Energy Bands in Solids:



(i) r = Od (>> Oa):

Each of N atoms has its own energy levels. The energy levels are identical, sharp, discrete and distinct.

The outer two sub-shells (3s and 3p of M shell or n = 3 shell) of silicon atom contain two s electrons and two p electrons. So, there are 2N electrons completely filling 2N possible s levels, all of which are at the same energy.

Of the 6N possible p levels, only 2N are filled and all the filled p levels have the same energy.

(iii) r = Oc:

The interaction between the outermost shell electrons of neighbouring silicon atoms becomes appreciable and the splitting of the energy levels commences.

(iv) Ob < r < Oc:

The energy corresponding to the s and p levels of each atom gets slightly changed. Corresponding to a single s level of an isolated atom, we get 2N levels. Similarly, there are 6N levels for a single p level of an isolated atom.

Since N is a very large number ($\approx 10^{29}$ atoms / m^3) and the energy of each level is of a few eV, therefore, the levels due to the spreading are very closely spaced. The spacing is $\approx 10^{-23}$ eV for a 1 cm^3 crystal.

The collection of very closely spaced energy levels is called an energy band.

(v) r = Ob:

The energy gap disappears completely. 8N levels are distributed continuously. We can only say that 4N levels are filled and 4N levels are empty.

(v) r = Oa:

The band of 4N filled energy levels is separated from the band of 4N unfilled energy levels by an energy gap called forbidden gap or energy gap or band gap.

The lower completely filled band (with valence electrons) is called the valence band and the upper unfilled band is called the conduction band.

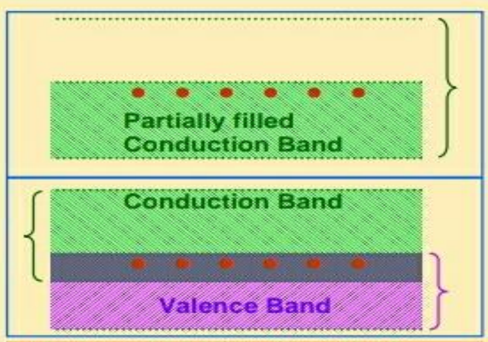
Note:

1. The exact energy band picture depends on the relative orientation of atoms in a crystal.
2. If the bands in a solid are completely filled, the electrons are not permitted to move about, because there are no vacant energy levels available.

Metals:

The first possible energy band diagram shows that the conduction band is only partially filled with electrons.

With a little extra energy the electrons can easily reach the empty energy levels above the filled ones and the conduction is possible.



The second possible energy band diagram shows that the conduction band is overlapping with the valence band.

This is because the lowest levels in the conduction band needs less energy than the highest levels in the valence band.

The electrons in valence band overflow into conduction band and are free to move about in the crystal for conduction.

The highest energy level in the conduction band occupied by electrons in a crystal, at absolute 0 temperature, is called Fermi Level.

The energy corresponding to this energy level is called Fermi energy.

If the electrons get enough energy to go beyond this level, then conduction takes place.