7.4 ENERGY LEVELS AND ENERGY BANDS

In an atom, the electrons revolve around the nucleus in almost circular orbits (Bohr's model). Energy of electrons in each subshell is definite. These definite energy values are called energy levels

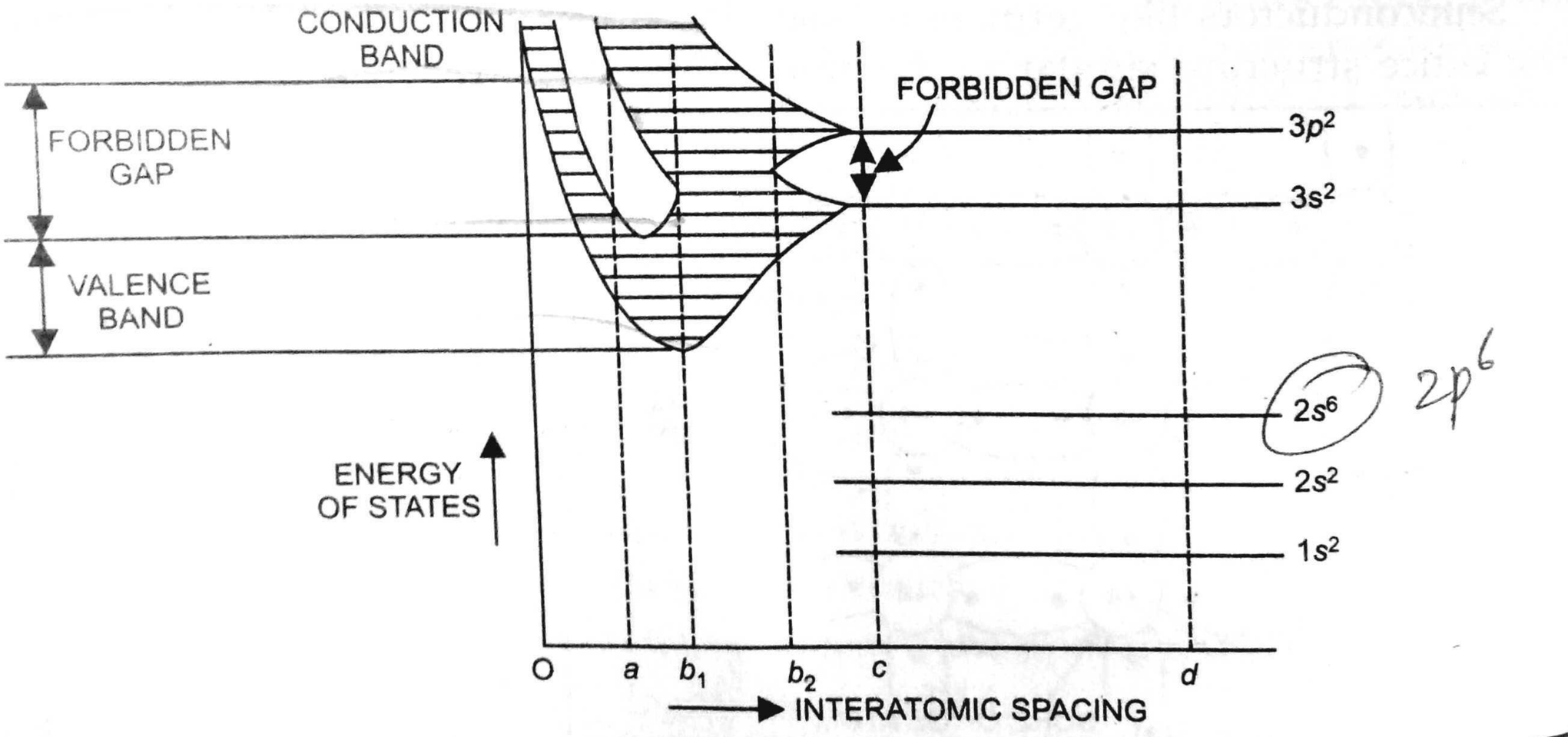

Fig. 7.3. Energy band of silicon lattice as a function of interatomic spacing.

of the atoms. But in crystals atoms are arranged in a regular and periodic manner. A solid crystal contains about 10^{23} atoms/cm^3 . So each atom is in the electrostatic field of neighbouring atoms and due to interaction between the atoms and modification of energy level takes place. The maximum effect of the interaction is on the valence electron and the energy E becomes E + ΔE. Thus each energy level becomes broad. This broadening of energy level is called energy band. The electrons in the inner shell are strongly bound to the nuclei, so they slightly affected by the presence of neighbouring atoms. They are called core levels. If an energy band consists of as much electrons as permitted by Pauli's exclusion principle, then it is said to be completely filled band, and in such a band there will be no free electrons for conduction of electricity, while for a partially filled band conduction is possible.

In order to understand how the modification of energy level takes place, let us consider a single crystal of Si having N atoms. The electronic configuration of Si is $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^2$. The energy levels of Si atom in isolated state as well as in the crystal form are shown in Fig. 7.3. Here the inter atomic spacing is r and distance 'a' corresponds to the crystal lattice spacing. The process of splitting is summarised as the follows :

1. *When $r > c$.*

The atomic spacing is sufficiently wide, so the interaction between atoms is negligible and practically, there is no modification of 3s and 3p energy sublevels.

2. *When $r = c$.*

When atoms are brought further close to each other, their interaction increases and the real splitting of the sublevels starts. The energy difference between 3s and 3p sublevels is denoted by double arrow and is called forbidden gap.

3. *When $r < c$.*

The forbidden gap decreases and reduces to zero at $r = b_2$. So at $r = b_2$, the two bands overlap. At a distance between b_2 and c instead of single 3s or 3p level, we get a large number of closely packed levels. The number N is very large so this collection of closely spaced levels is called an energy band.

4. *When $b_1 < r < b_2$.*

When the atomic spacing is further reduced, the 3s and 3p levels remain merged into each other and thus there is no restriction on the electrons to move from 3s sublevel to 3p sublevel or vice-versa. The energy gap between 3s and 3p disappears, and the two bands overlap. In this situation all 8N levels (2 from s and 6 from p) are now continuously distributed. Here we cannot distinguish between the electrons belonging to 3s and 3p sublevels. At such a situation one can only say the 4N sublevels are filled and 4N sublevels are empty.

5. *When $r = a$.*

This is known as equilibrium distance because the atoms in crystal lie at this interatomic separation. Here the bands divide and spread widely. Here we find that the bands of filled energy level and empty energy level are separated by an energy gap called forbidden gap or forbidden band. The lower band which is completely filled up is known as valence band and the upper band which is normally (at 0K) empty, is referred to as the conduction band.

Fig. 7.4. Band model of insulator and semiconductor at 0K and at TK.

The gap between valence band and conduction band is called forbidden band and it is a measure of energy E_g. Thus E_g is the amount of energy that should be given to electron in valence band so that it could jump to the conduction band. For insulators it is of the order of 5 to 10 eV, is extremely large and as such, it cannot be overcome by the valence electrons by ordinary means. Fig. 7.4 (a). The energy gap of a semiconductor like germanium is about 0.72 eV Fig. 7.4 (b). This small gap of 0.72 eV may easily be overcome by the action of external agency like heat or light. Thus, in this material the conduction of electric current may take place simply with the rise of temperature. In term of energy band we may express the same idea by stating that at absolute zero all energy levels in the valence band are filled up, while all the energy levels in the conduction band are vacant as shown in Fig. 7.4 (c).

On increasing the temperature of semiconductor the valence electrons are thermally excited and may become free on absorption of energy more than E_g. The number of valence electrons which excite from valence band to conduction band leave behind an equal number of electron vacancies (holes) in the valence band of the intrinsic semiconductor. Thus the number of electrons in the conduction band is exactly equal to the number of holes in the valence band Fig. 7.4 (c).

In conduction band, the charge carriers are electrons and in valence band, the charge carriers are holes. Since the number density of electrons is very large and the motion of electrons is random, so at a given temperature the energy levels occupied by electrons can be determined statistically. The probability f (E) of a state corresponding to energy being occupied by an electron at temperature TK is given by

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)} \qquad ...(7.1)$$

Where k is Boltzmann constant. E_F is known as Fermi energy, here it is given in eV.

At $T = 0K, f(E) = 0$ for $E > E_F$ (empty energy state)

and $f(E) = 1$ for $E < E_F$ (occupied energy state)

At $T \neq 0K, f(E) = \frac{1}{2}$ for $E = E_F$ (50% occupied energy state)

As conduction band is completely empty at T = 0K, hence E_F must be less than the lowest level of conduction band. Similarly, the electron state in valence band are occupied at T = 0K, hence E_F must be greater than the energy of the upper most state in valence band. On increasing the temperature, the probability of finding an electron above Fermi level with an equal probability of finding a hole below Fermi level increases. So in intrinsic semiconductors, the Fermi level should be situated in the middle of the forbidden gap Fig. 7.4 (d) and the position of Fermi level is independent of temperature.