Ionization Energy

We can calculate the approximate distance of the donor electron from the donor impurity

ion, and also the approximate energy required to elevate the donor electron into the conduction band. This energy is referred to as the ionization energy. We will use the Bohr model of the atom for these calculations. The justification for using this model is that the most probable distance of an electron from the nucleus in a hydrogen atom, determined from quantum mechanics, is the same as the Bohr radius. The energy levels in the hydrogen atom determined from quantum mechanics are also the same as obtained from the Bohr theory.

In the case of the donor impurity atom, we may visualize the donor electron orbiting the donor ion, which is embedded in the semiconductor material. We will need to use the permittivity of the semiconductor material in the calculations rather than the permittivity of free space as is used in the case of the hydrogen atom. We will al use the effective mass of the electron in the calculations. The analysis begins by setting the coulomb force of attraction between the electron and ion equal to the centripetal force of the orbiting electron. This condition give a steady orbit. We can calculate ionization energy and bonding energy for donner atom by using Bohr theory but after small change in permittivity constant of medium and effective mass m^* . $(\varepsilon = \varepsilon_o \varepsilon_r)$

$$E_n = \frac{me^4}{8h^2\varepsilon_o^2} . \frac{1}{n^2} ----\rightarrow (1)$$

$$E_d = \frac{me^4}{8h^2\varepsilon_o^2\varepsilon_r^2} . \frac{1}{n^2} ----\rightarrow (1)$$

We see that E_d related with ε_r^2 and with m^*

$$T = \frac{1}{2} mv^2$$

$$F_c = \frac{e^2}{4\pi\varepsilon r_n^2} = \frac{m^* v^2}{r_n}$$

Due to the quantization of angular momentum

$$l = n\hbar = r_n(m^* . v) ----\rightarrow (2)$$

$$\frac{e^2}{4\pi\varepsilon r_n^2} = \frac{m^*}{r_n}\left(\frac{n\hbar}{r_n m^*}\right)^2 = \frac{n^2\hbar^2}{r_n^3 m^*} ----\rightarrow (3) \qquad r_n \propto n^2$$

$$r_n = \frac{4\pi\varepsilon n^2\hbar^2}{e^2 m^*} = n^2\varepsilon_r\left(\frac{m_o}{m^*}\right) a_o ----\rightarrow (4) \qquad a_o\text{: Bohr radius}$$

$$a_o = \frac{4\pi\varepsilon_o\hbar^2}{m_o e^2} = 0.53\ \text{A}^o$$

We can normalize the radius of the donor orbital to that of the Bohr radius, which give

$$\frac{r_n}{a_o} = n^2 \varepsilon_r \left(\frac{m_o}{m^*}\right) - - - - -\rightarrow (5)$$

where $\boldsymbol{\varepsilon_r}$ is the relative dielectric constant of the semiconductor material, $\boldsymbol{m_o}$ is rest mass of an electron, and m^* is the conductivity effective mass of the electron the semiconductor.

The total energy of the orbiting electron is given by

$$E = T + V \ - - - - - -\rightarrow (6)$$

where T is the kinetic energy and V is the potential energy of the electron. The kinetic

energy is $T = \frac{1}{2} m^* v^2$

Using the velocity u from Equation (2) and the radius r,, from Equation (4), the kinetic energy becomes

$$T = \frac{m^* e^4}{2(n\hbar)^2 (4\pi\epsilon)^2}$$

The potential energy $V = \dfrac{-e^2}{4\pi\epsilon r_n} = \dfrac{-m^* e^4}{(n\hbar)^2 (4\pi\epsilon)^2}$

The total energy is the sum of the kinetic and potential energies, so that

$$E = T + V = \frac{-m^* e^4}{2(n\hbar)^2 (4\pi\epsilon)^2}$$

For the hydrogen atom, $\boldsymbol{m'} = m_o$ and $\varepsilon = \varepsilon_o$ **.** The ionization energy of the hydrogen atom in the lowest energy state is then E = - 13.6 eV. If we consider silicon, the ionization energy is E = -25.8 meV, much less than the bandgap energy of silicon . We defined an intrinsic semiconductor as a material with no impurity atoms presence in the crystal. An **extrinsic semiconductor** is defined as a semiconductor in controlled amounts of specific dopant or impurity atoms have been added so that thermal-equilibrium electron and hole concentrations are different from the intrinsic carrier concentration.

Equilibrium Distribution of Electrons and Holes

Adding donor or acceptor impurity atoms to a semiconductor will change the distribution

of electrons and holes in the material. Since the Fermi energy is related to the distribution function, the Fermi energy will change as dopant atoms are added. If the Fermi energy changes from near the midgap value, the density of electrons in the conduction band and the density of holes in the valence band will change.

These effects are shown in Figures 4.8 and 4.9. Figure 4.8 shows the case for $\boldsymbol{E_F} > \boldsymbol{E_{Fi}}$ and Figure 4.9 shows the case for $E_F < E_{Fi}$ When $E_F > \boldsymbol{E_{Fi}}$, the electron concentration is larger than the hole concentration, and when $EF < Ew$, the hole concentration

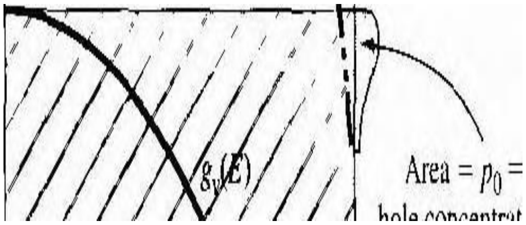

Figure 5.a Density of states functions. Fermi-Dirac probability function, and areas representing electron and hole concentrations for the case when ***EF*** is **above** the intrinsic Fermi energy.
b. Density of states functions, Fermi-Dirac probability function, and areas representing electron and hole concentrations for the casc when ***E,*** is below the intrinsic Fermi energy

n-type semiconductor

When the density of electrons in CB is greater than the density of holes in VB

☐ **p-type semiconductor**

When the density of holes in VB is greater than the density of electrons in CB.

Example 4 thermal equilibrium concentrations

Find the thermal equilibrium electron &hole concentrations for Si if the band gap 1.12 eV Fermi energy is 0.25 eV below conduction band , $Nc = 2.8 \times 10^{19}\ cm^{-3} and$

$$N_v = 1.04 \times 10^{19} cm^{-3}$$

Solution:

$$n_o = n_c = N_c\, exp\left(\frac{E_f - E_c)}{K_\beta T}\right) = 2.8 \times 10^{19} \exp\left(\frac{-0.25}{0.0259}\right) = 1.8 \times 10^{15} cm^{-3}$$

$$p_o = n_v = N_v exp\left(\frac{E_v - E_f)}{K_\beta T}\right) = 1.04 \times 10^{19} \exp\left(\frac{-0.87}{0.0259}\right) = 2.7 \times 10^{4} cm^{-3}$$

Another form of equations for n_o and p_o

n-type $n_o = n_c = N_c \, exp\left(\frac{E_f - E_c)}{K_\beta T}\right)$

Intrinsic $n_o = n_c = n_i = N_c \, exp\left(\frac{E_{fi} - E_c)}{K_\beta T}\right)$

$$n_o = n_c = N_c \, exp\left(\frac{E_f - E_c)}{K_\beta T}\right) = N_c \, exp\left(\frac{E_f - E_{fi})}{K_\beta T}\right) \; for \; n - type \; n_o > n_i, E_f > E_{fi}$$

$$p_o = n_v = N_v exp\left(\frac{E_v - E_f)}{K_\beta T}\right) = N_v exp\left(\frac{E_{fi} - E_f)}{K_\beta T}\right) for \; p - type \; n_o < n_i, E_f < E_{fi}$$

The change in the Fermi level is actually a function of the donor or acceptor impurity concentrations that are added to the semiconductor However, this example shows that electron and hole concentrations change by orders of magnitude from the intrinsic carrier concentration as the Femi energy changes by a few tenths of an electron-volt