Electrons and holes in semiconductors

intrinsic and extrinsic carriers; variations in E_F

July 1, 2021

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- Without the crystal lattice, the hole cannot exist. It is an artifact of the periodic potential (Ep) created by the crystal
- Hole is positively charged and can move, and for this is different from ionised atoms don't.

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- We can evaluate the carrier concentrations in the conduction band using the concept of DOS and the fermi-Dirac distribution:

$$\begin{aligned} n &= \int_{E_c}^{+\infty} Dos(\epsilon) f(\epsilon) d\epsilon \\ &= 2\left(\frac{m_e^* k_b T}{2\pi\hbar^2}\right)^{\frac{3}{2}} e^{\frac{E_{F_i} - E_c}{k_b T}} = N_c e^{\frac{E_{F_i} - E_c}{k_b T}} \end{aligned} \tag{1}$$

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- And proceeding as above we obtaining the concentration p of holes in the valence band:

$$p = \int_{-\infty}^{E_v} Dos(\epsilon) \left(1 - f(\epsilon)\right) d\epsilon$$
$$= 2\left(\frac{m_h^* k_b T}{2\pi\hbar^2}\right)^{\frac{3}{2}} e^{\frac{E_v - E_{F_i}}{k_b T}} = N_v e^{\frac{E_v - E_{F_i}}{k_b T}} \quad (2)$$

where N_v is a temperature dependent constant called the effective density of states of the valence band.

Intrinsic carrier concentration

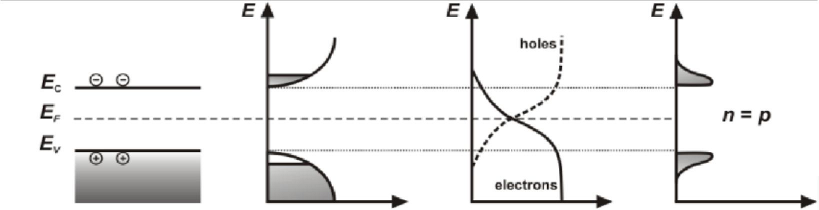

Figure 1: This figure shows the intrinsic behaviour of a semiconductor

Intrinsic carrier concentration

- In physics we usually look for constant of the system, we obtain one of it if we multiply equation (1) and equation (2):

$$np = 4\left(\frac{k_b T}{2\pi\hbar^2}\right)^3 (m_e^* m_h^*)^{\frac{3}{2}} e^{-\frac{E_g}{k_b T}} = n_i^2$$

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- Then we have $n = p = n_i$. This is because the product of the electron and hole concentration is a constant, not depending on the impurity concentration at given temperature. The introduction of a small proportion of a suitable impurity to increase n, say, must decrease p.

Intrinsic carrier concentration

- The property $n = p$ in an intrinsic semiconductor gives us the possibility to estimate the so called intrinsic Fermi energy, equalling equation (1) and equation (2):

$$n = p$$

$$N_c e^{\frac{E_{F_i} - E_c}{k_b T}} = N_v e^{\frac{E_v - E_{F_i}}{k_b T}}$$

$$E_{F_i} = \frac{E_c + E_v}{2} + \frac{3}{4} k_b T ln \left(\frac{m_h^*}{m_e^*} \right)$$

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- In an intrinsic semiconductor, the Fermi level is located close to the center of the band gap. Mote that this quantity depends only on the band gap and on the electron and hole effective masses.

Extrinsic semiconductor

- In an extrinsic semiconductor, the general behaviour is slightly different, with the dopants fully ionized, there is an imbalance in the electron and hole concentration. This is reflected in the Fermi level position being shifted from the center of the band gap towards either the conduction band for an n-type or valence band for an p-type.

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- The doped semiconductor has to satisfy the charge neutrality:

$$p + N_d^+ = n + N_a^-$$

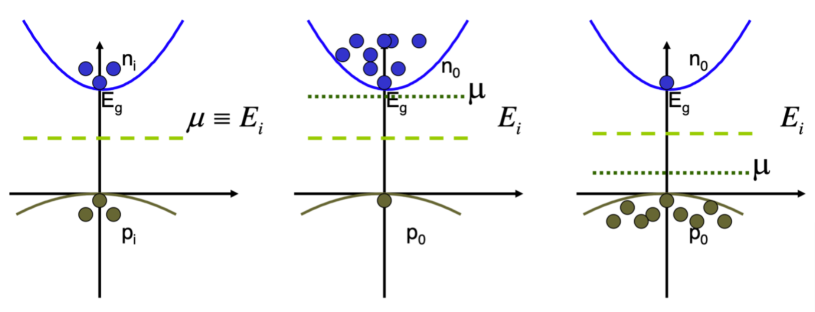

Figure 2: The first plot shows the intrinsic case. The second figure shows the case of n-type doped material. The last one shows the case of p-type doped material.

Fermi energy extrinsic semiconductor

- The carrier concentration is calculated as in equation (1), but this time we have a different Fermi energy, depending on the donor concentration.

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- Where N_d^+ is the number of ionised donors:

$$N_d^+ = Nd\left(1 - f(E_D)\right) = N_d \left(1 - \frac{1}{1 + g^{-1} e^{\frac{(E_D - E_f)}{k_b T}}}\right) = \frac{N_d}{1 + g e^{\frac{(E_F - E_D)}{k_b T}}}$$

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- The neutrality equations becomes:

$$n_i e^{\frac{E_{F_i} - E_F}{k_b T}} + \frac{N_d}{1 + 2e^{\frac{E_F - E_D}{k_b T}}} = n_i e^{\frac{E_F - E_{F_i}}{k_b T}} \tag{5}$$

Fermi energy extrinsic semiconductor

- An analytic solutions can only be found in special limiting cases. But it is possible to solve it numerically. In the case of silicon we have that:

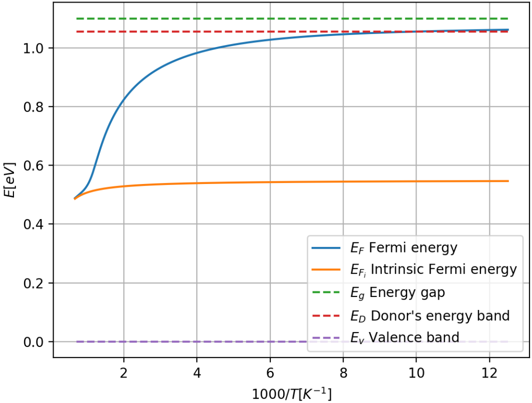
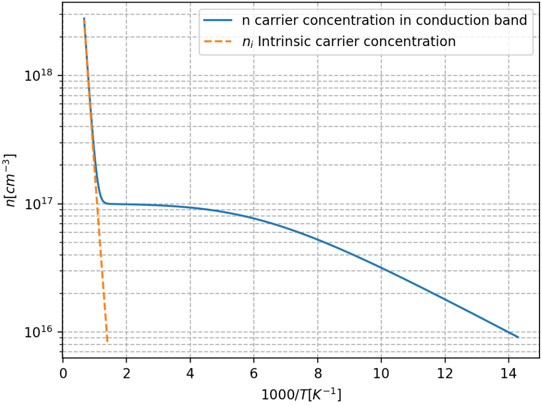


Figure 3: Caption

Intrinsic and extrinsic carrier concentration

- once we obtained the Fermi energy we can compute the electron carrier concentration in a doped semiconductor using equation (3).



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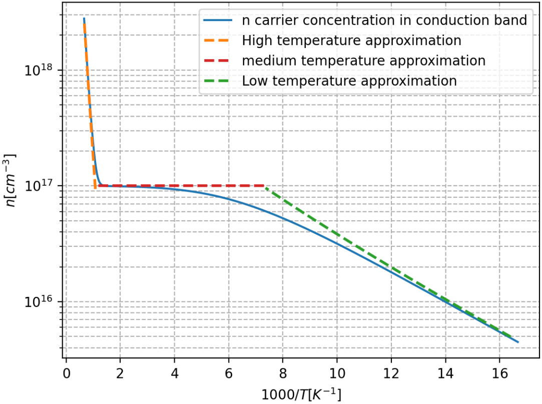

Figure 5: Caption

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$$N_d^+ \approx n$$

This equation is simpler and it can be solved analytically. Find the fermi energy and then substitute it in the carrier concentration formula.

$$n = N_c e^{\frac{E_F - E_c}{k_b T}} = \sqrt{\frac{N_d N_c}{2}} e^{-\frac{E_c - E_D}{2 k_b T}}$$

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- For low temperatures we expect that the concentration of holes is much lower than that of electrons (given mainly from the donor), and becomes very low when N_d becomes very large, in fact $p = \frac{n_i^2}{N_d^+} \ll N_d^+$.

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- Hence, we expect that the carrier concentration is flattened out at N_d, as it is shown in figure 5 .
- There is a saturation range where the concentration is determined by doping and all the impurities are ionised: this is where usually lies the working range of the device.

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- If this is the case, in this temperature domain the energy is enough to promote an electron from the valence band to the conduction band.
- Now the main contribution on the carrier concentration is given by n_i ($n \approx N_d^+ + p \approx n_i$). In fact at too high temperature, the concentration is essentially given by the intrinsic one (n_i), making the doping useless.