Chapter 3.

SEMICONDUCTOR MATERIALS

FOR SOLAR CELLS

3.1   Solar cell structure

In most of today solar cells the absorption of photons, which results in the generation of the charge carriers, and the subsequent separation of the photo-generated charge carriers take place in **semiconductor materials**. Therefore, the semiconductor layers are the most important parts of a solar cell; they form the hart of the solar cell. There are a number of different semiconductor materials that are suitable for the conversion of energy of photons into electrical energy, each having advantages and drawbacks. In this chapter the most important semiconductor properties that determine the solar cell performance will be discussed.

The crystalline silicon (c-Si) solar cell, which dominates the PV market at present, has a simple structure, and provides a good example of a typical solar cell structure. Figure 3.1 shows the essential features of c-Si solar cells. An absorber material is typically a moderately-doped p-type square wafer having thickness around 300 µm and an area of 10×10 cm^2 or 12.5×12.5 cm^2. On both sides of the c-Si wafer a highly doped layer is formed, n^+-type on the top side and p^+-type on the back side, respectively. These highly doped layers help to separate the photo-generated charge carriers from the bulk of the c-Si wafer. The trend in the photovoltaic industry is to reduce the thickness of wafers up to 250 µm and to increase the area to 20×20 cm^2.
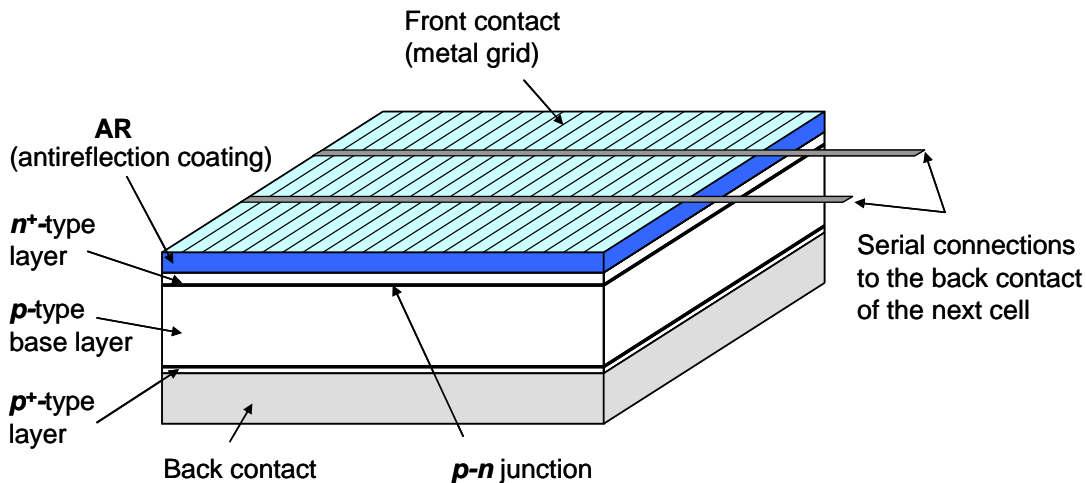
Figure 3.1. A typical structure of a c-Si solar cell.

In addition to semiconductor layers, solar cells consist of a top and bottom metallic grid or another electrical contact that collects the separated charge carriers and connects the cell to a load. Usually, a thin layer that serves as an antireflective coating covers the topside of the cell in order to decrease the reflection of light from the cell. In order to protect the cell against the effects of outer environment during its operation, a glass sheet or other type of transparent encapsulant is attached to both sides of the cell. In case of thin-film solar cells, layers that constitute the cell are deposited on a substrate carrier. When the processing temperature during the deposition of the layers is low, a wide range of low-cost substrates such as glass sheet, metal or polymer foil can be used.

The first successful solar cell was made from c-Si and c-Si is still the most widely used PV material. Therefore we shall use c-Si as an example to explain semiconductor properties that are relevant to solar cell operation. This gives us a basic understanding of how solar cells based on other semiconductor materials work. The ***central semiconductor parameters*** that determine the design and performance of a solar cell are:

i) concentrations of doping atoms, which can be of two different types; donor atoms which *donate* free electrons, N_D, or acceptor atoms, which *accept* electrons, N_A. The concentrations determine the width of a space-charge region of a junction.

ii) mobility, μ, and diffusion coefficient, D, of charge carriers that characterize carriers transport due to drift and diffusion, respectively.

iii) lifetime, τ, and diffusion length, L, of the excess carriers that characterize the recombination-generation processes.

iv) band gap energy, E_G, absorption coefficient, α, and refractive index, n, that characterize the ability of a semiconductor to absorb visible and other radiation.

3.2   Semiconductor properties

3.2.1   Atomic structure

The atomic number of Si atom is 14, it means there are 14 electrons orbiting the nucleus. In ground state configuration a Si atom has four valence electrons. These valence electrons are most important because they form the bonds with other Si atoms. Two Si atoms are bonded together when they share each other's valence electron. This is the so called covalent bond that is formed by two electrons. Since Si atom has four valence electrons it can be covalently bonded to four other Si atoms. In the crystalline form each Si atom is covalently bonded to four neighbouring Si atoms. All bonds have the same length and the angles between the bonds are equal. The number of bonds that an atom has with its immediate neighbours in the atomic structure is called the **coordination number** or **coordination**. Thus, in single crystal silicon, the coordination number for all Si atoms is four, we can also say that Si atoms are fourfold coordinated. A **unit cell** can be defined, from which the crystal lattice can be reproduced by duplicating the unit cell and stacking the duplicates next to each other. Such a regular atomic arrangement is described as a structure with **long range order**.

A diamond lattice unit cell represents the real lattice structure of single crystal silicon. Figure 3.2a shows the arrangement of the unit cell and Figure 3.2b the atomic structure of single crystal silicon. One can determine from Figure 3.2a that there are effective eight Si atoms in the volume of the unit cell. When a lattice constant of c-Si is 5.4 Å one can easily calculate that there are approximately 5×10^{22} Si atoms per cm^3. Figure 3.2 shows the crystalline Si atomic structure with no foreign atoms. In practice, a semiconductor sample always contains some impurity atoms. When the concentration of impurity atoms in a semiconductor is insignificant we refer to such semiconductor as an **intrinsic semiconductor**.

At practical operational conditions, for example room temperature, there are always some of the covalent bonds broken. The breaking of the bonds results in liberating the valence electrons from the bonds and making them mobile through the crystal lattice. We refer to these electrons as free electrons (henceforth simply referred as electrons). The position of a missing electron in a bond, which can be regarded as positively charged, is referred to as a hole. This situation can be easily visualized by using the **bonding model** shown in Figure 3.3.
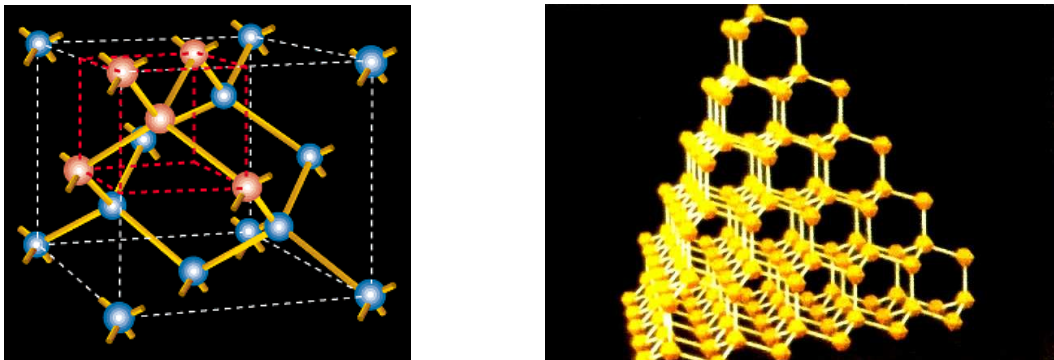

Figure 3.2. (a) A diamond lattice unit cell representing a unit cell of single crystal Si, (b) the atomic structure of a part of single crystal Si.

In the bonding model the atomic cores (atoms without valence electrons) are represented by circles and the valence or bonding electrons are represented by lines interconnecting the circles. In case of c-Si one Si atom has four valence electrons and four nearest neighbours. Each of the valence electron is equally shared with the nearest neighbour. There are therefore eight lines terminating on each circle. In an ideal Si crystal at 0°K all valence electrons take part in forming covalent bonds between Si atoms and therefore are no free electrons in the lattice. This situation is schematically shown in Figure 3.3a. At temperatures higher than 0°K the bonds start to break due to absorbing thermal energy. This process results in creation of mobile electrons and holes. Figure 3.3b shows a situation when a covalent bond is broken and one electron departs from the bond leaving a hole behind. A single line between the atoms in Figure 3.3b represents the remaining electron of the broken bond. When a bond is broken and a hole created, a valence electron from a neighbouring bond can "jump" into this empty position and restore the bond. The consequence of this transfer is that at the same time the jumping electron creates an empty position in its original bond. The subsequent "jumps" of a valence electron can be viewed as a motion of the empty position, hole, in the direction opposite to the motion of the valence electron through the bonds.

Because breaking of a covalent bond leads to the formation of an electron-hole pair, in intrinsic semiconductors the concentration of electrons is equal to the concentration of holes. At 300°K there are approximately 1.5×10^{10} broken bonds per cm^3 in the intrinsic c-Si. This number then gives also the concentration of holes, p, and electrons, n, in the intrinsic c-Si. It means, that at 300°K $n = p = 1.5 \times 10^{10}$ cm^{-3}. This concentration is called the ***intrinsic carrier concentration*** and is denoted n_i.
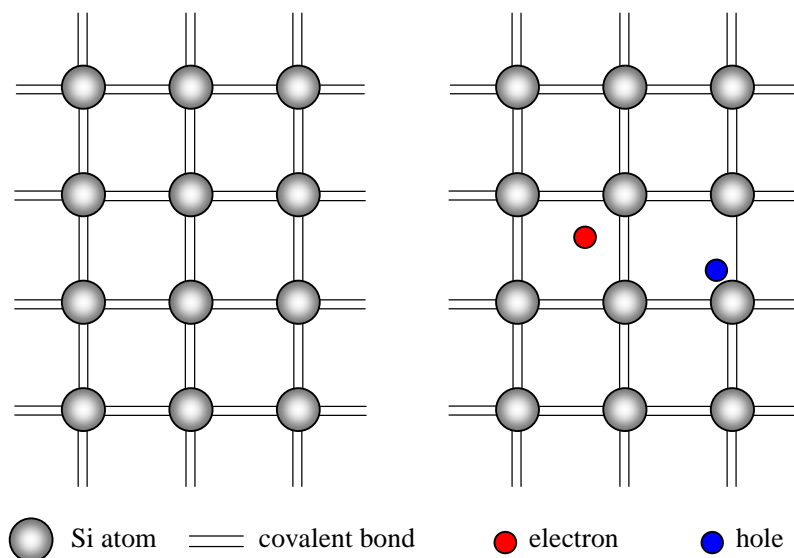

Figure 3.3. The bonding model for c-Si. (a) No bonds are broken. (b) A bond between two Si atoms is broken resulting in a mobile electron and hole.

3.2.2 Doping

The concentrations of electrons and holes in c-Si can be manipulated by doping. By doping c-Si we understand that atoms of appropriate elements substitute Si atoms in the crystal lattice. The substitution has to be carried out by atoms with three or five valence electrons, such as boron or phosphorous, respectively. The doping action can best be understood with the aid of the bonding model and is demonstrated in Figure 3.4.

When introducing phosphorous atom into the c-Si lattice, four of the five phosphorous atom valence electrons will readily form bonds with the four neighbouring Si atoms. The fifth valence electron cannot take part in forming a bond and becomes rather weakly bound to the phosphorous atom. It is easily liberated from the phosphorous atom by absorbing the thermal energy, which is available in the c-Si lattice at room temperature. Once free, the electron can move throughout the lattice. In this way the phosphorous atom that substitutes a Si atom in the lattice "*donates*" a free (mobile) electron into the c-Si lattice. The impurity atoms that enhance the concentration of electrons are called ***donors***. We donate the concentration of donors N_D.

An atom with three valence electrons such as boron cannot form all bonds with four neighbouring Si atoms when it substitutes a Si atom in the lattice. However, it can readily "*accept*" an electron from a nearby Si-Si bond. A thermal energy that the c-Si lattice contains at room temperature is sufficient to enable an electron from a nearby Si-Si bond to attach itself to the boron atom and complete the bonding to the four Si neighbours. In this process a hole is

(a)   (b)

$\oplus$ ionised P_4^+ atom $\ominus$ ionised B_4^- atom

Figure 3.4. The doping process illustrated using the bonding model. (a) A P atom substitutes a Si atom in the lattice resulting in the positively-ionised P atom and a free electron, (b) A B atom substitutes a Si atom resulting in the negatively ionised B atom and a hole.

created that can move around the lattice. The impurity atoms that enhance the concentration of holes are called **acceptors**. We denote the concentration of donors N_A. Note that by substituting Si atoms with only one type of impurity atoms, the concentration of only one type of mobile charge carriers is increased. Charge neutrality of the material is nevertheless maintained because the sites of the bonded and thus fixed impurity atoms become charged. The donor atoms become positively ionised and the acceptor atoms become negatively ionised.

A possibility to control the electrical conductivity of a semiconductor by doping is one of most important semiconductor features. The electrical conductivity in semiconductors depends on the concentration of electrons and holes and their mobility. The concentration of electrons and holes is influenced by the amount of the impurity atoms that are introduced into the atomic structure of semiconductor. Figure 3.5 shows the range of doping that is used in case of c-Si. We denote a semiconductor a **p-type** or **n-type** when holes or electrons, respectively, dominate its electrical conductivity. In case that one type of charge carriers has a higher concentration than the other type these carriers are called **majority** carriers (holes in the *p*-type and electrons in the *n*-type), while the other type with lower concentration are then called **minority** carriers (electrons in the *p*-type and holes in the *n*-type).
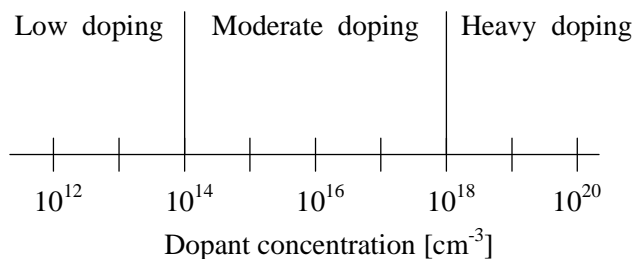

Figure 3.5. The range of doping levels used in c-Si.

3.2.3   Carrier concentrations

Any operation of a semiconductor device depends on the carriers that carry charge inside the semiconductor and cause electrical currents. In order to determine and/or to understand device operation it is important to know the precise number of these charge carriers. In the following section the concentrations of charge carriers inside a semiconductor are derived assuming the semiconductor is under **equilibrium**. The term equilibrium is used to describe the unperturbed state of a system, to which no external voltage, magnetic field, illumination, mechanical stress, or other perturbing forces are applied. In the equilibrium state the observable parameters of a semiconductor do not change with time.

In order to determine the carrier concentration one has to know the function of density of allowed energy states of electrons and the occupation function of the allowed energy states. The density of energy states function, *g(E)*, describes the number of allowed states per unit

volume and energy. The occupation function is the well known Fermi-Dirac distribution function, $f(E)$, which describes the ratio of states filled with an electron to total allowed states at given energy E. In an isolated Si atom, electrons are allowed to have only discrete energy values. The periodic atomic structure of single crystal silicon results in the ranges of allowed energy states for electrons that are called **energy bands** and the excluded energy ranges, **forbidden gaps** or **band gaps**. Electrons that are liberated from the bonds determine the charge transport in a semiconductor. Therefore, we further discuss only those bands of energy levels, which concern the valence electrons. Valence electrons, which are involved in the covalent bonds, have their allowed energies in the **valence band** (VB) and the allowed energies of electrons liberated from the covalent bonds form the **conduction band** (CB). The valence band is separated from the conduction band by a band of forbidden energy levels. The maximum attainable valence-band energy is denoted E_V, and the minimum attainable conduction-band energy is denoted E_C. The energy difference between the edges of these two bands is called the band gap energy or band gap, E_G, and it is an important material parameter.

$$E_G = E_C - E_V \qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.1)$$

The band gap of the single crystal silicon is of 1.12 eV at room temperature. An electron-volt is equal to the energy, which an electron acquires when it passes through a potential of 1 volt in vacuum ($1eV = 1.602 \times 10^{-19}$ J). A plot of allowed electron energy states as a function of position is called the energy band diagram and for intrinsic c-Si is shown in Figure 3.6.
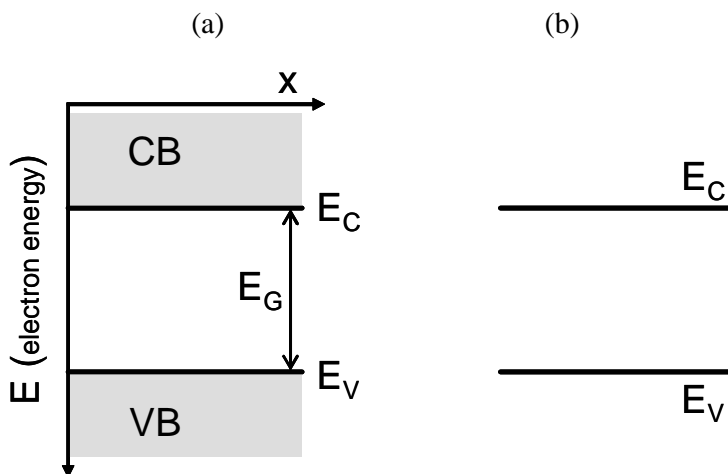

Figure 3.6. (a) The basic energy band diagram and (b) widely used simplified version of the energy diagram.

The density of energy states at an energy E in the conduction band close to E_c and in the valence band close to E_v are given by Eqs. (3.1).

$$g_C(E) = \left(\frac{4\sqrt{2}\,\pi m_n^*}{h^3}\right)^{3/2} (E - E_C)^{1/2} \qquad\qquad (3.2a)$$

$$g_V(E) = \left(\frac{4\sqrt{2}\,\pi m_p^*}{h^3}\right)^{3/2} (E - E_V)^{1/2} \qquad\qquad (3.2b)$$

where m_n^* and m_p^* is the effective mass of electrons and holes, respectively, averaged over different directions to take anisotropy into account. The Fermi-Dirac distribution function is given by

$$f(E) = \frac{1}{1 + \exp\left[(E - E_F)/kT\right]} \qquad\qquad (3.3)$$

where k is Boltzmann's constant ($k = 1.38 \times 10^{-23}$ JK^{-1}) and E_F is the so-called Fermi energy. kT is expressed in eV and equals to 0.0258 eV at 300°K. The **Fermi energy** is the electrochemical potential of the electrons in a material and in this way it represents the averaged energy of electrons in the material. The Fermi-Dirac distribution function is shown in Figure 3.7 for different temperatures.
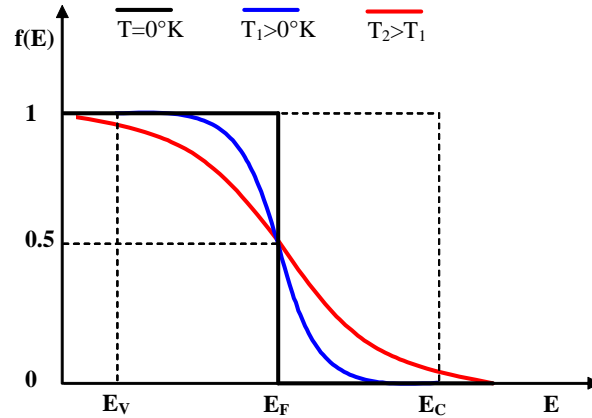
Figure 3.7. The Fermi-Dirac distribution function. For T = 0°K, all allowed states bellow the Fermi level are occupied by two electrons. At T > 0°K not all states below the Fermi level are occupied and there are some states above the Fermi level that are occupied.

The carriers that contribute to charge transport are electrons in the conduction band and holes in the valence band. The total concentration of electrons in the conduction band and the total concentration of holes in the valence band is obtained by multiplying the appropriate

density of states function with the appropriate distribution function and integrate over the whole energy band.

$$n = \int_{E_C}^{E_{top}} g_C(E) f(E) dE \tag{3.4a}$$

$$p = \int_{E_{bottom}}^{E_V} g_V(E) \left[1 - f(E)\right] dE \tag{3.4b}$$

Substituting the density of states and the Fermi-Dirac distribution function into Eq. (3.4) the resulting expressions for n and p are obtained after solving the equations. The full derivation can be found for example in reference [1].

$$n = N_C \exp\left[(E_F - E_C)/kT\right] \qquad \text{for } E_C - E_F \geq 3kT \tag{3.5a}$$

$$p = N_V \exp\left[(E_V - E_F)/kT\right] \qquad \text{for } E_F - E_V \geq 3kT \tag{3.5b}$$

where N_C and N_V are the effective density of conduction band states and the effective density of valence band states, respectively. In c-Si $N_C = 3.22 \times 10^{19}$ cm^{-3} and $N_V = 1.83 \times 10^{19}$ cm^{-3} at 300°K. When the requirement that the Fermi level lies in the band gap more than $3kT$ from either band edge is satisfied the semiconductor is referred to as **nondegenerate**.

In an intrinsic semiconductor in the equilibrium $n = p = n_i$. When multiplying the corresponding sides of Eqs. (3.5) one obtains

$$np = n_i^2 = N_C N_V \exp\left[(E_V - E_C)/kT\right] = N_C N_V \exp\left[-E_g/kT\right], \tag{3.6}$$

which is independent of the position of the Fermi level and is valid also for doped semiconductors. When we denote the position of the Fermi level in the intrinsic material E_i one can write

$$n_i = N_C \exp\left[(E_i - E_C)/kT\right] = N_V \exp\left[(E_V - E_i)/kT\right] \tag{3.7}$$

From Eq. (3.7) we can easily the position of E_i, which is given by

$$E_i = \frac{E_C + E_V}{2} + \frac{kT}{2} \ln\left(\frac{N_V}{N_C}\right) = E_C - \frac{E_g}{2} + \frac{kT}{2} \ln\left(\frac{N_V}{N_C}\right) \tag{3.8}$$

The Fermi level E_i lies close to the midgap; a slight shift is caused by the difference in the effective densities of the valence and conduction band.

It has been already mentioned in Section 3.2.2 that the concentrations of electrons and holes in c-Si can be manipulated by doping. The concentration of electrons and holes is

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[1] .F. Pierret. Advanced Semiconductor Fundamentals, in Modular series on solid state devices, Vol. **6**, Adison-Wesley Publishing Company, Inc., 1987.

influenced by the amount of the impurity atoms that substitute silicon atoms in the lattice. Under assumption that the semiconductor is uniformly doped and in equilibrium a simple relationship between the carrier and dopant concentrations can be established. We assume that at room temperature the dopant atoms are ionized. Inside a semiconductor the local charge density is given by:

$$\rho = q\left(p + N_D^+ - n - N_A^-\right) \tag{3.9}$$

where q is the elementary charge ($q = 1.602 \times 10^{-19}$ C). Under equilibrium conditions, in the uniformly doped semiconductor the local charge is zero, which means that the semiconductor is everywhere charge-neutral. One can write:

$$p + N_D^+ - n - N_A^- = 0 \tag{3.10}$$

As previously discussed, the thermal energy available at room temperature is sufficient to ionise almost all the dopant atoms. Under this assumption, $N_D^+ \approx N_D$ and $N_A^+ \approx N_A$, one obtains

$$p + N_D - n - N_A = 0 \tag{3.11}$$

which is the common form of the ***charge neutrality equation***.

Let's consider now an *n*-type material. At room temperature almost all donor atoms N_D are ionised and donate an electron into the conduction band. Under the assumption that $N_A = 0$, Eq. (3.11) becomes

$$p + N_D - n = 0 . \tag{3.12}$$

Under the assumption that

$$N_D \approx N_D^+ \approx n \tag{3.13}$$

we can expect that the concentration of holes is lower than that of electrons, and becomes very low when N_D becomes very large. We can calculate more accurate the concentration of holes in the *n*-type material from Eq. (3.6).

$$p = \frac{n_i^2}{n} = \frac{n_i^2}{N_D} \ll n \tag{3.14}$$

In case of a *p*-type material almost all acceptor atoms N_A are ionised at room temperature and accept an electron and leaving a hole in the valence band. Under the assumption that $N_D = 0$, Eq. (3.11) becomes

$$p - n - N_A = 0 . \tag{3.15}$$

Under the assumption that

$$N_A \approx N_A^- \approx p \tag{3.16}$$

we can expect that the concentration of electrons is lower than that of holes. We can calculate more accurate the concentration of electrons in the p-type material from Eq. (3.6).

$$n = \frac{n_i^2}{p} = \frac{n_i^2}{N_A} \ll p \tag{3.17}$$

Inserting donor and acceptor atoms into the lattice of crystalline silicon introduces allowed energy levels into the forbidden bandgap. For example, the fifth valence electron of the phosphorous atom does not take part in forming a bond, is rather weakly bound to the atom and easily liberates from the phosphorous atom. The energy of the liberated electron lies in the CB. The energy levels, which we denote E_D, of the weakly-bound valence electrons of the donor atoms have to be positioned close the CB. Notice that a dashed line represents the E_D. This means, that an electron that occupies the E_D level, is localized to the vicinity of the donor atom. Similarly, the acceptor atoms introduce allowed energy levels E_A close to the VB. Doping also influences the position of the Fermi energy. When increasing the concentration of electrons by increasing the concentration donors the Fermi energy will increase, which is represented by bringing the Fermi energy close to the CB in the band diagram. In the p-type material the Fermi energy is moving closer the VB. A change in the Fermi-energy position and the introduction of the allowed energy level into the bandgap due to the doping is illustrated in Figure 3.8.

The position of the Fermi level in an n-type semiconductor can be calculated using Eq. (3.5a) and the assumption (3.13) and in a p-type semiconductor using Eq. (3.5b) and Eq. (3.16), respectively.

$$E_C - E_F = kT \ln\left(N_C / N_D\right) \qquad \text{for } n\text{-type} \tag{3.18a}$$

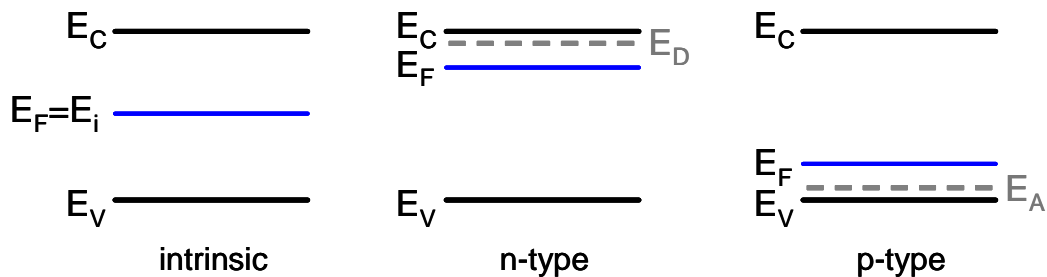$$E_F - E_V = kT \ln\left(N_V / N_A\right) \qquad \text{for } p\text{-type} \tag{3.18b}$$

Figure 3.8. A shift of the position of the Fermi energy in the band diagram and the introduction of the allowed energy level into the bandgap due to the doping.

EXAMPLE.
This example demonstrates how much the concentration of electrons and holes can be manipulated by doping. A c-Si wafer is uniformly doped with 1×10^{17} cm^{-3} phosphorous atoms. Phosphorous atoms act as donors and therefore at room temperature the concentration of electrons is almost equal to the concentration of donor atoms:

$$n = N_D^+ \approx N_D = 1\times 10^{17} \ cm^{-3}.$$

The concentration of holes in the n-type material is calculated from Eq. (3.13)

$$p = n_i^2 \big/ n = \left(1.5 \times 10^{10}\right)^2 \big/ 1 \times 10^{17} = 2.25\times 10^3 \ cm^{-3}.$$

We notice that there is a difference of 14 orders between n (1×10^{17} cm^{-3}) and p (2.25×10^3 cm^{-3}). It is now obvious why electrons are called in the n-type material the majority carriers and holes the minority carriers. We can calculate the change in the Fermi energy due to the doping. Let's assume that the reference energy level is the bottom of the conduction band, $E_c=0$ eV. Using Eq. (3.8) we calculate the Fermi energy in the intrinsic c-Si.

$$E_i = E_C - E_G\big/2 + kT\big/2 \ln\left(N_v\big/N_c\right) = -1.12\big/2 + 0.0258\big/2 \ln\left(1.83\times 10^{19}\big/3.22\times 10^{19}\right) = -0.57 \,\mathrm{eV}.$$

The Fermi energy in the n-type doped c-Si wafer is calculated from Eq. (3.5a)

$$E_F = E_c + kT \ln\left(n\big/N_c\right) = 0.0258 \ln\left(1\times 10^{17}\big/3.22\times 10^{19}\right) = -0.15 \,\mathrm{eV}.$$

We notice that the doping with phosphorous atoms has resulted in the shift of the Fermi energy towards the B. Note that when $n > N_c$, the $E_F > E_c$ and the Fermi energy lies in the CB.

3.2.4   Transport properties

In contrast to the equilibrium conditions, under operational conditions a net electrical current flows through a semiconductor device. The electrical currents are generated in a semiconductor due to the transport of charge from place to place by electrons and holes. The two basic transport mechanisms in a semiconductor are *drift* and *diffusion*.

Drift

Drift is charged-particle motion in response to an electric field. In an electric field the force acts on the charged particles in a semiconductor, which accelerates the positively charged holes in the direction of the electric field and the negatively charged electrons in the direction opposite to the electric field. Because of collisions with the thermally vibrating lattice atoms and ionised impurity atoms, the carrier acceleration is frequently disturbed. The resulting motion of electrons and holes can be described by average drift velocities $\mathbf{v}_{dn}$ and $\mathbf{v}_{dp}$ for electrons and holes, respectively. In case of low electric fields, the average drift velocities are directly proportional to the electric field as expressed by Eqs. (3.19). The proportionality factor is called *mobility*, μ, and is a central parameter that characterises electron and hole transport due to drift.

$$\mathbf{v}_{dn} = -\mu_n \xi \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.19a)$$

$$\mathbf{v}_{dp} = \mu_p \xi \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.19b)$$

Although the electrons move in the opposite direction to the electric field, because the charge of an electron is negative the resulting electron drift current is in the same direction as the electric field. This is illustrated in Figure 3.9.
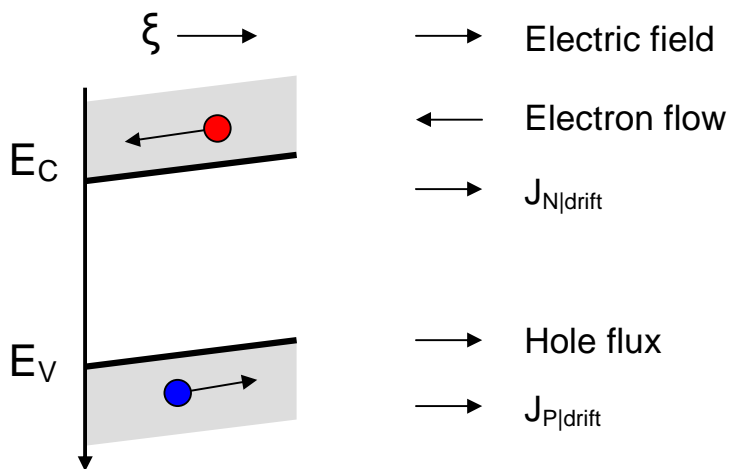

Figure 3.9. Visualization of carrier drift using the band diagram.

The electron and hole drift-current densities are defined by Eqs. (3.20) and the total drift current by Eq. (3.21).

$$\mathbf{J}_{N|drift} = -q\,n\,\mathbf{v}_{dn} = q\,n\,\mu_n\,\xi \tag{3.20a}$$

$$\mathbf{J}_{P|drift} = q\,p\,\mathbf{v}_{dp} = q\,p\,\mu_p\,\xi \tag{3.20b}$$

$$\mathbf{J}_{drift} = q\,(p\,\mu_p + n\,\mu_n)\,\xi \tag{3.21}$$

Mobility is a measure of how easily the charge particles can move through a semiconductor material. For example, at 300 K, $\mu_n \approx 1360$ cm^{2}V^{-1}s^{-1} and $\mu_p \approx 460$ cm^{2}V^{-1}s^{-1} in c-Si doped with N_D and N_A equal to 10^{14} cm^{-3}, respectively. As mentioned earlier, the motion of charged carriers is frequently disturbed by collisions. When number of collisions increases, the mobility decreases. Increasing the temperature increases the collisions of charged carriers with the vibrating lattice atoms, which results in a lower mobility. Increasing the doping concentration of donors or acceptors leads to more frequent collisions with the ionised dopant atoms, which again results in a lower mobility. The dependence of mobility on doping and temperature is in more detailed discussed in standard textbooks for semiconductor physics and devices [1,2].

Diffusion

Diffusion is a process whereby particles tend to spread out from regions of high particle concentration into regions of low particle concentration as a result of random thermal motion. A gradient in concentration of particles in a semiconductor is the driving force for the transport of particles associated with diffusion. On the contrary to the drift transport mechanism, the particles need not be charged to be involved in the diffusion process. Currents resulting from diffusion are proportional to the gradient in particle concentration and are expressed by Eqs (3.22) and the total diffusion current by Eq. (3.23). The total current due to both drift and diffusion is expressed by Eq. (3.24).

$$\mathbf{J}_{N|diff} = q\,D_N\nabla n \tag{3.22a}$$

$$\mathbf{J}_{P|diff} = -q\,D_P\nabla p \tag{3.22b}$$

$$\mathbf{J}_{diff} = q\left(D_N\nabla n - D_P\nabla p\right) \tag{3.23}$$

$$\mathbf{J} = \mathbf{J}_{drift} + \mathbf{J}_{diff} = q\,(p\,\mu_p + n\,\mu_n)\,\xi + q\left(D_N\nabla n - D_P\nabla p\right) \tag{3.24}$$

The constants of proportionality, D_N and D_P, are referred to as electron and hole *diffusion coefficients*, respectively. The diffusion coefficients of electrons and holes are linked with the mobilities of the corresponding charge carriers by the Einstein relationship, which is expressed by Eqs. (3.25).

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[2] D.A. Neaman, Semiconductor Physiscs and Devices: Basic principles, McGraw-Hill, 2003.

$$\frac{D_N}{\mu_n} = \frac{kT}{q} \tag{3.25a}$$

$$\frac{D_P}{\mu_p} = \frac{kT}{q} \tag{3.25b}$$

The visualization of the diffusion process and the resulting directions of particle fluxes and current are shown in Figure 3.10.
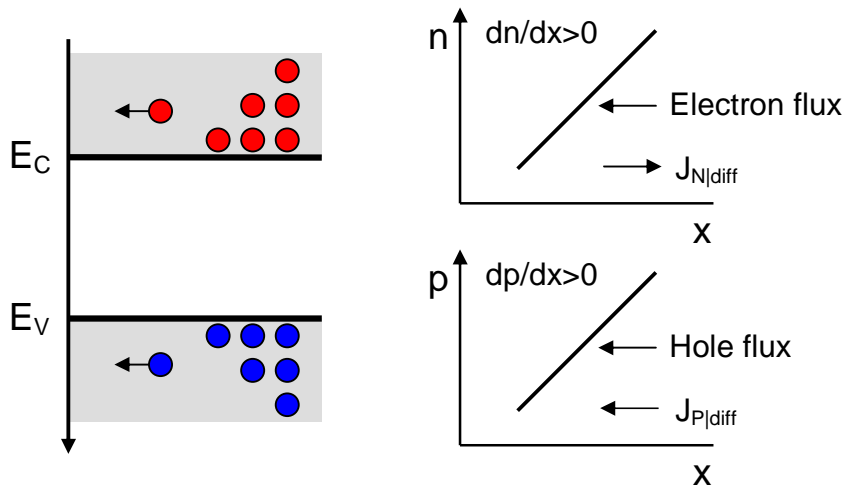

Figure 3.10. Visualization of carrier diffusion using the band diagram.

EXAMPLE. To obtain some idea about values of diffusion coefficients, let us assume Si sample at room temperature, doped with donors $N_D = 10^{14}$ cm^{-3}. According to Eq. (3.25a)

$$D_N = (kT/q)\mu_n = 0.0258\,\mathrm{V} \times 1360\,\mathrm{cm^2 V^{-1} s^{-1}} = 35\,\mathrm{cm^2\,s^{-1}}.$$

3.2.5   Recombination and generation

When a semiconductor is disturbed from the equilibrium state the electron and hole concentrations change from their equilibrium values. A number of processes start within the semiconductor after the perturbation in order to restore the equilibrium conditions. We call these processes recombination-generation (R-G) processes and they take care that a carrier excess or deficit is eliminated (if the perturbation is removed) or stabilized (if the perturbation is maintained). Generation is a process whereby electrons and holes are created. Recombination is a process whereby electrons and holes are annihilated or destroyed. As mentioned earlier, several processes can occur in a semiconductor, which lead to the generation or annihilation of the electrons and holes. In the following we shall describe only some of them, which are visualized in Figure 3.11.

1. **Band-to-band generation** (Figure 3.11a). The generation of an electron-hole pair can occur when the energy to break a bond is delivered by a photon (photogeneration) or by heat (direct thermal generation). This process can be visualized in terms of the band diagram as the excitation of an electron from the valence band into the conduction band.

2. **Band-to-band recombination** (Figure 3.11b). This process involves the direct annihilation of a conduction-band electron with a valence-band hole and is often called direct thermal recombination. It is typically a *radiative* process, in which a photon is emitted that carries an excess energy released in the recombination process.

3. **R-G center recombination or** indirect thermal recombination (Figure 3.11c). As the name suggests the annihilation or creation of electrons and holes does not occur directly but it is facilitated by a ***R-G center***. The R-G centers can be special impurity atoms or lattice defects. Their concentration is usually small compared to the acceptor or donor concentrations. The R-G centers introduce allowed energy levels (E_T) near the centre of the forbidden gap. An electron is trapped at the R-G center and consequently annihilated by a hole that is attracted by the trapped electron. Though this process seems to be less likely than the direct thermal recombination, it is at most operational conditions the dominant recombination-generation process in semiconductors. The process is typically non-radiative and the excess energy is dissipated into the lattice in form of heat.

The major effect of R-G processes in a semiconductor is to produce a change in the carrier concentration. In this way the R-G processes indirectly affects current flow in semiconductors by manipulating the concentrations of carriers that are involved in the drift and diffusion processes. The R-G processes change the carrier concentrations and this is mathematically characterized by the time rate of change in the carrier concentration ($\partial n/\partial t$ and $\partial p/\partial t$). In case of photogeneration, in which always an excess of an equal number of electrons and holes are created per second, one can write

$$\left.\frac{\partial n}{\partial t}\right|_{\text{light}} = \left.\frac{\partial p}{\partial t}\right|_{\text{light}} = G_L \qquad\qquad\qquad (3.26)$$

G_L is the generation rate due to light and its unit is (number/cm^3 s). G_L is a function of the distance in the material, depends in general on the absorption coefficient of the material, which is a function of the wavelength of light.
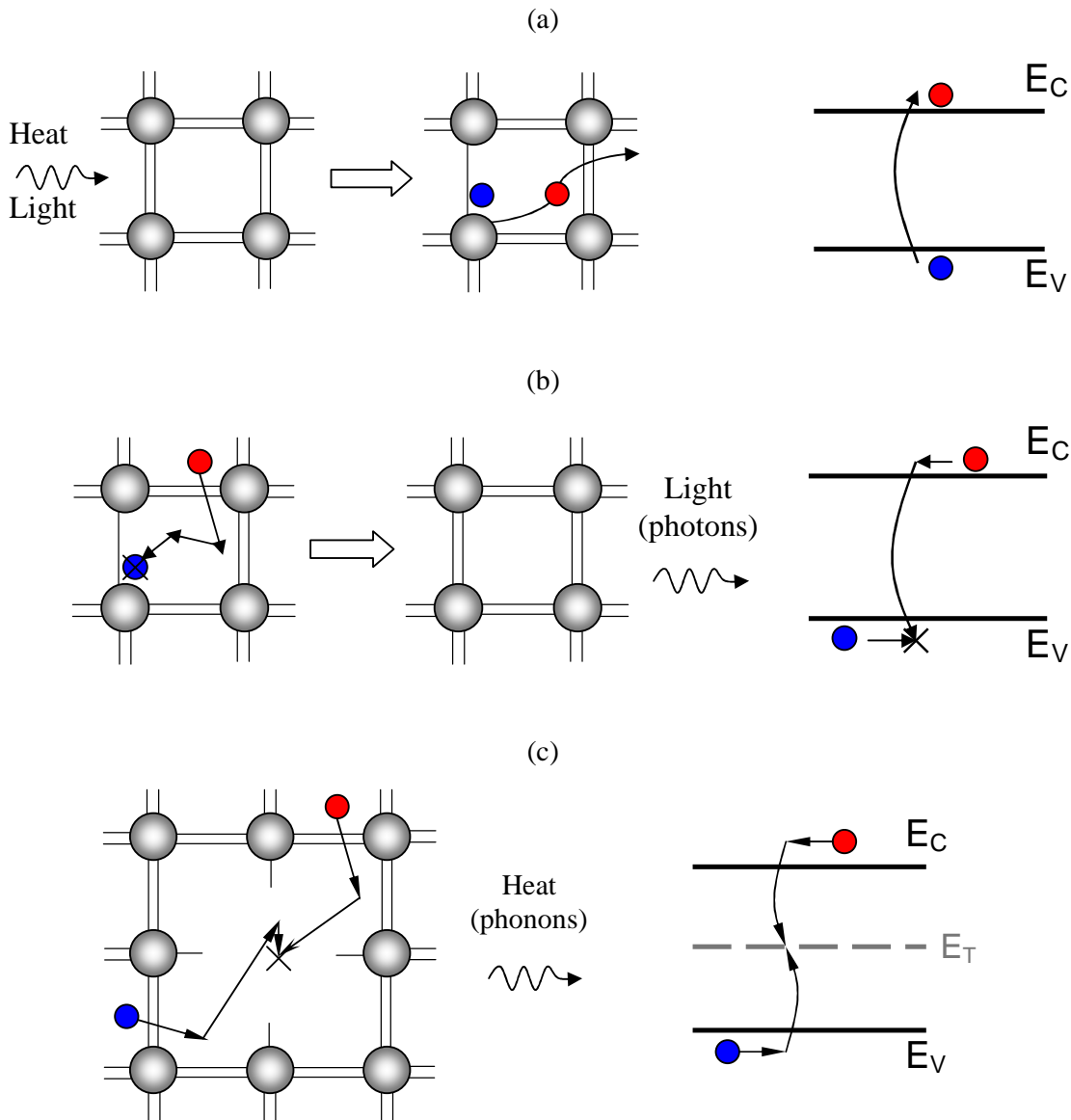
(a)

(b)

(c)

Figure 3.11. Visualization of some of the recombination-generation processes using the bonding model and the energy band diagram. (a) photogeneration and direct thermal generation, (b) direct thermal recombination, (c) R-G center (indirect thermal) recombination.

We shall introduce the equations describing the rate of change in the carrier concentration due to the dominant thermal R-G process for a semiconductor under following condition:
(1) the semiconductor is *n*- or *p*-type and
(2) the perturbation causes only *low level injection*.

The low injection means that

$\Delta n \ll p_0$, $p \cong p_0$ in a *p*-type material;

$\Delta p \ll n_0$, $n \cong n_0$ in an *n*-type material.

In case of the dominant thermal R-G process, which is recombination-generation involving R-G centres, the time rate of change in the carrier concentration depends on the excess or deficit of electrons and holes, in respect to their equilibrium values, $\Delta n = n - n_0$ and $\Delta p = p - p_0$, respectively, and the concentration of the R-G centers, N_T.

$$\left.\frac{\partial n}{\partial t}\right|_{\substack{\text{thermal}\\\text{R-G}}} = -c_n \, N_T \, \Delta n \qquad\qquad \text{for electrons in a } p\text{-type material} \qquad\qquad (3.27a)$$

$$\left.\frac{\partial p}{\partial t}\right|_{\substack{\text{thermal}\\\text{R-G}}} = -c_p \, N_T \, \Delta p \qquad\qquad \text{for holes in an } n\text{-type material} \qquad\qquad (3.27b)$$

where c_n and c_p are proportionality constants and are referred to as the electron and hole capture coefficients, respectively. The minus sign is introduced in Eqs. (3.27) because $\partial n / \partial t$ and $\partial p / \partial t$ decreases (is negative) when $\Delta n > 0$ and $\Delta p > 0$. We introduce the time constants

$$\tau_n = \frac{1}{c_n \, N_T} \qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.28a)$$

$$\tau_p = \frac{1}{c_p \, N_T} \qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.28b)$$

which, when substituted into Eqs. (3.27), yield

$$\left.\frac{\partial n}{\partial t}\right|_{\substack{\text{thermal}\\\text{R-G}}} = -\frac{\Delta n}{\tau_n} \qquad\qquad \text{for electrons in a } p\text{-type material} \qquad\qquad (3.29a)$$

$$\left.\frac{dp}{dt}\right|_{\substack{\text{thermal}\\\text{R-G}}} = -\frac{\Delta p}{\tau_p} \qquad\qquad \text{for holes in an } n\text{-type material} \qquad\qquad (3.29b)$$

The time constants τ_n and τ_p are the central parameters associated with recombination-generation. They can be interpreted as the *average time* an excess minority carrier will survive among majority carriers. The time constants τ_n and τ_p are referred to as ***minority-carrier lifetimes***. The values of the minority-carrier lifetimes can vary a lot. When the R-G center concentration is reduced to a very low level in c-Si, a τ_n (τ_p) can achieve ~ 1 ms. On the other hand, the intentional introduction of gold atoms into Si, which introduce efficient R-G centers into Si, can decrease a τ_n (τ_p) to ~ 1 ns. Typical minority-carrier lifetimes in most c-Si devices are usually ~ 1 μs. For an efficient collection of photo-generated carriers in c-Si solar cells the minority carrier lifetimes should be in range of tens of milliseconds.

When an excess of generated carriers is not uniform throughout a semiconductor, diffusion of the excess carriers takes place. The excess carriers will diffuse in the semiconductor till they do not recombine. We define the average distance that the minority carriers can diffuse among majority carries before being annihilated as ***minority-carrier-diffusion length***. The minority-carrier-diffusion lengths are defined as:

$$L_N = \sqrt{D_N \, \tau_n} \qquad\qquad \text{for electrons in a } p\text{-type material} \qquad\qquad (3.30a)$$

$$L_P = \sqrt{D_P \, \tau_p} \qquad\qquad \text{for holes in an } n\text{-type material} \qquad\qquad (3.30b)$$

EXAMPLE. To get an idea about the diffusion lengths, let us assume room temperature, mobility of electrons in a p-type c-Si wafer to be $\mu_n \approx 1250$ cm^{2}V^{-1}s^{-1}, which corresponds to doping of $N_A = 10^{14}$ cm^{-3}, and $\tau_n = 10^{-6}$ s. For the given conditions, the electron diffusion length in the p-type c-Si can be calculated from Eq. (3.30a).

$$L_N = \sqrt{D_N \, \tau_n} = \sqrt{(kT/q)\mu_n \, \tau_n} = \sqrt{0.02586\,\text{V} \times 1250\,\text{cm}^2\text{V}^{-1}\text{s}^{-1} \times 10^{-6}\,\text{s}} = 5.7 \times 10^{-3}\ \text{cm} = 57\,\mu\text{m}.$$

3.2.6   Optical properties

Absorption of light in a semiconductor material represents a complex interaction of light with the semiconductor atomic structure. Only such interactions that lead to the generation of free charge carriers in a semiconductor, electrons and holes, contribute to the transformation of energy carried by light into electrical energy. The generation of charge carriers is a result of breaking of the atomic bonds, when the electron-hole pairs are created. The process of generating an electron-hole pair can be visualized in the energy band diagram as transferring an electron from the valence energy band to the conduction energy band. The light particles, photons, have to carry at least the energy equal to the **band gap energy** of a semiconductor in order to free an electron from a covalent bond. Photons with energy higher than the band gap energy generate electron-hole pairs. Since the electrons and holes tend to occupy energy levels at the bottom of the conduction band and the top of the valence band, respectively, the extra energy that the electron-hole pairs receive from the photons is released as heat into the semiconductor lattice in the **thermalization** process. The process of creation of an electron-hole pair by absorbing a photon and the process of thermalization are illustrated in Figure 3.12.
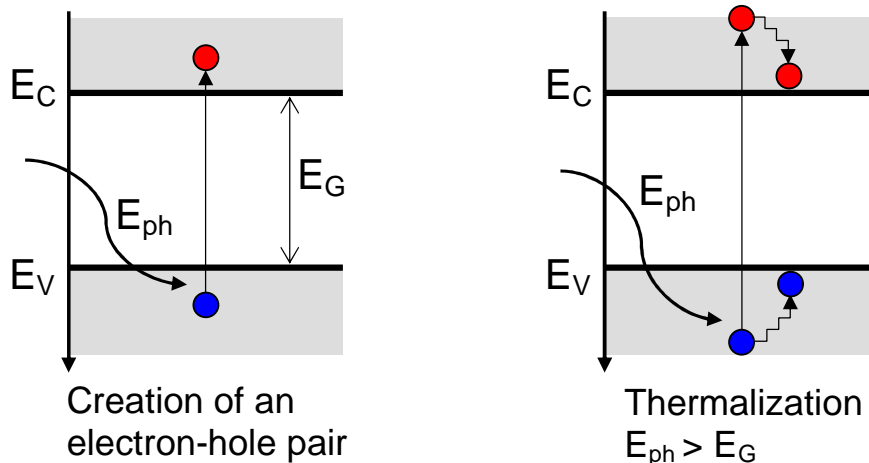

Figure 3.12. Visualization of the process of creation of an electron-hole pair by absorbing a photon and the process of thermalization using the energy band diagram.

An important key for obtaining an efficient solar cell is to minimize the heat losses due to the thermalization by choosing semiconductors with appropriate band gaps. When taking into account the energy distribution of the solar spectrum the most effective materials for solar energy conversion have band gap energies in the range of 1.0 to 1.8 eV (electron-volts).

The photon energy, E_{ph}, depends on the wavelength of light and is calculated using the following formula:

$$E_{ph} = hc/\lambda \tag{3.31}$$

where h is the Planck constant ($h = 6.625 \times 10^{-34}$ Js) , c is the speed of light ($c = 2.998 \times 10^{8}$ ms^{-1}), and λ is the wavelength of light. The entire spectrum of sunlight, from infrared to ultraviolet, covers a range of about 0.5 eV to about 4.0 eV. About 55% of the energy of sunlight cannot be used by most solar cells because this energy is either lower than the band gap or it is higher and the excess energy is lost by thermalization.

While the band gap energy of a semiconductor provides us with information, which part of the solar spectrum is absorbed, the ***complex refractive index***, $\tilde{n} = n - ik$, describes how efficient the photons of a particular energy are absorbed in the material. The real part n is called the refractive index, and the imaginary part k is called the extinction coefficient. The extinction coefficient is related to the absorption coefficient α by:

$$k = \frac{\alpha \lambda}{4 \pi} \qquad (3.32)$$

The n and k are called ***optical constants***, although they are functions of the wavelength of light or the photon energy. The wavelength, λ is related to the photon energy, $h\nu$ as,

$$h\nu = \frac{h}{q} \frac{c}{\lambda} \qquad (3.33)$$

where the photon energy is represented in eV.

When light impinges on an interface between two media that are characterized by their complex refractive indices, a part of the light is reflected from and the other part is transmitted through the interface. The interface is therefore characterized by the reflectance and transmittance. Reflectance is the ratio of the energy reflected from the surface of the interface to the total incident energy. Transmittance is the ratio of the energy transmitted through the interface to the total incident energy.

When light arrives at the optical interface at normal incidence, the reflectance and transmittance can be calculated by using the amplitude reflection and transmission coefficients also known as Fresnel amplitude coefficients ($\tilde{r}$, $\tilde{t}$)[3]:

$$\tilde{r} = \frac{\tilde{n}_0 - \tilde{n}_1}{\tilde{n}_0 + \tilde{n}_1} \qquad (3.34)$$

$$\tilde{t} = \frac{2\tilde{n}_0}{\tilde{n}_0 + \tilde{n}_1} \qquad (3.35)$$

The $\tilde{n}_0$ and $\tilde{n}_1$ are the complex refractive indices of the first and second medium. The Fresnel amplitude coefficients are also complex numbers. The reflectance and transmittance of the interface are:

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[3] J.M. Bennett and H.E. Bennett, *Polarization.* in Handbook of Optics, eds. W.G. Driscoll and W. Vaughan, Chap. 10, Mc Graw-Hill, 1978.

$$R = \left| \tilde{r} \right|^2 = \left| \frac{\tilde{n}_0 - \tilde{n}_1}{\tilde{n}_0 + \tilde{n}_1} \right|^2 \tag{3.36}$$

$$T = \left| \frac{\tilde{n}_1}{\tilde{n}_0} \right| \left| \tilde{t} \right|^2 = \frac{4 \left| \tilde{n}_0 \, \tilde{n}_1 \right|}{\left| \tilde{n}_0 + \tilde{n}_1 \right|^2} \tag{3.37}$$

When light penetrates into a material it will be absorbed as it propagates through the material. The absorption profile in the material depends on the absorption coefficient of the material, which is wavelength dependent. The most frequent approach to calculate the absorption profile of photons in semiconductor devices is by using the Lambert-Beer absorption formula. The Lambert-Beer formula states that a photon flux density after passing a distance x in a film with absorption coefficient $\alpha(\lambda)$ is reduced with a factor $e^{-\alpha(\lambda)x}$,

$$\Phi(x, \lambda) = \Phi^0(\lambda) \exp(-\alpha(\lambda)x), \tag{3.38}$$

where $\Phi^0(\lambda)$ is the incident photon flux density. The photon flux density is the number of photons per unit area per unit time and per unit wavelength. It is related to the spectral power density $P(\lambda)$ associated with the solar radiation by:

$$\Phi^0(\lambda) = P(\lambda) \frac{\lambda}{hc} \tag{3.39}$$

The spectral generation rate $g_{sp}(x, \lambda)$, which is the number of electron-hole pairs generated at a depth x in the film per second per unit volume per unit wavelength, by photons of wavelength λ, is calculated according to the following formula, on the assumption of zero reflection:

$$g_{sp}(x, \lambda) = \eta_g \Phi^0(\lambda) \, \alpha(\lambda) \, e^{-\alpha(\lambda)x} \tag{3.40}$$

where η_g is the generation quantum efficiency, usually assumed to equal unity. This assumption means that every photon generates one and only one electron-hole pair. The optical generation rate $G_L(x)$ is calculated from the spectral generation rate by integrating over a desired wavelength spectrum:

$$G_L(x) = \int_{\lambda_1}^{\lambda_2} g_{sp}(x, \lambda) \, d\lambda \tag{3.41}$$

The optical generation rate is related to the absorption profile, $A(x)$, in the film:

$$G_L(x) = \eta_g \, A(x) \tag{3.42}$$

$$A(x) = \int_{\lambda_1}^{\lambda_2} \Phi^0(\lambda) \, \alpha(\lambda) \, e^{-\alpha(\lambda)x} \, d\lambda \tag{3.43}$$

EXAMPLE.

Let's calculate how much light is reflected from the air/c-Si interface. Lets assume that the incident light has a wavelength of 500 nm. For this wavelength the complex refractive index of air is $\tilde{n}_0$ = 1.0 –0.0 i and for c-Si $\tilde{n}_1$ = 4.293 – 0.045 i. The reflectance is calculated from Eq. 3.36.

$$R = \left|\frac{\tilde{n}_0 - \tilde{n}_1}{\tilde{n}_0 + \tilde{n}_1}\right|^2 = \left|\frac{1.0 - 0.0i - (4.293 - 0.045i)}{1.0 - 0.0i + 4.239 - 0.045i}\right|^2 = \left|\frac{-3.293 - 0.045i}{5.293 - 0.045i}\right|^2 = 0.38.$$

It means 38% of light with the wavelength of 500 nm is reflected from the air/c-Si interface. In case of c-Si solar cells, over 30% of the incident light in the range of interest is reflected. In order to make solar cells with a high conversion efficiency, antireflection coatings are used to reduce the reflection from c-Si solar cells.

EXAMPLE.

Let's calculate the total absorption in a 300 μm thick c-Si wafer for light characterised by wavelength of 500 nm. The optical constants of c-Si for light with 500 nm are: refractive index is n = 4.293, extinction coefficient k = 0.045 and absorption coefficient α = 1.11 × 10⁴ cm⁻¹. The incident irradiance is 1000 W/m².

First we calculate the photon flux density at 500 nm corresponding to the irradiance of 1000 W/m². Using the Eq. 3.38 we obtain

$$\Phi^0 = P \times (\lambda/hc) = 1000\,\mathrm{Wm}^{-2} \times 500 \times 10^{-9}\,\mathrm{m} / (6.625 \times 10^{-34}\,\mathrm{Js} \times 2.998 \times 10^8\,\mathrm{ms}^{-1}) = 2.5 \times 10^{21}\,\mathrm{m}^{-2}\mathrm{s}^{-1}.$$

From Eq. 3.36 we calculate how many incident photons are reflected from the surface

$$R = \left|\frac{\tilde{n}_0 - \tilde{n}_1}{\tilde{n}_0 + \tilde{n}_1}\right|^2 = \left|\frac{1.0 - 0.0i - (4.293 - 0.045i)}{1.0 - 0.0i + 4.239 - 0.045i}\right|^2 = \left|\frac{-3.293 - 0.045i}{5.293 - 0.045i}\right|^2 = 0.38$$

Using Lambert-Beer formula (Eq. (3.38)) we calculate the photon flux density at the backside of the wafer, it means at the distance 300 μm from the surface. We take the reflected light into account by adapting Eq. (3.38).

$$\Phi(x) = \Phi^0(1-R)\exp(-\alpha x) = 2.5 \times 10^{21}\,\mathrm{m}^{-2}\mathrm{s}^{-1} \times (1-0.38)\exp(-1.11 \times 10^6\,\mathrm{m}^{-1} \times 300 \times 10^{-6}\mathrm{m}) \simeq 0$$

The total absorption in the wafer is the difference between the photon flux density at the surface after reflection and the photon flux density at the back of the wafer.

$$A = \Delta\Phi = \Phi^0(1-R) - \Phi(x) = 2.5 \times 10^{21}\,\mathrm{m}^{-2}\mathrm{s}^{-1} \times (1-0.38) - 0 = 1.55 \times 10^{21}\,\mathrm{m}^{-2}\mathrm{s}^{-1}$$

When we assume that all the absorbed photons generate one electron-hole pair (η_g=1), we can calculate how large photocurrent density corresponds to the absorbed photons.

$$J_{ph} = qA = 1.602 \times 10^{-19}\,\mathrm{C} \times 1.55 \times 10^{21}\,\mathrm{m}^{-2}\mathrm{s}^{-1} = 248.31\,\mathrm{Cm}^{-2}\mathrm{s}^{-1} = 248.31\,\mathrm{A\,m}^{-2}$$

3.2.7   Carrier concentrations in non-equilibrium

When a semiconductor is illuminated additional electrons and holes are generated in the material by the absorption of photons. The photo-generated carriers interact with the semiconductor lattice. The extra energy that the electron-hole pairs receive from the photons that have energy larger than the band gap of the semiconductor is released into the lattice in form of heat. After this so called **thermalization** process, which is very fast and takes approximately 10^{-12} s, the carrier concentrations achieve a steady-state. In this non-equilibrium state the electron and hole concentrations are different than those in the equilibrium state. In non-equilibrium states two Fermi distributions are used to describe the electron and hole concentrations. One Fermi distribution with the **quasi-Fermi energy for electrons**, E_{FC}, describes the occupation of states in the conduction band with electrons. Another Fermi distribution with the **quasi-Fermi energy for holes**, E_{FV}, describes the occupation of states in the valence band with electrons, and therefore determines also the concentration of holes. Using the band diagram with the quasi-Fermi levels the process of creation of electron-hole pairs and their subsequent thermalization that describe the carrier concentration under illumination is illustrated in Figure 3.13. The difference between the quasi-Fermi levels is the electrochemical energy, μ_{eh}, of the generated electron-hole pairs which represents the measure for the conversion efficiency of solar radiation.

The density of electrons and holes under non-equilibrium conditions is described by

$$n = N_C \exp\left[\left(E_{FC} - E_C\right)/kT\right] \tag{3.44a}$$

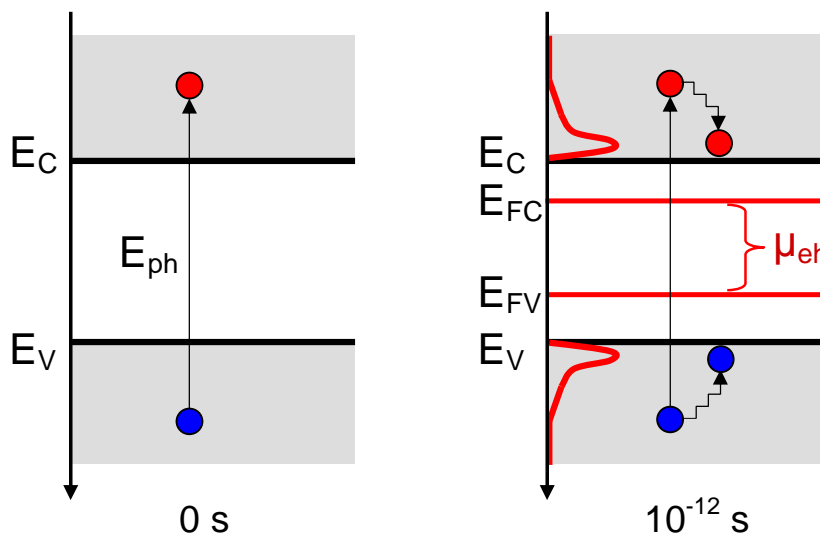$$p = N_V \exp\left[\left(E_V - E_{FP}\right)/kT\right] \tag{3.44b}$$

Figure 3.13. Thermalization photo-generated electron-hole pairs resulting in non-equilibrium charge-carrier concentrations described by the quasi-Fermi levels.

It then follows that under non-equilibrium conditions

$$n\,p = N_C\,N_V\,\exp\left[\frac{E_V - E_C}{kT}\right]\exp\left[\frac{E_{FC} - E_{FP}}{kT}\right] = n_i^2\,\exp\left[\frac{E_{FC} - E_{FP}}{kT}\right] \tag{3.45}$$

By using the quasi-Fermi level formalism for describing the concentration of charge carriers in non-equilibrium conditions the electron and hole current densities inside a semiconductor, $\mathbf{J}_N$ and $\mathbf{J}_P$, can be expressed by following equations:

$$\mathbf{J_N} = n\,\mu_n\nabla E_{FC} \tag{3.46a}$$

$$\mathbf{J_P} = p\,\mu_p\nabla E_{FV} \tag{3.46b}$$

One can notice from Eq. (3.46) that when a quasi-Fermi level varies with position ($dE_{FC}/dx \neq 0$ or $dE_{FV}/dx \neq 0$) the current is flowing inside the semiconductor. By checking the position dependence of the quasi-Fermi levels in an energy band diagram, one can easily determine whether current flows inside the semiconductor.

3.3 Basic equations of device physics

In the previous section, semiconductor material properties and the carrier transport, creation and annihilation taking place inside a semiconductor were discussed and described. The results from the drift, diffusion, and recombination-generation analysis are put together into a set of equations, which form a general three-dimensional mathematical model for semiconductor device operation.

3.3.1 Continuity Equations

Drift, diffusion, and recombination-generation processes give rise to a change in the carrier concentrations in time. Nevertheless, there must be a spatial and time continuity in the carrier concentrations. The combined effect of all types of carrier action within a semiconductor is described by the following continuity equation for electrons (Eq. (3. 47a) and holes (Eq. (3.47b), respectively

$$\frac{\partial n}{\partial t} = \left.\frac{\partial n}{\partial t}\right|_{\text{drift}} + \left.\frac{\partial n}{\partial t}\right|_{\text{diff}} + \left.\frac{\partial n}{\partial t}\right|_{\substack{\text{thermal}\\ \text{R-G}}} + \left.\frac{\partial n}{\partial t}\right|_{\substack{\text{other processes}\\ \text{(photogeneration)}}} \tag{3.47a}$$

$$\frac{\partial p}{\partial t} = \left.\frac{\partial p}{\partial t}\right|_{\text{drift}} + \left.\frac{\partial p}{\partial t}\right|_{\text{diff}} + \left.\frac{\partial p}{\partial t}\right|_{\substack{\text{thermal}\\ \text{R-G}}} + \left.\frac{\partial p}{\partial t}\right|_{\substack{\text{other processes}\\ \text{(photogeneration)}}} \tag{3.47b}$$

The continuity equations can be written in a more compact form when introducing substitutions

$$\left.\frac{\partial n}{\partial t}\right|_{\substack{\text{thermal}\\\text{R-G}}} = -R_N \; ; \qquad\qquad \left.\frac{dp}{dt}\right|_{\substack{\text{thermal}\\\text{R-G}}} = -R_P \qquad\qquad (3.48\text{a,b})$$

$$\left.\frac{\partial n}{\partial t}\right|_{\text{other processes}} = G_N \; ; \qquad\qquad \left.\frac{\partial p}{\partial t}\right|_{\text{other processes}} = G_P \qquad\qquad (3.49\text{a,b})$$

and noting

$$\left.\frac{\partial n}{\partial t}\right|_{\text{drift}} + \left.\frac{\partial n}{\partial t}\right|_{\text{diff}} = \frac{1}{q}\nabla\cdot\mathbf{J}_N \qquad\qquad (3.50\text{a})$$

$$\left.\frac{\partial p}{\partial t}\right|_{\text{drift}} + \left.\frac{\partial p}{\partial t}\right|_{\text{diff}} = -\frac{1}{q}\nabla\cdot\mathbf{J}_P \qquad\qquad (3.50\text{b})$$

In these equations $\partial n/\partial t$ ($\partial p/\partial t$) is the time rate change in the electron (hole) concentration, $\mathbf{J}_N$ ($\mathbf{J}_P$) is the electron (hole) current density, R_N (R_P) denotes the net recombination-generation rate of electrons (holes), G_N (G_P) is the generation rate of electrons (holes) due to other processes, such as photogeneration. Substituting Eqs. (3.48) through (3.50) into (3.47), we obtain

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla\cdot\mathbf{J}_N - R_N + G_N \qquad\qquad (3.51\text{a})$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla\cdot\mathbf{J}_P - R_P + G_P \qquad\qquad (3.51\text{b})$$

3.3.2   Current-Density Equations

The electron and hole current densities inside a semiconductor, $\mathbf{J}_N$ and $\mathbf{J}_P$, are obtained by adding the current densities due to drift and diffusion.

$$\mathbf{J}_N = q\,n\,\mu_n\,\xi + q\,D_N\nabla n \qquad\qquad (3.52\text{a})$$

$$\mathbf{J}_P = q\,p\,\mu_p\,\xi - q\,D_p\nabla p \qquad\qquad (3.52\text{b})$$

3.3.3   Poisson's Equation

The Poisson's equation (3.53) relates the divergence of the electric field to the space charge density, ρ.

$$\nabla\cdot\xi = \frac{\rho}{\varepsilon_r\varepsilon_0} \qquad\qquad (3.53)$$

In this equation ε_r is the semiconductor dielectric constant and ε_0 is the permittivity of the vacuum. The permittivity of the vacuum $\varepsilon_0 = 8.854 \times 10^{-14}$ F/cm and for c-Si $\varepsilon_r = 11.7$. Free electrons, holes and ionised dopant atoms are the main contributors to the charge density inside a semiconductor. It has been mentioned that impurities other than dopants and defects can be present in a semiconductor and act as charge capture centres. However, the concentration of such imperfections is kept small in semiconductors used for solar cells. The space charge density is therefore sufficiently described by Eq. (3.9):

$$\rho = q\left(p + N_D^+ - n - N_A^-\right).$$

3.3.4   Equations summary

Since the operation of a solar cell can be sufficiently described by processes taking place in one direction, the set of basic semiconductor equations will be given in one-dimensional form.

$$\left.\begin{aligned}
\frac{d\xi}{dx} &= \frac{\rho}{\varepsilon_r \varepsilon_0} \\[2mm]
J_N &= q\, n\, \mu_n\, \xi + q\, D_N \frac{dn}{dx} \\[2mm]
J_P &= q\, p\, \mu_p\, \xi - q\, D_P \frac{dp}{dx} \\[2mm]
\frac{\partial n}{\partial t} &= \frac{1}{q}\frac{dJ_N}{dx} - R_N + G_N \\[2mm]
\frac{\partial p}{\partial t} &= -\frac{1}{q}\frac{dJ_P}{dx} - R_P + G_P
\end{aligned}\right\} \qquad (3.54)$$