

6

Basic Semiconductor Physics

6.1 Introduction

With this chapter we start with the discussion of some important concepts from *semiconductor physics*, which are required to understand the operation of solar cells. After giving a brief introduction into semiconductor physics in this chapter, we will discuss the most important *generation and recombination* mechanisms in Chapter 7. Finally, we will focus on the physics of *semiconductor junctions* in Chapter 8.

The first successful solar cell was made from crystalline silicon (c-Si), which still is by far the most widely used PV material. Therefore we shall use c-Si as an example to explain the concepts of semiconductor physics that are relevant to solar cell operation. This discussion will give 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:

1. Concentrations of doping atoms, which can be of two different types: *donor atoms*, which donate free electrons or *acceptor atoms*, which accept electrons. The concentrations of donor and acceptor atoms are denoted by N_D and N_A , respectively, and determine the width of the space-charge region of a junction, as we will see in Chapter 8.
2. The mobility μ and the diffusion coefficient D of charge carriers is used to characterise the transport of carriers due to drift and diffusion, respectively, which we will discuss in Section 6.5.
3. The lifetime τ and the diffusion length L of the *excess carriers* characterise the recombination-generation processes, discussed in Chapter 7.

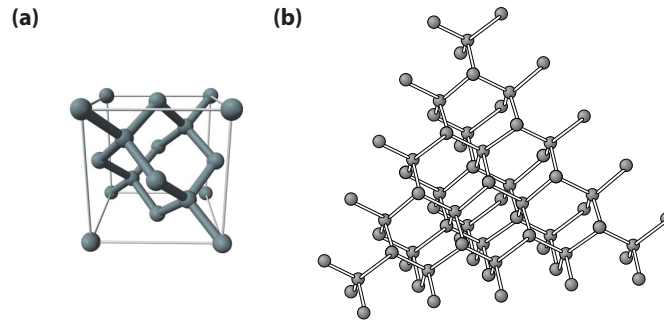


Figure 6.1: (a) A diamond lattice unit cell representing a unit cell of single crystal Si [30], (b) the atomic structure of a part of single crystal Si.

4. The band gap energy E_g , and the complex refractive index $n - ik$, where k is linked to the absorption coefficient α , characterise the ability of a semiconductor to absorb electromagnetic radiation.

6.2 Atomic structure

The *atomic number* of silicon is 14, which means that 14 electrons are orbiting the nucleus. In ground state configuration, two electrons are in the first shell, both in the 1s orbital. Further, eight electrons are in the second shell, two in the 2s and six in the 2p orbitals. Hence, four electrons are in the third shell, which is the outermost shell for a Si atom. Only these four electrons interact with other atoms, for example via forming chemical bonds. They are called the *valence electrons*.

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 atoms have four valence electrons, they can be covalently bonded to four other Si atoms. In the crystalline form each Si atom is covalently bonded to four neighbouring Si atoms, as illustrated in Fig. 6.1.

In the ground state, two valence electrons live in the 3s orbital and the other two are present in the three 3p orbitals (p_x , p_y and p_z). In this state only the two electrons in the 3p orbitals can form bonds as the 3s orbital is full. In a silicon crystal, where every atom is *symmetrically* connected to four others, the Si atoms are present as so-called *sp_3 hybrids*. The 3p and 3s orbitals are mixed forming 4 sp_3 orbitals. Each of these four orbitals is occupied by one electron that can form a covalent bond with a valence electron from a neighbouring atom.

All bonds have the same length and the angles between the bonds are equal to 109.5° . 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 monocrystalline silicon. Figure 6.1 (a) shows the arrangement of the unit cell and Fig. 6.1 (b) the atomic structure of single crystal silicon. One can determine from Fig. 6.1 (a) that there are eight Si atoms in the volume of the unit cell. Since the lattice constant of c-Si is 543.07 pm, one can easily calculate that the density of atoms is approximately $5 \times 10^{22} \text{ cm}^{-3}$. Figure 6.1 (a) 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, e.g. at room temperature,¹ 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 to 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 visualised by using the *bonding model* illustrated in Fig. 6.2.

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 electrons 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 no free electrons are present in the lattice. This situation is schematically shown in Fig. 6.2 (a).

At temperatures higher than 0 K the bonds start to break due to the absorption of thermal energy. This process results in the creation of mobile electrons and holes. Figure 6.2 (b) shows a situation when a covalent bond is broken and one electron departs from the bond leaving a so-called *hole* behind. A single line between the atoms in Fig. 6.2 (b) 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 hole, a positive charge representing the empty position, in the direction opposite to the motion of the valence electron through the bonds.

Since the 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. In intrinsic silicon at 300 K approximately $1.5 \times 10^{10} \text{ cm}^{-3}$ broken bonds are present. This number then gives also the concentration of holes, p , and electrons, n . Hence, at 300 K, $n = p = 1.5 \times 10^{10} \text{ cm}^{-3}$. This concentration is called the *intrinsic carrier concentration* and is denoted as n_i .

¹In semiconductor physics most of the time a temperature of 300 K is assumed.

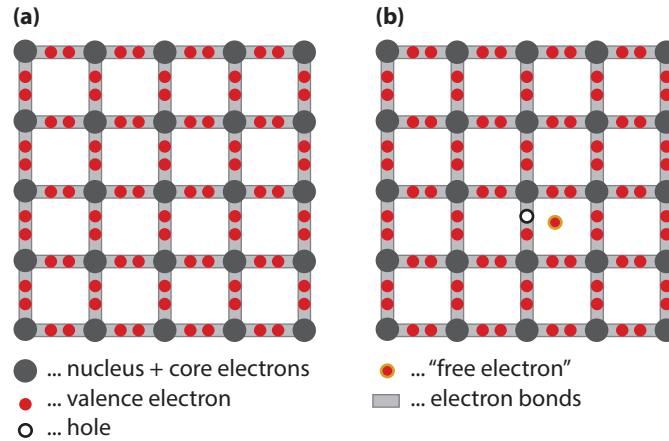


Figure 6.2: The bonding model for c-Si. (a) No bonds are broken. (b) A bond between two Si atoms is broken resulting in a free electron and hole.

6.3 Doping

The concentrations of electrons and holes in c-Si can be manipulated by *doping*. Doping of silicon means that atoms of other elements substitute Si atoms in the crystal lattice. The substitution has to be carried out by atoms with three or five valence electrons, respectively. The most used elements to dope c-Si are boron (B) and phosphorus (P), with atomic numbers of 5 and 15, respectively.

The process of doping action can best be understood with the aid of the bonding model and is illustrated in Fig. 6.3. When introducing a phosphorus atom into the c-Si lattice, four of the five phosphorus 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 phosphorus atom. It is easily liberated from the phosphorus 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 phosphorus 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 denote the concentration of donors by 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. The 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 created that can move around the lattice. The impurity atoms that enhance the concentration of holes are called *acceptors*. We denote the concentration of acceptors by 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

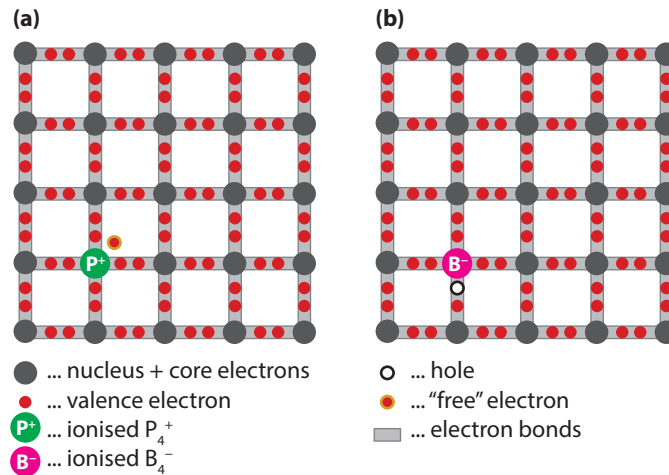


Figure 6.3: The doping process illustrated using the bonding model. (a) A phosphorus (P) atom substitutes a Si atom in the lattice resulting in the positively-ionised P atom and a free electron, (b) A boron (B) atom substitutes a Si atom resulting in the negatively ionised B atom and a hole.

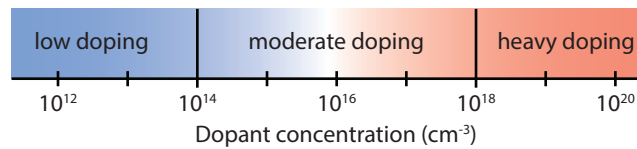


Figure 6.4: The range of doping levels used in c-Si.

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.

The possibility to control the electrical conductivity of a semiconductor by doping is one of the most important semiconductor features. The electrical conductivity in semiconductors depends on the concentration of electrons and holes as well as their mobility. The concentration of electrons and holes is influenced by the amount of the doping atoms that are introduced into the atomic structure of the semiconductor. Figure 6.4 shows the range of doping that is used in case of c-Si. We denote a semiconductor as *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).