

1 Review of semiconductor materials and physics

1.1 Executive summary

Semiconductor devices are fabricated using specific materials that offer the desired physical properties. There are three classes of solid state materials: insulators, semiconductors and conductors. This distinction is based on the electrical conductivity of these materials with insulators having the lowest and conductors having the highest conductivity. Semiconductors fall in between and their conductivity is affected by several factors such as temperature, the incidence of light, the application of a magnetic field and impurities. This versatility makes semiconductors very important in electronics and optoelectronics applications.

Semiconductors themselves are divided into two classes: elemental and compound. Each type has distinctive physical properties which are exploited in device design. Typical elemental semiconductor device materials are silicon and germanium; examples of compound semiconductors are GaAs, InP, AlGaAs and SiGe. The single crystal structure of these materials is that of a periodic lattice and this determines the properties of the semiconductors. Silicon has the diamond crystal structure and the compound semiconductors have the zincblende lattice structure. The bonding between atoms in a crystal of the semiconductors is termed *covalent bonding*, where electrons are shared between atoms. Fundamental principles of quantum mechanics are applied to determine the energy band structure of the semiconductor.

The basic device physics involves the description of the energy band structure, the density of states, the carrier concentration and the definition of donors and acceptors. Semiconductors are categorised as direct or indirect depending on the bandgap. The absorption mechanism is described and radiation and recombination processes important to device performance are detailed. The two carrier transport processes are drift and diffusion. The currents due to these transport processes are expressed in terms of the applied electric field, the carrier mobility and the carrier concentration. The junction formed by p-type semiconductor (excess holes) and n-type semiconductor (excess electrons) is described and the characteristics of such a junction are given. The important Schottky diode, a junction formed by a metal and a semiconductor layer (n-doped in this case) is characterised.

Heterostructures formed by dissimilar semiconductors are important in device design. The properties of heterojunctions of semiconductor materials are presented. Silicon–germanium heterojunctions are of particular interest as high performance electronic

Table 1.1 Portion of the periodic table showing semiconductor material elements

Period	Group III	Group IV	Group V
2	B Boron	C Carbon	N Nitrogen
3	Al Aluminium	Si Silicon	P Phosphorus
4	Ga Gallium	Ge Germanium	As Arsenic
5	In Indium	Sn Tin	Sb Antimony

Table 1.2 Elemental and binary compound semiconductors

Elements	IV–IV Binary compounds	III–V Binary compounds
Si Silicon	SiC Silicon carbide	AlAs Aluminium arsenide
Ge Germanium	SiGe Silicon germanium	AlP Aluminium phosphide
		AlSb Aluminium antimonide
		BN Boron nitride
		GaAs Gallium arsenide
		GaN Gallium nitride
		GaSb Gallium antimonide
		InAs Indium arsenide
		InP Indium phosphide
		InSb Indium antimonide

Table 1.3 Ternary and quaternary semiconductors

Ternary compounds	Quaternary compounds
$\text{Al}_x\text{Ga}_{1-x}\text{As}$ Aluminium gallium arsenide	$\text{Al}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$ Aluminium gallium arsenic antimonide
$\text{GaAs}_{1-x}\text{P}_x$ Gallium arsenic phosphide	$\text{Ga}_x\text{In}_{1-x}\text{As}_{1-y}\text{Py}$ Gallium indium arsenic phosphide

devices have been designed using this material alloy. This chapter gives a detailed discussion of these heterojunctions.

1.2 Semiconductor materials

Materials used for semiconductors fall into two categories: elemental semiconductors and compound semiconductors. Table 1.1 shows the section in the periodic table which has the semiconductor elements and Table 1.2 lists examples for elemental and binary compound semiconductors. Some ternary and quaternary semiconductors are listed in Table 1.3.

1.3 Types of solids

There are three types of solids: crystalline, polycrystalline and amorphous. The arrangement of atoms is periodic in three dimensions in a crystalline solid with forces binding the atoms together. This periodicity exists over the entire crystal and it will appear the same regardless of the region where the crystal is viewed. If the periodicity of the atoms occurs over a small region of the solid and changes in different regions of the solid, the solid is termed to be *polycrystalline*. Atoms in amorphous solids exhibit no periodicity. Figure 1.1 shows the three different types of solids.

1.4 Crystal structure

Semiconductor materials such as Si, Ge and GaAs that are to be used for devices are crystalline, that is, a single crystal. This periodic arrangement of atoms in a crystal is termed a *lattice* and the distance between the atoms is the *lattice constant*. The unit cell is a fundamental unit in the crystal and a repetition of the unit cell generates the entire lattice. The unit cell is not unique and can be chosen in various ways as shown in Figure 1.2(a). This is a two-dimensional representation of the crystal lattice. The entire lattice can be constructed by translations of any of the three unit cells in two coordinate directions. The primitive unit cell is the smallest unit cell. A generalised primitive three-dimensional unit cell is shown in Figure 1.2(b). The coordinate directions are **a,b,c**. In cubic structures, these would be the rectangular coordinates. The basic cubic crystal structures are (a) the simple cubic, (b) the body-centred cubic and

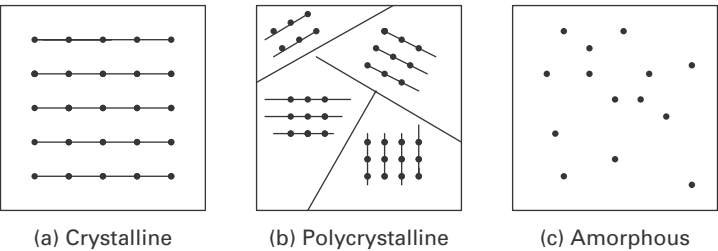


Fig. 1.1 Schematic arrangement of atoms in solids.

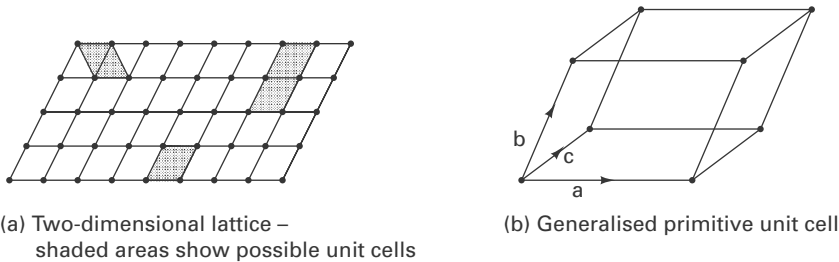


Fig. 1.2 Unit cells.

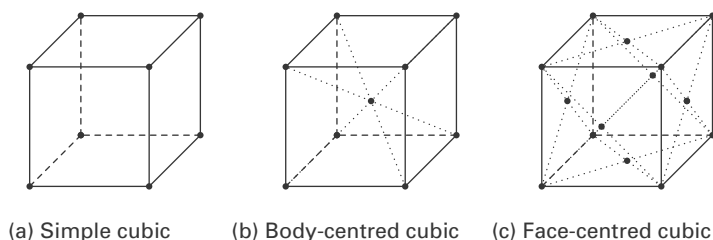


Fig. 1.3 Types of cubic lattices.

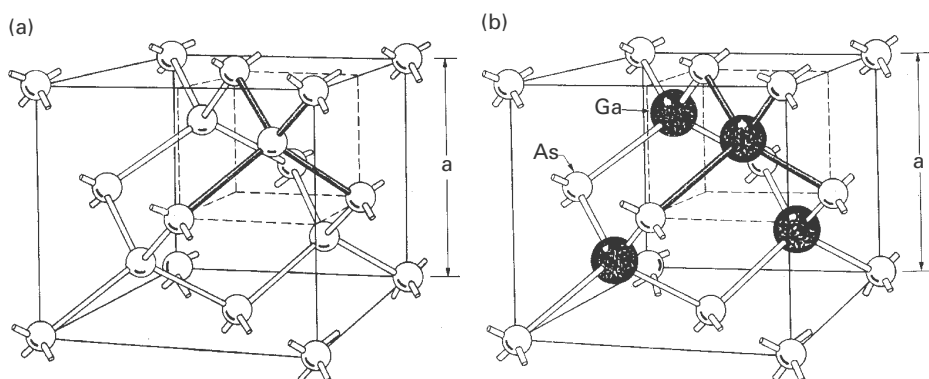


Fig. 1.4 (a) Diamond lattice and (b) Zincblende lattice. (S. M. Sze, *Semiconductor Devices: Physics and Technology*, John Wiley & Sons, 1985). Reprinted with permission of John Wiley & Sons, Inc.

(c) the face-centred cubic shown in Figure 1.3. The simple cubic lattice has an atom at each corner of the cube, where the length of a side of the cube is a , the lattice constant. The body-centred cubic lattice (BCC) has an additional atom in the centre of the cube and the face-centred cubic lattice (FCC) has an additional atom in the centre of each face of the cube. The two most important semiconductor crystal structures are the diamond lattice structure and the zincblende structure. Silicon and germanium have the diamond lattice structure and most of the binary compound semiconductors such as GaAs have the zincblende lattice structure. The only difference between the diamond and the zincblende structures is that the latter has two different types of atoms as seen in Figure 1.4. The diamond structure consists of two inter-penetrating FCC sublattices of atoms. The second FCC cube is shifted by one-fourth of the body diagonal, which is the longest diagonal. In the zincblende structure of GaAs, one sublattice has gallium atoms and the other has arsenic atoms.

1.5 Crystal directions and planes

Crystals are of finite size and hence have surfaces. It is necessary to define the planes at the crystal surfaces and the crystallographic directions, both of which determine the

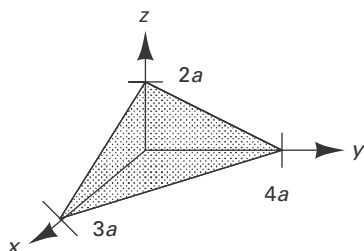


Fig. 1.5 Representation of plane with Miller indices $[6, 5, 8]$.

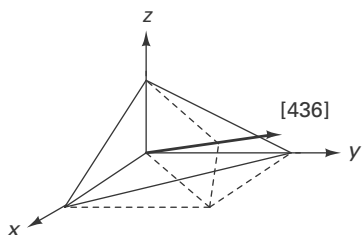


Fig. 1.6 Representation of direction with Miller indices $[6, 5, 8]$.

properties of semiconductor devices. The rectangular coordinate system defines the cubic crystal and the plane surfaces and directions are described by a set of indices called the *Miller indices*. Planes are described by the indices (h,k,l) and the directions perpendicular to these planes are described by the same indices $[hkl]$.

Example: Find the Miller indices of the plane which makes intercepts $3a, 4a, 2a$ along the coordinate axes in a cubic crystal, where a is the lattice constant. Draw the direction vector with the same Miller indices.

Solution: The intercepts are 3, 4 and 2. The reciprocals are $1/3, 1/4$ and $1/2$. Multiplication by the lowest common denominator, which is 12, yields $(4,3,6)$. These are the Miller indices which define the plane shown in Figure 1.5. It can be shown that parallel planes are described by the same Miller indices.

The Miller indices of the direction are given as $[436]$. The intercepts on the three coordinate axes are 3, 4 and 2. The direction vector is drawn and seen to be perpendicular to the planes shown in Figure 1.6.

The basic planes in cubic crystals are shown in Figure 1.7. It is also important to describe specific directions in a crystal in addition to the planes. As in the case of the crystal plane, a crystal direction is also described by three integers which are the components of a vector drawn in the particular crystal direction. The crystal planes and directions of most interest are shown in Figure 1.8. The $[hkl]$ direction is perpendicular to the (hkl) plane.

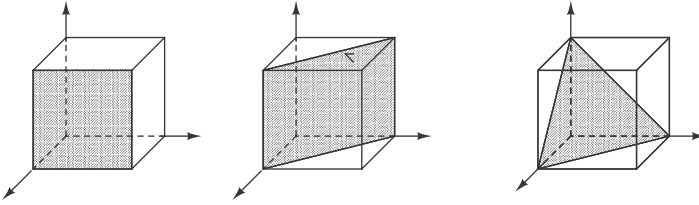


Fig. 1.7 Basic crystal planes.

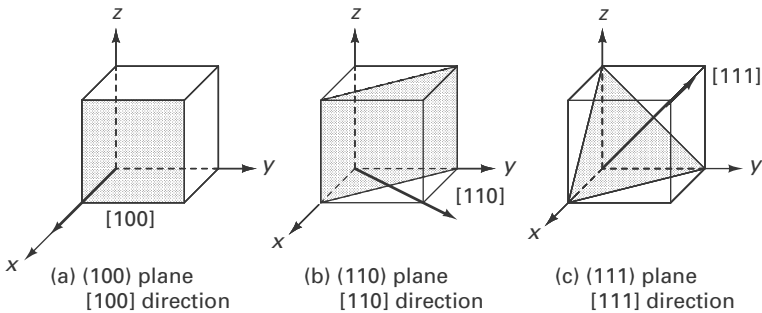


Fig. 1.8 Important crystal planes and directions.

1.6 Atomic bonding

Atoms are held together by bonding forces to form solids. When the attractive and repulsive forces are equivalent, the atoms are in equilibrium and maintain the spacing characterised by the lattice constant, a . There are different bonding classifications which are described by the dominant force of attraction. When one of the atoms gives up an electron in the outer shell to another atom, positive and negative ions are produced. There is a Coulomb interaction force of attraction between them. This is termed *ionic bonding*. At equilibrium, the forces of attraction and repulsion are equivalent. Sodium chloride (NaCl) and Potassium chloride (KCl) are examples of ionic bonding after the formation of the Na^+ and Cl^- ions.

1.6.1 Covalent bonding

This type of bonding results when electrons are shared by neighbouring atoms. The hydrogen atom is the simplest example of covalent bonding. Each of the two electrons bonds with the other to complete the lowest energy shell as shown in Figure 1.9.

Each atom in a diamond or zincblende lattice has four nearest neighbours. Each atom has four electrons in the outer orbit. These are the valence electrons and each atom shares these valence electrons with its four neighbours. The interaction between the shared electrons results in bonding forces which are quantum mechanical in nature. In other words, each electron pair constitutes a covalent bond. Elements in group IV such as Si and Ge have four valence electrons as shown in the references [8, 14, 15]. These are available for bonding as seen in Figure 1.10. Compound semiconductors such as



Fig. 1.9 Covalent bonding in hydrogen.

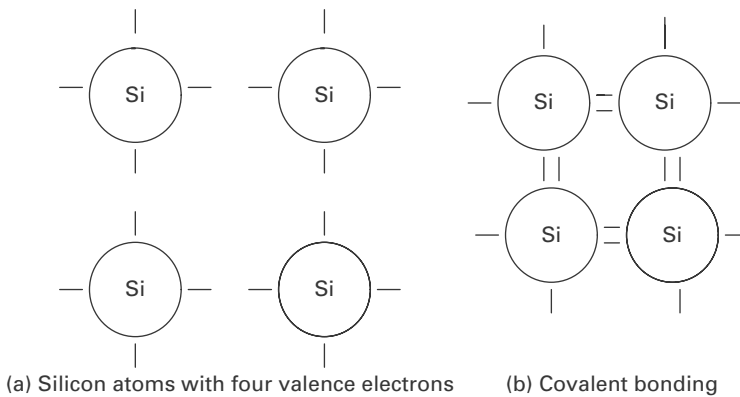


Fig. 1.10 Covalent bonding in silicon.

GaAs exhibit both covalent as well as ionic bonding. This is due to the fact that Ga and As occur in two different groups in the periodic table and hence there is a transfer of charge resulting in some ionic bonding.

1.7 Atomic physics

The theories of atomic physics were based on experimental observations. These theories subsequently explained the experiments and led to the understanding of atoms in matter.

1.7.1 The photoelectric effect

The measurements of Planck on a heated sample of material indicated that energy is radiated in discrete units called *quanta* as shown in Equation (1.1).

$$E = h\nu, \quad (1.1)$$

where h (Planck's constant) = $6.63 \times 10^{-34} \text{ J} \cdot \text{s}$ and ν is the frequency of the radiation. Heinrich Hertz discovered the photoelectric effect in 1887. The experiments performed by Philipp Lenard, a former student of Hertz, showed that if light shines on a metal surface in vacuum, some of the electrons receive enough energy so that they are emitted from the surface into the vacuum. They were interpreted by Albert Einstein, who received the Nobel Prize for his work in 1921. This is termed the *photoelectric effect* and the maximum energy is a function of the frequency of the incident light. The quantised units of light energy are called *photons*.

Based on further experimental observations of Davisson and Germer (USA) and Thompson (UK) on the diffraction of electrons by the atoms in a crystal, de Broglie related the wavelength of a particle of momentum $p = mv$, where m is the mass of the particle as seen in Equation (1.2):

$$\lambda = \frac{h}{p} = \frac{h}{mv}. \tag{1.2}$$

1.7.2 The Bohr model of the atom

A model of the atom was first proposed by Bohr. In his model, the electrons move in stable circular orbits about the nucleus and the electron may move to an orbit of higher or lower energy. The electron would either gain energy or lose energy by the absorption or emission of a photon of energy $h\nu$. Bohr further proposed that the angular momentum of the electron moving in a circular orbit was an integral multiple of Planck’s constant as seen in Equation (1.3).

$$p_{\theta} = \frac{nh}{2\pi} = n\hbar, \quad n = 1, 2, 3, \dots \tag{1.3}$$

The hydrogen atom with one electron and the nucleus illustrates this concept in a simple manner as seen in Figure 1.11.

Assuming that the electron of mass m rotates in a stable orbit of radius r with velocity v , the angular momentum is written in Equation (1.4):

$$p_{\theta} = mvr = n\hbar. \tag{1.4}$$

The electrostatic force between the charge on the nucleus and the charge on the electron must be equal to the centripetal force for the electron to remain in stable orbits. This yields the expression in Equation (1.5) for the energy of the electron [15]:

$$E_n = -\frac{mq^4}{2(4\pi\epsilon_0)^2n^2\hbar^2}. \tag{1.5}$$

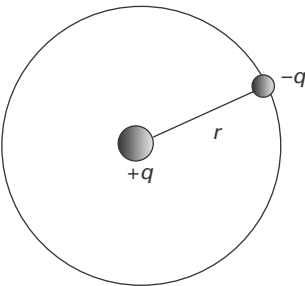


Fig. 1.11 Bohr model of the hydrogen atom.

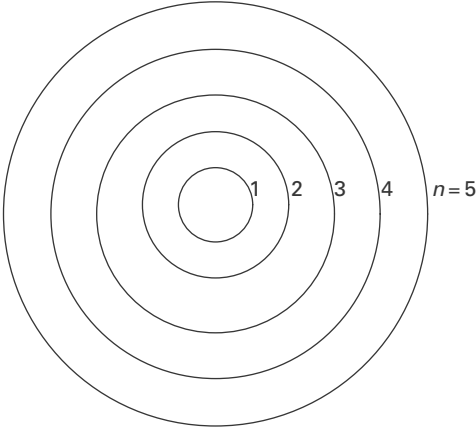


Fig. 1.12 Electron orbits in Bohr model (not to scale).

The electron orbits in the Bohr model are shown in Figure 1.12.

1.8 The de Broglie relation

The initial theoretical and experimental results of Planck, Einstein and Bohr laid the foundation for the development of quantum mechanics. It was de Broglie, however, who first postulated that if waves were seen to behave as particles then it could be that particles might behave like waves.

In the Bohr formulation, the electron which travels in a circular orbit of radius r is assumed to behave like a wave with a wavelength λ . It travels in a circular path equal in length to the circumference $2\pi r$, which will be an integral number of wavelengths so that

$$n\lambda = 2\pi r. \quad (1.6)$$

The Bohr formulation yielded the linear velocity of the electron to be

$$v = \frac{q^2}{4\pi\epsilon_0 n \hbar}. \quad (1.7)$$

Using this velocity relation, the wavelength can be written as

$$\lambda = \frac{h}{mv} = \frac{h}{p}, \quad (1.8)$$

where p is the linear momentum of the electron. Thus, de Broglie postulated that the relationship between the wavelength and the linear momentum p of a particle is given by Equation (1.2).

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \frac{2\pi}{\lambda} = \hbar k. \quad (1.9)$$

This is the *de Broglie relationship*. For free electrons, the energy–momentum relationship is as follows:

$$E = \frac{mv^2}{2} = \frac{p^2}{2m}; \quad p = \sqrt{2mE}. \quad (1.10)$$

Hence, the experiments of Davisson and Germer and of Thompson were verified by the de Broglie relationship.

1.9 Quantum mechanics

Newtonian mechanics can be used to describe physical behaviour that is macroscopic. Typical examples of this are planetary motion, the classical electromagnetic fields and fluid motion. The motion of electrons and the interaction of electrons in atoms in semiconductor materials cannot, however, be described thus since we are dealing with microscopic behaviour. This physical behaviour on the atomic scale can only be described by quantum mechanics rather than Newtonian mechanics. Quantum or wave mechanics had as its basis the physical understanding developed by Planck and de Broglie. The classical laws of the conservation of energy, momentum and angular momentum are also assumed to be valid in quantum mechanics. Hence, the physics involved in the interaction between atoms can be described mathematically by quantum mechanics.

1.9.1 Probability and the uncertainty principle

When the motion of the particle is microscopic, the parameters cannot be described exactly but rather in terms of average (expectation) values. Hence we have, for example, the expectation values of position, momentum and energy of an electron. So, we have a probabilistic rather than an exact description of the particle behaviour. There is, thus, an inherent uncertainty in the position and momentum of the particle. This was formulated by Heisenberg and is termed the *Heisenberg uncertainty principle*. The uncertainty in the measurement of the position and momentum of particle motion is given as

$$(\Delta x)(\Delta p_x) \geq \hbar. \quad (1.11)$$

The uncertainty in energy is related to the time at which the energy was measured and is given by

$$(\Delta E)(\Delta t) \geq \hbar. \quad (1.12)$$

These equations show that the simultaneous measurements of position and momentum on the one hand and energy and time on the other hand cannot be performed with arbitrary accuracy.

It follows that we can only determine the probability of finding an electron in a certain position or having a certain momentum. This leads to the definition of a probability density function. The probability of finding a particle in a range, say, from x to $x + dx$ is given by