CHAPTER 1 BACKGROUND ON MICROELECTRONICS

1.1 INTRODUCTION

Material processing, mainly semiconductor and metal, and related physics to fabricate (make) nanostructures and electronic devices, such as transistors, are the subject matter of microelectronics. As such, before proceeding with nanostructure physics in Chap. 2, it is imperative to get acquainted with some basics of microelectronics in this chapter. This chapter begins with elemental, binary, ternary, and quaternary semiconductors, then concludes with a discussion on bandgap engineering, semiconductor heterojunctions and heterostructures, and the idea of effective mass. For a coherent text on microelectronics, see Chowdhury (2014).

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1.2 INTRINSIC SEMICONDUCTORS

The energy bands of intrinsic semiconductors are broad and the gaps are narrow. For intrinsic semiconductors, Fermi energy is given by

$$E_F = \frac{E_c + E_v}{2} \tag{1.1}$$

at 0 K. At 0 K, the valence band (VB) is completely filled, and the conduction band (CB) is completely empty. Above 0 K, the VB is partially empty, and the CB is partially filled. See Fig. 1.1. Appreciable electrical conduction is then possible by electrons in the CB and by holes in the VB. The conduction increases with increasing temperature. Above 0 K, the Fermi energy is given by

$$E_F = \frac{E_g}{2} + \frac{3}{4} k_B T \ \ln\left(\frac{m_h^*}{m_e^*}\right). \tag{1.2}$$

So $E_F \approx \frac{E_g}{2}$ and rises above $\frac{E_g}{2}$ as the temperature is raised.

For semiconductors (intrinsic or extrinsic), electron concentration in the CB is given by

$$n_e = 2\left(\frac{2\pi \ m_e^* k_B T}{h^2}\right)^{3/2} e^{(E_F - E_g)/(k_B T)} \tag{1.3}$$

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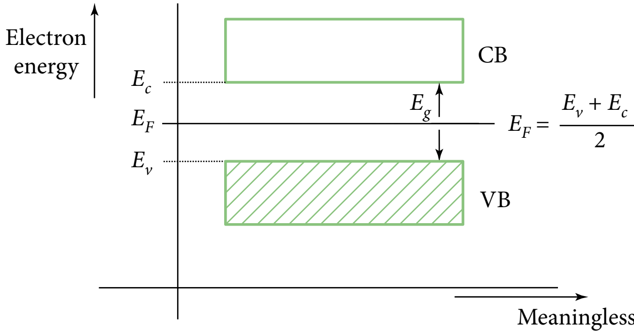

FIG. 1.1
Band model of intrinsic semiconductor (at 0 K).

or

$$n_e = 2\left(\frac{2\pi k_B T}{h^2}\right)^{3/2}(m_e^* m_h^*)^{3/4} e^{-E_g/(2k_BT)}. \quad (1.4)$$

$n_e \sim 10^{10}/\text{cm}^3$ for intrinsic Si crystal at 300 K. There are $\sim 10^{22}$ atoms/cm^3 in Si crystal.

The hole concentration in the VB is given by

$$n_h = 2\left(\frac{2\pi\ m_h^* k_B T}{h^2}\right)^{3/2} e^{-E_F/(k_BT)} \quad (1.5)$$

or

$$n_h = 2\left(\frac{2\pi\ k_B T}{h^2}\right)^{3/2}(m_e^* m_h^*)^{3/4} e^{-E_g/(2k_BT)}. \quad (1.6)$$

Equations (1.3) to (1.6) hold if $E_c - E_F \gg k_BT$ and $E_F - E_v \gg k_BT$, or, taken together, $E_g \gg k_BT$. At 300 K, $k_BT \approx 25$ meV. $E_g = 1.12$ eV for Si and 0.66 eV for Ge. So $E_g \gg k_BT$ for both Si and Ge.

1.3 SEMICONDUCTORS: ELEMENTAL AND BINARY

Table 1.1
Properties of Si and Ge.

Property	Si	Ge
Energy gap (eV)	1.12	0.66
Electron mobility (cm^{2}V^{-1}s^{-1})	1500	3900
Hole mobility (cm^{2}V^{-1}s^{-1})	450	1900
Transition	Indirect	Indirect
Lattice structure	Diamond	Diamond
Lattice constant (Å)	5.43	5.66
Dielectric constant	11.9	16.2
Density (gm/cm^3)	2.33	5.32
Melting point (°C)	1415	936

The most widely used elemental semiconductors are Si and Ge. Their notable properties (at 300 K) are given in Table 1.1.

Si and Ge have some important drawbacks:

1. Energy gaps are indirect.
2. Energy gaps are small.

Si, considered by many as a universal semiconductor material, cannot perform many important functions. It was natural to turn to other materials, notably compound semiconductor materials, which offer many desired properties and can be synthesized without much difficulty.

Compound semiconductors are made from elements of different columns of the periodic table. Examples are III–V and II–VI compounds. Group III–V compounds are most widely used. Table 1.2 shows a list of elements of group III and V of the periodic table generally used to obtain III–V compound semiconductors.

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Table 1.2
Elements of group III and V of the periodic table generally used to obtain III–V compound semiconductors.

Group III elements	Group V elements
B	N
Al	P
Ga	As
In	Sb
Te	Bi

Examples of III–V compound semiconductors are GaAs and InP. InSb was the first III–V compound semiconductor discovered in 1950. Compound semiconductors have some particular features that attracted interest:

1. Ease with which these can be synthesized.
2. High mobility of electrons.

Compared to Si and Ge, GaAs and InP have a high mobility of electrons and a high velocity of electrons. These properties are extremely important for development of high-speed electronic devices. Their (GaAs and InP) bandgaps are direct, which is also useful. Table 1.3 provides a comparison of properties of elemental and binary semiconductors (at 300 K).

Table 1.3
Comparison of properties of elemental and binary semiconductors.

Property	Si	GaAs	InP
Energy gap (eV)	1.12	1.42	1.34
Electron mobility ($cm^2V^{-1}s^{-1}$)	1500	9000	5000
Hole mobility ($cm^2V^{-1}s^{-1}$)	450	400	100
Transition	Indirect	Direct	Direct
Lattice structure	Diamond	Zinc blende	Zinc blende
Lattice constant (Å)	5.43	5.65	5.87
Dielectric constant	11.9	13.2	12.6
Atoms/cm^3	5×10^{22}	4.42×10^{22}	–
Density (gm/cm^3)	2.33	5.32	4.8
Atomic weight	28	144	145
Melting point (°C)	1415	1238	–
Breakdown field (V/cm)	$\approx 3 \times 10^5$	$\approx 4 \times 10^5$	–
Effective mass of electron (m^*/m_e)	–	0.067	0.077
Intrinsic carrier concentration (cm^{-3})	1.45×10^{10}	1.8×10^6	10^6
Intrinsic resistivity (Ω-cm)	2.3×10^5	10^8	–

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1.4 ALLOY SEMICONDUCTORS (TERNARY AND QUATERNARY)

An attractive feature of binary compounds is that they can be combined or alloyed to form ternary or quaternary compounds, or mixed-crystal or alloy semiconductors. The "solid solution" of binary compounds can form ternary or quaternary alloys. For example, a ternary III–V semiconductor $A_xB_{1-x}C$ is made of binary compounds AC and BC in a solid solution.

$A_xB_{1-x}C$ consists of 100x atoms of element A and $100(1-x)$ atoms of element B randomly distributed in every 100 sites of group III sublattice. Atoms of element C occupy all sites of group V sublattice. x can be varied continuously between 0 and 1.

A typical example is $Al_xGa_{1-x}As$, a ternary alloy semiconductor of great technological importance. In $Al_xGa_{1-x}As$, atoms of Al and Ga are randomly distributed in a group III sublattice, and atoms of As occupy all sites of the group V sublattice.

Another form of ternary alloy is $AB_{1-y}C_y$, where all group III sublattice sites are occupied by atoms of element A, and sites of group V are randomly occupied by atoms of element B and C. An example of this type of ternary compound is $GaAs_{1-x}P_x$, which is also technologically important and made of GaAs and GaP in a solid solution.

In a similar manner, quaternary alloy semiconductors are formed by mixing atoms of four different elements. Such a compound can consist of atoms of two group III elements A and B randomly distributed in group III sublattice sites and atoms of two group V elements C and D randomly distributed in group V sublattice sites to give the compound $A_xB_{1-x}C_yD_{1-y}$. An example is $In_xGa_{1-x}As_yP_{1-y}$.

If atoms of three group III elements A, B, C randomly occupy group III sublattice sites and atoms of only one group V element are present in group V sublattice sites, a quaternary compound $A_xB_yC_zD$ is formed. The composition is more conveniently expressed as $(A_xB_{1-x})_yC_{1-y}D$, where x and y can be varied from 0 to 1. An example is $(In_xGa_{1-x})_yAl_{1-y}As$ or $In_xGa_yAl_zAs$.

Alloy semiconductors are formed by mixing in group III sublattice or group V sublattice or both. But mixing in group V sublattice with accurate control of alloy composition is more difficult to achieve than mixing in group III sublattice.

1.5 BANDGAP ENGINEERING

1. Ternary alloy semiconductors are made of two binary semiconductors. Alloy semiconductors lie on the lines joining binary compounds (see Fig. 1.2). For example, $In_xGa_{1-x}As$ lies on the tie line between InAs and GaAs.

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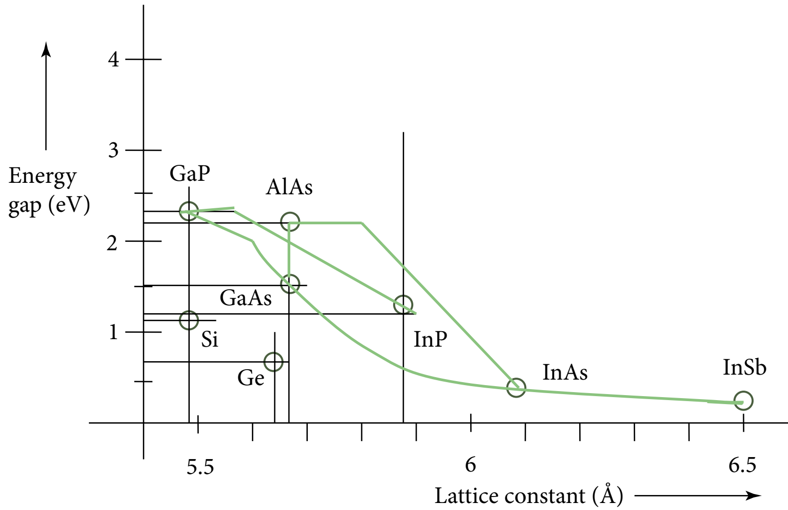

FIG. 1.2
Bandgap engineering. On tie line between a pair of binary compounds lies the ternary.

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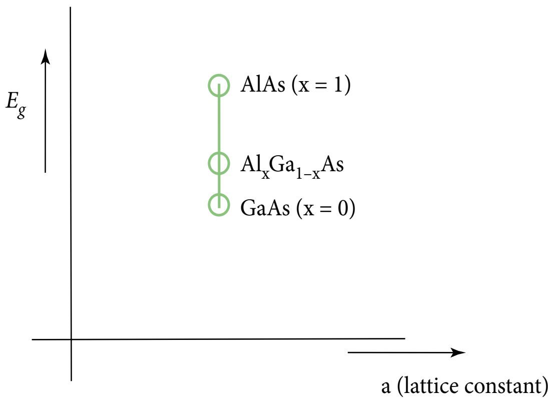

FIG. 1.3
AlGaAs lies on the tie line between GaAs and AlAs.

2. By choosing different binary compounds, it is possible to get ternary compounds of desired bandgaps.
3. By alloying, it is possible to vary the bandgap continuously and monotonically by varying the composition. As an example, the bandgap of the ternary alloy $Al_xGa_{1-x}As$ ($0 \leq x \leq 1$) depends on x. The (minimum) bandgap can be varied continuously from 1.43 eV (GaAs, $x = 0$) to 2.17 eV (AlAs, $x = 1$); see Eqs. (1.8) and (1.9). (See Fig. 1.3.) Among the common ternary and quaternary alloys, properties of $Al_xGa_{1-x}As$ have been most thoroughly investigated. See Fig. 1.4 for the case with $In_xGa_{1-x}As$.

An empirical relation usually gives bandgap E_g for the ternary alloy $A_xB_{1-x}C$ semiconductor as a function of x:

$$E_g(x) = E_{g0} + bx + cx^2, \tag{1.7}$$

where E_{g0} is the bandgap of BC, the lower bandgap binary; $E_{g0} + b + c$ is the bandgap of AC, the upper bandgap binary; b is a fitting parameter; and c is called the bowing parameter, which may be calculated theoretically or determined experimentally.

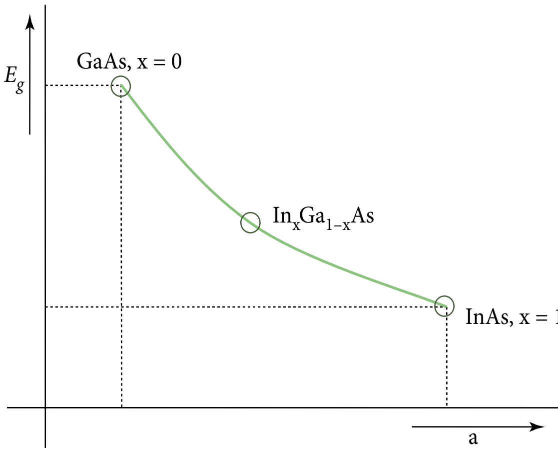

FIG. 1.4
InGaAs lies on the tie line between GaAs and InAs.

Variation of direct and indirect bandgaps of $Al_xGa_{1-x}As$ with the composition are approximately given (in eV) by

$$\begin{aligned} E_g^{\Gamma}(x) &= 1.424 + 1.247x \quad \text{for } x < 0.45 \\ &= 1.656 + 0.215x + 1.147x^2 \quad \text{for } x > 0.45 \\ &= 1.424 \quad \text{for GaAs} \quad \text{and} \quad 3.018 \quad \text{for AlAs.} \end{aligned} \tag{1.8}$$

$$\begin{aligned} E_g^{X}(x) &= 1.9 + 0.125x + 0.143x^2 \\ &= 2.168 \quad \text{for } x = 1. \end{aligned} \tag{1.9}$$

$$\begin{aligned} E_g^{L} &= 1.708 + 0.642x \\ &= 2.350 \quad \text{for } x = 1. \end{aligned} \tag{1.10}$$

1.6 SEMICONDUCTOR HETEROJUNCTIONS AND HETEROSTRUCTURES

A semiconductor heterojunction is a junction of two different semiconductors of unequal bandgap, and this combination of semiconductors is called a heterostructure. See Fig. 1.5. Figure 1.6 shows a band model of the (undoped) GaAs–AlGaAs heterostructure having an abrupt (sharp) junction. The discontinuity in the valence band edge ΔE_v and in the conduction band edge ΔE_c are not equal.

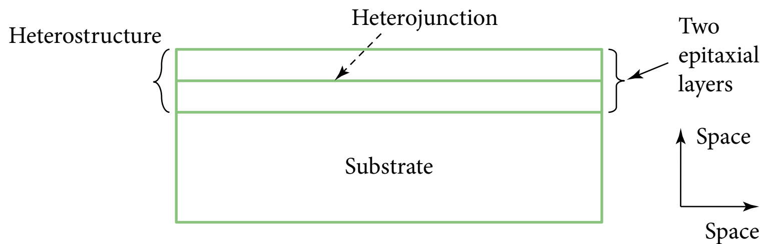

FIG. 1.5
Schematic diagram of a semiconductor heterostructure.

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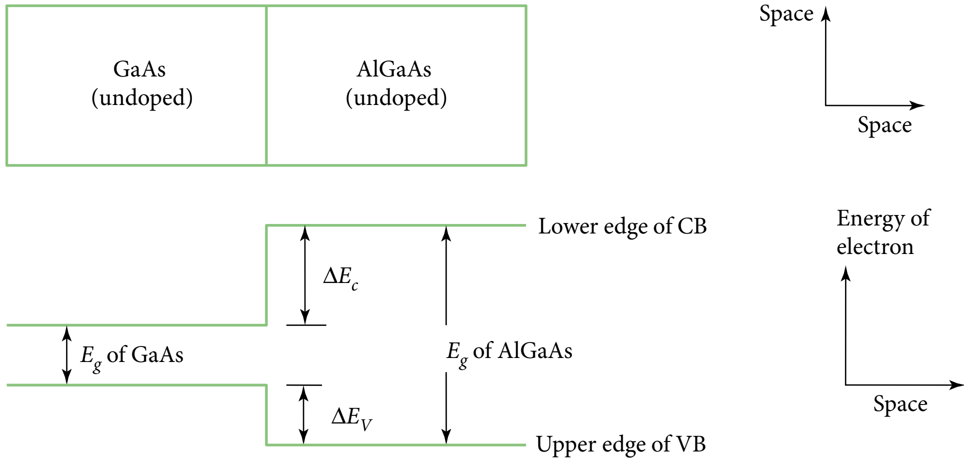

FIG. 1.6
Band model of GaAs–AlGaAs heterostructure, $\Delta E_c > \Delta E_v$.

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1.7 EFFECTIVE MASS

The velocity of an electron (in a periodic potential) is defined as the group velocity of the associated matter wave packet:

$$v = \frac{1}{\hbar}\frac{dE}{dk}. \tag{1.11}$$

Otherwise, the electron will soon be at a location where there is no matter wave. Here, E is the energy of the electron, and k is the momentum of the electron in the unit of $\hbar$. If we have E as a function of k, we can find the velocity as a function of k using Eq. (1.11).

Newton's law gives

$$F = \frac{d(\hbar k)}{dt}$$

or

$$F = \hbar\frac{dk}{dt}. \tag{1.12}$$

Using Eq. (1.11), we can write $\frac{dv}{dt} = a = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right)$ for acceleration.

Thus,

$$a = \frac{1}{\hbar}\frac{d}{dk}\left(\frac{dE}{dk}\right)\frac{dk}{dt} = \frac{1}{\hbar}\left(\frac{d^2E}{dk^2}\right)\frac{dk}{dt}. \tag{1.13}$$

Effective mass m^* is the ratio of the force F and the acceleration a. Hence,

$$m^* = \frac{F}{a} = \frac{\hbar\frac{dk}{dt}}{\left(\frac{1}{\hbar}\right)\left(\frac{d^2E}{dk^2}\right)\frac{dk}{dt}}$$

or

$$m^* = \frac{1}{\frac{1}{\hbar^2}\left(\frac{d^2E}{dk^2}\right)}. \tag{1.14}$$

Equation (1.14) is used to calculate the effective mass of an electron in a periodic potential. If we have E as a function of k, we can find the effective mass m^* as a function of k using Eq. (1.14). This value of m^* depends on the value of k. Usually, we use values of m^* for values of k at the extrema of the E vs k curve, because carriers usually reside there. Electrons reside at the minimum of the E vs k curve for the conduction band to stay at lower energy.

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REFERENCE

Chowdhury, S., *Nanostructure Physics and Microelectronics* (Narosa/Alpha Science, New Delhi, 2014).