1 Basic Properties of Semiconductors

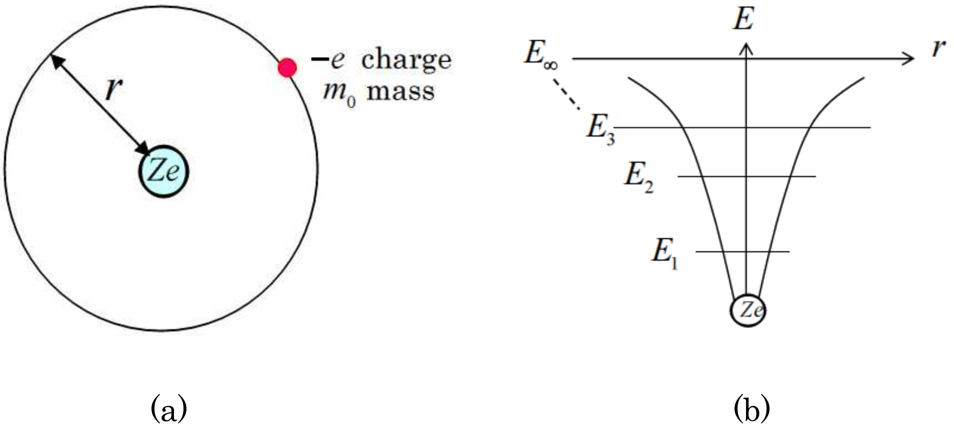
1.1 Crystal Structure

The atoms that make up materials are composed of a nucleus and the electrons that surround it. Figure 1.1 shows (a) the Bohr model of the atom and (b) the appearance of the discrete energies E. An electron of charge $-e$ and mass m_0 is moving around a nucleus of charge Ze in a circular orbit of radius r in vacuum (dielectric constant ε_0). In this case, the possible energy E of the electron is given by the following equation, which is a discrete value (see Appendix A for the derivation of the equation).

$$E = -\frac{m_0 Z^2 e^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} \tag{1.1}$$

n ; principal quantum number $n = 1, 2, 3, \cdots$

h ; Planck constant $h = 6.626 \times 10^{-34} \left[J \cdot S\right]$



(a) (b)

Figure 1.1 (a) Bohr model of the atom and (b) discrete energies E

According to quantum mechanics, strictly speaking, in addition to the principal quantum number n, there are the following quantum numbers

l, m, s.

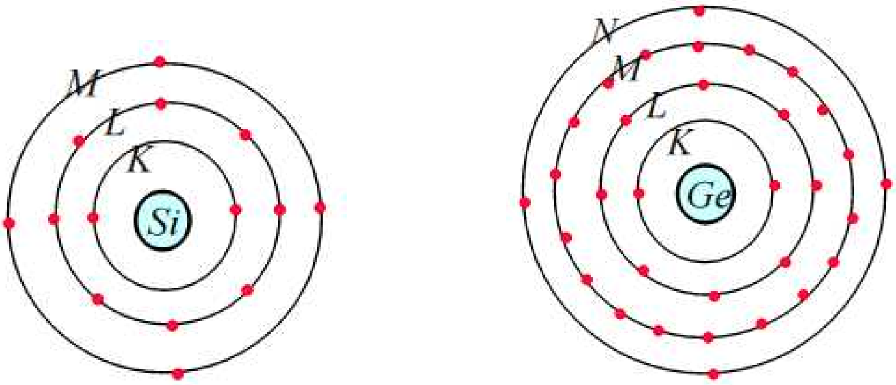
l ; azimuthal quantum number $l = 0, 1, \cdots, n-1$
m ; magnetic quantum number $m = 0, \pm 1, \cdots, \pm l$
s ; spin quantum number $s = \pm \frac{1}{2}$

The electron is a Fermi particle, and each quantum state determined by n, l, m, s can be occupied by only one electron, and there is no distinction between electrons. Table 1.1 shows the specific quantum states and the number of electrons that can occupy them in an atom. The principal quantum numbers n are called shells, and $n = 1,2,3,4$ are called $K, L. M, N$ shells. The azimuthal quantum numbers l are called sub-shells, and $l = 0,1,2,3$ are called s, p, d, f shells. The sub-shells are denoted by appending the principal quantum numbers.

Table 1.1 Quantum states and the number of electrons that can occupy them in an atom

Shell	Quantum number				Sub-shell	Number of occupied electrons	
	n	l	m	s			
K	1	0	0	±1/2	1s	2	2
L	2	0 1	0 0, ±1	±1/2	2s 2p	2 6	8
M	3	0 1 2	0 0, ±1 0, ±1 , ±2	±1/2	3s 3p 3d	2 6 10	18
N	4	0 1 2 3	0 0, ±1 0, ±1 , ±2 0, ±1 , ±2 , ±3	±1/2	4s 4p 4d 4f	2 6 10 14	32

As an example, Figure 1.2 shows the shells and electrons of (a) Si and (b) Ge atoms. In the figure, the red circles represent electrons. The properties of an atom are related to the number of electrons in its outermost shell. The Si and Ge atoms have four outermost electrons and are called group IV atoms. Group IV atoms are materials that constitute semiconductors on their own.



(a) (b)

Figure 1.2 Shells and electrons of (a) *Si* and (b) *Ge* atoms

Semiconductors are also composed of compounds of group III atoms with three outermost electrons and group V atoms with five. These are called compound semiconductors. Table 1.2 shows the atoms in the group III-V portion of the periodic table. Generally, semiconductors are made by combining these atoms.

Table 1.2 Atoms in Groups III-V

Group	Ⅲ	Ⅳ	Ⅴ
Number of outermost electrons	3	4	5
	B Boron	C Carbon	N Nitrogen
	Al Aluminum	Si Silicon	P Phosphorus
	Ga Gallium	Ge Germanium	As Arsenic
	In Indium	Sn Tin	Sb Antimony

In the case of *Si* or *Ge* atoms with four electrons in the outermost shell, the crystal is a diamond-shaped crystal structure with covalent bonds. Figure 1.3 shows the three-dimensional (3D) structure of a *Si* crystal (one cell).

Each Si atom is covalently bonded at four locations to form a diamond-shaped crystal.

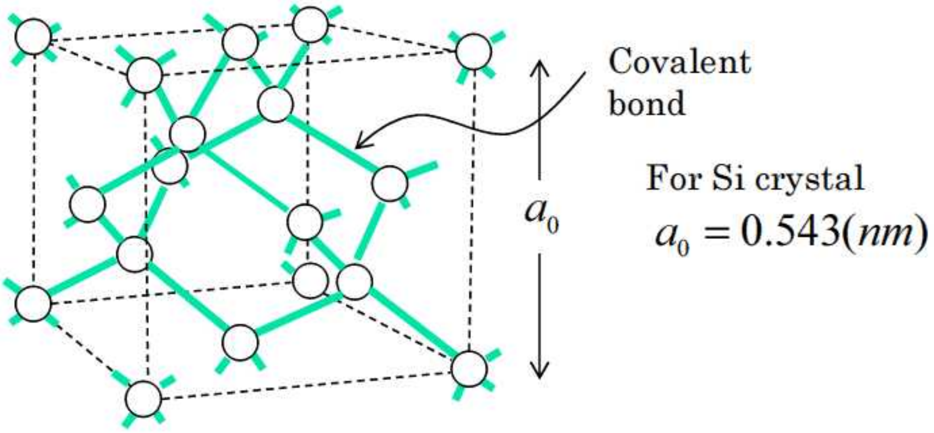


Figure 1.3 3D structure of Si crystal (diamond-shaped crystal)

When studying the operation of semiconductors, a two-dimensional (2D) structural model that represents the crystal structure in planar form is used for convenience. Figure 1.4 shows 2D structural model of a Si crystal. The red circles in the figure represent outermost electrons. Neighboring Si atoms emit their outermost electrons to each other, forming a covalent bond.

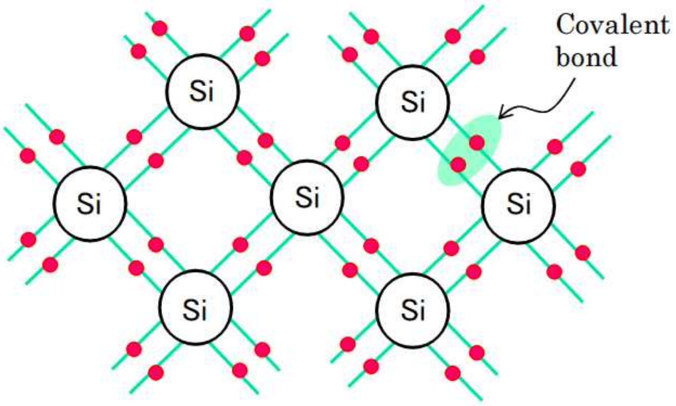


Figure 1.4 2D structural model of Si semiconductor crystal

$GaAs$ semiconductors are well-known compound semiconductors. Figure 1.5 shows 3D structural model of a $GaAs$ semiconductor crystal (for one cell), and Figure 1.6 shows 2D structural model. One of the five outer-most electrons of the group V *As* atom is lent to the group III *Ga* atom, resulting in a diamond-like crystal structure with four covalent bonds between the *Ga* and *As* atoms. It also has the property of ionization bonding because of the lending and borrowing of electrons. This crystal structure is called a sphalerite crystal structure.

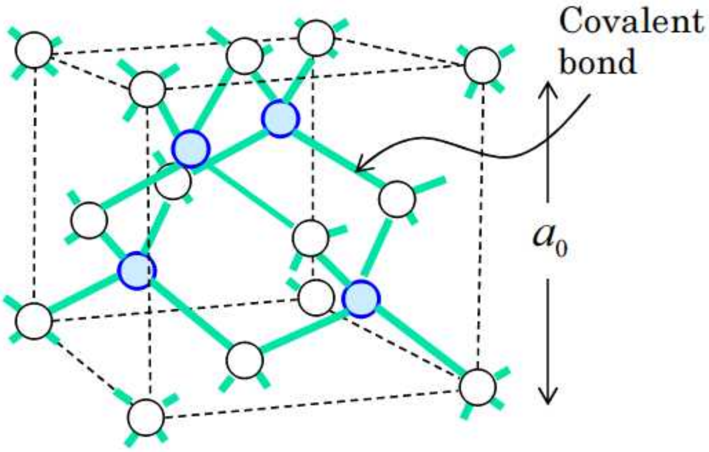


Figure 1.5 3D structural model of a *GaAs* semiconductor crystal (sphalerite crystal)

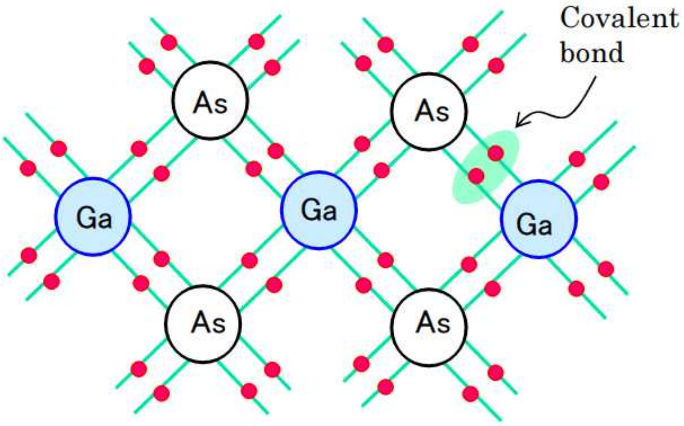


Figure 1.6 2D structural model of GaAs compound semiconductor crystal

1.2 Energy Band

Semiconductor crystals form periodic structure potentials in which the nuclei are potential wells. In the case of a semiconductor crystal composed of N atoms, the total number of outermost electrons in it is $4N$ ($2N$ in the sub-shell s and $2N$ in the sub-shell p). The $4N$ outermost electrons are used for covalent bonding, but they also operate under the influence of each other in the field of the periodic structure potential of the crystal. In this case, all $4N$ electrons must be in different quantum states.

Figure 1.7 shows the energy levels in a semiconductor crystal as the interatomic distance is narrowed (the figure is based on calculations for a Si crystal). As the interatomic distance is narrowed, the degeneracy of the energy levels of a single atom is resolved and broadened, forming energy bands. These energy bands are called allowed bands because electrons can exist in them, while the forbidden bands between the allowed bands, where electrons cannot exist, are called band gaps. Note that a_0 in the figure corresponds to the interatomic distance (strictly speaking, the cell dimension). At cryogenic temperatures ($\approx 0K$), the $4N$ outermost electrons are all in the lower energy state of the allowed band (in the case of a Si semiconductor).

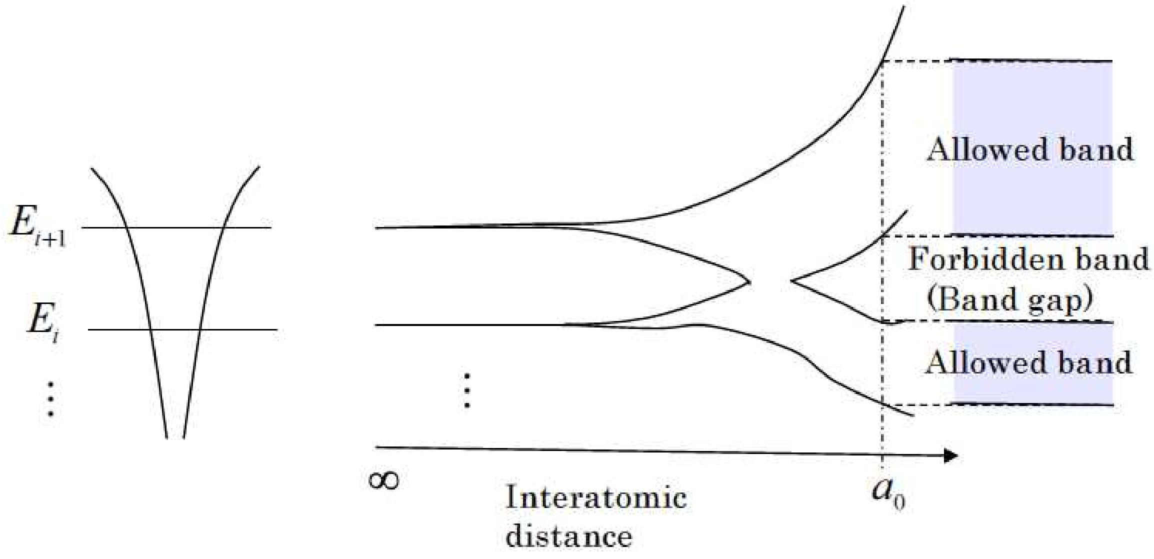
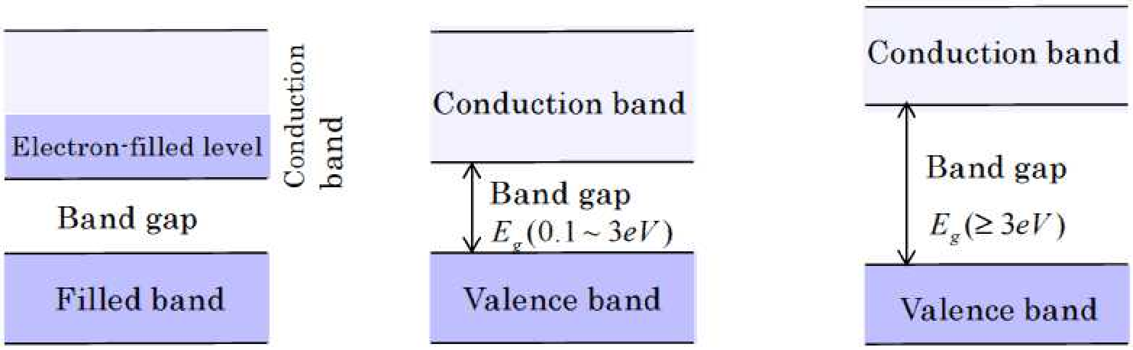


Figure 1.7 Energy bands of a single atom and a crystal with narrower atomic spacing.

The size of the energy bands (gaps) in the allowable and forbidden bands, and the circumstances under which electrons exist, vary depending on the materials that make up the crystal. Figure 1.8 shows the energy bands (gaps) and the presence of electrons for (a) conductors, (b) semiconductors, and (c) insulators.



(a) Conductor (b) Semiconductor (c) Insulator

Figure 1.8 Conduction band, band gap, and valence band of (a) a conductor, (b) a semiconductor, and (c) an insulator, and appearance of electrons

The upper energy band of the allowable bands is called the conduction band, and the electrons in it are called conduction electrons, which can move freely in a crystal. On the other hand, the lower energy band is called the valence band, where electrons are bound to the atoms that make up the crystal and cannot move freely within the crystal. In conductors, conduction electrons exist in the conduction band, whereas in semiconductors and insulators, all electrons exist in the valence band at cryogenic temperatures. In semiconductors, the band gap is relatively small, and a small amount of energy (heat) will produce conduction electrons and allow current to flow. In contrast, insulators have a large band gap and produce few conduction electrons, making them highly resistive.

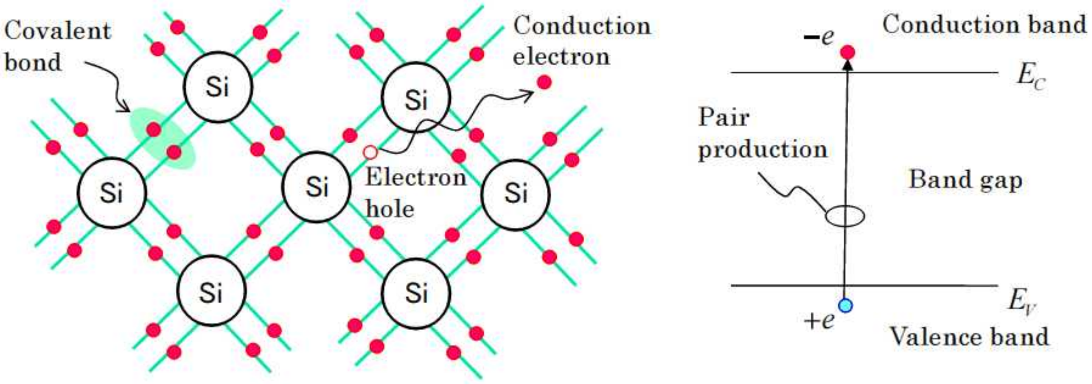
1.3 Intrinsic and Impurity Semiconductors

Semiconductors are classified by the presence or absence of impurity (additive) implantation as follows

- Semiconductor
  - Intrinsic semiconductor — i-type semiconductor (free of impurities)
  - Impurity semiconductor
    - N-type semiconductor (replace some of the Si (group IV) atoms with group V atoms such as As)
    - P-type semiconductor (replace some of the Si (group IV) atoms with group III atoms such as B)

(1) Intrinsic semiconductor - i-type semiconductor

Semiconductors that do not contain impurities (additives) are called intrinsic semiconductors. It is also called an i-type semiconductor from the English name intrinsic semiconductor. Figure 1.9 shows (a) 2D structural model and (b) the energy band diagram of an intrinsic semiconductor using Si as an example.



(a) (b)

Figure 1.9 (a) 2D structural model and (b) the energy band diagram of an intrinsic semiconductor

In semiconductors, when given energy above the forbidden band energy gap, covalently bonded electrons become conduction electrons (electrons in the conduction band), which can move around in the crystal. On the other hand, the hole through which a covalently bonded electron has left is called an electron hole. Electron holes in the valence band can also move around in the crystal. From this, conduction electrons and electron holes are called carriers as they carry charge (negative charge $-e$ for conduction electrons and positive charge $+e$ for electron holes). In intrinsic semiconductors, carrier creation of conduction electrons and electron holes occurs only by pair generation. Thus, at thermal equilibrium, the conduction electron density n and the electron hole density p are equal (a characteristic of the intrinsic semiconductor).

(2) N-type semiconductor

The name N-type semiconductor comes from the fact that the charge carriers are negatively charged conduction electrons Note *1. N-type semiconductors made of group IV atoms (e.g.,Si) are created by injecting a small amount of group V atoms (e.g.,As) as impurities (additives) during crystal growth and replacing some group IV atoms (Si) with group V atoms (As). Figure 1.10 shows (a) 2D structural model and (b) the energy band diagram of an N-type Si semiconductor.

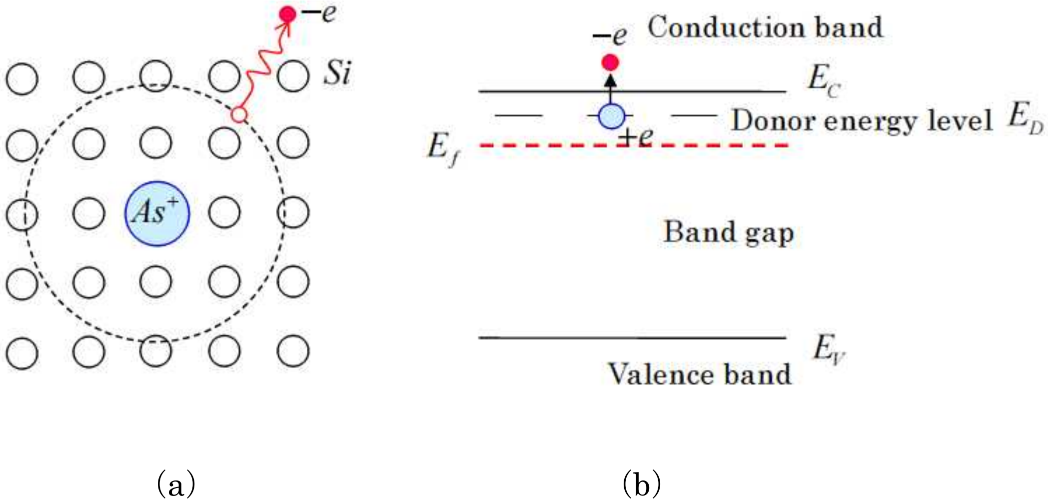
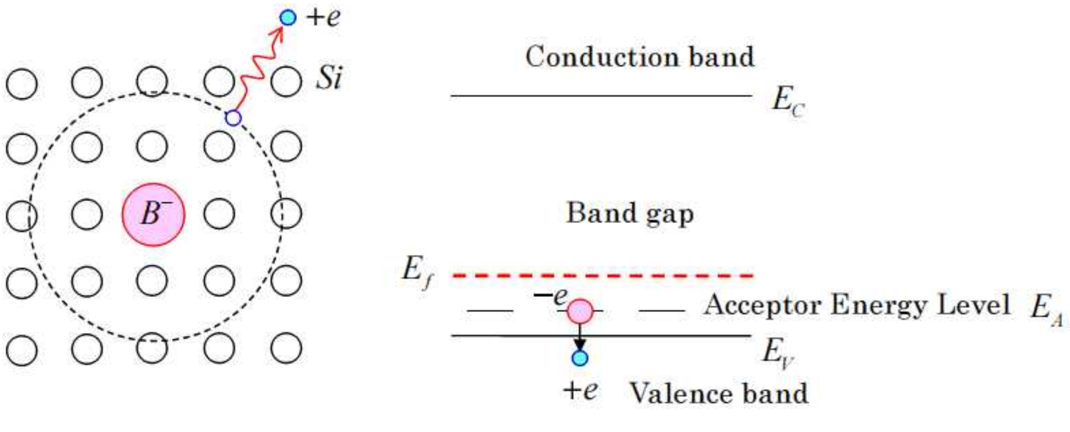


Figure 1.10 (a) 2D structural model and (b) the energy band diagram of an N-type Si semiconductor.

Four of the outermost electrons of the As atom are used for covalent bonding with the Si atom, and the remaining one electron is weakly bound to the As atom. These electrons leave the As atom boundaries and become conduction electrons that can move around in the crystal after obtaining only a small amount of thermal energy at room temperature. On the other hand, an As atom that loses an electron becomes a positive ion. In the energy band diagram, this means that electrons bound to the donor level E_D in the band gap, which is at a slightly lower energy level than the energy level E_C at the bottom of the conduction band, are excited to the conduction band by a small gain of energy. Impurities that give conduction electrons in the crystal, such as As atoms, are called donors.

(3) P-type semiconductor

The name P-type semiconductor comes from the fact that charge carriers are positively charged electron holes Note *1. P-type semiconductors made of group IV atoms (e.g., Si) are created by injecting a small amount of group III atoms (e.g., B) as impurities (additives) during crystal growth and replacing a portion of group IV atoms (Si) with group III atoms (B). Figure 1.11 shows (a) 2D structural model and (b) the energy band diagram of a P-type Si semiconductor.



(a) (b)

Figure 1.11 (a) 2D structural model and (b) the energy band diagram of a P-type Si semiconductor.

The B atom has three outermost electrons, which is not enough for covalent bonding with the Si atom. The missing one electron is covered by the transfer of an electron from the valence band used for other $Si - Si$ covalent bonds. The holes through which electrons leave the valence band are called electron holes, and at low temperatures they are weakly bound around the B atom. These electron holes leave the B atom boundaries and become electron holes that can move around in the crystal after obtaining only a small amount of thermal energy at room temperature. In the case of electron flow, electrons in the valence band, which are used for covalent bonding, are excited by a small amount of thermal energy and fill the holes (electron holes) bound in the vicinity of the B atom. This creates a new electron hole (a hole through which an electron has left) in the valence band that can move around in the crystal. On the other hand, the B atom, which had maintained its charge balance by having an electron hole in its neighborhood, becomes a negative ion when the electron hole in its neighborhood disappears.

In the energy band diagram, electrons in the valence band are excited to the acceptor level E_A in the band gap, which is at a slightly higher energy level than the energy level E_V at the top of the valence band, and in the valence band, electron holes (holes through which electrons have escaped) are created that can move around in the crystal. Negatively ionized B atoms remain in the acceptor level E_A. In Figures (a) and (b), the arrows indicate the flow of electron holes. Impurities that provide electron holes in the crystal, such as B atoms, are called acceptors.

Note *1

N- and P-type names were originally determined by the negative and positive charge carriers. Then, if a P-type semiconductor is used, as in a MOSFET (to be discussed later), but the carriers that carry the charge are electrons, is it called an N-type semiconductor? By the original definition, this would be called an N-type, but that would be confusing. In this case, it is called an n-channel MOSFET (commonly known as nMOS). A similar idea, using an N- type Si semiconductor but with electron holes as charge carriers, is called a p-channel MOSFET (commonly known as pMOS).

1.4 Effective Mass

All matters have duality (being both a particle and a wave), and this property becomes more pronounced for microscopic particles such as electrons. The momentum P and energy E of an electron can be expressed in terms of wave parameters as follows. Note that momentum is originally a vector quantity, but here we consider one-dimensional motion and express it as a scalar.

$$P = \frac{h}{\lambda} = \hbar k \tag{1.2}$$

$$E = \hbar\omega \tag{1.3}$$

where $\hbar = \frac{h}{2\pi}$, k is the wavenumber, λ is the wavelength, and ω is the angular frequency of the wave corresponding to wavelength λ.

The wavenumber k is the same as that introduced for electromagnetic waves and is related to the wavelength λ by the following equation. It means the number of waves in a unit length$\times 2\pi$.

$$k = \frac{2\pi}{\lambda} \tag{1.4}$$

The motion of conduction electrons in a crystal is represented by the motion of the wave packet of the wave function ψ in quantum mechanics. That is, the motion of the wave packet gives the motion of the electrons. The velocity of the wave packet in the wave function ψ is called the group velocity v_g and is given in the following equation (thus the velocity of the conduction electrons in the crystal is also given by v_g).

$$v_g = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk} \tag{1.5}$$

When an external force F is applied to an electron by an electric field for dt time, the electron moves a distance ds, resulting in an energy change dE. From this, the following equation is obtained.

$$dE = Fds = F\frac{ds}{dt}dt = Fv_g dt \longrightarrow \frac{dE}{dt} = Fv_g \tag{1.6}$$

$\frac{dE}{dt}$ can also be expressed as follows using equation (1.5).

$$\frac{dE}{dt} = \frac{dE}{dk}\frac{dk}{dt} = \hbar v_g \frac{dk}{dt} \tag{1.7}$$

From equations (1.6) and (1.7), we obtain

$$\frac{dE}{dt} = Fv_g = \hbar v_g \frac{dk}{dt} \longrightarrow \frac{dk}{dt} = \frac{F}{\hbar} \tag{1.8}$$

Differentiating v_g in Eq. (1.5) by t gives the acceleration α_g of the conduction electrons in the crystal as

$$\alpha_g = \frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right) = \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt} \tag{1.9}$$

Here, using equation (1.8), we obtain

$$\alpha_g = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}F = \frac{F}{m^*} \tag{1.10}$$

$$m^* = \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1} \tag{1.11}$$

The m^* given by equation (1.11) has the dimension of mass and is called the effective mass. If the crystals are not isotropic and the E property varies with the crystal axial direction, then m^* is the tensor quantity given by

$$m_{i,j}^* = \hbar^2 \left(\frac{d^2E}{dk_i dk_j} \right)^{-1} \tag{1.12}$$

When a force F acts on a conduction electron in a crystal, the electron behaves as if it were a particle with mass m^*. In other words, for conduction electrons in a crystal, the usual equation of motion can be applied by using the effective mass m^* as the mass.

The above discussion is for conduction electrons, but effective masses can also be obtained for electron holes. The effective masses of conduction electrons and electron holes are denoted by m_e^* and m_h^*, respectively. The effective mass has different values depending on the semiconductor crystal material. Table 1.3 shows examples of effective masses of conduction electrons and electron holes in semiconductors.

Table 1.3 Examples of effective masses of conduction electrons and electron holes in semiconductors

	Si $\langle 100 \rangle$ crystal axis	*Ge* $\langle 111 \rangle$ crystal axis	*GaAs* isotropic	*InAs* isotropic	*InP* isotropic
m_e^* / m_0	0.19 †1 0.92 †2	0.08 †1 1.59 †2	0.066	0.026	0.073
m_h^* / m_0 †3	0.52	0.34	0.5	0.41	0.4

$m_0 = 9.1 \times 10^{-31}\,Kg$ (electron mass)

†1 transverse mass †2 vertical mass †3 heavy hole mass

(Data are from Ref. [10], p. 302)

-- Column 1 --

Why should the mass of conduction electrons in a crystal be intentionally expressed in terms of energy E, as in equation (1, 11) ?

This is because the influence of the potential energy E_p due to the crystal lattice must be taken into account. If the energy E is given only by the kinetic energy E_K ($E_P = 0$), then $E = E_K = \frac{p^2}{2m_0} = \frac{\hbar^2 k^2}{2m_0}$ and the effective mass m^* obtained by substituting in equation (1, 11) is the electron mass m_0 itself ($m^* = m_0$).

The conduction electrons in a crystal are affected by collisions with and scattering from the crystal lattice (roughly, the atoms that make up the crystal), but when the crystal lattice is perfectly periodic, this effect can be considered to be incorporated by the fact that the mass of the conduction electrons becomes the effective mass m^*.

1.5 Electron Statistics and Carrier Density

(1) Conduction-band density of states $g_e(E)$

The conduction energy band of a semiconductor crystal is composed of a collection of (discrete) energy levels with different quantum states in which electrons are allowed to exist. The density of energy levels (the number of energy levels per unit energy width) in the conduction energy band of a unit volume of semiconductor crystal in which electrons are allowed to exist is called the density of states $g_e(E)$ of the conduction energy band and is given by (see Appendix B for equation derivation)

$$g_e(E) = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{\frac{3}{2}} (E - E_C)^{\frac{1}{2}} \tag{1.13}$$

Figure 1.12 shows the relationship between $g_e(E)$ and energy bands. Using E_C as a base point, the density of states increases as the energy increases.

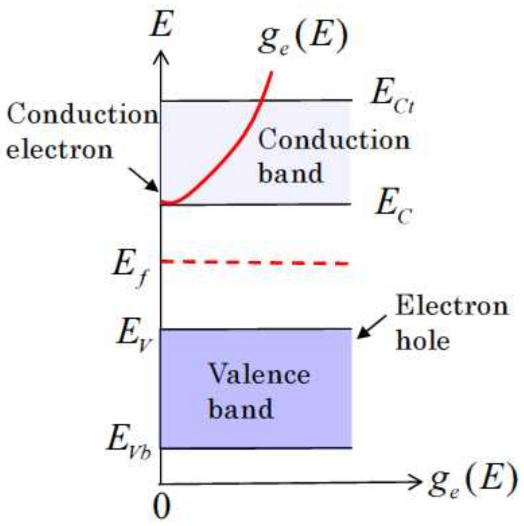


Figure 1.12 Relationship between density of states $g_e(E)$ and energy bands

(2) Electron occupancy probability $f_e(E)$

The probability of an electron occupying an energy level E with given quantum state (electron occupancy probability) $f_e(E)$ is given by the following equation according to the Fermi-Dirac statistics (the principle formula for Fermi particles in quantum mechanics)

$$f_e(E) = \frac{1}{1 + \exp\left(\frac{E - E_f}{k_B T}\right)} \tag{1.14}$$

$k_\mathrm{B} = 1.38 \times 10^{-23} \left[J / K \right]$; Boltzmann constant

T ; absolute temperature

E_f ; Fermi level

Figure 1.13 shows the relationship between electron occupancy probability $f_e(E)$ and energy bands.

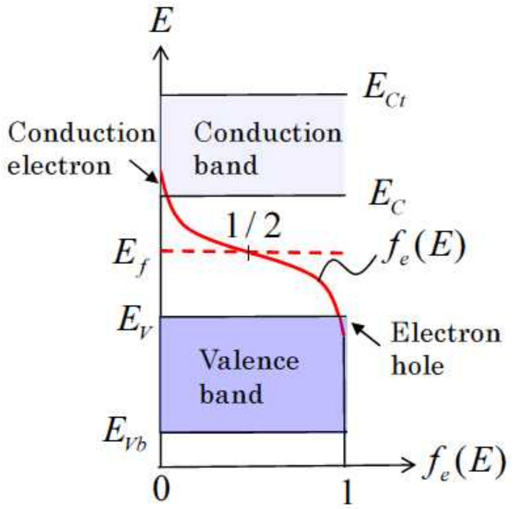


Figure 1.13 Relationship between electron occupancy probability $f_e(E)$ and energy bands

The figure shows that the electron occupancy probability $f_e(E)$ is a value between 0 and 1. When the energy E is the Fermi level E_f ($E = E_f$), the probability of electron occupation is 1/2. Conversely, the energy E at which the probability of electron occupation is 1/2 is the Fermi level E_f. At cryogenic temperatures ($T \approx 0$), the probability of electron occupancy is 0 for $E \geq E_f$ and 1 for $E \leq E_f$. As temperature increases, the electron occupancy probability becomes a smooth characteristic. In the valence band, the part of the probability of electron occupancy that is less than 1 gives the probability of hole occupancy.

(3) Conduction electron density n

In a unit volume of semiconductor crystal, the number of conduction electrons $N_e(E)dE$ occupying energies $E \sim E + dE$ is given by the following equation using $g_e(E)$ and $f_e(E)$

$$N_e(E)dE = g_e(E) f_e(E) dE \tag{1.15}$$

From this, the total number of electrons in the conduction band in a unit volume of semiconductor crystal (conduction electron density) n is given by

$$n = \int_{E_C}^{E_{Ct}} N_e(E)dE = \int_{E_C}^{E_{Ct}} g_e(E) f_e(E) dE \tag{1.16}$$

where E_{Ct} is the energy at the top of the conduction band

Using equations (1.13) and (1.14) and approximating $E_{Ct} \rightarrow \propto$, we obtain n as follows

$$\begin{aligned} n &= \int_{E_C}^{\infty} \frac{1}{2\pi^2} \left(\frac{2m_e^*}{\hbar^2} \right)^{\frac{3}{2}} \left(E - E_C \right)^{\frac{1}{2}} \frac{1}{1 + \exp\left(\dfrac{E - E_f}{k_B T} \right)} dE \\ &= N_C \exp\left(-\frac{E_C - E_f}{k_B T} \right) \end{aligned} \tag{1.17}$$

where $N_C = 2 \left(\dfrac{m_e^* k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}}$ (1.18)

(4) Electron hole density p

The electron hole density p can be obtained in the same way. The density of states $g_h(E)$ for electron holes in the valence band is given as

$$g_h(E) = \frac{1}{2\pi^2} \left(\frac{2m_h^*}{\hbar^2} \right)^{\frac{3}{2}} \left(E_V - E \right)^{\frac{1}{2}} \tag{1.19}$$

As the probability $f_h(E)$ of an electron hole occupying energy E in the valence band is equal to the probability of an electron being empty, it follows that

$$f_h(E) = 1 - f_e(E) = 1 - \frac{1}{1+\exp\left(\frac{E-E_f}{k_B T}\right)} = \frac{1}{1+\exp\left(\frac{E_f-E}{k_B T}\right)} \quad (1.20)$$

In a unit volume of semiconductor crystal, the number of electron holes $N_h(E)dE$ occupying energies $E \sim E + dE$ in the valence band is given by

$$N_h(E)dE = g_h(E) f_h(E) dE \quad (1.21)$$

From this, the total number of electron holes in the valence band in a unit volume of semiconductor crystal (electron hole density) p is given by

$$\begin{aligned} p &= \int_{E_{Vb}}^{E_V} N_h(E)dE = \int_{E_{Vb}}^{E_V} g_h(E) f_h(E) dE \\ &= \int_{-\infty}^{E_V} \frac{1}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{\frac{3}{2}} \left(E_V - E\right)^{\frac{1}{2}} \frac{1}{1+\exp\left(\frac{E_f-E}{k_B T}\right)} dE \quad (1.22) \\ &= N_V \exp\left(-\frac{E_f - E_V}{k_B T}\right) \end{aligned}$$

$$\text{where} \quad N_V = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} \quad (1.23)$$

The density of states $g_e(E)$, $g_h(E)$, occupancy probability $f_e(E)$, $f_h(E)$, carrier density n, and p for conduction electrons and electron holes described above are summarized in Figure 1.14.

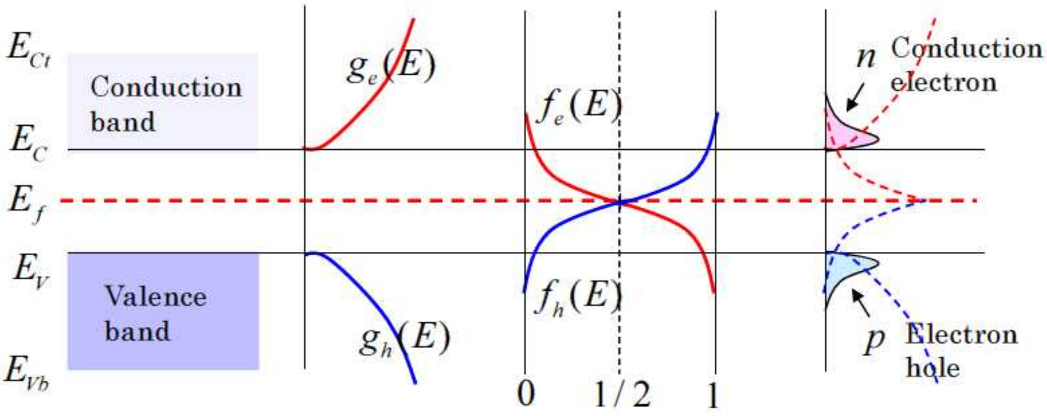


Figure 1.14 The density of states $g_e(E)$, $g_h(E)$, occupancy probability $f_e(E)$, $f_h(E)$, carrier density n and p for conduction electrons and electron holes

(5) np product

From equations (1.17) and (1.22), the following np product is obtained.

$$\begin{aligned} np &= N_C \exp\left(-\frac{E_C - E_f}{k_B T}\right) N_V \exp\left(-\frac{E_f - E_V}{k_B T}\right) \\ &= 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 (m_e^* m_h^*)^{\frac{3}{2}} \exp\left(-\frac{E_G}{k_B T}\right) = n_i^2 \end{aligned} \tag{1.24}$$

where $E_G = E_C - E_V$ (band gap energy)

In semiconductors, the values of carrier densities n and p are determined by the value of the Fermi level E_f, including the case of N- and P-type semiconductors obtained by impurity injection, but the above equation does not include E_f. This implies that the value of the np product is independent of E_f. In other words, in the steady state, the np product is determined to a certain value once the semiconductor material is determined (E_G is determined) and the temperature T is determined. Furthermore, it does not depend on the presence or absence of impurities. For example, even if the majority carrier density n is extremely large in an N-type semiconductor, there is always a certain amount of minority carrier density p, and this value must satisfy $np = n_i^2$. In the case of an intrinsic semiconductor with $n = p$ the following holds.

$$n = p = n_i = \sqrt{N_C N_V} \exp\left(-\frac{E_G}{2k_B T}\right) \tag{1.25}$$

As described below, even N- or P-type semiconductors containing impurities will have $n \approx p$ at higher temperatures and behave the same as an intrinsic semiconductor.

1.6 Fermi Energy

Using equations (1.17) and (1.22), p/n can be expressed as follows

$$\frac{p}{n} = \frac{N_V \exp\left(-\frac{E_f - E_V}{k_B T}\right)}{N_C \exp\left(-\frac{E_C - E_f}{k_B T}\right)} = \left(\frac{m_h^*}{m_e^*}\right)^{\frac{3}{2}} \exp\left(\frac{E_C + E_V - 2E_f}{k_B T}\right) \tag{1.26}$$

From the above equation, E_f can be expressed as

$$E_f = \frac{E_C + E_V}{2} + \frac{k_B T}{2} \ln\left(\frac{n}{p}\right) + \frac{3k_B T}{4} \ln\left(\frac{m_h^*}{m_e^*}\right) \tag{1.27}$$

However, since n and p are originally functions of E_f, it is generally difficult to solve E_f analytically from the above equation, and it must be obtained by numerical calculation.

The main focus here is on understanding the properties of E_f, and we will try to obtain this analytically, although we will use a relatively rough approximation. In the following, we will consider two cases: (a) the case of an intrinsic semiconductor and (b) the case of an impurity semiconductor.

(a) For an intrinsic semiconductor

Since $n = p$ for an intrinsic semiconductor, the second term on the right-hand side of Eq. (1.27) is 0, and E_f can be calculated by substituting the physical constants of the semiconductor. Furthermore, in general, the value of the third term on the right-hand side is sufficiently so small that, neglecting it, E_f can be given approximately as follows.

$$E_f \approx \frac{E_C + E_V}{2} \tag{1.28}$$

(b) For an impurity semiconductor

Figure 1.15 shows a schematic diagram showing the number of impurity atoms (donors and acceptors) and carriers (conduction electrons and electron holes) in a unit volume of a semiconductor crystal.

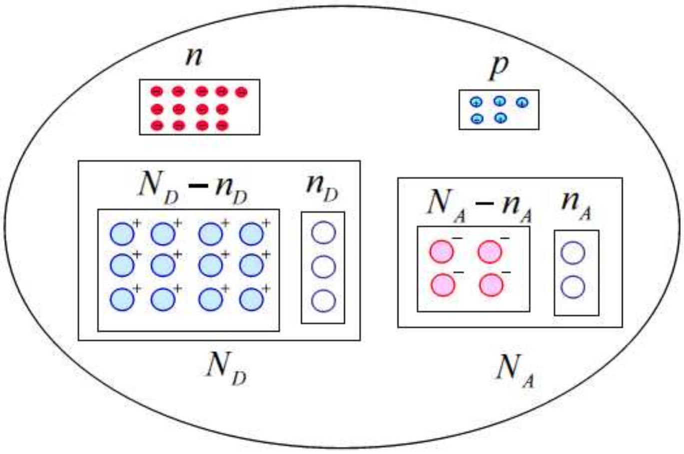


Figure 1.15 Schematic diagram showing the number of impurity atoms (donors and acceptors) and carriers (conduction electrons and electron holes) in a unit volume of a semiconductor crystal.

The symbols in the figure mean the following

N_D: Number of donor atoms
n_D: Number of non-ionized donor atoms

n: Number of conduction electrons
N_A: Number of acceptor atoms
n_A: Number of non-ionized acceptor atoms
p: Number of electron holes

Since the total charge in the semiconductor is 0 (neutral) in thermal equilibrium, the following equation must hold

$$\underbrace{N_D - n_D + p}_{\text{Positive charge}} = \underbrace{N_A - n_A + n}_{\text{Negative charge}} \tag{1.29}$$

Let us consider an ideal N- type semiconductor and assume that

$$N_A = n_A = 0 \tag{1.30}$$

Furthermore, if we assume that $p = 0$ as an approximation (although in practice there is a small amount of p to satisfy the np product), then equation (1.29) becomes

$$N_D - n_D = n \tag{1.31}$$

This equation indicates that the conduction electrons are given by the ionization of the donor atom. Figure 1.16 shows this schematically in the energy band structure. In the figure, E_D is the energy value of the donor level, n_D is the number of donor levels occupied by electrons, and $N_D - n_D = n$ is the number of donor levels not occupied by electrons and the number of conduction electrons.

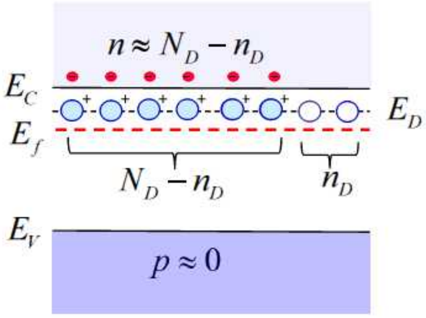


Figure 1.16 Conduction electrons and donor atoms in an ideal N- type semiconductor.

The $n(= N_D - n_D)$ electrons originally in the donor level become conduction electrons in the conduction band, leaving behind ionized donor atoms. The number of non-ionized donor atoms n_D means the number of electrons occupying the donor level E_D. From this, n_D is given by the occupancy probability $f_e(E_D)$ at energy E_D and the number of states N_D as follows

$$n_D = N_D f_e(E_D) = N_D \frac{1}{1+\exp\left(\frac{E_D - E_f}{k_B T}\right)} \tag{1.32}$$

On the other hand, the number of conduction electrons n is given by

$$n = N_C \exp\left(-\frac{E_C - E_f}{k_B T}\right) \qquad \text{(1.33) (see Eq. (1.17))}$$

Substituting equations (1.32) and (1.33) into equation (1.31), we obtain

$$N_D \frac{\exp\left(\frac{E_D - E_f}{k_B T}\right)}{1+\exp\left(\frac{E_D - E_f}{k_B T}\right)} = N_C \exp\left(-\frac{E_C - E_f}{k_B T}\right) \tag{1.34}$$

This equation (1.34) is used to obtain E_f. First, since $E_f < E_C$, the right-hand side of equation (1.34) is ≈ 0 at cryogenic temperatures ($T \approx 0$). From this, the left-hand side must also be ≈ 0, and for this reason, it must be $E_D < E_f$.

Next, consider increasing the temperature. For sufficiently high temperatures, the left-hand denominator of equation (1.34) is approximated roughly as follows

$$1+\exp\left(\frac{E_D - E_f}{k_B T}\right) \approx 2 \qquad (1.35)$$

Substituting this into the original equation (1.34), we obtain

$$\frac{N_D}{2}\exp\left(\frac{E_D - E_f}{k_B T}\right) \approx N_C \exp\left(-\frac{E_C - E_f}{k_B T}\right)$$

$$\longrightarrow \quad \frac{N_D}{2N_C} \approx \exp\left(\frac{2E_f - E_C - E_D}{k_B T}\right) \qquad (1.36)$$

Solving for E_f yields the following equation

$$E_f \approx \frac{E_C + E_D}{2} - \frac{k_B T}{2}\ln\left(\frac{2N_C}{N_D}\right) \qquad (1.37)$$

Since the value of the donor density N_D is usually chosen to be sufficiently small compared to N_C Note *2 , $\ln\left(\frac{2N_C}{N_D}\right)$ in the second term on the right side of equation (1.37) is positive. From this, we can say that the value of E_f decreases as temperature rises.

Note *2

For example, if N_C is calculated with $T = 300K$ and $m_e^* \approx 0.1 m_0 = 0.1 \times 9.1 \times 10^{-31} (Kg)$, then $N_C = 2\left(\frac{m_e^* k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} \approx 0.8\times10^{24}(m^{-3})$ ·

In summary, the properties of the Fermi energy level E_f are as follows.

(a) At cryogenic temperatures ($T \approx 0$), E_f becomes

$$E_D < E_f \approx \frac{E_C + E_D}{2} < E_C$$

(b) E_f becomes smaller (lower level) as temperature increases.

(c) At the same temperature, the smaller N_D is, the smaller (lower) E_f is.

Figure 1.17 shows schematically how E_f depends on T and N_D.

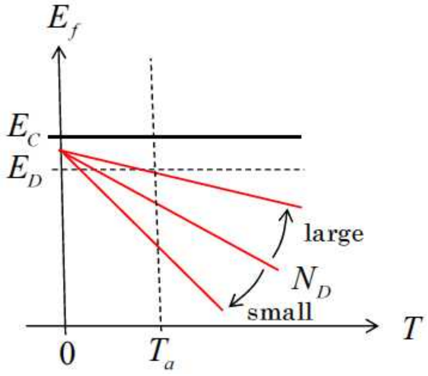


Figure 1.17　Dependence of E_f on T and N_D

1.7　Temperature Characteristics of Carrier Density

Figure 1.18 shows schematically the carrier densities n and p and the Fermi level E_f in an N-type semiconductor as the temperature T is varied.

In the figure, (a) is at cryogenic temperatures, (b) at low to room temperatures, and (c) at high temperatures. Figure 1.19 shows an example calculation of the temperature T dependent characteristics of the carrier (conduction electron) density n of an N-type semiconductor. The characteristics of parts (a), (b), and (c) in Figure 1.19 correspond to the states (a), (b), and (c) in Figure 1.18. The operation of parts (a), (b), and (c) of Figures 1.18 and 1.19 is described as follows.

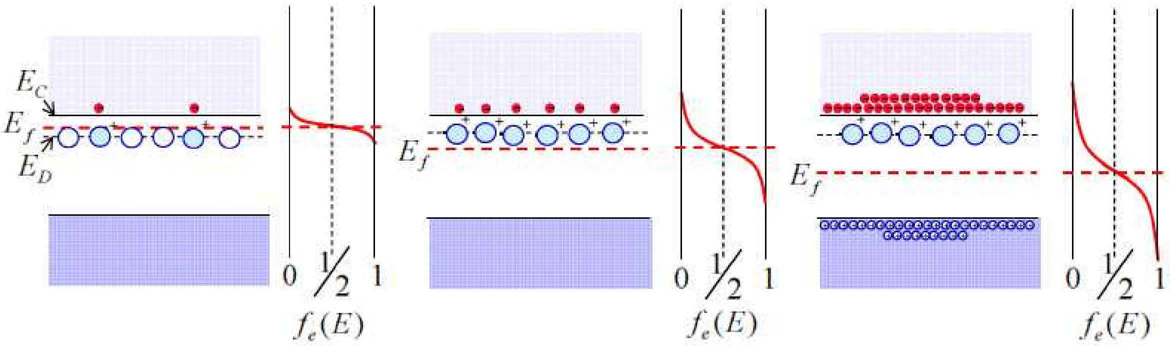
(a) At cryogenic temperatures, the Fermi level becomes $E_f \approx \frac{E_C + E_D}{2}$ and k_BT is small. At this time, n varies according to the following equation, with $n << N_D$ (see Appendix C).

$$n = \sqrt{N_C N_D} \exp\left(-\frac{E_C - E_D}{2k_BT}\right) \tag{1.38}$$

(b) As the temperature increases, $E_f < E_D$ and k_BT also increases. At this time, $n \approx N_D$, the electrons from the donor are almost exhausted. This state continues for a while even when the temperature changes.

(c) At higher temperatures, when k_BT exceeds the band gap energy E_G, carrier generation by electron-hole pair production becomes dominant, and the behavior is the same as that of an intrinsic semiconductor. In this case, n and p are given by

$$n \approx p \approx n_i = \sqrt{N_C N_V} \exp\left(-\frac{E_G}{2k_BT}\right) >> N_D \qquad \text{(1.39) (see Eq. (1.25))}$$



(a) cryogenic temp. (b) low to room temp. (c) high temp.

$n<<N_D$ $n \approx N_D$ $n \approx p \approx n_i >> N_D$

Figure 1.18 Carrier densities n, p, and Fermi level E_f of N-type semiconductor

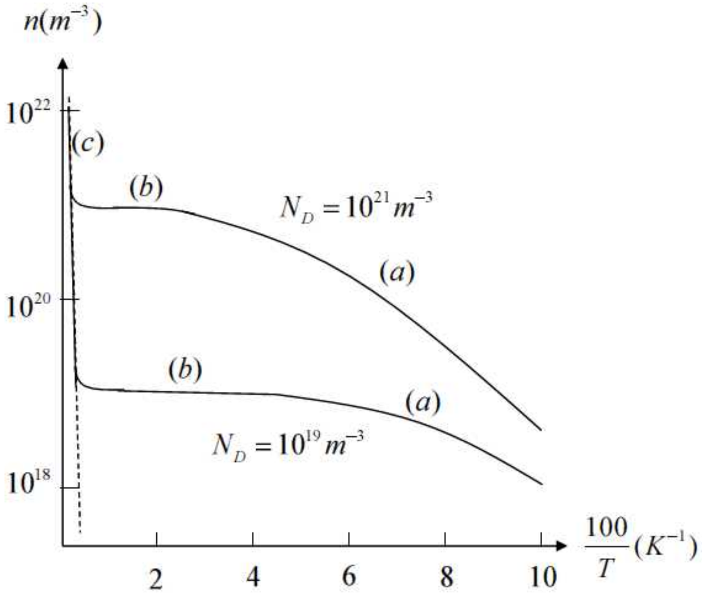


Figure 1.19 Example of calculation of the temperature dependence of the conduction electron density n of an N-type semiconductor (According to Ref. [4], p.170)

Appendix A Bohr's Atomic Model

Consider an electron of charge $-e$ and mass m_0 is moving around a nucleus of charge Ze in a circular orbit of radius r in vacuum (dielectric constant ε_0), as shown in Figure A-1.

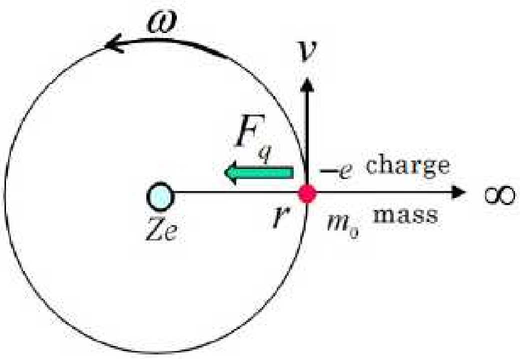


Figure A.1 Bohr's atomic model

When a nucleus of charge Ze and an electron of charge $-e$ exist at a distance r apart, the following Coulomb force F_q acts

$$F_q = -\frac{Ze^2}{4\pi\varepsilon_0 r^2} \tag{A.1}$$

At this time, electrons rotate with F_q as the centripetal force. From the relationship between the speed of rotation v and the centripetal force, the following equation holds.

$$F_q = -\frac{Ze^2}{4\pi\varepsilon_0 r^2} = -m_0\frac{v^2}{r} \longrightarrow v^2 = \frac{Ze^2}{4\pi\varepsilon_0 r m_0} \tag{A.2}$$

The electron kinetic energy E_K is given below using equation (A.2).

$$E_K = \frac{P^2}{2m_0} = \frac{1}{2} m_0 v^2 = \frac{Ze^2}{8\pi\varepsilon_0 r} \tag{A.3}$$

On the other hand, the potential energy E_P of an electron is defined as the amount of work done by the electron during its slow (velocityless) movement to infinity, and is given by

$$E_P = \int_r^\infty F_q dr = \int_r^\infty -\frac{Ze^2}{4\pi\varepsilon_0 r^2} dr = -\frac{Ze^2}{4\pi\varepsilon_0 r} \tag{A.4}$$

From this, the total energy E of the electron is given by

$$E = E_P + E_K = -\frac{Ze^2}{8\pi\varepsilon_0 r} \tag{A.5}$$

Here, from the duality of the electron in quantum mechanics (being both a particle and a wave), the wavelength λ of the electron is given by

$$\lambda = \frac{h}{P} = \frac{h}{m_0 v} \tag{A.6}$$

In addition, for an electron to rotate on a circumference of radius r, the following quantum conditions must be satisfied,

$$2\pi r = n\lambda \qquad (n = 1, 2, \cdots) \tag{A.7}$$

From equations (A.2), (A.6), and (A.7), the following equation is obtained.

$$r = \frac{h^2 \varepsilon_0}{\pi m_0 Z e^2} n^2 \qquad (n = 1, 2, \cdots) \tag{A.8}$$

Also, from equations (A.5) and (A.8), the following equation is obtained.

$$E = -\frac{m_0 Z^2 e^4}{8\varepsilon_0{}^2 h^2}\frac{1}{n^2} \qquad (n = 1, 2, \cdots) \tag{A.9}$$

Appendix B Derivation of Density of States $g_e(E)$

Consider a one-dimensional periodic potential well $U(r)$ in length L, as shown in Figure B.1, in which N conduction electrons exist.

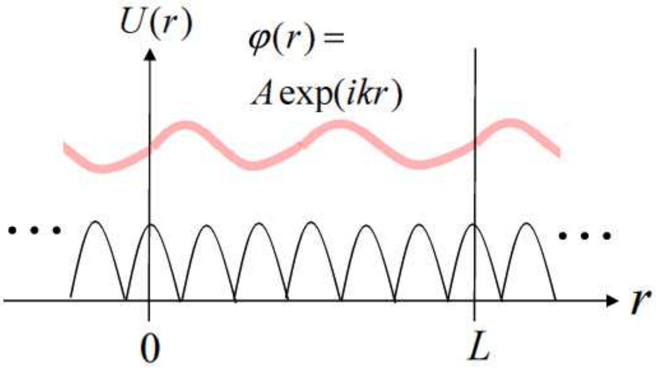


Figure B.1 One-dimensional periodic potential well $U(r)$ in a length L, in which N conduction electrons exist

Considering the wave function $\varphi(r) = A\,exp(jkr)$ (wavenumber k) of the electrons in this well, from the period boundary condition $\varphi(0) = \varphi(L)$ of the wave function, the possible values of k are

$$k = \frac{2\pi}{L}n \tag{B.1}$$

Here, consider the first Brillouin region, and let n take N integer values in the range $-\frac{N}{2} \sim \frac{N}{2}$. In this case, the number of states dN in the wavenumber $k \sim k + dk$ is

$$dN = \frac{L}{2\pi} dk \tag{B.2}$$

Extending to 3-dimensional crystals, the number of states $dN_V{}'$ in a small volume $dk_x dk_y dk_z$ of $\boldsymbol{k}$ -space is

$$dN_V{}' = \left(\frac{L}{2\pi}\right)^3 dk_x dk_y dk_z \tag{B.3}$$

The number of states per unit volume is obtained by dividing by the volume L^3 , and furthermore, taking into account the electron spin, the number of states (per unit volume) dN_V in the box of a small volume $dk_x dk_y dk_z$ of $\boldsymbol{k}$ -space shown in Figure B.2 is

$$dN_V = \frac{2}{L^3} dN_V' = \frac{2}{(2\pi)^3} dk_x dk_y dk_z \tag{B.4}$$

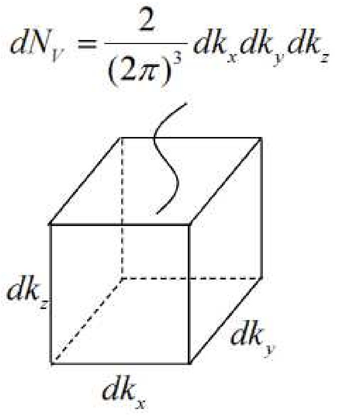


Figure B.2 Number of states (per unit volume) dN_V contained in a box of microvolume $dk_x dk_y dk_z$

From this, the number of states (per unit volume) N_V contained in a sphere of radius $k(= \sqrt{k_x^2 + k_y^2 + k_z^2})$ is given by

$$N_V = \frac{2}{(2\pi)^3} \frac{4\pi}{3} k^3 \tag{B.5}$$

Further from this, the number of states (per unit volume) dN_V contained in the spherical shell of radius $k \sim k + dk$ shown in Figure B.3 is

$$dN_V = \frac{2}{(2\pi)^3} 4\pi k^2 dk \tag{B.6}$$

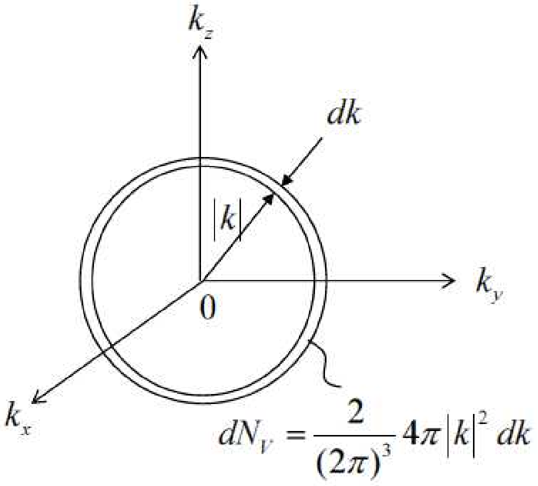


Figure B.3 Number of states (per unit volume) dN_V contained in a spherical shell of radius $k \sim k + dk$

On the other hand, there exists a relationship between the wavenumber k and the energy E as follows.

$$E = \frac{P^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*} \tag{B.7}$$

m^* is the effective mass of the carrier, $\hbar = \frac{h}{2\pi}$ (h is Planck's constant)

From this, by expressing k in equation (B.6) in terms of E, we obtain

$$dN_V = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E}dE \tag{B.8}$$

The above equation gives the number of states (per unit volume) in the energy range $E \sim E + dE$. Assuming that the density of states at energy E is $g(E)$, from equation (B.8), $g(E)$ can be expressed as

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E} \tag{B.9}$$

Here, when the carrier is a conduction electron, the symbols are converted to $g(E) \rightarrow g_e(E)$ and $m^* \rightarrow m_e^*$. Since the kinetic energy of the conduction electrons is given by the energy difference from the energy level E_C at the bottom of the conduction band, we convert $E \rightarrow E - E_C$. As a result, the density of states $g_e(E)$ of the conduction electrons is given by

$$g_e(E) = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{\frac{3}{2}}\left(E - E_C\right)^{\frac{1}{2}} \tag{B.10}$$

Appendix C Derivation of Equation (1.38)

The conduction electron density n in an N-type semiconductor at cryogenic temperatures is approximately given by

$$n = N_D - n_D = N_D(1 - f_e(E_D)) \tag{C.1}$$

Transforming equation (C.1), we obtain

$$N_D - n = N_D f_e(E_D) \tag{C.2}$$

Dividing each side of equations (C.1) and (C.2), respectively, the following equation is obtained.

$$\frac{n}{N_D - n} = \frac{1}{f_e(E_D)} - 1 = \exp\left(\frac{E_D - E_f}{k_B T}\right) \tag{C.3}$$

Multiplying each side of the above equation (C.3) by each side of $n = N_C \exp\left(-\frac{E_C - E_f}{k_B T}\right)$ yields

$$\frac{n^2}{N_D - n} = N_C \exp\left(-\frac{E_C - E_D}{k_B T}\right) \tag{C.4}$$

Since $n \ll N_D$ at cryogenic temperatures, the above equation (C.4) can be approximated as follows

$$\frac{n^2}{N_D - n} \approx \frac{n^2}{N_D} = N_C \exp\left(-\frac{E_C - E_D}{k_B T}\right)$$

$$\longrightarrow \qquad n = \sqrt{N_C N_D} \exp\left(-\frac{E_C - E_D}{2 k_B T}\right) \tag{C.5}$$